

Quantum criticality in the two-dimensional Hubbard model

A dynamical cluster approximation and numerical renormalization group study

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Zusammenfassung

(Summary in German)

In dieser Arbeit verwenden wir die dynamische Clusterapproximation in Kombination mit der numerischen Renormierungsgruppenmethode als Störstellenmodelll ser, um das zweidimensionale Hubbard-Modell zu untersuchen, da dieses eine Minimalbeschreibung der CuO₂-Ebene in Kupratmaterialien liefert. Ziel ist es, die seit Langem offene Frage nach Quantenkritikalit t im endlichen Dotierungsbereich zwischen Fermi-Fl ssigkeit und Pseudogap-Phase zu beantworten.

Die Berechnungen bleiben aufgrund des exponentiellen Wachstums des Hilbertraums mit zunehmender Clustergr  e numerisch sehr aufwendig. Daher beschr nken sich unsere Rechnungen auf ein eingebettetes 2×2 -Cluster. Dennoch zeigen unsere Ergebnisse eine Rekonstruktion der Fermifl che von einer geschlossenen Fermifl che zu Fermib gen bei einer kritischen Dotierung $p^* \simeq 0.14$, die mit dem Verschwinden der Fermi-Fl ssigkeitsskala bei $T = 0$ in verschiedenen Korrelationsfunktionen einhergeht und damit einen Nachweis f r Quantenkritikalit t bei p^* liefert. Die divergierenden Korrelationsfunktionen deuten auf kurzreichweitige antiferromagnetische Korrelationen als treibende Kraft hinter dem quantenkritischen  bergang hin. Dar ber hinaus beobachten wir koh rente Anregungen zusammengesetzter elektronischer Quasiteilchen in der Pseudogap-Phase, was das Verschwinden des spektralen Gewichts beim  ffnen des Pseudogaps erkl rt.

Wir finden einen scharfen  bergang an den antinodalen Punkten, w hrend die nodalen Punkte scheinbar unbeeinflusst bleiben, was mit ARPES-Experimenten an Kupraten  bereinstimmt. Dar ber hinaus zeigen innerhalb des quantenkritischen Kegels sowohl die Temperaturabh ngigkeit der lokalen Spin-Suszeptibilit t als auch der lokale Beitrag zur optischen Leitf higkeit eine plancksche Skalierung. Letztere stimmt mit Transportexperimenten  berein und weist auf einen linear-in- T -Widerstand hin. Ferner deutet die nodale Selbstenergie in unseren Ergebnissen auf ein marginales Fermi-Fl ssigkeitsverhalten hin, mit $\Sigma''_{(0,0)}(\omega, T) \sim \max(\omega, T)$.

Im Rahmen der Nachbearbeitung haben wir verschiedene Interpolationsmethoden untersucht, um eine glatte Impulsabh ngigkeit innerhalb der Clusterapproximation wiederherzustellen. Dies f hrte zur Entwicklung eines neuartigen Verfahrens, bei dem Liouvillian-Matrixelemente interpoliert werden und die Kausalit t konstruktionsbedingt erhalten bleibt. Die Liouvillian-Matrixelemente werden mittels einer Kettenbruchentwicklung der Selbstenergie bestimmt, was die Idee zur Entwicklung einer vollst ndig diskreten dynamischen Molekularfeldtheorie angesto en hat.

Summary

(Summary in English)

In this thesis, we use the dynamical cluster approximation in combination with the numerical renormalization group as an impurity solver to study the two-dimensional Hubbard model, as it provides a minimal description of the CuO_2 plane in cuprate materials. The goal is to address the long-standing question of quantum criticality in the finite doping regime between the Fermi liquid and pseudogap phases.

The computations remain numerically very expensive due to the exponential growth of the Hilbert space with increasing cluster size. Therefore, our calculations are limited to an embedded cluster of 2×2 sites. Nevertheless, we observe a Fermi surface reconstruction from a full Fermi surface to Fermi arcs at a critical doping $p^* \simeq 0.14$, which is accompanied by a vanishing Fermi-liquid scale at $T = 0$ in various correlation functions, providing evidence for quantum criticality at p^* . The diverging correlation functions indicate short-ranged antiferromagnetism as the driving mechanism behind the quantum critical transition. We also observe the emergence of coherent composite electronic quasiparticles in the pseudogap phase, explaining the loss of spectral weight associated with the opening of the pseudogap.

We find a sharp transition at the antinodal points, while the nodal points remain largely unaffected, consistent with ARPES experiments on cuprates. Moreover, within the quantum critical cone, the temperature dependence of the local spin susceptibility and the local contribution to the optical conductivity exhibit Planckian scaling. The latter is consistent with transport experiments, and indicates linear-in- T resistivity. Furthermore, the nodal self-energy in our results suggests marginal Fermi-liquid behavior, with $\Sigma''_{(0,0)}(\omega, T) \sim \max(\omega, T)$.

During post-processing, we explored various interpolation methods to restore smooth momentum dependence within our cluster approximation. This led to the development of a novel scheme in which Liouvillian matrix elements are interpolated while preserving causality by construction. These Liouvillian matrix elements are obtained via a continued-fraction expansion of the self-energy, which further inspired the development of a fully discrete dynamical mean-field theory.

Publications

This dissertation is based on the following journal articles, listed in order of publication date:

- [P1] *Liouvillian interpolation of the self-energy of cluster dynamical mean-field theories*
Mathias Pelz, Jan von Delft and Andreas Gleis
 Sec. 2.4 / [arXiv:2602.16351](#) to APS Open Science
- [P2] *Symmetric estimator for discrete self-energy of discrete many-body systems*
 Aleksandrs Zacinskis, Frank T. Ebel, **Mathias Pelz**, Fabian B. Kugler, Karsten Held, Jan von Delft, Maurits W. Haverkort, and Andreas Gleis
 Sec. 2.5 / [arXiv:2605.04974](#) to Physical Review B
- [P3] *Quantum criticality in the two-dimensional Hubbard model*
Mathias Pelz, Gabriel Kotliar, Jan von Delft, and Andreas Gleis
 Sec. 3.2 / [arXiv:2605.15059](#) to Proceedings of the National Academy of Sciences
- [P4] *Dynamical scaling near the pseudogap quantum critical point of the two-dimensional Hubbard model*
Mathias Pelz, Gabriel Kotliar, Jan von Delft, and Andreas Gleis
 Sec. 3.3 / [arXiv:2605.15060](#) to Physical Review Letters

I further contributed to the following publications which have not been included in this thesis:

- [P5] *Testing the parquet equations and the $U(1)$ Ward identity for real-frequency correlation functions from the multipoint numerical renormalization group*
 Nepomuk Ritz, Anxiang Ge, Markus Frankenbach, **Mathias Pelz**, Jan von Delft and Fabian B. Kugler
[arXiv:2504.05910v2](#) [Phys. Rev. Res. 7, 33139 \(2025\)](#)
- [P6] *Compressing local vertex functions from the multipoint numerical renormalization group using quantics tensor cross interpolation*
 Markus Frankenbach, Marc K. Ritter, **Mathias Pelz**, Nepomuk Ritz, Jan von Delft and Anxiang Ge
[arXiv:2506.13359v3](#) [Phys. Rev. Res. 7, 043032 \(2025\)](#)

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My family has always provided a place to retreat to in times of need, even if they were not very present during my time in Munich.

Completing this PhD marks the end of an important and formative chapter of my life. While this journey has deepened my appreciation for scientific research, it has also led me to reflect on my personal and professional priorities. I have therefore decided to pursue my future path outside of academia. I am grateful for the experiences, challenges, and insights gained during this time, which will continue to shape my thinking and approach in the years ahead.

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1 Introduction

This chapter provides an overview of the cuprate class of materials and the models used to describe them from a theoretical point of view. Section 1.1 provides a brief summary of research conducted over the last decades since the discovery of the cuprates, as well as our motivation for this study. The following Section 1.2 gives an overview of commonly used models to describe cuprate physics.

1.1 Cuprate class of materials

Since the discovery in the 1980's [BM86; Haz+87; Tar+88; She+88; SH88a; SH88b; Shi+89; GF87; Var+89] the cuprates are a puzzling class of materials, and are still to this day.

These materials form intricate heterostructures, as illustrated in Fig. 1.1(a) for four representative examples. Layered copper oxides consist of CuO_2 planes separated by insulating spacer layers, which largely suppress interlayer hopping and render the electronic structure quasi two-dimensional. All cuprates share this copper–oxygen plane as their fundamental structural unit, which gives the class its name. The low-energy electronic degrees of freedom arise predominantly from the hybridization between a hole on the Cu $3dx^2 - y^2$ orbital and the planar O $2p_x$ and $2p_y$ orbitals, as shown in Fig. 1.1(b). Within the CuO_2 planes, this strong orbital overlap results in pronounced electronic confinement and enhanced Coulomb interactions on the copper sites. Consequently, cuprates are prototypical strongly correlated electron systems and are commonly described within multi-band Hubbard-type models (Emery model) or their effective single-band reductions. Both are detailed in Sec. 1.2.

These strong correlations lead to a variety of phases depending on the doping level p . Figure 1.2 shows a cuprate phase diagram as a function of hole doping. Most prominently, it features a high- T_c superconducting dome at finite doping p . The origin of this superconductivity and the mechanism behind Cooper pair formation are still debated.

At very low temperatures, to the left of the dome at small doping $p < p_{\min}$, the system exhibits a Mott-insulating phase with antiferromagnetic order, while at large doping $p > p_{\max}$ it becomes a textbook Fermi liquid.

In between these two phases and above the superconducting dome, two additional phases are observed. At lower doping, the pseudogap phase emerges, which remains a subject of intense debate within the community, as it exhibits Fermi arcs measured by angle-resolved photoemission spectroscopy (ARPES) [NDR+98; TS99; KKN+15; RPS+12; Kor15; He+11; Che+19; RZP+19; Vis+10]. In contrast to a conventional Fermi surface, Fermi arcs do not form closed contours in momentum space, in apparent contradiction to standard band theory [Wan+11; SKK+22]. On the other hand, transport measurements suggest the formation of pocket-like Fermi surface structures [Bar+13; Bar+19; Kun+20; Yan+19]. The Fermi arcs observed in ARPES could therefore arise from thermal excitations and finite experimental resolution, which may smear out closed pockets and make them appear arc-like. From a theoretical perspective, however, Fermi arcs also emerge in numerical studies of strongly correlated systems, for instance within

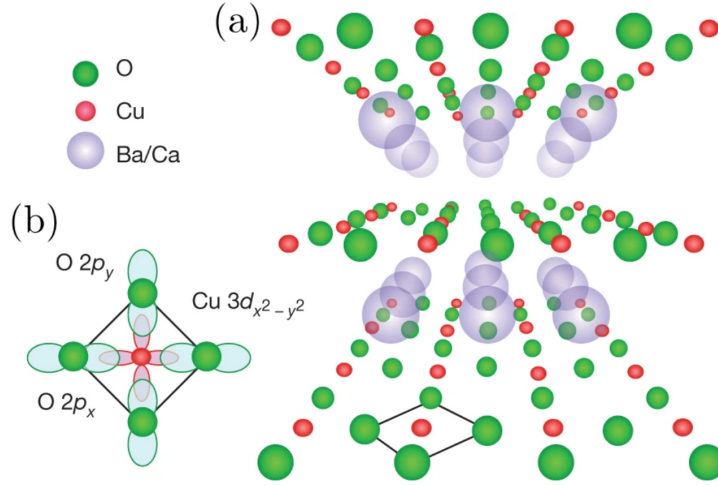


Figure 1.1 (a) Cuprate heterostructure consisting of multiple CuO₂-planes with indicated CuO₂-plane unit cell. (b) Detailed view on the unit cell showing the atomic orbitals for oxygen $2p_x$, $2p_y$ and copper $3d_{x^2-y^2}$, respectively, in green and red. Adopted from Fig. 3 of Ref. [KKN+15].

the Hubbard model treated using dynamical mean-field theory [Wu+18; Qin+22; Fer+09; SK06a].

The second phase above the superconducting dome is the strange metal phase, which exhibits a broad crossover regime into the pseudogap phase. The strange metal, or non-Fermi liquid, is a metallic state characterized by unconventional ω/T -scaling [MBR+23]. In general, response functions in this phase deviate from Fermi liquid theory; for example, the resistivity scales linearly with temperature, $\rho \propto T$ [Coo+09; Leg+19; Gri+21], the specific heat coefficient shows logarithmic behavior, $\gamma = C_V/T \propto \ln T$ [Gir+21; TS23].

1.1.1 Motivation

It has been suggested early on that the emergence of the aforementioned strange metal phase is linked to a quantum critical point (QCP) concealed beneath the superconducting dome [CDG95; Var97; Var99; Tal+99; Sac10]. In this scenario, a phase transition occurs at a critical doping p_{c2} of Fig. 1.2, separating the Fermi-liquid (FL) phase at $p > p_{c2}$ from the pseudogap (PG) phase at $p < p_{c2}$. Across this transition, a Fermi surface reconstruction is expected, involving a change from a hole-like Fermi surface in the FL regime to the reconstructed Fermi surface topology characteristic of the PG phase. However, a Fermi-surface reconstruction alone does not constitute proof of a QCP. A necessary condition would be the vanishing of the Fermi-liquid coherence scale at a critical doping p_{c2} , which should manifest itself in the critical behavior of various susceptibilities.

Experimentally, probing such behavior is highly challenging due to the extremely low temperatures required and the presence of superconductivity masking the putative transition. On the theoretical side, the unusual properties of the pseudogap phase have motivated a wide range of phenomenological approaches [RYZ11; Wor+24; YRZ06; SCI16; ZS20; YI11; Fab22; Rob+19; Sad+05], as well as extensive numerical studies [Hus+01; Civ+05; Mai+05; TKS06; Kyu+06; SK06a; Mac+06; HK07; Fer+09; Gul+09; LT09; Mik+09; Vid+09; Gul+10; Kha+10; Yan+11; SHT10; SHT11; Sor+12a; Sor+12b; Sor+13; Sor+19; Sch+18; Wu+18; WWT22; Qin+22; Mei+24].

In this thesis, we address the open question of quantum criticality, taking advantage of our numerical renormalization-group impurity solver, which enables computations

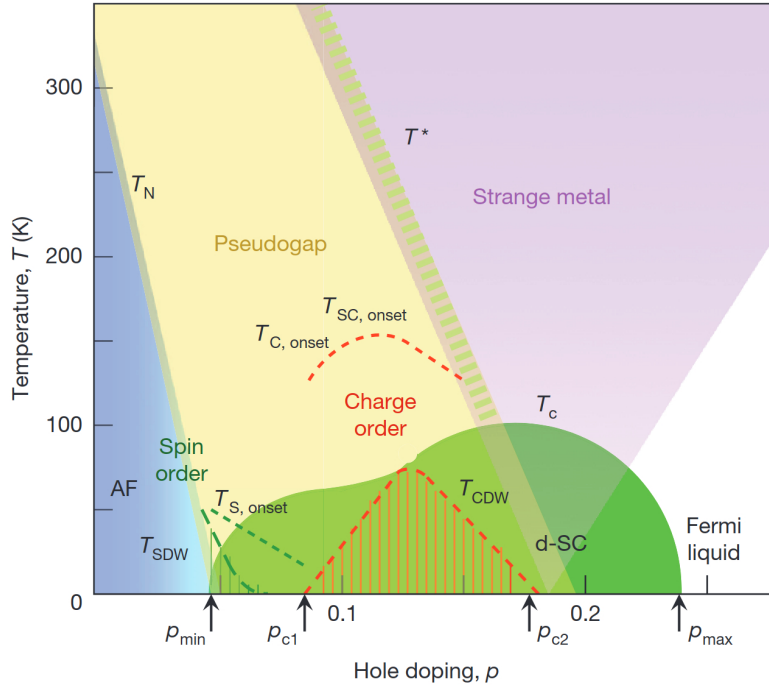


Figure 1.2 General cuprate phasediagram as function of doping p , exhibiting various phases: an anti-ferromagnetic Mott insulator (AF), a pseudogap phase, a strange metal, a Fermi liquid and a superconducting dome (d-SC). Lines indicate observed spin and charge order regions, respectively, in green and red. Adopted from Fig. 2 of Ref. [KKN+15].

of real-frequency spectra at arbitrarily low temperatures. Combined with dynamical mean-field theory and its cluster extensions, this approach allows us to solve the lattice problem while incorporating the necessary momentum dependence.

1.2 Model descriptions

The lattice problem we aim to solve is defined by the strongly correlated CuO_2 -plane. Its unit cell contains two oxygen orbitals, p_x and p_y , as well as a copper $d_{x^2-y^2}$ orbital, which allows it to be described by an effective three-band model.

1.2.1 Emery model

The Emery model [Mai+99; Ave+13; WGV14; Zha+25] is defined as

$$\begin{aligned}
 H_{\text{Emery}} = & \epsilon_d \sum_{i,\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \epsilon_p \sum_{j,\sigma} p_{j\sigma}^\dagger p_{j\sigma} + \sum_{\langle i,j \rangle, \sigma} t_{pd}^{ij} (d_{i\sigma}^\dagger p_{j\sigma} + \text{h.c.}) \\
 & + \sum_{\langle i,j' \rangle, \sigma} t_{pp}^{jj'} (p_{j\sigma}^\dagger p_{j'\sigma} + \text{h.c.}) + U_d \sum_i n_{d,i\uparrow} n_{d,i\downarrow} + U_p \sum_j n_{p,j\uparrow} n_{p,j\downarrow} .
 \end{aligned} \tag{1.1}$$

Here, $d_{i\sigma}^{(\dagger)}$ and $p_{j\sigma}^{(\dagger)}$ denote annihilation (creation) operators for electrons in the Cu $d_{x^2-y^2}$ and O p_x , p_y orbitals, respectively. The corresponding number operators are defined as $n_{d,i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ and $n_{p,j\sigma} = p_{j\sigma}^\dagger p_{j\sigma}$. The on-site energies of the orbitals are given by ϵ_d and ϵ_p , while t_{dp}^{ij} and $t_{pp}^{jj'}$ describe the hopping amplitudes between copper and oxygen

sites and between neighboring oxygen sites, respectively. The local Coulomb interactions on copper and oxygen are parametrized by U_d and U_p .

As it stands, accounting for all energy scales in the Emery model poses a significant numerical challenge, particularly when high momentum resolution is required. One common approximation to simplify the calculations is to neglect comparatively small energy scales, such as $U_p \ll U_d$; however, even then, numerical simulations remain demanding. An alternative strategy to further reduce the complexity of the model is a Schrieffer-Wolff transformation [KK90], i.e., constructing an effective one-band model that describes the low-energy physics of the CuO_2 plane yielding

$$H_{\text{eff}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U_{\text{eff}} \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1.2)$$

Here $U_{\text{eff}} \approx U_d$, $t = t_{pd}^2/\Delta_\epsilon$ and $t' = t(t_{pp}/\Delta_\epsilon)$ are effective energies incorporating the three-band energy structure.

The reduction is controlled when $t_{pd} \ll U_d$ and $t_{pd} \ll \Delta_\epsilon$, where the charge-transfer energy is defined as $\Delta_\epsilon = \epsilon_d - \epsilon_p$. For cuprates, these conditions are only moderately satisfied. As a result, the mapping works qualitatively but is not quantitatively accurate. Because the separation of energy scales is not strong, it remains debated whether the single-band Hubbard model provides a sufficient minimal description of the cuprates. This issue will also be discussed in this work.

1.2.2 Hubbard model

To describe cuprate physics, we employ the Hubbard model of Eq. 1.2 rewritten as:

$$H = \sum_{\mathbf{r}\mathbf{r}'\sigma} -t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} - \mu \sum_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} \quad (1.3)$$

$$= \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \quad (1.4)$$

where $\mathbf{r}$ and $\mathbf{k}$ denote lattice sites in real space and wave vectors in momentum space, respectively, for a square lattice. The hopping matrix $t_{\mathbf{r}\mathbf{r}'}$ includes nearest-neighbor (t) and next-nearest-neighbor (t') hopping between lattice sites $\mathbf{r}$ and $\mathbf{r}'$. Upon Fourier transformation, this yields the tight-binding dispersion $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$. The second and third terms in the Hamiltonian correspond to the chemical potential μ and the on-site Coulomb interaction U , respectively.

Throughout this thesis, we simulate cuprate physics using t as the unit of energy and $U = 7t$ to model the strong Coulomb interaction on the copper orbital. We perform computations for several negative values of $t'/t = \{-0.30, -0.25, -0.20, -0.15\}$. The chemical potential μ is used to tune the doping p . We scan across the hole-doped regime at $T = 10^{-10}t$ and perform temperature sweeps at fixed values of μ slightly above and below the critical point.

It is well established in the literature that momentum correlations play an important role in the emergence of criticality [Gul+10; Niu24; Fer+09; Wu+18]. To solve the Hubbard model while incorporating the necessary momentum dependence, we employ a cluster extension of dynamical mean-field theory (DMFT), namely the dynamical cluster approximation (DCA). For this approach the lattice model is reduced to an effective

cluster representation:

$$H_{\text{imp}} = \sum_{\mathbf{R}\mathbf{R}'\sigma} -t_{\mathbf{R}\mathbf{R}'} c_{\mathbf{R}\sigma}^\dagger c_{\mathbf{R}'\sigma} - \mu \sum_{\mathbf{R}\sigma} n_{\mathbf{R}\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow} \quad (1.5)$$

$$= \sum_{\mathbf{K}\sigma} (\epsilon_{\mathbf{K}} - \mu) n_{\mathbf{K}\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow}, \quad (1.6)$$

where $\mathbf{R}$ and $\mathbf{K}$ denote cluster sites in real space and $\mathbf{k}$ -averages in momentum space, respectively.

1.3 Scope and Outline

The main focus of this thesis is the study of the Hubbard model defined in Eq. 1.4. To solve the lattice problem, we employ cluster dynamical mean field theory (cDMFT) with the numerical renormalization group (NRG) as the impurity solver at its core. This approach enables the computation of real-frequency correlation functions at low temperatures.

In Sec. 2.1, we provide a description of dynamical mean-field theory (DMFT) and its cluster extensions. Of the two prominent extensions, cellular DMFT (CDMFT) and the dynamical cluster approximation (DCA), we employ the latter, as it is computationally slightly less demanding. Cluster calculations are particularly taxing when using NRG as the impurity solver. DCA operates in a diagonal $\mathbf{k}$ -space representation in terms of cluster momenta $\mathbf{K}$, which simplifies the numerical treatment and reduces the computational effort.

Thereafter, in Sec. 2.2, we introduce the numerical renormalization group (NRG) as our cluster impurity solver, as well as its multipoint extension, mpNRG [KLD21; LKD21]. Although mpNRG is not the main focus of this thesis, several side projects were developed during the course of this PhD, representing initial steps toward a real-frequency dynamical vertex approximation (DΓA). The corresponding publications [P5; P6] with fourth and third author contribution. Since these publications are not related to the topic of criticality in the Hubbard model and spawned from the development of a methodical extension of NRG, they are not reprinted in this thesis.

The post-processing of our initial results drew our attention to the issue of periodization or interpolation. The cluster reduction of the lattice breaks translational symmetry in CDMFT and introduces discontinuities between momentum-averaged regions in DCA. Resolving these artifacts often leads to violations of causality. Ref. [Ver+22a] inspired a new approach to address these issues through a novel interpolation scheme based on frequency-independent matrix elements of the Liouvillian $\mathcal{L}$. We introduce this topic and present the corresponding publication [P1] in Sec. 2.4. In Sec. 2.5 we reprint the publication [P2], which spawned from the development of the Liouvillian interpolation and shows how to compute self-energies in a purely discrete fashion, without involving any broadening.

In Sec. 3, we present our results for the DCA+NRG computations. We begin, in Sec. 3.1, with a benchmark of our method against Ref. [Fer+09] and Ref. [Gul+10], which report a two-site and four-site DCA+QMC study, respectively. We briefly discuss cluster size dependence referring to results of a master's thesis which I have co-supervised [Niu24], which compares two-site DCA+NRG calculations for the Hubbard and Emery models. Sec. 3.2 presents evidence for a quantum critical point (QCP) at finite doping, $p^* \simeq 0.14$, with the corresponding publication attached [P3]. We observe a vanishing Fermi liquid scale in various correlation functions, accompanied by a reconstruction of the Fermi

surface driven by the onset of antiferromagnetic correlations. A follow-up discussion of dynamical scaling as a function of temperature is provided in Sec. 3.3, based on Ref. [P4]. In Sec. 4.1 we provide a conclusion of our results and an outlook for related future research topics is given in Sec. 4.2.

2 Methods

In this chapter, we introduce the methods used to solve the Hubbard model within the cluster representation of Eq. (1.6) and the self-consistent dynamical mean-field theory (DMFT) framework in Sec. 2.1 and the single-site version in Sec. 2.1.1. Thereafter, in Sec. 2.1.2, we discuss the most commonly used cluster extensions of DMFT, namely cellular DMFT (CDMFT) and the dynamical cluster approximation (DCA), as we employ a four-site impurity cluster. In Sec. 2.1.3, we provide an overview of the lattice integration procedure used.

The impurity problem is solved using the real-frequency numerical renormalization group (NRG), which is detailed in Sec. 2.2. Furthermore, we briefly discuss the multipoint extension of NRG (mpNRG) in Sec. 2.2.1, as several side projects emerged from the capability to compute real-frequency four-point vertex functions.

2.1 Dynamical mean field theory

Dynamical mean field theory (DMFT) [MV89; GK92; Geo+96] provides an impurity embedding scheme in which a correlated lattice problem is mapped onto an effective quantum impurity model embedded in a self-consistent bath. The impurity problem is solved using a suitable impurity solver. For the reader's convenience, Fig. 2.1 provides a graphical illustration of the DMFT self-consistency cycle, described below.

Starting from an initial guess for the dynamical mean field (bath hybridization function), the impurity Green's function and the corresponding impurity self-energy are computed. The impurity self-energy is then used as an approximation to the lattice self-energy, assuming locality. Using this self-energy, the lattice Green's function is obtained via momentum integration over the Brillouin zone.

From the resulting local lattice Green's function, an updated bath hybridization function is constructed, which defines a new impurity problem for the next iteration. This self-consistency cycle is repeated until convergence is achieved. Self-consistency is reached when the impurity Green's function coincides with the local lattice Green's function, ensuring that the impurity is embedded in a bath that faithfully represents the surrounding lattice.

2.1.1 Single-site DMFT

Single-site DMFT refers to a self-consistency cycle in which a single interacting impurity is embedded in a non-interacting bath. The effective Hamiltonian reads

$$H_{\text{DMFT}} = H_{\text{imp}} + H_{\text{hyb}} + H_{\text{bath}} \quad \text{with} \quad (2.1)$$

$$H_{\text{imp}} = \sum_{\sigma} \epsilon_d c_{\sigma}^{\dagger} c_{\sigma} + U n_{\uparrow} n_{\downarrow} , \quad (2.2)$$

$$H_{\text{hyb}} = \sum_{\mathbf{k}, \sigma} V_{\mathbf{k}\sigma} \left(b_{\mathbf{k}\sigma}^{\dagger} c_{\sigma} + \text{h.c.} \right) , \quad (2.3)$$

$$H_{\text{bath}} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}\sigma} b_{\mathbf{k}\sigma}^{\dagger} b_{\mathbf{k}\sigma} . \quad (2.4)$$

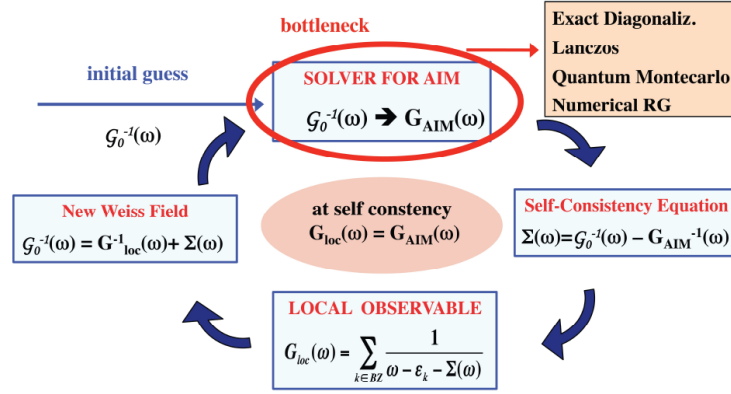


Figure 2.1 Schematic DMFT cycle, showing one iteration of the self-consistency scheme, where $\mathcal{G}_0(\omega)$, $G_{\text{AIM}}(\omega)$ and $G_{\text{loc}}(\omega)$ are bath, impurity and lattice Green's function, respectively. Figure taken from Ref. [Pel22].

Here, $c_\sigma^{(\dagger)}$ annihilates (creates) an electron on the impurity site, while $b_{\mathbf{k}\sigma}^{(\dagger)}$ acts on the bath degrees of freedom. The impurity number operator is $n_\sigma = c_\sigma^\dagger c_\sigma$. After integrating out the bath degrees of freedom, the impurity problem can be written in terms of an effective action,

$$S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^\dagger(\tau) \mathcal{G}_\sigma^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau) . \quad (2.5)$$

The non-interacting impurity (Weiss) Green's function is given in Matsubara frequency by

$$\mathcal{G}_\sigma^{-1}(i\omega_n) = i\omega_n + \mu - \epsilon_0 - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}\sigma}|^2}{i\omega_n - \epsilon_{\mathbf{k}\sigma}} = i\omega_n + \mu - \epsilon_0 - \Delta_\sigma(i\omega_n) , \quad (2.6)$$

where ϵ_0 is the local on-site energy of the lattice model and $\Delta_\sigma(i\omega_n)$ is the hybridization function. The impurity Green's function and self-energy are

$$G_{\sigma,\text{imp}}(\tau) = -\langle \mathcal{T} c_\sigma(\tau) c_\sigma^\dagger(0) \rangle_{S_{\text{eff}}} , \quad (2.7)$$

$$\Sigma_{\sigma,\text{imp}}(\omega) = \mathcal{G}_\sigma^{-1}(\omega) - G_{\sigma,\text{imp}}^{-1}(\omega) , \quad (2.8)$$

respectively, where $\mathcal{T}$ denotes the time-ordering operator. The impurity self-energy follows from the Dyson equation.

DMFT can be derived within the Baym–Kadanoff formalism [BK61; Bay62] as a stationary condition of the grand potential functional,

$$\Omega[G] = \Phi[G] + T \sum_{\mathbf{k},\sigma} [\ln G_{\mathbf{k}}(i\omega_n) - \Sigma_{\mathbf{k}}[G](i\omega_n) G_{\mathbf{k}}(i\omega_n)] , \quad (2.9)$$

where $\Phi[G]$ is the Luttinger–Ward (LW) functional [LW60; Pot03]. The stationary condition, $\delta\Omega/\delta G = 0$, leads to

$$\frac{\delta\Omega[G]}{\delta G_{\mathbf{k}}(i\omega_n)} = T \Sigma_{\mathbf{k}}[G](i\omega_n) + T G_{\mathbf{k}}^{-1}(i\omega_n) - T \mathcal{G}_{\mathbf{k}}^{-1}(i\omega_n) \stackrel{!}{=} 0 , \quad (2.10)$$

where the self-energy in the second term on the right-hand side is expressed via the Dyson equation, $\Sigma_{\mathbf{k}}(i\omega_n) = \mathcal{G}_{\mathbf{k}}^{-1}(i\omega_n) - G_{\mathbf{k}}^{-1}(i\omega_n)$. The variation of $\Phi[G]$ yields the self-energy as a functional of G ,

$$\frac{\delta\Phi[G]}{\delta G_{\mathbf{k}}(i\omega_n)} = T \Sigma_{\mathbf{k}}[G](i\omega_n). \quad (2.11)$$

Rearranging Eq. (2.10) gives the self-consistency condition

$$G_{\mathbf{k}}(i\omega_n) = \frac{1}{\mathcal{G}_{\mathbf{k}}^{-1}(i\omega_n) - \Sigma_{\mathbf{k}}[G](i\omega_n)}. \quad (2.12)$$

The DMFT approximation assumes the self-energy to be momentum-independent and local in U :

$$\Sigma_{\mathbf{r}\mathbf{r}'}(i\omega_n) = \delta_{\mathbf{r}\mathbf{r}'} \Sigma(i\omega_n) \quad \text{or} \quad \Sigma_{\mathbf{k}}(i\omega_n) = \Sigma(i\omega_n), \quad (2.13)$$

which in turn renders the Luttinger–Ward functional local, i.e., dependent only on the local Green’s function $G_{\text{loc}}(i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} G_{\mathbf{k}}(i\omega_n)$, so that

$$\Sigma[G](i\omega_n) = \frac{\delta\Phi[G_{\text{loc}}]}{\delta G_{\mathbf{k}}(i\omega_n)} = \frac{1}{N} \frac{\delta\Phi[G_{\text{loc}}]}{\delta G_{\text{loc}}(i\omega_n)} = \Sigma[G_{\text{loc}}](i\omega_n) \quad (2.14)$$

This leads to a local version of the self-consistency condition (Eq. (2.12)) when summing over $\mathbf{k}$:

$$G_{\text{loc}}(i\omega_n) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\mathcal{G}_{\mathbf{k}}^{-1}(i\omega_n) - \Sigma[G_{\text{loc}}](i\omega_n)}. \quad (2.15)$$

The computation of $\Sigma[G_{\text{loc}}](i\omega_n)$ for a given G_{loc} is provided by a reference impurity model with interaction U . Since the DMFT approximation to the lattice Luttinger–Ward functional is $\Phi[G] \approx \Phi[G_{\text{loc}}]$, solving the impurity model and computing its Green’s function $G_{\text{imp}}(i\omega_n)$ and self-energy $\Sigma_{\text{imp}}(i\omega_n)$ allows us to evaluate the DMFT Σ -functional:

$$\Sigma[G_{\text{imp}}](i\omega_n) = \Sigma_{\text{imp}}(i\omega_n). \quad (2.16)$$

Since we want to evaluate the functional at G_{loc} to solve the local self-consistency condition (Eq. (2.18)), a second self-consistency condition is required to match the impurity model to the lattice:

$$G_{\text{imp}}(i\omega_n) = G_{\text{loc}}(i\omega_n), \quad (2.17)$$

which is used to adjust the non-interacting (Weiss) Green’s function of the impurity model. This condition ensures that the impurity Green’s function converges iteratively to the local lattice Green’s function, effectively mapping the lattice problem onto the impurity model. The Weiss field can be written as $\mathcal{G}_{\text{imp}}^{-1}(i\omega_n) = i\omega_n + \mu - \epsilon_0 - \Delta(i\omega_n)$, where ϵ_0 is the local on-site energy of the lattice model, and the hybridization $\Delta(i\omega_n)$ describes the coupling of the impurity to the bath.

2.1.2 Cluster extensions of DMFT

The previous description of DMFT considers only a purely local self-energy. However, many applications including our investigation of cuprate physics using the Hubbard

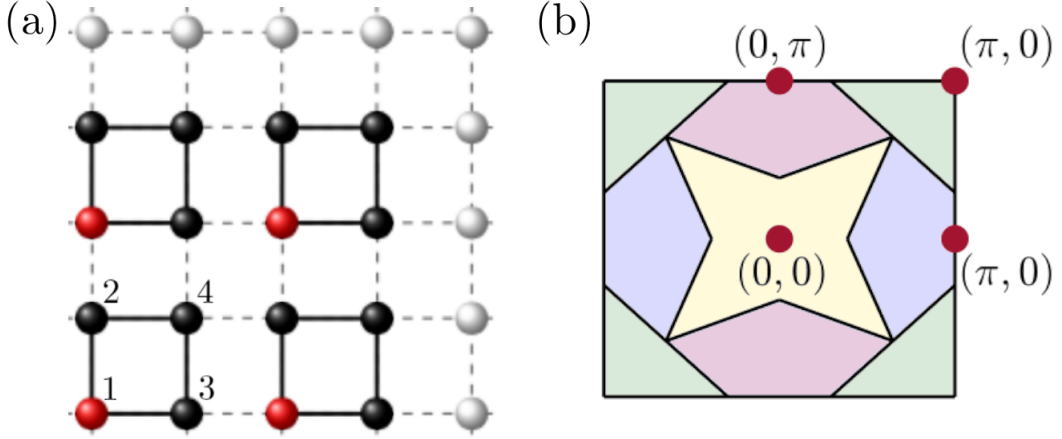


Figure 2.2 (a) Black real spaces cluster forms the impurity for a cellular DMFT extension. Here, a square lattice separated into 2×2 -site clusters, where red sites indicated the cluster origin in real space and a the basis of a single-site DMFT. Adapted from Ref. [Kle+20a]. (b) Cluster impurity in momentum space with $\mathbf{k}$ averaged patches forms cluster impurity for dynamical cluster approximation. Here, momentum space separation of the Brillouin zone of square lattice into four patches, where red dots mark the patch center and patch averaged momenta $\mathbf{K}$.

model require some momentum resolution. In the following, we discuss two commonly used extensions: (i) cellular DMFT (CDMFT) and (ii) dynamical cluster approximation (DCA). The basis of these extensions is the replacement of the single-site impurity with a cluster impurity, which allows short-range spatial correlations and partial momentum dependence of the self-energy to be captured [Mai+05; Pot18].

2.1.2.1 Cellular DMFT

Cellular DMFT (CDMFT) is a cluster method based on a real-space ansatz for the impurity [Kot+01; Mai+05; Sta+06]. The single-site impurity is extended to a cluster comprising multiple lattice sites, as illustrated in Fig. 2.2(a). As an example, we consider a square lattice partitioned into clusters of size 2×2 sites. In contrast to single-site DMFT, where the self-energy is assumed to be purely local, CDMFT allows for short-range spatial correlations within the cluster by promoting the self-energy to a matrix in the cluster-site indices. Correlations inside the cluster are therefore treated explicitly, while correlations beyond the cluster size are neglected. Since the construction is formulated in real space, translational symmetry of the original lattice is explicitly broken. Instead, the lattice is tiled by identical clusters, forming a superlattice whose unit cell consists of the entire cluster. Translational symmetry is thus preserved only with respect to translations between clusters, but not between individual lattice sites within a cluster.

The real-space formulation of CDMFT generalizes the single-site method to a matrix-valued description:

$$[G_{\text{loc}}(i\omega_n)]_{\mathbf{R}\mathbf{R}'} = \frac{1}{N} \sum_{\mathbf{k}} \left[\mathcal{G}_{\mathbf{k}}^{-1}(i\omega_n) - \Sigma[G_{\text{loc}}](i\omega_n) \right]_{\mathbf{R}\mathbf{R}'}^{-1}. \quad (2.18)$$

Here, the matrix indices $\mathbf{R}$, $\mathbf{R}'$ label the cluster sites or, more generally, additional internal degrees of freedom such as orbitals. This matrix structure distinguishes CDMFT from single-site DMFT, where all quantities are scalar, and from the dynamical cluster approximation (DCA), where momentum-space coarse graining is employed and lattice translational symmetry of the original lattice is maintained.

2.1.2.2 Dynamical cluster approximation

The dynamical cluster approximation (DCA) is a cluster extension of DMFT formulated in momentum space [Het+98; Het+00; Mai+05]. Instead of partitioning the lattice into real-space clusters as in CDMFT, the Brillouin zone is divided into N_c momentum patches. Each patch is represented by a cluster momentum $\mathbf{K}$, and the lattice self-energy is approximated as being constant within each patch, $\Sigma_{\mathbf{k}}(i\omega_n) \approx \Sigma_{\mathbf{K}}(i\omega_n)$, for all $\mathbf{k}$ belonging to the patch centered around $\mathbf{K}$. As illustrated in Fig. 2.2(b), a common choice is a four-site cluster with star-like patching of the Brillouin zone. In this construction, the Brillouin zone is divided into four momentum sectors centered at the high-symmetry points $\mathbf{K} = (0, 0)$, $\mathbf{K} = (0, \pi)$, $\mathbf{K} = (\pi, 0)$ and $\mathbf{K} = (\pi, \pi)$, respectively. The term star patching refers to grouping together all momenta that are related by the point-group symmetries of the lattice into symmetry-equivalent sectors (“stars”) around these cluster momenta. All lattice momenta within a given sector share the same self-energy, which provides a piecewise-constant approximation to $\Sigma_{\mathbf{k}}(i\omega_n)$. The DCA self-consistency condition is obtained by coarse graining the lattice Green’s function over each momentum patch,

$$G_{\mathbf{K}}(i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \text{patch } \mathbf{K}} \frac{1}{\mathcal{G}_{\mathbf{k}}^{-1}(i\omega_n) - \Sigma_{\mathbf{K}}(i\omega_n)}. \quad (2.19)$$

This coarse-grained Green’s function defines the cluster impurity problem, whose solution yields the cluster self-energy $\Sigma_{\mathbf{K}}(i\omega_n)$. In contrast to CDMFT, the construction of DCA preserves the translational symmetry of the original lattice, since the approximation is performed in reciprocal space rather than real space. Consequently, the self-energy remains diagonal in momentum space and periodic in the original Brillouin zone. Spatial correlations are incorporated up to a length scale set by the cluster size, while the momentum resolution improves systematically with increasing N_c . For the four-site star patching shown in Fig. 2.2(b), this momentum differentiation already captures the essential distinction between nodal and antinodal regions of the Brillouin zone, which is particularly relevant for studies of the Hubbard model and cuprate physics. In the following, we therefore adopt DCA as our method of choice, as it provides direct momentum resolution while preserving lattice translational symmetry.

2.1.3 Lattice integrals of the Green’s function

Since we use DCA as method of choice the following section is formulated in terms of DCA. In DCA, the lattice Green’s function entering the self-consistency condition is obtained by coarse graining over momentum patches. For a given cluster momentum $\mathbf{K}$, one computes

$$G_{\mathbf{K}}(i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \text{patch } \mathbf{K}} \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{K}}(i\omega_n)}, \quad (2.20)$$

where $\epsilon_{\mathbf{k}}$ is the lattice dispersion and $\Sigma_{\mathbf{K}}(i\omega_n)$ is assumed constant within the patch. This expression represents a coarse-grained lattice integration, i.e., an average of the lattice Green’s function over all momenta belonging to the patch centered at $\mathbf{K}$.

Since the self-energy is constant inside each patch, the only momentum dependence in the denominator arises from the dispersion $\epsilon_{\mathbf{k}}$. Therefore, the momentum sum can be rewritten as an integral over the partial density of states (DOS) associated with the patch.

Defining the patch-resolved density of states $\rho_{\mathbf{K}}(\epsilon) = \frac{N_c}{N} \sum_{\mathbf{k} \in \text{patch } \mathbf{K}} \delta(\epsilon - \epsilon_{\mathbf{k}})$, the coarse-grained Green's function becomes

$$G_{\mathbf{K}}(i\omega_n) = \int \frac{d\epsilon \rho_{\mathbf{K}}(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_{\mathbf{K}}(i\omega_n)}. \quad (2.21)$$

Thus, the Brillouin-zone sum is transformed into a one-dimensional energy integral weighted by the patch DOS.

2.1.3.1 Asymmetric estimator for lattice integration

We use a DOS integration of Eq. (2.21) for a stable computation of the local Green's function. To update the hybridization $\Delta_{\mathbf{K}}(i\omega_n)$ for the next DCA iteration we use an asymmetric estimator approach [Kug22; BSB22],

$$\Delta_{\mathbf{K}}(i\omega_n) = \frac{F_{\mathbf{K}}(i\omega_n)}{G_{\mathbf{K}}(i\omega_n)} - \epsilon_{\mathbf{K}} \quad (2.22)$$

with

$$F_{\mathbf{K}}(i\omega_n) = \int \frac{d\epsilon \rho_{\mathbf{K}}(\epsilon) \epsilon}{i\omega_n + \mu - \epsilon - \Sigma_{\mathbf{K}}(i\omega_n)} \quad \text{and} \quad \epsilon_{\mathbf{K}} = \int d\epsilon \rho_{\mathbf{K}}(\epsilon). \quad (2.23)$$

Eq. (2.22) is derived from the DCA approximation of the $\mathbf{k}$ -dependent local lattice Green's function

$$G_{\mathbf{K}}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon(\mathbf{k}) - \Sigma_{\mathbf{K}}(i\omega_n)}, \quad (2.24)$$

where $\epsilon(\mathbf{k})$ is the lattice dispersion. Rewriting and averaging over patches gives

$$[i\omega_n + \mu - \Sigma_{\mathbf{K}}(i\omega_n)] G_{\mathbf{K}}(i\omega_n) - F_{\mathbf{K}}(i\omega_n) = 1, \quad (2.25)$$

where

$$G_{\mathbf{K}}(i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \text{patch } \mathbf{K}} G_{\mathbf{K}}(\mathbf{k}, i\omega_n), \quad (2.26a)$$

$$F_{\mathbf{K}}(i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \text{patch } \mathbf{K}} \epsilon(\mathbf{k}) G_{\mathbf{K}}(\mathbf{k}, i\omega_n). \quad (2.26b)$$

Adding the identity $0 = \epsilon_{\mathbf{K}} + \Delta_{\mathbf{K}}(i\omega_n) - \epsilon_{\mathbf{K}} - \Delta_{\mathbf{K}}(i\omega_n)$ to the first term of Eq. (2.25) gives

$$[G_{\mathbf{K}}^{-1}(i\omega_n) + \epsilon_{\mathbf{K}} + \Delta_{\mathbf{K}}(i\omega_n)] G_{\mathbf{K}}(i\omega_n) - F_{\mathbf{K}}(i\omega_n) = 1, \quad (2.27)$$

where $G_{\mathbf{K}}^{-1}(i\omega_n) = i\omega_n + \mu - \epsilon_{\mathbf{K}} - \Delta_{\mathbf{K}}(i\omega_n) - \Sigma_{\mathbf{K}}(i\omega_n)$. Rearranging this expression leads to the asymmetric estimator for the hybridization, Eq. (2.22).

Eq. (2.22) provides a more stable computation of the hybridization than the Dyson equation $\Delta_{\mathbf{K}}(i\omega_n) = i\omega_n + \mu - \epsilon_{\mathbf{K}} - \Sigma_{\mathbf{K}}(i\omega_n) - G_{\mathbf{K}}^{-1}(i\omega_n)$. Inverting numerical zeros of $G_{\mathbf{K}}(i\omega_n)$ and subtracting these from $\Sigma_{\mathbf{K}}(i\omega_n)$ in the Dyson equation leads to large peak heights, that scale with numerical errors. Consequently, this approach can produce large errors near the poles of $\Sigma_{\mathbf{K}}(i\omega_n)$. In contrast, these errors cancel in the quotient form of Eq. (2.22), keeping numerical errors small.

Similar to this approach a symmetric estimator approach or general cavity scheme can be set up using a third estimator

$$I_{\mathbf{K}}(i\omega_n) = \frac{N_c}{N} \sum_{\mathbf{k} \in \text{patch } \mathbf{K}} \epsilon(\mathbf{k}) G_{\mathbf{K}}(\mathbf{k}, i\omega_n) \epsilon(\mathbf{k}). \quad (2.28)$$

This yields an established way, which is detailed in Ref. [BSB22] to compute the hybridization

$$\Delta_{\mathbf{K}}(i\omega_n) = I_{\mathbf{K}}(i\omega_n) - F_{\mathbf{K}}^\dagger(i\omega_n) G_{\mathbf{K}}^{-1}(i\omega_n) F_{\mathbf{K}}(i\omega_n). \quad (2.29)$$

In addition to a more stable computation of the hybridization, it allows the inclusion of spatial correlation to the DMFT cycle (see Ref. [BSB22]). Very recently, it was recognized that this expression can be recast into an even more computationally stable form using the Schur complement formula, see Sec. [P2]. This approach (not used in the present work) makes it possible to devise a DMFT self-consistency loop involving purely discrete representations of the hybridization function and self-energy. In this work, we employ the asymmetric, continuous scheme rather than the symmetric one, as the latter entails higher computational costs. For future work, however, we recommend using the more stable symmetric approach, re-expressed via the Schur complement formula.

2.2 Numerical renormalization group

In DCA, each cluster momentum $\mathbf{K}$ is mapped onto an effective impurity model with a hybridization function $\Delta_{\mathbf{K}}(z)$ (here we use $z = \omega + i\eta$ as frequency argument, since NRG is a real frequency impurity solver) that encodes the coupling of the cluster impurity to the self-consistent bath. To solve this impurity problem, we employ the numerical renormalization group (NRG) [Wil75; BCP08; LW16; AS05; Sta+16; KWW80; Mit+14], which is particularly suited for resolving low-energy excitations of strongly correlated systems.

The continuous bath defined by $\Delta_{\mathbf{K}}(z)$ is discretized on a logarithmic grid in order to resolve low-energy excitations near the Fermi level with high accuracy. Using a discretization parameter $\Lambda > 1$, the hybridization is divided into intervals whose widths decrease logarithmically toward the Fermi energy. Within each interval, the bath degrees of freedom are represented by a single effective orbital. This procedure transforms the impurity problem into a one-dimensional tight-binding chain with nearest-neighbor hopping, which is called a Wilson chain [Wil75]. The resulting Hamiltonian reads

$$H_{\text{chain}, \mathbf{K}} = H_{\text{loc}} + \sum_{n=0}^{\infty} t_n (f_n^\dagger f_{n+1} + \text{h.c.}) + \sum_{n=0}^{\infty} \epsilon_n f_n^\dagger f_n, \quad (2.30)$$

where H_{loc} contains the interacting cluster degrees of freedom (e.g., the Hubbard interaction U), and the Wilson chain parameters t_n and ϵ_n are obtained from the hybridization function $\Delta_{\mathbf{K}}(z)$ via a tridiagonalization procedure. The impurity couples only to the first Wilson site f_0 , which encodes the full hybridization to the bath.

Each Wilson chain site f_n represents a discretized bath orbital associated with a characteristic energy scale $\sim \Lambda^{-n/2}$. The hopping amplitudes t_n decrease exponentially with increasing n , generating a separation of energy scales along the chain. This hierarchical structure enables the iterative diagonalization scheme of NRG: at each iteration, one additional Wilson site is added and high-energy states are truncated, while the

low-energy sector, with N_{keep} multiples, is retained. As a consequence, the method systematically resolves the many-body spectrum from high energies down to arbitrarily low temperatures.

To improve the efficiency of the NRG calculations, we exploit the symmetries of the Hamiltonian, which allows for a block-diagonal decomposition into quantum number sectors and significantly reduces the effective Hilbert space size. The symmetry handling is implemented using the QSpace library [Wei12a; Wei12b; Wei20; Wei24b; Wei24a], which incorporates Abelian and non-Abelian symmetries. In our DCA+NRG calculations, we explicitly employ U(1) charge conservation and SU(2) spin symmetry.

In cluster impurity problems, such as those arising in DCA, multiple bath channels couple to different cluster momenta. A straightforward Wilson mapping would generate several independent Wilson chains that are added simultaneously at each iteration, leading to an exponential growth of the Hilbert space with the number of channels. To mitigate this, we employ interleaved NRG (iNRG) [Mit+14; Sta+16], in which the Wilson chains corresponding to different bath channels are interwoven into a single effective chain. Instead of adding one site per channel at each iteration, the sites of the different channels are added sequentially in an interleaved fashion. This preserves the logarithmic energy scale separation while reducing the growth of the Hilbert space at each iteration, thereby significantly improving numerical efficiency. Interleaving is particularly advantageous for multiorbital or cluster DMFT calculations, where it enables the treatment of several hybridization functions $\Delta_{\mathbf{K}}(z)$ within a single NRG flow while maintaining controlled truncation and accurate low-energy resolution.

Real-frequency Green's functions are constructed from the matrix elements of impurity operators between eigenstates obtained at successive NRG iterations. Within the Lehmann representation, the corresponding discrete spectral function reads

$$A_{\text{disc},\mathbf{K}}(\omega) = \sum_{m,n} |\langle m | c_{\mathbf{K}}^{\dagger} | n \rangle|^2 \delta(\omega - E_n + E_m) (e^{-\beta E_n} + e^{-\beta E_m}), \quad (2.31)$$

where $|m\rangle$, $|n\rangle$ denote many-body NRG eigenstates with energies E_m , E_n , respectively. The Boltzmann factors ensure the correct thermal weighting at finite temperature. Due to the logarithmic discretization of the bath, each NRG iteration contributes spectral weight on an exponentially decreasing energy scale. As a result, the spectral function consists of a set of logarithmically spaced discrete δ -peaks, which naturally provide very high resolution at low frequencies while remaining coarser at high energies.

The contributions from all iterations are combined using the complete Anders-Schiller basis [AS05], ensuring proper sum rules and thermodynamic consistency. Although the NRG truncates the Hilbert space at each iteration by retaining only the lowest-energy states, completeness is restored by systematically incorporating the discarded states from all iterations. At iteration N , the eigenstates are split into kept and discarded states; while only the kept states are propagated forward, the collection of all discarded states, together with the remaining Wilson chain degrees of freedom, forms an exact resolution of the identity of the full Hilbert space. Correlation functions are computed within this complete basis, assigning spectral contributions to the iteration whose characteristic energy scale matches the excitation energy. This guarantees exact sum rules, thermodynamic consistency, and controlled finite-temperature dynamics.

To obtain continuous real-frequency Green's functions, the discrete spectrum is subsequently broadened using a logarithmic Gaussian (log-Gaussian) kernel adapted to the underlying energy grid [LW16]. This controlled broadening preserves the high resolution near the Fermi level while avoiding artificial oscillations at higher energies. The resulting

continuous spectral function is then used to reconstruct the retarded Green's function via Kramers–Kronig relations.

To obtain the impurity self-energy $\Sigma_{\mathbf{K}}(z)$ in a numerically stable manner, we employ the symmetric improved estimator [Kug22], derived from the equation of motion $\langle\{A, B\}\rangle = \langle\langle zA - [A, H], B \rangle\rangle_z$. We compute three correlators using NRG:

$$G(z) = \langle\langle c, c^\dagger \rangle\rangle_z, \quad F(z) = \langle\langle c, q^\dagger \rangle\rangle_z, \quad I(z) = \langle\langle q, q^\dagger \rangle\rangle_z, \quad (2.32)$$

where $q = [c, H_{\text{int}}]$ and H_{int} denotes the interacting part of the impurity Hamiltonian. The self-energy is then obtained from

$$\Sigma(z) = I(z) - F^\dagger(z)G^{-1}(z)F(z). \quad (2.33)$$

This formulation avoids the direct Dyson inversion of the Green's function and significantly improves numerical stability, particularly near zeros of $G(z)$. Eq. (2.33), too, can be recast into a numerically more stable form using the Schur complement formula, see Sec. [P2]. For future work, we recommend following that approach.

2.2.1 Multipoint NRG

Beyond computing single-particle Green's functions and self-energies with NRG, one often requires higher-order correlation functions, such as three- and four-point correlators, to describe multiparticle excitations, response functions, vertex functions, and effective interactions in strongly correlated systems. The multipoint NRG (mpNRG), introduced in Refs. [KLD21; LKD21; Lih+24], provides a numerically exact strategy for computing these multipoint correlators in Matsubara and Keldysh formalism corresponding to imaginary and real frequency descriptions, respectively.

The multipoint correlators are expressed in terms of partial spectral functions (PSFs), which encode the contributions of various particle combinations to correlated dynamics. Multipoint NRG calculates these PSFs by generalizing the NRG approach used for two-point functions to three- and four-point functions. The method systematically resolves multiparticle excitations down to the lowest energy scales by evaluating matrix elements involving multiple creation and annihilation operators on the Wilson chain basis produced by the NRG iterative diagonalization.

Convolution kernels are applied to the PSFs to construct full multipoint correlators in different frequency formalisms.

The new implementation of multipoint NRG within our NRG library opens a promising avenue for future research, e.g. for a real frequency dynamical vertex approximation (DFA). During the course of this thesis, several side projects emerged, including tests of Ward identity fulfillment within the mpNRG and improvements in vertex computations using a tensor cross interpolation (TCI) algorithm [Rit+24; Roh+25]. The computation of partial spectral functions (PSFs) and vertex functions led to third- and fourth-author contributions to the publications [P5; P6].

2.3 Cluster DMFT interpolation

The analysis and post-processing of DCA results typically involve interpolation schemes that restore a smooth $\mathbf{k}$ -dependence across the Brillouin zone [SPP02; SK06b; BK02; BPK04; Kle+20b]. Since DCA yields quantities that are constant within each momentum patch, the resulting lattice functions exhibit artificial discontinuities at patch boundaries. To reconstruct a continuous momentum dependence, one introduces smooth $\mathbf{k}$ -dependent

interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}$, which distribute the cluster quantities $Q_{\mathbf{K}}(z)$ over the full Brillouin zone, where $Q(z)$ denotes a frequency-dependent quantity, such as the self-energy $\Sigma(z)$ or cumulant $M(z) = [z + \mu - \Sigma(z)]^{-1}$. The interpolated quantity is then given by

$$Q_{\mathbf{k}}(z) = \sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} Q_{\mathbf{K}}(z). \quad (2.34)$$

The interpolation weights $\alpha_{\mathbf{k},\mathbf{K}}$ are constructed to satisfy normalization, $\sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} = 1$, and to reproduce the original patch averages upon $\mathbf{k}$ averaging.

A similar post-processing procedure is used in CDMFT to recover the translational symmetry that is inherently broken by the cluster construction. In this periodization scheme, the lattice quantity is reconstructed from the cluster Green's function, self-energy, or cumulant as

$$Q_{\mathbf{k}}(z) = \sum_{\mathbf{r},\mathbf{r}'} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} Q_{\mathbf{r}-\mathbf{r}'}(z), \quad (2.35)$$

where $Q_{\mathbf{r}-\mathbf{r}'}(z)$ is defined on the cluster sites, and the sum runs over all cluster site pairs. Periodization restores a smooth $\mathbf{k}$ -dependence over the Brillouin zone while preserving the local correlations captured by the cluster.

Different choices of Q for instance can lead to slight variations in the reconstructed lattice quantities. Cumulant periodization often provides better analytic properties and improved momentum-space interpolation, particularly in strongly correlated systems.

Both approaches, CDMFT periodization and DCA interpolation, can suffer from causality issues. The cluster quantities contain only a truncated portion of the full lattice information, limited by the cluster size. Reconstructing frequency dependent quantities from these finite clusters via periodization or interpolation can produce ringing artifacts, which violate causality [Oka+03].

Several strategies have been proposed to enforce causality, such as superlattice averaging or rescaling the interpolation functions. However, these procedures introduce additional approximations and can distort the spectral features of the lattice Green's function or self-energy. The limitations of these approaches and their impact on spectral accuracy are discussed in detail in Ref. [Ver+22b].

These shortcomings, together with the findings of Ref. [Ver+22b], inspired us to develop a new approach to periodization and interpolation, where “interpolation” serves as an umbrella term for both CDMFT periodization and DCA interpolation. Our method is based on the interpolation of irreducible Liouvillian matrix elements, providing a novel scheme for cluster methods [P1]. In this work, we show how to extract the irreducible Liouvillian matrix elements of the self-energy via a Lanczos recursion, representing the self-energy as a continued fraction expansion (CFE).

By interpolating these physical, frequency-independent matrix elements, causality is strictly preserved, since the Liouvillian $\mathcal{L}$ remains Hermitian after interpolation. An additional advantage is that the nonlinear frequency dependence of the CFE naturally distributes spectral weight more efficiently, avoiding the artifacts and limitations of previous interpolation methods.

2.3.1 Discrete representation of the self-energy

To use our interpolation scheme we determine a continued fraction expansion of the self-energy to extract the matrix elements of the one-particle irreducible part of the Liouvillian. To this end, we compute the discrete self-energy from the Green's function through a

discrete version of the self-energy trick of Ref. [Kug22], using the Schur-complement. This computation sparked the idea of a fully discrete dynamical mean field theory. This would eliminate any broadening artifacts from discrete impurity solvers such as NRG or ED.

At the same time a similar idea was proposed by A. Zacinskis and M. W. Haverkort. This lead to a collaboration between multiple groups and a publication with third author contribution [P2].

Liouvillian interpolation of the self-energy of cluster dynamical mean field theories

by

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Liouvillian interpolation of the self-energy of cluster dynamical mean-field theories

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Two widely-used non-local extensions of dynamical mean field theory (DMFT), cellular DMFT (CDMFT) and the dynamical cluster approximation (DCA), both yield self-energies marred by having some unphysical properties: CDMFT yields real-space self-energies that are not translationally invariant, and DCA yields momentum-space self-energies with discontinuities in their momentum dependence. It is often desirable to remove these flaws by post-processing cluster DMFT results, using strategies called periodization for CDMFT and interpolation for DCA—for brevity, we refer to both cases as *interpolation*. However, traditional interpolation approaches struggle to capture intricate structures such as hole pockets in the hole-doped square-lattice Hubbard model, as highlighted in [Phys. Rev. B **105**, 35117 \(2022\)](#). Further, these approaches interpolate frequency-dependent functions, which may lead to causality violations. Here, we propose *Liouvillian interpolation*, a novel, intuitive, and robust scheme for interpolating cluster DMFT results. Our key idea is to interpolate frequency-independent matrix elements of the single-particle irreducible part of the Liouvillian, obtained from a continued-fraction expansion of the cDMFT self-energy. We demonstrate that the ingredients of such an expansion possess a more local Fourier expansion than the functions involved in traditional interpolation schemes, and that Liouvillian interpolation inherently conserves causality. We illustrate our method for the one-dimensional Hubbard model using CDMFT, and for the two-dimensional Hubbard model using four-patch DCA. For the latter, we find that $\mathcal{L}$ -interpolation can (depending on doping) yield Fermi and Luttinger arcs which together form a closed surface.

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I. INTRODUCTION

Cluster dynamical mean-field theories (cDMFT) [1–14] are commonly used to describe strong but short-ranged non-local correlations beyond single-site dynamical mean-field theory (DMFT) [15]. They effectively capture strongly correlated phenomena that may be driven by short-ranged correlations, such as the pseudogap phase in cuprates [5, 11, 12, 16–20], certain types of heavy-fermion quantum criticality [21–23], strange metals [24–27], Hund’s coupling [28, 29] or multi-orbital systems [30, 31].

The most commonly used cDMFT methods are cellular DMFT (CDMFT) [2], which couples a real-space cluster of sites to self-consistent baths, thereby breaking translation symmetry; and the dynamical cluster approximation (DCA) [3, 4], which coarse-grains the Brillouin zone into patches and couples these to self-consistent baths, thereby introducing artificial discontinuities in momentum space. The lack of periodicity for CDMFT results (implying real-space discontinuities) and the lack of a smooth momentum dependence for DCA results are unphysical. Removing these flaws requires the cDMFT results to be post-processed. CDMFT results have to be periodized to restore real-space translational invariance;

loosely speaking, this amounts to interpolating across cluster boundaries to remove the real-space discontinuities associated with non-periodic behavior. DCA results have to be interpolated across DCA patch boundaries to restore a smooth momentum dependence [1, 8–12, 14]. For brevity, we will use “interpolation” as an umbrella term for both CDMFT periodization and DCA interpolation. It is to be understood that in the context of CDMFT, “interpolation” refers to “periodization”.

In this work, we will focus on interpolating the single-particle Green’s function, G , and related quantities like the self-energy, Σ , and the cumulant, M . In the momentum/frequency representation, they are related by

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)}, \quad (1a)$$

$$M_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \Sigma_{\mathbf{k}}(\omega)}. \quad (1b)$$

Instead of G , Σ or M , we will generically write Q for the quantity to be interpolated. In general, $Q_{\mathbf{k}}$ and $\tilde{Q}_{\mathbf{r}}$, the momentum and position representations of Q , are related by a Fourier transformation. However, approximate methods such as CDMFT or DCA yield $\tilde{Q}_{\mathbf{r}}$ only for a limited range of $\mathbf{r}$ values, say with $|\mathbf{r}| \leq R$, where the distance cutoff R is determined by the cluster size (for CDMFT) or the number of momentum patches (for DCA). Thus, interpolation schemes amount to approxi-

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mating $Q_{\mathbf{k}}$ by a *truncated* Fourier Ansatz,

$$Q_{\mathbf{k}}(\omega) \simeq \sum_{\mathbf{r}, |\mathbf{r}| \leq R} \bar{Q}_{\mathbf{r}}(\omega) e^{-i\mathbf{k} \cdot \mathbf{r}}. \quad (2)$$

Here, $\bar{Q}_{\mathbf{r}}$ has to be estimated from quantities computed on the cluster (for CDMFT) or the Brillouin zone patches (for DCA). In the case of CDMFT, commonly used schemes for this purpose are superlattice averaging [11] or center-focused extrapolation [32]. Other related quantities are then derived from Q ; for example, when Σ is interpolated via Eq. (2), that also determines G and M .

It is common knowledge among practitioners of cDMFT that the quality and reliability of the interpolation scheme is quite sensitive to the choice of Q . A particularly striking example was recently pointed out by Verret *et al.* [33]. They analyzed the limitations of existing choices for Q in the context of a long-standing question on the pseudogap phase of underdoped cuprates: Does the Fermi surface exhibit hole or electron pockets, as deduced from various transport experiments [34, 35], or disconnected Fermi arcs, as indicated by angle-resolved photoemission spectroscopy (ARPES) [36, 37]? Verret *et al.* [33] have argued that “contrary to previous claims [11, 12, 16, 38], cDMFT schemes cannot discriminate between Fermi arcs and hole pockets” (with the implication that previous cDMFT work attempting to answer the aforementioned question is inconclusive). They illustrated this for a Yang-Rice-Zhang (YRZ) [39] toy-model self-energy with built-in hole pockets: when they approximated its self-energy in CDMFT fashion and then periodized it, their M - and G -periodization schemes both yielded Fermi arcs [33] instead of reproducing the hole pockets. Verret *et al.* argued that this failure is due to “neglecting the self-energy between clusters”. They then presented a so-called *compact tiling* scheme that includes estimates of these neglected parts, see Ref. 33 for details. For the YRZ toy model, compact tiling successfully recovers the expected hole pockets. However, their scheme was formulated in a manner not applicable to general cDMFT calculations.

The fact that the quality of interpolated cDMFT results depends strongly on the choice of Q can be expected on general grounds. In Eq. (2), the Fourier truncation at $|\mathbf{r}| \leq R$ introduces errors. To limit these, it is preferable for $\bar{Q}_{\mathbf{r}}(\omega)$ to have (i) a short-ranged dependence on $\mathbf{r}$, and (ii) a weak (or no) dependence on ω . Different choices for Q satisfy these criteria to different degrees, leading to errors of differing severity. Regarding (ii), we note that if $\bar{Q}_{\mathbf{r}}(\omega)$ does depend significantly on ω , then the truncation of the Fourier series can cause unintended (even unacceptable) modifications in the analytic structure of $Q_{\mathbf{k}}(\omega)$. An example is Σ -interpolation: if $\tilde{\Sigma}_{\mathbf{r}}(\omega)$ depends strongly on ω , the truncation to $|\mathbf{r}| \leq R$ can cause $\text{Im}\Sigma_{\mathbf{k}}(\omega)$ to become positive for some values of ω and $\mathbf{k}$, implying a violation of causality for $G_{\mathbf{k}}(\omega)$ [10, 38].

In this paper, we propose the Liouvillian, $\mathcal{L}$, as a new and previously unexplored quantity for interpolation (i.e. we choose $Q = \mathcal{L}$). Our scheme, which we

call $\mathcal{L}$ -interpolation, is based on a general, exact relation between the self-energy and the Liouvillian: if the self-energy is expressed through a continued-fraction expansion (CFE), its CFE coefficients are matrix elements of the single-particle irreducible part of the Liouvillian in a Krylov space obtainable via a Lanczos scheme. For a lattice model, these matrix elements are generically translation-invariant and smooth functions of $\mathbf{k}$. However, when Liouvillian matrix elements are extracted from the CFE expansion of a self-energy computed using CDMFT or DCA, they either do not satisfy translation invariance or exhibit discontinuities in $\mathbf{k}$ -space, respectively. Our $\mathcal{L}$ -interpolation scheme restores translation invariance or smooth $\mathbf{k}$ -dependence by interpolating the single-particle irreducible Liouvillian matrix elements obtained from CDMFT or DCA self-energies, respectively: using superlattice averaging [11] for CDMFT or a self-consistency condition for DCA, respectively, we obtain estimates for the matrix elements of $\tilde{\mathcal{L}}_{\mathbf{r}}$, and insert these into the truncated Fourier ansatz (2) for $\mathcal{L}_{\mathbf{k}}$. The resulting matrix elements of $\mathcal{L}_{\mathbf{k}}$ serve as interpolated CFE coefficients – we insert them into the CFE of the self-energy, thereby obtaining an interpolated self-energy and Green’s function.

$\mathcal{L}$ -interpolation has two properties that are very favorable: (i) $\tilde{\mathcal{L}}_{\mathbf{r}}$ appears to be shorter-ranged than $\tilde{\Sigma}_{\mathbf{r}}$ or $\tilde{M}_{\mathbf{r}}$ (according to some case studies presented below). (ii) Since the Liouvillian is, by definition, independent of frequency, its interpolated version remains hermitian, thus ensuring causality for the resulting self-energy. From a more general perspective: interpolating $\mathcal{L}$ corresponds to directly interpolating the time-evolution generator for operators. This ensures that unitarity of the time evolution and therefore causality are preserved.

For the phenomenological YRZ self-energy ansatz of Ref. 33, $\mathcal{L}$ -interpolation (along with a suitable choice of $\tilde{\mathcal{L}}_{\mathbf{r}}$) is equivalent to compact tiling; indeed, compact tiling served as inspiration for our strategy to use Liouvillian matrix elements as the objects to be periodized.

This paper is structured as follows: In Sec. II, we discuss the basic properties of the Liouvillian and its relation to the single-particle Green’s function and self-energy. Section III introduces $\mathcal{L}$ -interpolation in great detail. In Sec. IV, we use the 1d Hubbard model as a testbed for $\mathcal{L}$ -interpolation of CDMFT results (where “interpolation” refers to periodization). Using matrix product state (MPS) techniques, we obtain numerically exact results for this model. In Sec. IV A we show that a truncated Fourier expansion of $\mathcal{L}$ has much more favorable convergence properties than that of Σ or M . In Sec. IV B, we then show that $\mathcal{L}$ -interpolation yields faster convergence with cluster size for this model than M - or Σ -interpolation.

In Sec. V, we illustrate the advantages of $\mathcal{L}$ - over Σ - and M -interpolation for DCA results. These were obtained from a 4-patch DCA+NRG treatment of the 2-dimensional Hubbard model for three choices of doping, corresponding to Fermi-liquid, pseudo-gap and Mott

regimes. We show that $\mathcal{L}$ -interpolation is the interpolation scheme that most convincingly mimics the original discontinuous DCA+NRG results for the shape and spectral weight distribution along the FS (see Fig. 16, whose rightmost column is the interpolation that best mimics the discontinuous structures of the leftmost one). Moreover, this section also contains the main physical result of this paper: remarkably, $\mathcal{L}$ -interpolation can yield Fermi and Luttinger arcs that together form a closed surface (see Fig. 19), with a smooth crossover between Fermi and Luttinger arcs (see Figs. 17 and 18). The aforementioned figures vividly illustrate the capability of $\mathcal{L}$ -interpolation to generate intricate structures in non-trivial contexts; we invite the reader to briefly preview them before studying the formal developments below.

Section VI offers a summary and outlook. The Appendices provide additional details and computational aspects of $\mathcal{L}$ -interpolation, and (in App. G) an application to the pseudogap phase of the 2-dimensional Hubbard model treated using CDMFT and exact diagonalization (CDMFT+ED).

II. CFE REPRESENTATION OF LIOUVILLIAN DYNAMICS

The use of Liouvillian methods for obtaining CFEs of 2-point functions and their self-energies has a long history [40–49]. In this section, we recapitulate some central ideas and results. Our presentation, building on those of Refs. 46–49, is self-contained and emphasizes aspects relevant for the $\mathcal{L}$ -interpolation strategy in later sections.

Concretely, we (re)derive two central results. The first is formal: (i) The CFE coefficients of a Green’s function or its self-energy are given by matrix elements of the Liouvillian in an orthonormal Krylov basis obtained via a Lanczos scheme involving repeated applications of the Liouvillian; this can be shown by resolving the Green’s function in this Krylov basis. The second central result is a numerical recipe: (ii) If the spectral function of the Green’s function or its self-energy is assumed known (analytically or numerically), the CFE coefficients can be computed numerically using a Lanczos scheme to build a basis of polynomials that are orthonormal with respect to said spectral function. These polynomials can also be used to define residual functions for terminating a CFE exactly at any finite depth.

These findings are embodied in three sets of equations that constitute the main results of this section: Eqs. (28) and (31) express CFE coefficients of the self-energy through matrix elements of the single-particle irreducible part of the Liouvillian; Eqs. (38) show how to compute CFE coefficients numerically from a known spectral function; and Eqs. (43) do the same for residual functions that terminate the CFE exactly according to Eq. (42). Readers familiar with these results may choose to skip this section.

In subsequent sections we propose an interpolation

scheme based on both results (i) and (ii): taking cDMFT Green’s functions or self-energies as input, we numerically compute their CFE coefficients via (ii), then interpolate these, arguing via (i) that this amounts to interpolating the Liouvillian itself, thereby ensuring causality.

A. Liouvillian: basic notions

We begin by recalling some basic definitions and properties involving the Liouvillian. Consider a quantum system with Hamiltonian H acting in a Hilbert space $\mathbb{V}$. Linear operators acting on $\mathbb{V}$ form a vector space, too, to be denoted $\mathbb{W} = \mathbb{V} \otimes \mathbb{V}^*$. We use a round-bracket ket notation, $|\cdot\rangle$, for its elements, representing a linear operator O acting in $\mathbb{V}$ by $|O\rangle \in \mathbb{W}$ (the so-called Choi-Jamiołkowski transformation [50, 51]).

The Heisenberg equation of motion for operators, $-\mathrm{i}\partial_t O(t) = [H, O(t)]$, is linear in $O(t)$. Therefore, it can be expressed in the form $-\mathrm{i}\partial_t |O(t)\rangle = \mathcal{L}|O(t)\rangle$, with solution

$$|O(t)\rangle = e^{i\mathcal{L}t}|O(0)\rangle, \quad (3)$$

where the Liouvillian $\mathcal{L} \in \mathbb{W} \otimes \mathbb{W}^*$ is a linear operator on $\mathbb{W}$ whose action is defined through $\mathcal{L}O = [H, O]$, or

$$\mathcal{L}|O\rangle = |[H, O]\rangle. \quad (4)$$

For systems in thermal equilibrium, it is useful to define an inner product on $\mathbb{W}$ through [49]

$$(A|B) = \langle \{A^\dagger, B\} \rangle, \quad (5)$$

where $\{\cdot, \cdot\}$ denotes an anti-commutator, $\langle O \rangle = \mathrm{Tr}[\rho O]$ a thermal average and $\rho = e^{-H/T}/Z$ the thermal density matrix at temperature $T \neq 0$. This inner product ($|\cdot\rangle$) of Eq. (5) is well-defined if ρ has full rank. That is true for $T \neq 0$, but not for $T = 0$. We discuss the latter case in App. A. Since $[\rho, H] = 0$, the Liouvillian is hermitian w.r.t. this inner product, $(A|\mathcal{L}B) = (\mathcal{L}A|B)$.

B. Liouvillian representation of Green’s functions

We next recall how fermionic single-particle Green’s functions and self-energies can be expressed in terms of the Liouvillian. We begin with some standard definitions.

We consider a system described by a general fermionic Hamiltonian, $H = H_0 + H_{\mathrm{int}}$, containing quadratic and quartic parts,

$$H_0 = \sum_{\alpha\beta} \epsilon_{\alpha\beta} c_\alpha^\dagger c_\beta, \quad H_{\mathrm{int}} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} U_{\alpha\gamma,\delta\beta} c_\alpha^\dagger c_\gamma^\dagger c_\delta c_\beta. \quad (6)$$

Here, the fermionic operators satisfy $\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha\beta}$, where $\alpha = 1, \dots, M$ is a composite single-particle index encompassing, e.g., spin, orbital, and position or momentum indices. Let $\mathbf{G}^{\mathrm{R/A}}(t)$ and $\mathbf{G}^{\mathrm{R/A}}(\omega)$ denote

$M \times M$ matrices of retarded/advanced single-particle Green's functions and their Fourier transforms, respectively, with elements

$$\tilde{G}_{\alpha\beta}^{R/A}(t) = \mp i\theta(\pm t)\langle\{c_\alpha(0), c_\beta^\dagger(-t)\}\rangle, \quad (7a)$$

$$G_{\alpha\beta}^{R/A}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega^\pm t} \tilde{G}_{\alpha\beta}^{R/A}(t), \quad (7b)$$

where $\omega^\pm = \omega \pm i0^+$, and $\mathbf{G}^A(\omega) = \mathbf{G}^{R\dagger}(\omega)$. The Fourier-domain Green's functions can be viewed as analytic continuations, $\mathbf{G}^{R/A}(\omega) = \mathbf{G}(z \rightarrow \omega^\pm)$, of a function $\mathbf{G}(z)$ defined through the spectral representation

$$\mathbf{G}(z) = \int_{-\infty}^{\infty} d\omega \frac{\mathbf{A}(\omega)}{z - \omega}, \quad z \in \mathbb{C}, \quad (8a)$$

$$\mathbf{A}(\omega) = \frac{i}{2\pi} [\mathbf{G}^R(\omega) - \mathbf{G}^A(\omega)], \quad (8b)$$

with a hermitian spectral function, $\mathbf{A}(\omega) = \mathbf{A}^\dagger(\omega)$.

The non-interacting Green's function reads $\mathbf{G}_0(z) = (\mathbf{z} - \boldsymbol{\epsilon})^{-1}$, with $\mathbf{z} = z\mathbf{1}$, where $\boldsymbol{\epsilon}$ and $\mathbf{1}$ are $M \times M$ matrices with elements $\epsilon_{\alpha\beta}$ and $\delta_{\alpha\beta}$, respectively. The full Green's function can be expressed through the Dyson equation,

$$\mathbf{G}(z) = [\mathbf{G}_0^{-1}(z) - \boldsymbol{\Sigma}(z)]^{-1} = \frac{\mathbf{1}}{\mathbf{z} - \boldsymbol{\epsilon} - \boldsymbol{\Sigma}(z)}, \quad (9)$$

thereby defining the self-energy $\boldsymbol{\Sigma}(z)$.

We now express the above functions in terms of the Liouvillian. First, note that Eq. (7a) can be written as

$$\tilde{G}_{\alpha\beta}^{R/A}(t) = \mp i\theta(\pm t)(\mathbf{c}_\alpha^\dagger | e^{-i\mathcal{L}t} | \mathbf{c}_\beta^\dagger). \quad (10)$$

For notational brevity, we gather all $|\mathbf{c}_\alpha^\dagger\rangle$ into a row or *block* of M operators, denoted

$$|\mathbf{c}^\dagger\rangle = (|c_1^\dagger\rangle, \dots, |c_M^\dagger\rangle) \in \mathbb{W}^{\oplus M}. \quad (11)$$

(This choice is appropriate for Hamiltonians with U(1) charge symmetry, as in Eq. (6). Footnote [52] discusses the modifications required if H_{int} also contains $c^\dagger c^\dagger$ and cc , as needed to describe mean-field superconductivity.) The relations $\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha\beta}$ imply the $M \times M$ matrix equation $(\mathbf{c}^\dagger | \mathbf{c}^\dagger) = \mathbf{1}$. Then, Eqs. (7) can be expressed as

$$\tilde{\mathbf{G}}^{R/A}(t) = \mp i\theta(\pm t)(\mathbf{c}^\dagger | e^{-i\mathcal{L}t} | \mathbf{c}^\dagger), \quad (12)$$

$$\mathbf{G}^{R/A}(\omega) = (\mathbf{c}^\dagger | \frac{\mathbf{1}}{\omega^\pm - \mathcal{L}} | \mathbf{c}^\dagger). \quad (13)$$

The latter can be viewed as analytic continuation of

$$\mathbf{G}(z) = (\mathbf{c}^\dagger | \frac{\mathbf{1}}{z - \mathcal{L}} | \mathbf{c}^\dagger), \quad (14a)$$

having a spectral representation of the form (8), with

$$\mathbf{A}(\omega) = (\mathbf{c}^\dagger | \delta(\omega - \mathcal{L}) | \mathbf{c}^\dagger). \quad (14b)$$

The spectral function $\mathbf{A}(\omega)$ has unit weight, $\int d\omega \mathbf{A}(\omega) = \mathbf{1}$, as already follows from Eqs. (7) and (8).

C. The single-particle irreducible subspace $\mathbb{W}_{\bar{\epsilon}}$

In Eq. (12), $e^{-i\mathcal{L}t}$ acts on the subspace of fermionic single-particle creation operators, $\mathbb{W}_c = \text{span}\{|c_\beta^\dagger\rangle\}$. We call these “charge-1” operators, since when acting on particle number eigenstates, they increase the charge by +1. Since $e^{-i\mathcal{L}t}$ can be expressed as an infinite power series, the Green's function is governed by the “dynamically relevant charge-1” subspace that is spanned by all operators in $\mathbb{W}_c$ and all operators obtainable from them through repeated action with the Liouvillian. We denote this subspace by $\mathbb{W}_1(\mathcal{L}) \subset \mathbb{W}$. Importantly (and in contrast to $\mathbb{W}$) it depends on the Liouvillian; we will henceforth refrain from indicating this explicitly. (For brevity, we will refer to $\mathbb{W}_1$ simply as the “charge-1” subspace, even though operators with charge +1 may exist that are not in $\mathbb{W}_1$ [53].) $\mathbb{W}_1$ may have additional subspace structure, depending on the symmetries of the system at hand. For example, in a system with U(1) spin symmetry or translation symmetry, we could, in principle, define separate subspaces for spin $\uparrow$ and $\downarrow$ operators, or for operators with different momenta $\mathbf{k}$, respectively.

To express the self-energy through the Liouvillian, we need to exploit additional structure. We decompose the charge-1 operator space as $\mathbb{W}_1 = \mathbb{W}_c \oplus \mathbb{W}_{\bar{\epsilon}}$, where $\mathbb{W}_{\bar{\epsilon}}$ is the orthogonal complement of $\mathbb{W}_c$ in $\mathbb{W}_1$. It contains all charge-1 operators that are *single-particle irreducible*, i.e. orthogonal to $\mathbb{W}_c$. For example, if the Hamiltonian contains a quartic term such that $|c_\alpha^\dagger c_\beta c_\gamma^\dagger\rangle \in \mathbb{W}_1$, then the operator $|O_{\alpha\beta\gamma}\rangle = |c_\alpha^\dagger c_\beta c_\gamma^\dagger\rangle - |c_\alpha^\dagger\rangle\langle c_\beta c_\gamma^\dagger| - |c_\gamma^\dagger\rangle\langle c_\alpha c_\beta|$ is in $\mathbb{W}_{\bar{\epsilon}}$, since $(c_\delta^\dagger | O_{\alpha\beta\gamma}\rangle = 0$. We denote the projectors to the operator spaces $\mathbb{W}_c$ and $\mathbb{W}_{\bar{\epsilon}}$ by

$$\mathcal{P}_c = |\mathbf{c}^\dagger\rangle\langle\mathbf{c}^\dagger| = \sum_\alpha |c_\alpha^\dagger\rangle\langle c_\alpha^\dagger|, \quad (15a)$$

$$\mathcal{P}_{\bar{\epsilon}} = 1 - \mathcal{P}_c = |\bar{\mathbf{c}}^\dagger\rangle\langle\bar{\mathbf{c}}^\dagger| = \sum_{\bar{\alpha}} |\bar{c}_{\bar{\alpha}}^\dagger\rangle\langle\bar{c}_{\bar{\alpha}}^\dagger|, \quad (15b)$$

where $\{|\bar{c}_{\bar{\alpha}}^\dagger\rangle\}$ is an arbitrary orthonormal basis of $\mathbb{W}_{\bar{\epsilon}} = \text{span}\{|\bar{c}_{\bar{\alpha}}^\dagger\rangle\}$. The Liouvillian can thus be expressed as

$$\mathcal{L} = \sum_{x, \bar{x} \in \{c, \bar{c}\}} \mathcal{L}_{x\bar{x}} = \sum_{\mathbf{x}, \bar{\mathbf{x}} \in \{c, \bar{c}\}} |\mathbf{x}^\dagger\rangle\langle\mathbf{x}^\dagger| [\mathcal{L}]_{\mathbf{x}\bar{\mathbf{x}}} |\bar{\mathbf{x}}^\dagger|, \quad (16)$$

Here, $\mathcal{L}_{x\bar{x}} = \mathcal{P}_x \mathcal{L} \mathcal{P}_{\bar{x}}$ are projections of $\mathcal{L}$ to the subspaces $\mathbb{W}_x$, $\mathbb{W}_{\bar{x}}$, and the blocks $[\mathcal{L}]_{\mathbf{x}\bar{\mathbf{x}}} = (\mathbf{x}^\dagger | \mathcal{L} | \bar{\mathbf{x}}^\dagger)$ are their representation in the bases spanning these subspaces. W.r.t. these, the Liouvillian has a 2×2 block structure, $\begin{pmatrix} cc & c\bar{c} \\ \bar{c}c & \bar{c}\bar{c} \end{pmatrix}$.

Since $\mathcal{P}_{\bar{\epsilon}} |\mathbf{c}^\dagger\rangle = 0$, $(\mathbf{c}^\dagger | \mathcal{P}_{\bar{\epsilon}} = 0$, the Green's function $\mathbf{G}(z)$ of Eq. (14a) equals $[(z - \mathcal{L})^{-1}]_{cc}$, the cc block of $(z - \mathcal{L})^{-1}$. It can be found using the matrix identity (C1):

$$\begin{aligned} \mathbf{G}(z) &= (\mathbf{c}^\dagger | \left[z - \mathcal{L}_{cc} - \mathcal{L}_{c\bar{c}} \frac{1}{z - \mathcal{L}_{\bar{c}\bar{c}}} \mathcal{L}_{\bar{c}c} \right]^{-1} | \mathbf{c}^\dagger) \\ &= \left[\mathbf{z} - (\mathbf{c}^\dagger | \mathcal{L}_{cc} | \mathbf{c}^\dagger) - (\mathbf{c}^\dagger | \mathcal{L}_{c\bar{c}} \frac{1}{z - \mathcal{L}_{\bar{c}\bar{c}}} \mathcal{L}_{\bar{c}c} | \mathbf{c}^\dagger) \right]^{-1}. \end{aligned} \quad (17)$$

Comparing this to the Dyson equation (9), we obtain an

expression for the self-energy involving the Liouvillian:

$$\Sigma(z) = \Sigma^{\text{HF}} + \Sigma^{\text{dyn}}(z), \quad (18a)$$

$$\Sigma^{\text{HF}} = \epsilon_0 - \epsilon, \quad \epsilon_0 = (\mathbf{c}^\dagger | \mathcal{L}_{cc} | \mathbf{c}^\dagger), \quad (18b)$$

$$\Sigma^{\text{dyn}}(z) = (\mathbf{c}^\dagger | \mathcal{L}_{c\bar{c}} \frac{1}{z - \mathcal{L}_{\bar{c}\bar{c}}} \mathcal{L}_{\bar{c}c} | \mathbf{c}^\dagger). \quad (18c)$$

The z -independent part, Σ^{HF} , is the Hartree-Fock (HF) term. Since $\langle \{c_\alpha, [H_0, c_\beta^\dagger]\} \rangle = \epsilon_{\alpha\beta}$, its elements are

$$[\Sigma^{\text{HF}}]_{\alpha\beta} = \langle \{c_\alpha, [H_{\text{int}}, c_\beta^\dagger]\} \rangle = \sum_{\gamma\delta} \langle c_\gamma^\dagger c_\delta \rangle U_{\alpha\gamma, \delta\beta}. \quad (19)$$

Evidently, they are governed by the single-particle density matrix [54]. By contrast, the dynamical part of the self-energy, $\Sigma^{\text{dyn}}(z)$, is determined by the one-particle dynamics in the single-particle irreducible subspace $\mathbb{W}_{\bar{c}}$. From Eq. (18c), it is immediately evident that it has the same analytic properties as $\mathbf{G}(z)$.

We can further simplify Eq. (18c) by defining a set of operators that are normalized versions of $\mathcal{L}_{\bar{c}c} | \mathbf{c}^\dagger \rangle$. Their definition involves the *principal square root* of a matrix, hence we briefly digress to recall its definition and properties. For a positive semidefinite matrix $\mathbf{M}$, the principal square root $\mathbf{M}^{\frac{1}{2}}$ is the unique positive semidefinite hermitian matrix satisfying $\mathbf{M}^{\frac{1}{2}} \mathbf{M}^{\frac{1}{2}} = \mathbf{M}$. Given the eigendecomposition $\mathbf{M} = \mathbf{U} \mathbf{D} \mathbf{U}^\dagger$, the principal square root is obtained as $\mathbf{M}^{\frac{1}{2}} = \mathbf{U} \mathbf{D}^{\frac{1}{2}} \mathbf{U}^\dagger$.

If $\mathbf{M}$ is full rank (all eigenvalues nonzero), the inverse of $\mathbf{M}^{\frac{1}{2}}$ is $\mathbf{M}^{-\frac{1}{2}} = \mathbf{U} \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^\dagger$. If $\mathbf{M}$ is rank-deficient (some eigenvalues zero), the principal square root can be expressed as $\mathbf{M}^{\frac{1}{2}} = \tilde{\mathbf{U}} \tilde{\mathbf{D}}^{\frac{1}{2}} \tilde{\mathbf{U}}^\dagger$, where $\tilde{\mathbf{D}}$, $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{U}}^\dagger$ are truncated versions of $\mathbf{D}$, $\mathbf{U}$ and $\mathbf{U}^\dagger$, obtained by dropping the columns and/or rows corresponding to zero eigenvalues. Then, the inverse of the principal square root can be defined only in the image space of $\tilde{\mathbf{U}} \tilde{\mathbf{U}}^\dagger$, namely as the pseudoinverse $\mathbf{M}^{-\frac{1}{2}} = \tilde{\mathbf{U}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{U}}^\dagger$. Moreover, then $\mathbf{M}^{-\frac{1}{2}} \mathbf{M}^{\frac{1}{2}} = \tilde{\mathbf{M}}^{\frac{1}{2}} \tilde{\mathbf{M}}^{-\frac{1}{2}} = \tilde{\mathbf{U}} \tilde{\mathbf{U}}^\dagger$ is not a unit matrix, but a projector onto the subspace spanned by the eigenvectors with nonzero eigenvalues.

Returning to Eq. (18c), we define a block (or row vector) of single-particle irreducible operators $|\mathbf{q}_1\rangle$ as

$$|\mathbf{q}_1\rangle = \mathcal{L}_{\bar{c}c} | \mathbf{c}^\dagger \rangle \mathbf{t}_1^{-1} \quad (20a)$$

$$\mathbf{t}_1 \mathbf{t}_1 = (\mathbf{c}^\dagger | \mathcal{L}_{c\bar{c}} \mathcal{L}_{\bar{c}c} | \mathbf{c}^\dagger). \quad \mathbf{t}_1 = \mathbf{t}_1^\dagger \geq 0, \quad (20b)$$

Here, the notation $\mathbf{t}_1 = \mathbf{t}_1^\dagger \geq 0$ is shorthand for stating that the *weight matrix* $\mathbf{t}_1$ is a hermitian positive definite matrix. Thus, Eq. (20b) defines $\mathbf{t}_1$ as the principal square root of the positive semidefinite hermitian matrix $\mathbf{M} = (\mathbf{c}^\dagger | \mathcal{L}_{c\bar{c}} \mathcal{L}_{\bar{c}c} | \mathbf{c}^\dagger)$. Note that the right spaces of the operators $|\mathbf{q}_1\rangle$ and $|\mathbf{c}^\dagger\rangle$ are characterized by the same set of (physically motivated) spin and orbital quantum numbers, since $\mathbf{U} \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^\dagger$ or $\tilde{\mathbf{U}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{U}}^\dagger$ involve transformations out of and back into the right spaces of $|\mathbf{c}^\dagger\rangle$. This important property motivates the use of the principal square root here. If $\mathbf{M}$ is full rank, Eq. (20a)

yields a block (or row vector) of M orthonormal operators $|\mathbf{q}_1\rangle \in \mathbb{W}_{\bar{c}}^M$, with $(\mathbf{q}_1 | \mathbf{q}_1) = \mathbf{1}$.

In many cases, $\mathbf{M}$ is rank deficient for the simple reason that some of the single-particle orbitals are non-interacting; then, $\mathbf{M}$ is zero on the entire block of non-interacting orbitals. In these cases, the rank deficiency of $\mathbf{M}$ simply reflects the well-known fact that the single-particle irreducible self-energy of non-interacting orbitals is zero. Prominent—and for our work very relevant—examples are impurity models, where the bath orbitals are non-interacting, and $\mathbf{M}$ is zero on the entire bath block.

If $\mathbf{M}$ is rank deficient in the space of interacting orbitals, we take $\mathbf{t}_1^{-1}$ to be the pseudoinverse of $\mathbf{t}_1$ in that space, such that $(\mathbf{q}_1 | \mathbf{q}_1) = \tilde{\mathbf{U}} \tilde{\mathbf{U}}^\dagger$. If $\mathbf{t}_1$ has rank 0, then $|\mathbf{q}_1\rangle = 0$. In the present work, we never encountered a partial rank-deficiency in the space of interacting operators: $\mathbf{t}_1$ was either full rank or had rank 0 in this space.

Using the definitions (20), we can express $\Sigma^{\text{dyn}}(z)$ as

$$\Sigma^{\text{dyn}}(z) = \mathbf{t}_1 \mathbf{S}(z) \mathbf{t}_1, \quad (21a)$$

$$\mathbf{S}(z) = (\mathbf{q}_1 | \frac{1}{z - \mathcal{L}_{\bar{c}\bar{c}}} | \mathbf{q}_1). \quad (21b)$$

Hence, the frequency dependence of the self-energy is determined by $\mathbf{S}(z)$, a propagator in the single-particle irreducible subspace $\mathbb{W}_{\bar{c}}$. Let us introduce a spectral representation for $\mathbf{S}(z)$ analogous to Eqs. (8a) and (14b) for $\mathbf{G}(z)$ and $\mathbf{A}(\omega)$,

$$\mathbf{S}(z) = \int_{-\infty}^{\infty} d\omega \frac{\mathbf{W}(\omega)}{z - \omega}, \quad (22a)$$

$$\mathbf{W}(\omega) = (\mathbf{q}_1 | \delta(\omega - \mathcal{L}_{\bar{c}\bar{c}}) | \mathbf{q}_1), \quad (22b)$$

with $\int d\omega \mathbf{W}(\omega) = \mathbf{1}$ and $\mathbf{W}(\omega) = \mathbf{W}^\dagger(\omega)$. Correspondingly, if we express the retarded/advanced self-energies $\Sigma^{\text{R/A}}(\omega) = \Sigma(\omega^\pm)$ as $\Sigma'(\omega) \mp i\pi \Sigma''(\omega)$, then

$$\Sigma''(\omega) = \frac{i}{2\pi} [\Sigma^{\text{R}}(\omega) - \Sigma^{\text{A}}(\omega)] = \mathbf{t}_1 \mathbf{W}(\omega) \mathbf{t}_1, \quad (23a)$$

$$\Sigma'(\omega) = \Sigma^{\text{HF}} + P \int_{-\infty}^{\infty} d\omega' \frac{\Sigma''(\omega')}{z - \omega'}. \quad (23b)$$

Note that $\int d\omega \Sigma''(\omega) = \mathbf{t}_1 \mathbf{t}_1$, which identifies $\mathbf{t}_1$ as the principal square root of the total spectral weight of the retarded self-energy. We will call $\mathbf{W}(\omega)$ the *normalized spectral function* and $\mathbf{t}_1$ the *weight matrix* of $\Sigma^{\text{dyn}}(z)$.

Equations (17), (18) and (21a) together imply

$$\mathbf{G}(z) = \frac{1}{z - \epsilon_0 - \mathbf{t}_1 \mathbf{S}(z) \mathbf{t}_1}. \quad (24)$$

Together with Eq. (21b), this constitutes the first step of CFEs of the Green's function and self-energy, respectively, as explained in more detail in the next subsection.

The above relations are general and exact. When dealing with fermionic many-body systems, $\mathbb{W}_c$ can usually be handled with reasonable effort, whereas $\mathbb{W}_{\bar{c}}$ has to

be dealt with in an approximate manner. The Hartree-Fock approximation treats the self-energy solely within $\mathbb{W}_c$, approximating Σ by Σ^{HF} . It thus sets $\Sigma^{\text{dyn}} = 0$ and completely ignores $\mathbb{W}_c$. For long-ranged interactions, Σ^{HF} is non-local, for on-site interactions it is local. This is also true within DMFT. Additionally, DMFT incorporates single-particle irreducible contributions from $\mathbb{W}_c$ by including Σ^{dyn} , but approximates it as local. Thus, $\mathcal{L}_{\bar{c}\bar{c}}$ and $\mathbf{t}_1$ are approximated as local in DMFT.

Cluster extensions of DMFT additionally incorporate non-local but short-ranged matrix elements in $\mathcal{L}_{\bar{c}\bar{c}}$ and $\mathbf{t}_1$. In CDMFT, matrix elements are fully considered within each real-space cluster, while inter-cluster matrix elements are neglected. As a result, translation symmetry is broken. DCA, on the other hand, tiles the Brillouin zone (BZ) into N_p patches and approximates $\mathcal{L}_{\bar{c}\bar{c}}$ and $\mathbf{t}_1$ as constant within each patch. As a result, DCA is translation invariant, but the self-energy is not a smooth function of $\mathbf{k}$. Our goal in this work is to reinstate the translation invariance in CDMFT or a smooth $\mathbf{k}$ -dependence in DCA by interpolating (periodizing or interpolating, respectively) $\mathbf{t}_1$ and the matrix elements of $\mathcal{L}_{\bar{c}\bar{c}}$.

In the remaining subsections of this section, we show how a matrix representation of $\mathcal{L}_{\bar{c}\bar{c}}$ within $\mathbb{W}_c$ can be constructed, yielding a CFE for $\mathbf{S}(z)$ and thus also for $\Sigma^{\text{dyn}}(z)$. Then, we will switch perspective, assume that the spectral function $\mathbf{W}(\omega)$ of $\mathbf{S}(z)$ is known analytically or numerically, and show how a CFE for the latter can be constructed, thereby also obtaining a CFE for $\Sigma^{\text{dyn}}(z)$. In Sec. III we will then interpolate the self-energy by interpolating its CFE coefficients.

D. CFE for the self-energy

A CFE for the dynamical part of the self-energy, $\Sigma^{\text{dyn}}(z) = \mathbf{t}_1 \mathbf{S}(z) \mathbf{t}_1$, can be obtained by representing $\mathbf{S}(z)$ in a Krylov space constructed via an iterative Lanczos procedure [49, 55]. According to Eq. (21), $\mathbf{S}(z)$ involves the projection of the Liouvillian to the single-particle irreducible subspace, $\mathcal{L}_{\bar{c}\bar{c}}$. We thus define the Krylov space $\mathbb{K}_N = \text{span}\{|\mathbf{q}_1\rangle, \mathcal{L}_{\bar{c}\bar{c}}|\mathbf{q}_1\rangle, \dots, \mathcal{L}_{\bar{c}\bar{c}}^N|\mathbf{q}_1\rangle\}$, with $|\mathbf{q}_1\rangle$ given by Eq. (20a), and use an $(N-1)$ -step *block*-Lanczos procedure to obtain an orthonormal basis of operator blocks such that $\mathbb{K}_N = \text{span}\{|\mathbf{q}_1\rangle, |\mathbf{q}_2\rangle, \dots, |\mathbf{q}_N\rangle\}$ and

$$(\mathbf{q}_n|\mathbf{q}_{n'}) = [\mathbb{1}]_{nn'} = \delta_{nn'} \mathbf{1}. \quad (25)$$

The blocks for $n \geq 2$ are constructed iteratively by repeating four substeps that together constitute one step:

$$(1) \quad |\tilde{\mathbf{q}}_n\rangle = \mathcal{L}_{\bar{c}\bar{c}}|\mathbf{q}_{n-1}\rangle, \quad \epsilon_{n-1} = (\mathbf{q}_{n-1}|\tilde{\mathbf{q}}_n), \quad (26a)$$

$$(2) \quad |\mathbf{q}_n^\perp\rangle = |\tilde{\mathbf{q}}_n\rangle - \sum_{n'=0}^{n-1} |\mathbf{q}_{n'}\rangle(\mathbf{q}_{n'}|\tilde{\mathbf{q}}_n), \quad (26b)$$

$$(3) \quad \mathbf{t}_n \mathbf{t}_n = (\mathbf{q}_n^\perp|\mathbf{q}_n^\perp), \quad \mathbf{t}_n = \mathbf{t}_n^\dagger \geq 0, \quad (26c)$$

$$(4) \quad |\mathbf{q}_n\rangle = |\mathbf{q}_n^\perp\rangle \mathbf{t}_n^{-1} \quad (26d)$$

(1) applies $\mathcal{L}_{\bar{c}\bar{c}}$ to $|\mathbf{q}_{n-1}\rangle$ to obtain $|\tilde{\mathbf{q}}_n\rangle$ and computes its overlap with $|\mathbf{q}_{n-1}\rangle$; (2) orthogonalizes it w.r.t. all previous blocks to obtain $|\mathbf{q}_n^\perp\rangle$; (3) defines the $M \times M$ weight matrix $\mathbf{t}_n$ as the principal square root of the matrix $(\mathbf{q}_n^\perp|\mathbf{q}_n^\perp)$ (which is positive semidefinite, since $\mathcal{L}_{\bar{c}\bar{c}}$ is hermitian); and (4) normalizes $|\mathbf{q}_n^\perp\rangle$ to obtain $|\mathbf{q}_n\rangle$, where $\mathbf{t}_n^{-1}$ is the pseudoinverse of $\mathbf{t}_n$. The reasons for defining $\mathbf{t}_n$ using the principal square root are the same as those discussed for the construction of $|\mathbf{q}_1\rangle$ above. If $\mathbf{t}_n$ has rank 0, the iterative procedure terminates.

Using the convenient definition $|\mathbf{q}_0\rangle = 0$, the generated basis operators satisfy a three-term recursion relation,

$$\mathcal{L}_{\bar{c}\bar{c}}|\mathbf{q}_n\rangle = |\mathbf{q}_n\rangle \epsilon_n + |\mathbf{q}_{n+1}\rangle \mathbf{t}_{n+1} + |\mathbf{q}_{n-1}\rangle \mathbf{t}_n, \quad n \geq 1. \quad (27)$$

If at step $N-1$ one finds $|\mathbf{q}_N\rangle = 0$, the Lanczos iteration terminates automatically; otherwise one terminates it by hand after $N-1$ steps. Equation (27) implies that in the Krylov basis $\{|\mathbf{q}_1\rangle, \dots, |\mathbf{q}_N\rangle\}$, the single-particle irreducible projection of the Liouvillian is represented by a block-tridiagonal matrix (also known as Jacobi matrix),

$$[\mathbb{L}_N]_{\bar{c}\bar{c}} = \begin{pmatrix} \epsilon_1 & \mathbf{t}_2 & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{t}_2 & \epsilon_2 & \mathbf{t}_3 & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{t}_3 & \epsilon_3 & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \epsilon_{N-2} & \mathbf{t}_{N-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{t}_{N-1} & \epsilon_{N-1} & \mathbf{t}_N \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{t}_N & \epsilon_N \end{pmatrix}. \quad (28)$$

Its N^2 blocks are all $M \times M$ matrices, given by

$$[[\mathbb{L}_N]_{\bar{c}\bar{c}}]_{nn'} = (\mathbf{q}_n|\mathcal{L}_{\bar{c}\bar{c}}|\mathbf{q}_{n'}) = \begin{cases} \epsilon_n, & n' = n, \\ \mathbf{t}_{n+1}, & n' = n+1, \\ \mathbf{t}_n, & n' = n-1, \\ \mathbf{0} & \text{otherwise.} \end{cases} \quad (29)$$

Within $\mathbb{K}_N$, expression (21b) for $\mathbf{S}(z)$ is represented as

$$\mathbf{S}(z) \simeq [(\mathbb{z}_N]_{\bar{c}\bar{c}} - [\mathbb{L}_N]_{\bar{c}\bar{c}})^{-1}]_{n=1, n'=1}. \quad (30)$$

where $\mathbb{z}_N = z \mathbb{1}_N$ equals z times a block unit matrix, with $[\mathbb{1}_N]_{nn'} = \delta_{nn'} \mathbf{1}$. Using Eq. (C8), a formula for the 11- (upper-left) block of the inverse of a tridiagonal block matrix, we obtain the desired CFE (with $\mathbf{z}_n = \mathbf{z} - \epsilon_n$):

$$\mathbf{S}(z) \simeq \frac{1}{\mathbf{z}_1 - \mathbf{t}_2 \frac{1}{\mathbf{z}_2 - \cdots - \mathbf{t}_N \frac{1}{\mathbf{z}_N} \mathbf{t}_N}}. \quad (31)$$

We have thus established that the CFE coefficients ϵ_n and $\mathbf{t}_n$ of $\mathbf{S}(z)$ and hence of $\Sigma^{\text{dyn}}(z)$ are matrix elements of the single-particle irreducible Liouvillian $\mathcal{L}_{\bar{c}\bar{c}}$. The CFE (31) becomes exact for sufficiently large N , provided that the moment problem defined by the measure $\mathbf{W}(\omega)d\omega$ is determinate. This is the case if the support of $\mathbf{W}(\omega)$ is bounded, or if $\mathbf{W}(\omega)$ decays fast enough at high frequencies, see App. B for more details.

E. Computing CFE coefficients via polynomials

Above, we found that the CFE coefficients of $\mathbf{S}(z)$ correspond to matrix elements $(\mathbf{q}_n | \mathcal{L}_{\bar{c}\bar{c}} | \mathbf{q}_{n'})$ of the single-particle-irreducible projection of the Liouvillian. Since each Lanczos block $|\mathbf{q}_n\rangle$ is a linear combination of powers of $\mathcal{L}_{\bar{c}\bar{c}}$ applied to the initial block $|\mathbf{q}_1\rangle$, all such matrix elements are linear combinations of diagonal matrix elements of the form $(\mathbf{q}_1 | \mathcal{L}_{\bar{c}\bar{c}}^m | \mathbf{q}_1)$. Now, the latter correspond to moments of the spectral function $\mathbf{W}(\omega)$ of $\mathbf{S}(z)$, due to an identity following from Eq. (22b):

$$(\mathbf{q}_1 | \mathcal{L}_{\bar{c}\bar{c}}^m | \mathbf{q}_1) = \int d\omega \mathbf{W}(\omega) \omega^m. \quad (32)$$

It follows that if $\mathbf{W}(\omega)$ is known explicitly (analytically or numerically), the CFE coefficients of $\mathbf{S}(z)$ can be computed directly from the moments of $\mathbf{W}(\omega)$. This can be done by constructing a set of orthonormal vector-valued polynomials [42, 48, 49] using a Lanczos scheme completely analogous to that described in the previous subsection [55–58]. Below, we review this construction.

The block Lanczos scheme in Sec. IID is initialized by a length- M block or row vector of operators, $|\mathbf{q}_1\rangle$. Its entries, all vectors in $\mathbb{W}_{\bar{c}}$, are by definition mutually orthonormal, $(\mathbf{q}_1 | \mathbf{q}_1) = \mathbf{1}$. Each block of Lanczos vectors $|\mathbf{q}_n\rangle$ can be written as a linear combination of the form

$$|\mathbf{q}_n\rangle = \sum_{\bar{n}=0}^{n-1} \mathcal{L}_{\bar{c}\bar{c}}^{\bar{n}} |\mathbf{q}_1\rangle \mathbf{C}_{\bar{n}n}, \quad (33)$$

where for each $\bar{n}n$, $\mathbf{C}_{\bar{n}n}$ is an $M \times M$ matrix that right-multiplies the length- M row vector of operators $|\mathbf{q}_1\rangle$. When this representation is inserted into the orthonormality relations (25) and the matrix elements of Eq. (29), both $(\mathbf{q}_n | \mathbf{q}'_n)$ and $(\mathbf{q}_n | \mathcal{L}_{\bar{c}\bar{c}} | \mathbf{q}'_n)$ become linear combinations of matrix elements $(\mathbf{q}_1 | \mathcal{L}_{\bar{c}\bar{c}}^m | \mathbf{q}_1)$ involving various powers m of $\mathcal{L}_{\bar{c}\bar{c}}$. Using Eq. (32) to express these through moments of $\mathbf{W}(\omega)$, Eqs. (25) and (29) take the form

$$[\mathbb{1}]_{nn'} = \int d\omega \mathbf{p}_n^{(1)\dagger}(\omega) \mathbf{W}(\omega) \mathbf{p}_{n'}^{(1)}(\omega), \quad (34a)$$

$$[\mathbb{L}_{\bar{c}\bar{c}}]_{nn'} = \int d\omega \mathbf{p}_n^{(1)\dagger}(\omega) \mathbf{W}(\omega) \omega \mathbf{p}_{n'}^{(1)}(\omega), \quad (34b)$$

where we have defined the matrix polynomials

$$\mathbf{p}_n^{(1)}(\omega) = \sum_{\bar{n}=0}^{n-1} \omega^{\bar{n}} \mathbf{C}_{\bar{n}n}. \quad (35)$$

(The reason for the superscript (1) on $\mathbf{p}_n^{(1)}(\omega)$ will become clear below.) For each n , $\mathbf{p}_n^{(1)}(\omega)$ is an $M \times M$ matrix. Its columns, enumerated by $\alpha = 1, \dots, M$, are length- M column-vector-valued polynomials of degree $n-1$, which we denote by $p_{n,\alpha}^{(1)} : \mathbb{R} \rightarrow \mathbb{C}^M$, $\omega \mapsto p_{n,\alpha}^{(1)}(\omega)$. Note that $p_{n,\alpha}^{(1)}$ is constructed from column α of the matrix $\mathbf{C}_{\bar{n}n}$, which via Eq. (33) also defines entry α of the block

$|\mathbf{q}_n\rangle = (|q_{n,1}\rangle, \dots, |q_{n,M}\rangle)$. This yields a one-to-one correspondence, $p_{n,\alpha}^{(1)} \leftrightarrow |q_{n,\alpha}\rangle$, between length- M column-vector-valued polynomials and operators in $\mathbb{W}_{\bar{c}}$. The matrix $\mathbf{p}_n^{(1)}$ can thus be also be viewed as a length- M row vector of column-vector-valued polynomials, associated with the length- M row vector of operators $|\mathbf{q}_n\rangle$.

To compactify the notation, let

$$\langle f, g \rangle = \int d\omega f^\dagger(\omega) \mathbf{W}(\omega) g(\omega) \quad (36)$$

denote the inner product, with matrix-valued measure $\mathbf{W}(\omega)d\omega$, of two length- M column-vector-valued functions, $f : \mathbb{R} \rightarrow \mathbb{C}^M$, $\omega \mapsto f(\omega)$, and likewise for g . Then, equations (34) can be expressed as

$$\langle \mathbf{p}_n^{(1)}, \mathbf{p}_{n'}^{(1)} \rangle = \mathbb{1}_{nn'}, \quad (37a)$$

$$\langle \mathbf{p}_n^{(1)}, \hat{\mathcal{L}}_{\bar{c}\bar{c}} \mathbf{p}_{n'}^{(1)} \rangle = [\mathbb{L}_{\bar{c}\bar{c}}]_{nn'}, \quad (37b)$$

where $\hat{\mathcal{L}}_{\bar{c}\bar{c}}$ is the Liouvillian in function space, acting as $\hat{\mathcal{L}}_{\bar{c}\bar{c}} f(\omega) = \omega f(\omega)$. For given nn' , Eq. (37a) is an $M \times M$ matrix equation whose element $\alpha\alpha'$ reads $\langle p_{n,\alpha}^{(1)}, p_{n',\alpha'}^{(1)} \rangle = \delta_{nn'} \delta_{\alpha\alpha'}$; similarly for Eq. (37b).

Equation (37a) states that the $N \cdot M$ vector-valued polynomials $\{p_{n,\alpha}^{(1)}\}$ defined by the columns of all $\mathbf{p}_n^{(1)}(\omega)$, $n = 1, \dots, N$, are mutually orthonormal w.r.t. the matrix-valued measure $\mathbf{W}(\omega)d\omega$. (The superscript on $\mathbf{p}_n^{(1)}$ signifies that these are “associated polynomials of the first kind” relative to another set of orthonormal polynomials, namely those defined w.r.t. the measure $\mathbf{A}(\omega)d\omega$, see App. B.) The polynomials $\{p_{n,\alpha}^{(1)}\}$ thus form a basis for the space of all length- M column-vector-valued polynomials of degree $N-1$. Equation (37b) states that all matrix elements of $\mathbb{L}_{\bar{c}\bar{c}}$, and hence all CFE coefficients of $\mathbf{S}(z)$, can be expressed as matrix elements of the Liouvillian $\hat{\mathcal{L}}_{\bar{c}\bar{c}}$ in this basis.

For a given $\mathbf{W}(\omega)$, the relations (37), together with the initial condition $\mathbf{p}_1^{(1)}(\omega) = \mathbf{1}$, fully define the basis $\{p_{n,\alpha}^{(1)}\}$. It can be constructed iteratively via a block-Lanczos procedure (in complete analogy to that for $|\mathbf{q}_n\rangle$) which also generates to matrix elements $[\mathbb{L}_{\bar{c}\bar{c}}]_{nn'}$. It involves (1) multiplication by ω , (2) orthogonalization, (3) identification of a normalization matrix, and (4) normalization:

$$(1) \quad \tilde{\mathbf{p}}_n^{(1)}(\omega) = \omega \mathbf{p}_{n-1}^{(1)}(\omega), \quad \epsilon_{n-1} = \langle \mathbf{p}_{n-1}^{(1)}, \tilde{\mathbf{p}}_n^{(1)} \rangle, \quad (38a)$$

$$(2) \quad \mathbf{p}_n^{(1)\perp}(\omega) = \tilde{\mathbf{p}}_n^{(1)}(\omega) - \sum_{n'=0}^{n-1} \mathbf{p}_{n'}^{(1)}(\omega) \langle \mathbf{p}_{n'}^{(1)}, \tilde{\mathbf{p}}_n^{(1)} \rangle, \quad (38b)$$

$$(3) \quad \mathbf{t}_n \mathbf{t}_n = \langle \mathbf{p}_n^{(1)\perp}, \mathbf{p}_n^{(1)\perp} \rangle, \quad \mathbf{t}_n = \mathbf{t}_n^\dagger \geq 0, \quad (38c)$$

$$(4) \quad \mathbf{p}_n^{(1)}(\omega) = \mathbf{p}_n^{(1)\perp}(\omega) \mathbf{t}_n^{-1}. \quad (38d)$$

(On the right of Eq. (38b), the second term involves matrix multiplication of two $M \times M$ matrices, the matrix of polynomials $\mathbf{p}_{n'}^{(1)}(\omega)$ and the inner product matrix $\langle \mathbf{p}_{n'}^{(1)}, \tilde{\mathbf{p}}_n^{(1)} \rangle$.) Along the way, we obtain the CFE coefficients ϵ_{n-1} from Eq. (38a), and $\mathbf{t}_n$ as the principal square root of $\langle \mathbf{p}_n^{(1)\perp}, \mathbf{p}_n^{(1)\perp} \rangle$ in Eq. (38c), as in Eq. (26d).

The resulting polynomials and CFE coefficients satisfy a three-term recurrence relation analogous to Eq. (27):

$$\omega \mathbf{p}_n^{(1)} = \mathbf{p}_n^{(1)} \epsilon_n + \mathbf{p}_{n+1}^{(1)} \mathbf{t}_{n+1} + \mathbf{p}_{n-1}^{(1)} \mathbf{t}_n, \quad n \geq 1, \quad (39)$$

with $\mathbf{p}_0^{(1)}(\omega) = \mathbf{0}$, $\mathbf{p}_1^{(1)}(\omega) = \mathbf{1}$.

Equations (21) and (22) together imply that the dynamical part of the self-energy can be expressed as

$$\begin{aligned} \Sigma^{\text{dyn}}(z) &= \mathbf{t}_1 \langle \mathbf{p}_1^{(1)}, (z - \hat{\mathcal{L}}_{\text{cc}})^{-1} \mathbf{p}_1^{(1)} \rangle \mathbf{t}_1 \\ &= \mathbf{t}_1 [(z - \mathbb{L}_{\text{cc}})^{-1}]_{11} \mathbf{t}_1. \end{aligned} \quad (40)$$

The same argument that led from Eq. (30) to (31) then gives an approximate depth- N CFE (41) for $\Sigma^{\text{dyn}}(z)$ (with $\mathbf{z}_n = \mathbf{z} - \epsilon_n$):

$$\Sigma^{\text{dyn}}(z) \simeq \mathbf{t}_1 \frac{1}{z_1 - \mathbf{t}_2 \frac{1}{z_2 - \dots - \mathbf{t}_N \frac{1}{z_N} \mathbf{t}_N}} \mathbf{t}_1. \quad (41)$$

If the self-energy spectrum $\mathbf{W}(\omega)$ is discrete with a finite number of δ -peaks, as is the case for a finite-size system, $\Sigma^{\text{dyn}}(z)$ has an exact finite-depth CFE representation of the form (41). Otherwise, Eq. (41) is an approximation.

F. Exact termination of CFE

To replace Eq. (41) by an exact depth- N CFE, we subtract an $M \times M$ matrix function, the *residual function* $\mathbf{R}_N(z)$, from the denominator at depth N and *define* it by the requirement that the following equation is exact:

$$\Sigma^{\text{dyn}}(z) = \mathbf{t}_1 \frac{1}{z_1 - \mathbf{t}_2 \frac{1}{z_2 - \dots - \mathbf{t}_N \frac{1}{z_N - \mathbf{R}_N(z)} \mathbf{t}_N}} \mathbf{t}_1. \quad (42)$$

In other words, the residual function $\mathbf{R}_N(z)$ by definition terminates the CFE at level N in an exact manner. As shown in App. D, once the matrix polynomials $\mathbf{p}_{N-1}^{(1)}(\omega)$ and $\mathbf{p}_N^{(1)}(\omega)$ are known, they can be used to compute, $\mathbf{R}_{N-1}(z)$, which terminates the CFE exactly at depth $N-1$, as follows:

$$\mathbf{R}_{N-1}(z) = \mathbf{I}_N(z) - \mathbf{F}_N^L(z) \mathbf{G}_N^{-1}(z) \mathbf{F}_N^R(z), \quad (43a)$$

$$\mathbf{G}_N(z) = \int d\omega \mathbf{p}_{N-1}^{(1)\dagger}(\omega) \mathbf{W}(\omega) \mathbf{p}_{N-1}^{(1)}(\omega) / (z - \omega), \quad (43b)$$

$$\mathbf{F}_N^L(z) = \int d\omega \mathbf{p}_N^{(1)\dagger}(\omega) \mathbf{W}(\omega) \mathbf{p}_{N-1}^{(1)}(\omega) / (z - \omega), \quad (43c)$$

$$\mathbf{F}_N^R(z) = \int d\omega \mathbf{p}_{N-1}^{(1)\dagger}(\omega) \mathbf{W}(\omega) \mathbf{p}_N^{(1)}(\omega) / (z - \omega), \quad (43d)$$

$$\mathbf{I}_N(z) = \int d\omega \mathbf{p}_N^{(1)\dagger}(\omega) \mathbf{W}(\omega) \mathbf{p}_N^{(1)}(\omega) / (z - \omega). \quad (43e)$$

The CFE (42) can also be constructed iteratively via a sequence of depth-1 CFEs, each terminated by a residual function that serves as starting point for the next iteration. Initialize the process using $\mathbf{R}_0(z) = \Sigma^{\text{dyn}}(z)$ as input. Then, iteratively proceed as follows for $n \geq 1$: (a) Using $\mathbf{R}_{n-1}(z)$ as input, find its normalized spectral function $\mathbf{W}_{n-1}(\omega)$ and weight matrix $\mathbf{t}_n$, as follows:

$$\mathbf{R}_{n-1}''(\omega) = \frac{i}{2\pi} [\mathbf{R}_{n-1}(\omega^+) - \mathbf{R}_{n-1}^\dagger(\omega^+)], \quad (44a)$$

$$\mathbf{t}_n \mathbf{t}_n = \int d\omega \mathbf{R}_{n-1}''(\omega), \quad \mathbf{t}_n = \mathbf{t}_n^\dagger \geq 0, \quad (44b)$$

$$\mathbf{W}_{n-1}(\omega) = \mathbf{t}_n^{-1} \mathbf{R}_{n-1}''(\omega) \mathbf{t}_n^{-1}. \quad (44c)$$

(b) Use a one-step Lanczos scheme with measure $\mathbf{W}_{n-1}(\omega) d\omega$ to compute ϵ_n . (c) Express $\mathbf{R}_{n-1}(z)$ via the depth-1 version of Eq. (42), with $\{\Sigma^{\text{dyn}}, \mathbf{t}_1, \mathbf{z}_1, \mathbf{R}_1\}$ there replaced by $\{\mathbf{R}_{n-1}, \mathbf{t}_n, \mathbf{z}_n, \mathbf{R}_n\}$:

$$\mathbf{R}_{n-1}(z) = \mathbf{t}_n \frac{1}{z_n - \mathbf{R}_n(z)} \mathbf{t}_n. \quad (45)$$

(Concretely: Let us use a superscript (n) to tag objects obtained from the n -th one-step Lanczos scheme with measure $\mathbf{W}_{n-1}(\omega) d\omega$. Step (b) yields $\mathbf{p}_1^{(n)}(\omega) = \mathbf{1}$, $\tilde{\mathbf{p}}_2^{(n)} = \omega \mathbf{1}$, $\epsilon_1^{(n)}$, $\mathbf{p}_2^{(n)\perp} = \omega \mathbf{1} - \epsilon_1^{(n)}$. Step (c) yields $\mathbf{R}_1^{(n)}$ via Eqs. (43), with $\{\mathbf{W}, \mathbf{p}_{N-1}^{(1)}, \mathbf{p}_N^{(1)\perp}, \mathbf{R}_{N-1}\}$ there replaced by $\{\mathbf{W}_{n-1}, \mathbf{1}, \omega \mathbf{1} - \epsilon_1^{(n)}, \mathbf{R}_1^{(n)}\}$. Finally, set $\epsilon_n = \epsilon_1^{(n)}$ and $\mathbf{R}_n = \mathbf{R}_1^{(n)}$.) Concatenating N depth-1 CFEs of the form (45) yields a CFE of the form (42). The resulting CFE coefficients are identical to those obtained via an N -step Lanczos scheme.

To conclude this subsection, we note that a CFE for the self-energy implies a CFE for the corresponding Green's function: inserting Eqs. (18a) and (42) for the self-energy into the Dyson equation (9) for $\mathbf{G}(z)$, we obtain

$$\mathbf{G}(z) = \frac{1}{z_0 - \mathbf{t}_1 \frac{1}{z_1 - \mathbf{t}_2 \frac{1}{z_2 - \dots - \mathbf{t}_N \frac{1}{z_N - \mathbf{R}_N(z)} \mathbf{t}_N}} \mathbf{t}_1}. \quad (46)$$

This CFE can also be obtained directly by using a Lanczos scheme with measure $\mathbf{A}(\omega) d\omega$ to construct an orthogonal set of matrix polynomials $\{\mathbf{p}_n(\omega), n = 0, \dots, N\}$, initiated with $\mathbf{p}_0(\omega) = \mathbf{1}$. These polynomials differ from the $\{\mathbf{p}_n^{(1)}(\omega), n = 1, \dots, N\}$ obtained using the measure $\mathbf{W}(\omega) d\omega$, but the CFE coefficients $\epsilon_{n \geq 1}$ and $\mathbf{t}_{n \geq 2}$ are the same, as elaborated in App. B.

G. Quantum impurity models: separating hybridization function and self-energy

Quantum impurity models involve a small number N_d of impurity orbitals and a large number N_b of bath or-

bitals. We assemble their creation operators into length- N_d and length- N_b row vectors, denoted $|\mathbf{d}^\dagger\rangle$ and $|\mathbf{b}^\dagger\rangle$, respectively, and combine them as $|\mathbf{c}^\dagger\rangle = (|\mathbf{d}^\dagger\rangle, |\mathbf{b}^\dagger\rangle)$, a row vector of length $M = N_d + N_b$. Its entries span the single-particle subspace, $\mathbb{W}_c = \mathbb{W}_d \oplus \mathbb{W}_b$, of the impurity model. In analogy to Eq. (15a), we define the projectors

$$\mathcal{P}_d = |\mathbf{d}^\dagger\rangle\langle\mathbf{d}^\dagger|, \quad \mathcal{P}_b = |\mathbf{b}^\dagger\rangle\langle\mathbf{b}^\dagger|, \quad \mathcal{P}_{\bar{c}} = 1 - \mathcal{P}_c, \quad (47)$$

and denote the corresponding projections of the Liouvillian by $\mathcal{L}_{xx'} = \mathcal{P}_x \mathcal{L} \mathcal{P}_{x'}$, with $x, x' \in \{d, b, \bar{c}\}$. This more finely grained decomposition $\mathbb{W} = \mathbb{W}_d \oplus \mathbb{W}_b \oplus \mathbb{W}_{\bar{c}}$ induces a 3×3 block structure on $\mathcal{L}$, akin to Eq. (16), having blocks $[\mathcal{L}]_{\mathbf{x}\tilde{\mathbf{x}}} = (\mathbf{x}^\dagger | \mathcal{L} | \tilde{\mathbf{x}}^\dagger)$ with $\mathbf{x}, \tilde{\mathbf{x}} \in \{d, b, \bar{c}\}$. Since the bath is non-interacting, the action of $\mathcal{L}$ on $|\mathbf{b}^\dagger\rangle$ yields another single-particle operator, never reaching the single-particle irreducible space $\mathbb{W}_{\bar{c}}$, i.e. $\mathcal{L}|\mathbf{b}^\dagger\rangle \in \mathbb{W}_c$ and $\mathcal{L}_{\bar{c}b} = \mathcal{L}_{b\bar{c}} = 0$. Since $\mathbb{W}_{\bar{c}}$ is reached only when $\mathcal{L}$ acts on impurity orbitals, the dynamical part of single-particle irreducible self-energy, $\Sigma^{\text{dyn}}(z)$, is non-zero only for impurity orbitals, cf. Eq. (20). For impurity models, the right space of $|\mathbf{q}_1\rangle$ is thus implicitly constrained to the impurity block, where it is non-zero, and likewise for $\Sigma^{\text{dyn}}(z)$.

The full single-particle Green's function, $\mathbf{G} = (\mathbf{c}^\dagger | (z - \mathcal{L})^{-1} | \mathbf{c}^\dagger)$, is an $M \times M$ matrix containing both impurity and bath blocks. However, one typically only works with the impurity Green's function, $\mathbf{G}_{dd} = (\mathbf{d}^\dagger | (z - \mathcal{L})^{-1} | \mathbf{d}^\dagger)$, an $N_d \times N_d$ matrix. Its form, found via Eq. (C4), is

$$\mathbf{G}_{dd}(z) = \left[z - \epsilon_0 - \Delta(z) - \Sigma^{\text{dyn}}(z) \right]^{-1}, \quad (48a)$$

$$\epsilon_0 = (\mathbf{d}^\dagger | \mathcal{L} | \mathbf{d}^\dagger), \quad (48b)$$

$$\Delta(z) = (\mathbf{d}^\dagger | \mathcal{L}_{db} \frac{1}{z - \mathcal{L}_{bb}} \mathcal{L}_{bd} | \mathbf{d}^\dagger), \quad (48c)$$

$$\Sigma^{\text{dyn}}(z) = (\mathbf{d}^\dagger | \mathcal{L}_{d\bar{c}} \frac{1}{z - \mathcal{L}_{\bar{c}\bar{c}}} \mathcal{L}_{\bar{c}d} | \mathbf{d}^\dagger). \quad (48d)$$

The hybridization function $\Delta(z)$ encodes all relevant information about the impurity-bath coupling.

For the $\mathcal{L}$ -interpolation strategy to be presented in Sec. III, we are only interested in the Liouvillian matrix elements in the single-particle irreducible subspace, to be extracted from $\Sigma^{\text{dyn}}(z)$. These matrix elements cannot be extracted by a direct CFE of $\mathbf{G}_{dd}(z)$, since that mixes single-particle reducible contributions from $\Delta(z)$ with single-particle irreducible ones from $\Sigma^{\text{dyn}}(z)$. However, the contribution of $\Delta(z)$ can be subtracted either explicitly (as discussed in App. G) or implicitly, using Kugler's symmetric improved estimator strategy [59, 60] (as done for the results of Secs. IV and V).

H. CFE for NRG spectra

If the self-energy of a quantum impurity model is computed using NRG, as is the case for several results presented in later sections, a complication arises: The spectral function $\mathbf{W}(\omega)$ obtained from NRG possesses long

tails due to the log-Gaussian broadening used to obtain smooth spectral functions from discrete ones. As a result, the moment problem of the measure $\mathbf{W}(\omega)d\omega$ is indeterminate (see App. B), a problem artificially introduced by log-Gaussian broadening. This implies that it is not possible to uniquely determine the self-energy from its CFE coefficients without additional information. Below, we describe how such additional high-frequency information can be introduced via a regularized CFE.

Even without the problem of indeterminate moments, it is often desirable for the regularization scheme to be geared towards extracting low-energy information. Many-body systems often exhibit features that are separated by several orders of magnitude in frequency, and resolving all of those features would require a CFE with exponentially large depth N —unfeasible in numerical practice. Instead, we need a “logarithmic CFE”, featuring CFE coefficients whose magnitudes decrease exponentially with depth N , thus naturally terminating the CFE when N becomes large.

A strategy for constructing CFEs that both regularizes high-energy tails and yields exponentially decreasing CFE coefficients has been described in Ref. 61. There, a logarithmic CFE (log-CFE) was constructed for the hybridization function of an impurity model. This was achieved by an iterative procedure analogous to using Eq. (45), with one crucial difference: after each step the spectrum of the residual function $\mathbf{R}_n(z)$ is split into a high-energy part and a low-energy part, called, “fast” (F) and “slow” (S) modes, respectively, and only the slow modes are used for the next iteration. Here, we adapt that scheme to construct a logarithmic CFE of our self-energy via N one-step Lanczos schemes combined with fast/slow splitting.

We initialize the procedure by setting $\mathbf{R}_0^S(z) = \Sigma^{\text{dyn}}(z)$, i.e. we declare the input self-energy to be “all slow modes”. For iterations $n \geq 1$, we proceed as before for steps (a) to (c), now using $\mathbf{R}_{n-1}^S(z)$ as input, to compute $\mathbf{t}_n$, ϵ_n and $\mathbf{R}_n(z)$ and obtain the depth-1 CFE

$$\mathbf{R}_{n-1}^S(z) = \mathbf{t}_n \frac{1}{z_n - \mathbf{R}_n(z)} \mathbf{t}_n. \quad (49)$$

Thereafter comes a new step: (d) We split $\mathbf{R}_n(z)$ into “fast” and “slow” contributions, $\mathbf{R}_n(z) = \mathbf{R}_n^F(z) + \mathbf{R}_n^S(z)$, built from the high- or low-energy part of its spectrum,

$$\mathbf{R}_n^{F/S}(z) = \int_{-\infty}^{\infty} d\omega \frac{w_n^{F/S}(\omega) \mathbf{R}_n''(\omega)}{z - \omega}. \quad (50)$$

Here, the so-called splitting functions $w_n^{F/S}(\omega)$ satisfy $w_n^F(\omega) + w_n^S(\omega) = 1$ and monotonically increase/decrease with $|\omega|$ (see below). Then, we use only the slow-mode part, $\mathbf{R}_n^S(z)$, as input for the next iteration. Iterating,

we obtain an exact CFE of the following form:

$$\Sigma^{\text{dyn}}(z) = \begin{array}{ccc} & 1 & \\ t_1 & \text{-----} & t_1 \\ & 1 & \\ z_1 - \mathbf{R}_1^F(z) - t_2 & \text{-----} & t_2 \\ & z_2 - \mathbf{R}_2^F(z) - \dots & \\ & 1 & \\ & -t_N & \\ & z_N - \mathbf{R}_N(z) & t_N \end{array} \quad (51)$$

Each level contains an explicit fast-mode contribution $\mathbf{R}_n^F(z)$, except the last level, containing the full $\mathbf{R}_N(z)$. Note that $\mathbf{R}_n^F(z)$ will, in general, contain an imaginary part; therefore, some amount of broadening is present at each level, yielding a self-energy with a continuous spectrum. The fact that $\mathbf{R}_n^F(z)$ does not feed into the next iteration in effect regularizes the contribution from high-energy tails of the spectrum of $\mathbf{R}_n(z)$. Nevertheless, the representation (51) is exact—the fast-slow splitting does not neglect any information, it just distributes high- and low-energy information to different parts of the CFE.

To achieve a *logarithmic* CFE whose CFE coefficients decrease exponentially with N , we choose

$$w_n^S(\omega) = \frac{1}{1 + |\omega/\Omega_n|^\tau}, \quad \Omega_n = \Omega_{\text{max}} \Lambda^{1-n}. \quad (52)$$

This box-shaped function has height 1, half-width Ω_n and box corners whose rounding is controlled by $\tau > 2$. The scale Ω_n decreases exponentially with n , and we choose $\Lambda = (\Omega_{\text{max}}/\Omega_{\text{min}})^{1/(N-1)}$ such that Ω_n ranges between specified maximal and minimal values, $\Omega_1 = \Omega_{\text{max}}$ and $\Omega_N = \Omega_{\text{min}}$. The splitting function has weight $\int d\omega w_n^S(\omega) \sim \Lambda^{-n}$, resulting in exponentially decreasing CFE coefficients, $\epsilon_n, t_n \sim \Lambda^{-n}$ and the weight of the spectrum of $\mathbf{R}_n^F$ likewise scales $\sim \Lambda^{-n}$ (see Fig. 10 below, and App. E3 for numerical details.)

III. LIOUVILLIAN INTERPOLATION

In this section, we outline the basic ideas underlying Liouvillian interpolation. We start with a brief discussion of cDMFT approximations and traditional interpolation schemes, then introduce our $\mathcal{L}$ -interpolation scheme. Technical steps are spelled out in detail in Appendix E.

A. Cluster DMFT approximations

We begin with some general remarks. For computations in a real-space basis of N_{latt} lattice sites with M orbitals per site, the self-energy matrix $\tilde{\Sigma}(z)$ is a $N_{\text{latt}}M \times N_{\text{latt}}M$ matrix built from $N_{\text{latt}} \times N_{\text{latt}}$ blocks $[\tilde{\Sigma}(z)]_{\mathbf{r},\mathbf{r}'}$ labeled by site indices, with each block having dimension $M \times M$. If $\tilde{\Sigma}(z)$ is expressed through a block-CFE, its CFE coefficients $\tilde{\epsilon}_n$ and $\tilde{t}_n$ (i.e. Liouvillian matrix elements) are matrices too, built from $N_{\text{latt}} \times N_{\text{latt}}$ blocks $[\tilde{\epsilon}_n]_{\mathbf{r},\mathbf{r}'}$ and $[\tilde{t}_n]_{\mathbf{r},\mathbf{r}'}$, each of dimension $M \times M$.

For translationally invariant systems $[\tilde{\Sigma}(z)]_{\mathbf{r},\mathbf{r}'}$ depends only on the difference vector $\delta = \mathbf{r} - \mathbf{r}'$, as do $[\tilde{\epsilon}_n]_{\mathbf{r},\mathbf{r}'}$ and $[\tilde{t}_n]_{\mathbf{r},\mathbf{r}'}$. Then the Fourier transform block-diagonalizes $\tilde{\Sigma}$ w.r.t. spatial indices:

$$\Sigma_{\mathbf{k}}(z) = \sum_{\delta} [\tilde{\Sigma}(z)]_{\delta,0} e^{-i\mathbf{k} \cdot \delta}. \quad (53)$$

Here, $\Sigma_{\mathbf{k}}(z)$ is shorthand for the diagonal elements of a block-diagonal matrix with elements $[\Sigma(z)]_{\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k}\mathbf{k}'} \Sigma_{\mathbf{k}}(z)$ obtained by viewing the Fourier transform as a basis transformation $\Sigma = \mathbf{U} \tilde{\Sigma} \mathbf{U}^\dagger$ with matrix entries $[\mathbf{U}]_{\mathbf{k},\mathbf{r}} = e^{-i\mathbf{k} \cdot \mathbf{r}} / \sqrt{N_{\text{latt}}}$. The sum runs over all distinct difference vectors δ between two lattice sites. (Since the lattice includes site $\mathbf{0}$, this is equivalent to summing over all lattice sites.) For given $\mathbf{k}$, $\Sigma_{\mathbf{k}}(z)$ is an $M \times M$ matrix, as are its CFE coefficients,

$$\epsilon_{\mathbf{k}n} = \sum_{\delta} [\tilde{\epsilon}_n]_{\delta,0} e^{-i\mathbf{k} \cdot \delta}, \quad t_{\mathbf{k}n} = \sum_{\delta} [\tilde{t}_n]_{\delta,0} e^{-i\mathbf{k} \cdot \delta}. \quad (54)$$

In conventional single-site DMFT, the “impurity” is a single lattice site self-consistently embedded in its surrounding, the real-space self-energy is local, $[\tilde{\Sigma}(z)]_{\mathbf{r},\mathbf{r}'} = \delta_{\mathbf{r},\mathbf{r}'} \Sigma(z)$, and the momentum-space self-energy is $\mathbf{k}$ -independent, $\Sigma_{\mathbf{k}}(z) = \Sigma(z)$. The same is true for its $n > 0$ CFE coefficients: $[\tilde{\epsilon}_n]_{\delta,0} = \delta_{\delta,0} \epsilon_n$ and $\epsilon_{\mathbf{k}n} = \epsilon_n$, likewise for $\tilde{t}_n$ and $t_{\mathbf{k}n}$. Single-DMFT thus approximates the single-particle irreducible part of the Liouvillian of the lattice model by that of an effective impurity model.

For cellular DMFT (CDMFT), the real-space lattice is tiled into identical clusters, each containing N_c sites. The “impurity” is one of these clusters, which we denote by $\mathcal{C}$, and the real-space self-energy $[\tilde{\Sigma}(z)]_{\mathbf{r},\mathbf{r}'}$ is taken to be localized on $\mathcal{C}$ (with open boundary conditions): it contains non-local contributions only when both position arguments are on the same cluster, while intercluster terms are set to zero: $[\tilde{\Sigma}(z)]_{\mathbf{r},\mathbf{r}'} \neq 0$ only when $\mathbf{r}, \mathbf{r}' \in \mathcal{C}$. Therefore, the same is true for its $n > 0$ CFE coefficients $[\tilde{\epsilon}_n]_{\mathbf{r},\mathbf{r}'}$ and $[\tilde{t}_n]_{\mathbf{r},\mathbf{r}'}$. CDMFT thus explicitly breaks translation invariance.

By contrast, the dynamical cluster approximation (DCA) retains translational invariance at the cost of using coarse-grained momentum variables. The Brillouin zone (BZ) is partitioned into equally-sized patches labeled by patch momenta $\mathbf{K}$. The momentum-space self-energy is block-diagonal in $\mathbf{K}$, with diagonal blocks $\Sigma_{\mathbf{K}}(z)$, each of dimension $M \times M$. They are taken to depend only on the patch momentum $\mathbf{K}$ and are $\mathbf{k}$ -independent within each patch, with discontinuous jumps between patches. $\Sigma_{\mathbf{K}}(z)$ mimics the patch average of $\Sigma_{\mathbf{k}}(z)$. The same is true for its CFE coefficients, denoted $\epsilon_{\mathbf{K}n}$ and $t_{\mathbf{K}n}$.

interpolation schemes seek to restore translational invariance for CDMFT self-energies or a smooth momentum dependence for DCA self-energies. (As mentioned earlier, for CDMFT, our use of “interpolation” should be understood to refer to “periodization”.) In Sec. III C, we

propose $\mathcal{L}$ -interpolation as a unifying scheme, applicable to both CDMFT and DCA, capable of achieving these goals. Before that, in Sec. III B we briefly review the traditional schemes, Σ -, M -, and G -interpolation, since we will later present results comparing the performance of all these schemes.

B. Traditional interpolation

CDMFT: When applying traditional interpolation to our CDMFT data, we use a superlattice average [11] to guarantee causality. The superlattice is constructed translating a cluster $\mathcal{C}$ to tile the original lattice, treating $\mathcal{C}$ as a super-site carrying internal degrees of freedom. To interpolate a z -dependent $[\tilde{\mathbf{Q}}(z)]_{\mathbf{r},\mathbf{r}'}$ obtained from CDMFT as a real-space matrix, where $\tilde{\mathbf{Q}}$ stands for the self-energy $\tilde{\Sigma}$, cumulant $\tilde{\mathbf{M}}$ or Green's function $\tilde{\mathbf{G}}$, we make the CDMFT interpolation Ansatz

$$\mathbf{Q}_{\mathbf{k}}(z) \simeq \sum_{\delta} \bar{\mathbf{Q}}_{\delta}(z) e^{-i\mathbf{k} \cdot \delta}. \quad (55)$$

We estimate $\bar{\mathbf{Q}}_{\delta}(z)$ using a superlattice average [11]

$$\bar{\mathbf{Q}}_{\delta}(z) = \frac{1}{N_c} \sum_{\mathbf{r}' \in \mathcal{C}} [\tilde{\mathbf{Q}}(z)]_{\mathbf{r}', \mathbf{r}' + \delta}, \quad (56)$$

where the sum runs over a cluster with N_c sites. For $\tilde{\mathbf{Q}} = \tilde{\Sigma}$ or $\tilde{\mathbf{M}}$ (but not for $\tilde{\mathbf{G}}$), terms in Eq. (56) having $\mathbf{r}' + \delta \notin \mathcal{C}$ are zero. For $\tilde{\mathbf{Q}} = \tilde{\Sigma}$ or $\tilde{\mathbf{M}}$ (but not $\tilde{\mathbf{G}}$), we therefore have $\bar{\mathbf{Q}}_{\delta} = \mathbf{0}$ if $|\delta|$ exceeds the cluster size. For $\tilde{\mathbf{Q}} = \tilde{\Sigma}$ or $\tilde{\mathbf{M}}$, Eq. (55) thus is equivalent to a short-range-truncated Fourier Ansatz of the form (2), while for $\tilde{\mathbf{Q}} = \tilde{\mathbf{G}}$, Eq. (55) involves no short-ranged truncation.

Superlattice averaging as described above leads to causal self-energies or Green's functions [11]. However, these may become non-causal if the superlattice average is replaced, for instance, by a cluster average, i.e. if in Eq. (56) $1/N_c$ is replaced by $1/N_{\delta}$, where N_{δ} is the number of pairs of sites in the cluster having distance δ .

DCA: In DCA, the Brillouin zone (BZ) is partitioned into N_p disjoint patches labeled by a set of representative momenta $\{\mathbf{K}\}$. We write $V_{\text{BZ}} = \cup_{\mathbf{K}} V_{\mathbf{K}}$ for the union of their domains, and $\sum_{\mathbf{K}} |V_{\mathbf{K}}| = |V_{\text{BZ}}|$ for the sum of their volumes. The output of DCA computations are translationally invariant, momentum patch-averaged quantities.

$$\mathbf{Q}_{\mathbf{K}}(z) = \begin{cases} \Sigma_{\mathbf{K}}(z), \\ \mathbf{M}_{\mathbf{K}}(z) = [z + \mu - \Sigma_{\mathbf{K}}(z)]^{-1}. \end{cases} \quad (57)$$

These must be combined to yield a function $\mathbf{Q}_{\mathbf{k}}(z)$ defined throughout the BZ. “Bare” (non-interpolated) DCA does this using step functions, $\mathbf{Q}_{\mathbf{k}}(z) = \sum_{\mathbf{K}} \theta_{\mathbf{k},\mathbf{K}} \mathbf{Q}_{\mathbf{K}}(z)$, where $\theta_{\mathbf{k},\mathbf{K}} = 1$ if $\mathbf{k}$ lies in patch $\mathbf{K}$ and zero otherwise, resulting in artificial discontinuities in momentum space. The interpolation of $\mathbf{Q}_{\mathbf{K}}(z)$ amounts

to smearing out the discontinuities through an DCA interpolation Ansatz of the form

$$\mathbf{Q}_{\mathbf{k}}(z) = \sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} \mathbf{Q}_{\mathbf{K}}(z), \quad (58)$$

where for each patch $\mathbf{K}$ the “form factor” $\alpha_{\mathbf{k},\mathbf{K}}$ is an interpolation function of $\mathbf{k}$ defined on the entire BZ. Various choices for the form factors can be found in the literature, including splines [5] and low-order Fourier-Ansätze [62]. If $\mathbf{Q}_{\mathbf{K}}(z)$ depends on z (e.g. when it stands for $\Sigma_{\mathbf{K}}(z)$ or $\mathbf{M}_{\mathbf{K}}(z)$), interpolation can cause causality problems; a heuristic strategy for ameliorating these is to choose the form factors such that $\alpha_{\mathbf{k},\mathbf{K}} = 1$ [1, 6, 7].

Canonical DCA interpolation: For Liouvillian interpolation, the quantities to be interpolated are z -independent Liouvillian matrix elements, hence causality concerns do not arise (with one small caveat, discussed later). This affords us the freedom to focus on a formulation of a truncated Fourier expansion that is particularly well suited for our purposes. We will call it “canonical” DCA interpolation, since it ensures that the resulting $\mathbf{Q}_{\mathbf{k}}(z)$ possesses three canonical (clearly desirable) properties: (i) $\mathbf{Q}_{\mathbf{k}}(z)$ is invariant under the point-group symmetry operations (rotations, reflections, inversions) that leave the patches invariant. (ii) Averaging $\mathbf{Q}_{\mathbf{k}}(z)$ over patch $\mathbf{K}'$ yields $\mathbf{Q}_{\mathbf{K}'}(z)$, i.e. $\int_{V_{\mathbf{K}'}} \frac{d\mathbf{k}}{|V_{\mathbf{K}'}|} \mathbf{Q}_{\mathbf{k}}(z) = \mathbf{Q}_{\mathbf{K}'}(z)$. (iii) If $\mathbf{Q}_{\mathbf{K}}(z)$ does not depend on $\mathbf{K}$, $\mathbf{Q}_{\mathbf{K}}(z) = \mathbf{Q}(z)$, then $\mathbf{Q}_{\mathbf{k}}(z) = \mathbf{Q}(z)$. Below, we present a form factor construction that ensures these canonical properties. It expresses the form factors as linear combinations of lattice harmonics, using only ones that are invariant under the symmetry operations that leave all patches invariant. This construction is not new, but, for completeness, we explain its rationale nevertheless. (For some background on the definition of lattice harmonics, see App. F.)

For canonical DCA interpolation, we expand $\alpha_{\mathbf{k},\mathbf{K}}$ as

$$\alpha_{\mathbf{k},\mathbf{K}} = \sum_{j=1}^{N_p} \phi_{\mathbf{k},j} \Psi_{j,\mathbf{K}}. \quad (59)$$

Here, the $\phi_{\mathbf{k},j}$ are real-valued lattice harmonics chosen according to a criterion described below; j enumerates the chosen ones in order of increasing complexity, with $\phi_{\mathbf{k},1} = 1$; and the $\Psi_{j,\mathbf{K}}$ are real expansion coefficients, to be determined in manner described below.

To ensure property (i), we include in Eq. (59) only lattice harmonics $\phi_{\mathbf{k},j}$ that are invariant under the point group symmetries of the patches; that immediately implies the same for $\alpha_{\mathbf{k},\mathbf{K}}$. (The choice of $\phi_{\mathbf{k},j}$ may also depend on additional details of the chosen patching scheme and the physics it attempts to capture. A concrete example is given in Sec. V, where we consider 4-patch DCA results for a Hubbard model on a 2D square lattice and use $\phi_{\mathbf{k},j}$ functions constructed via Eq. (F4) in App. F.)

To ensure property (ii), we impose the condition

$$\int_{V_{\mathbf{K}'}} \frac{d\mathbf{k}}{|V_{\mathbf{K}'}|} \alpha_{\mathbf{k},\mathbf{K}} = \delta_{\mathbf{K}',\mathbf{K}}. \quad (60)$$

Inserting Ansatz (59) into condition (60) we obtain

$$\sum_{j=1}^{N_p} \Phi_{\mathbf{K}',j} \Psi_{j,\mathbf{K}} = \delta_{\mathbf{K}',\mathbf{K}}, \quad (61)$$

where the coefficients $\Phi_{\mathbf{K}',j} = \int_{V_{\mathbf{K}'}} \frac{d\mathbf{k}}{|V_{\mathbf{K}'}|} \phi_{\mathbf{k},j}$ encode information about patch shapes. Viewing Eq. (61) as an $N_p \times N_p$ matrix equation, $\Phi \cdot \Psi = \mathbb{1}$, we find $\Psi_{j,\mathbf{K}} = (\Phi^{-1})_{j,\mathbf{K}}$ (assuming Φ^{-1} exists). This completes the construction of the form factors $\alpha_{\mathbf{k},\mathbf{K}}$. Note that they are unchanged if the $\phi_{\mathbf{k},j}$ functions are replaced by linearly transformed combinations $\sum_{j'} \phi_{\mathbf{k},j'} T_{j'j}$ (assuming T is invertible), because by Eq. (61) that would just result in inversely transformed coefficients $\sum_{j''} T_{j,j''}^{-1} \Psi_{j'',\mathbf{K}}$.

Property (iii) holds, too, since the form factors satisfy

$$\sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} = 1 \quad (62)$$

by construction. This can be seen as follows. The only lattice harmonic whose BZ integral is nonzero is the constant one: $\int_{\text{BZ}} d\mathbf{k} \phi_{\mathbf{k},j} = |V_{\text{BZ}}| \delta_{j,1}$. Therefore,

$$\sum_{\mathbf{K}'} |V_{\mathbf{K}'}| \Phi_{\mathbf{K}',j} = \sum_{\mathbf{K}'} \int_{V_{\mathbf{K}'}} d\mathbf{k} \phi_{\mathbf{k},j} = |V_{\text{BZ}}| \delta_{j,1}. \quad (63)$$

Moreover, defining $\psi_j = \sum_{\mathbf{K}} \Psi_{j,\mathbf{K}}$, we find from Eq. (61),

$$\sum_{\mathbf{K}'} |V_{\mathbf{K}'}| \sum_{j=1}^{N_p} \Phi_{\mathbf{K}',j} \psi_j = \sum_{\mathbf{K}'} |V_{\mathbf{K}'}| \delta_{\mathbf{K}',\mathbf{K}} = |V_{\text{BZ}}|. \quad (64)$$

Inserting Eq. (63) into (64) we find $\psi_1 = 1$. Summing Eq. (61) over $\sum_{\mathbf{K}}$ we obtain $\sum_j \Phi_{\mathbf{K}',j} \psi_j = 1$, and since $\Phi_{\mathbf{K}',1} \psi_1 = 1 \cdot 1$, this implies $\sum_{j>1} \Phi_{\mathbf{K}',j} \psi_j = 0$. This linear combination of columns of Φ , which are linearly independent since was assumed to Φ^{-1} exist, can vanish only if all coefficients $\psi_{j>1}$ vanish, implying $\psi_j = \delta_{j,1}$. Thus $\sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} = \sum_j \phi_{\mathbf{k},j} \psi_j = \phi_{\mathbf{k},1} = 1$, proving Eq. (62).

Finally, we remark that the interpolation Ansatz of Eqs. (58) and (59) for $\mathbf{Q}_{\mathbf{k}}(z)$ and $\alpha_{\mathbf{k},\mathbf{K}}$ can be expressed as a truncated Fourier expansion having the form of Eq. (2), see App. F for details.

If canonical DCA interpolation is used to interpolate the self-energy or the cumulant, the resulting functions $\mathbf{Q}_{\mathbf{k}}(z)$ and $\mathbf{M}_{\mathbf{k}}(z)$ may exhibit frequency-dependent ringing effects that lead to violations of causality [63]. One possible remedy is to use a modified version of Eq. (59),

$$\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}} = \sum_{j=1}^{N_p} \frac{1}{N_j} \phi_{\mathbf{k},j} \Psi_{j,\mathbf{K}}, \quad (65)$$

where ϕ and Ψ are defined as above, and N_j is the number of sites in the real-space orbit O_j associated with $\phi_{\mathbf{k},j}$ (see App. F, Eq. (F4) for details). The factor $1/N_j$ reduces the contribution of the non-local Fourier coefficients $\phi_{\mathbf{k},j>1}$ relative to the local one, $\phi_{\mathbf{k},1}$, thereby counteracting their causality-violating tendencies. However,

it must be acknowledged that this prescription is somewhat arbitrary and spoils the above-mentioned canonical property (ii).

An alternative fix to ensure causality, already mentioned above, is to drop Eq. (60) and instead enforce $[\alpha_{\mathbf{k},\mathbf{K}}]_{\mathbf{k}=\mathbf{K}} = 1$ [1, 6, 7]. However, this prescription, too, involves arbitrariness, since the choice $\mathbf{k} = \mathbf{K}$ singles out one point in the patch and contains no information about the actual shape of the patch. Moreover, typically it does not guarantee canonical property (ii).

By contrast, when DCA interpolation is performed by $\mathcal{L}$ -interpolation, as presented in the next sections, such problems do not arise. Since $\mathcal{L}$ is Hermitian and its matrix elements are frequency-independent, $\mathcal{L}$ -interpolation respects causality by construction. It can thus be used in conjunction with canonical DCA interpolation, thus also ensuring the canonical properties (i)-(iii).

C. $\mathcal{L}$ -interpolation

Conceptually, our $\mathcal{L}$ -interpolation scheme is very simple: we compute the dynamical part of the self-energy, construct its CFE coefficients, and interpolate the latter using the same strategy as in Sec. III B—but now applied to n -dependent coefficients instead of z -dependent functions, which makes all the difference for ensuring causality. Concretely, we proceed as follows.

CDMFT: Using the Lanczos scheme of Sec. II E, we construct the CFE of the dynamical part of the CDMFT self-energy, $[\Sigma^{\text{dyn}}(z)]_{\mathbf{r},\mathbf{r}'}$ (see App. E 1 for numerical details), obtaining the corresponding hermitian CFE coefficients $[\tilde{\epsilon}_n]_{\mathbf{r},\mathbf{r}'}$ and $[\tilde{\mathbf{t}}_n]_{\mathbf{r},\mathbf{r}'}$. From these we estimate hermitian, real-space Liouvillian matrix elements of the lattice model using superlattice averaging as in Eq. (56):

$$\bar{\epsilon}_{\delta n} = \frac{1}{N_c} \sum_{\mathbf{r}' \in \mathcal{C}} [\tilde{\epsilon}_n]_{\mathbf{r}',\mathbf{r}'+\delta}, \quad \bar{\mathbf{t}}_{\delta n} = \frac{1}{N_c} \sum_{\mathbf{r}' \in \mathcal{C}} [\tilde{\mathbf{t}}_n]_{\mathbf{r}',\mathbf{r}'+\delta}. \quad (66)$$

They are cluster-range-limited, vanishing if $|\delta|$ exceeds the cluster size. Note that $\bar{\epsilon}_{\delta n} = \bar{\epsilon}_{-\delta n}^\dagger$ since by construction, $\epsilon_n = \epsilon_n^\dagger$, implying $[\tilde{\epsilon}_n]_{\mathbf{r},\mathbf{r}'} = [\tilde{\epsilon}_n^\dagger]_{\mathbf{r}',\mathbf{r}}$ for its matrix elements. Likewise for $\mathbf{t}_n$.

Finally, we define CDMFT-interpolated CFE coefficients in analogy to Eq. (55):

$$\epsilon_{\mathbf{k}n} \simeq \sum_{\delta} \bar{\epsilon}_{\delta n} e^{-i\mathbf{k} \cdot \delta}, \quad \mathbf{t}_{\mathbf{k}n} \simeq \sum_{\delta} \bar{\mathbf{t}}_{\delta n} e^{-i\mathbf{k} \cdot \delta}. \quad (67)$$

By construction, we have $\epsilon_{\mathbf{k}n} = \epsilon_{\mathbf{k}n}^\dagger$, $\mathbf{t}_{\mathbf{k}n} = \mathbf{t}_{\mathbf{k}n}^\dagger$.

The reason why in this work we use using superlattice averaging in Eq. (66) to estimate $\bar{\epsilon}_{\delta n}$ and $\bar{\mathbf{t}}_{\delta n}$ is that this provided the most favorable comparisons to benchmark results obtained using MPS methods (see Sec. IV). However, instead of superlattice averaging, one could in Eq. (66) also use cluster averaging, or some other scheme, as long as $\bar{\epsilon}_{\delta n} = \bar{\epsilon}_{-\delta n}^\dagger$ and $\bar{\mathbf{t}}_{\delta n} = \bar{\mathbf{t}}_{-\delta n}^\dagger$, ensuring that

$\epsilon_{\mathbf{k}n}$ and $\mathbf{t}_{\mathbf{k}n}$ and therefore also the CDMFT-interpolated Liouvillian are hermitian, leading to causal Green's functions and self-energies after interpolation. This is in stark contrast to periodization schemes based on frequency-dependent quantities such as the self-energy or the cumulant, as discussed above.

DCA: Here, we use the Lanczos scheme of Sec. II E to construct CFE coefficients $\epsilon_{\mathbf{K}n}$ and $\mathbf{t}_{\mathbf{K}n}$ from the dynamical part of the patch self-energies $\Sigma_{\mathbf{K}}^{\text{dyn}}(z)$. We then apply the canonical DCA interpolation of Sec. III B to the CFE coefficients, with $\alpha_{\mathbf{k},\mathbf{K}}$ constructed according to Eqs. (59)–(61), to define DCA-interpolated coefficients,

$$\epsilon_{\mathbf{k}n} = \sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} \epsilon_{\mathbf{K}n}, \quad \mathbf{t}_{\mathbf{k}n} = \sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} \mathbf{t}_{\mathbf{K}n}. \quad (68)$$

They are hermitian, since the CFE coefficients $\epsilon_{\mathbf{K}n}$ and $\mathbf{t}_{\mathbf{K}n}$ are hermitian by construction, and the $\alpha_{\mathbf{k},\mathbf{K}}$ are real.

Having constructed the interpolated coefficients $\epsilon_{\mathbf{k}n}$ and $\mathbf{t}_{\mathbf{k}n}$ from CDMFT or DCA as described above, we are ready to assemble the corresponding interpolated dynamical self-energy $\Sigma_{\mathbf{k}}^{\text{dyn}}(z)$. If the Lanczos iteration for finding CFE coefficients terminates automatically, i.e. for a discrete $\mathcal{L}_{\text{cc}}$ that is fully represented by Eq. (28), the CFE (41) is an exact representation of $\Sigma_{\mathbf{k}}^{\text{dyn}}(z)$. Its interpolated version, and in turn the interpolated self-energy $\Sigma_{\mathbf{k}}(z)$, follows from inserting the interpolated matrix elements $\epsilon_{\mathbf{k}n}$ and $\mathbf{t}_{\mathbf{k}n}$ into Eq. (41), thereby defining

$$\Sigma_{\mathbf{k}}^{\text{dyn}}(z) = \mathbf{t}_{\mathbf{k}1} \frac{1}{z_{\mathbf{k}1} - \mathbf{t}_{\mathbf{k}2} \frac{1}{z_{\mathbf{k}2} - \dots - \mathbf{t}_{\mathbf{k}N} \frac{1}{z_{\mathbf{k}N}}} \mathbf{t}_{\mathbf{k}N}} \mathbf{t}_{\mathbf{k}1}, \quad (69)$$

with $\mathbf{z}_{\mathbf{k}n} = \mathbf{z} - \epsilon_{\mathbf{k}n}$. If the CFE is terminated by a residual function $\mathbf{R}_N(z)$ as in Eq. (42), we construct its interpolated version $\mathbf{R}_{\mathbf{k}N}(z)$ via the traditional for CDMFT or DCA approaches of Sec. III B, using

$$[\tilde{\mathbf{Q}}(z)]_{\mathbf{r},\mathbf{r}'} = [\tilde{\mathbf{R}}_N(z)]_{\mathbf{r},\mathbf{r}'}, \quad \mathbf{Q}_{\mathbf{K}}(z) = \mathbf{R}_{\mathbf{K}N}(z), \quad (70)$$

respectively, and set $\mathbf{z}_{\mathbf{k}N} = \mathbf{z} - \epsilon_{\mathbf{k}N} - \mathbf{R}_{\mathbf{k}N}(z)$ in (69). For an NRG self-energy whose CFE involves F/S-splitting (cf. Sec. II H), we similarly interpolate the fast-mode terms $[\tilde{\mathbf{R}}_n^{\text{F}}(z)]_{\mathbf{r},\mathbf{r}'}$ or $\mathbf{R}_{\mathbf{K}n}^{\text{F}}(z)$ for CDMFT or DCA, and set $\mathbf{z}_{\mathbf{k}n} = \mathbf{z} - \epsilon_{\mathbf{k}n} - \mathbf{R}_{\mathbf{k}n}^{\text{F}}(z)$ for $n < N$ in (69).

We note that our suggestion to interpolate the z -dependent functions $\mathbf{R}_n^{(\text{F})}(z)$ using traditional schemes, can, in principle, lead to similar causality violations for $\Sigma_{\mathbf{k}}^{\text{dyn}}(z)$ as those discussed in Sec. III B for traditional periodizations of $\Sigma_{\mathbf{k}}(z)$ or $\mathbf{M}_{\mathbf{k}}(z)$. However, for the computations performed for this work, we find that the functions $\mathbf{R}_n^{(\text{F})}(z)$ are quite local, and that essentially all significantly non-local features of $\Sigma_{\mathbf{k}}^{\text{dyn}}(z)$ are encoded in ϵ_n and $\mathbf{t}_n$, see Sec. V A. As a result, we did not encounter any violations of causality. (In case DCA computations

do yield causality violations, we recommend using $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ of Eq. (65) when interpolating $\mathbf{R}_n^{(\text{F})}(z)$, thereby reducing the contribution of non-local Fourier coefficients.)

D. Discrete self-energies: interpolation before broadening

If the impurity solver used within cDMFT discretizes the bath, then both spectral functions and self-energies are discrete functions of frequency. They have to be broadened to estimate the corresponding continuous functions of the impurity model with a continuous bath. For some impurity solvers, such as NRG, discrete spectral functions are computed and broadened, but discrete self-energies are typically unavailable (see, however, Ref. 60). If discrete self-energies *are* available, it is advantageous to apply interpolation schemes directly to the discrete ones and broaden them *after* interpolation. We have done that for the CDMFT data in Sec. IV B, which was computed with a tangent-space Krylov (TaSK) impurity solver [64] where discrete self-energies are available. The same goes for the exact diagonalization data shown in App. G.

The discrete self-energy has a finite CFE, which can usually be computed exactly (otherwise, the discussion that follows does not apply). Interpolating the CFE coefficients according to our discussion above yields periodic self-energy with a discrete frequency dependence. To obtain a continuous frequency dependence, we simply broaden the discrete periodic self-energy for every $\mathbf{k}$ -point with the same broadening scheme used within the cDMFT calculation.

We close this section with a final remark. After the dynamical part of the cDMFT self-energy has been interpolated, DMFT defines the lattice Green's function as

$$\mathbf{G}_{\mathbf{k}}(z) = \frac{1}{\mathbf{z} - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}^{\text{HF}} - \Sigma_{\mathbf{k}}^{\text{dyn}}(z)}. \quad (71)$$

Here $\epsilon_{\mathbf{k}}$, representing the free single-particle Hamiltonian, is exact and does not require interpolation. The Hartree-Fock term $\Sigma_{\mathbf{k}}^{\text{HF}}$, unlike $\epsilon_{\mathbf{k}}$, depends on the density matrix used to evaluate inner products. For purely local interactions, as treated in this work, the HF term is local and identical to that of the impurity model, $\Sigma_{\mathbf{k}}^{\text{HF}} = \Sigma^{\text{HF}}$, so it does not need to be interpolated. With non-local interactions, however, the HF term does acquire a $\mathbf{k}$ -dependence (even without interpolation) that is only partially captured by the impurity model: it arises from lattice expectation values computed via $\mathbf{k}$ -sums over corresponding lattice Green's functions. However, for CDMFT/DCA, these lattice expectation values are generally not fully periodic/continuous, leading to a non-periodic/non-continuous HF contribution. To resolve this, we propose to recompute the HF term after interpolating the single-particle irreducible matrix elements, and to iterate this until self-consistency.

IV. BENCHMARK: CDMFT INTERPOLATION IN THE 1D HUBBARD MODEL

This section is devoted to benchmarking the $\mathcal{L}$ -interpolation of CDMFT data in a context in which essentially exact reference data is also available. By comparing the results of G -, Σ -, M - and $\mathcal{L}$ -interpolation schemes to the reference data, we establish which interpolation schemes perform best. (Reminder: in this section, “interpolation” stands for “periodization”, i.e. real-space interpolation.)

We consider the one-dimensional Hubbard model,

$$H = - \sum_{\ell\sigma} (c_{\ell\sigma}^\dagger c_{\ell+1\sigma} + \text{h.c.}) - \mu \sum_{\ell\sigma} n_{\ell\sigma} + U \sum_{\ell} n_{\ell\uparrow} n_{\ell\downarrow}, \quad (72)$$

for a chain of L sites. This model is challenging for DMFT-type approaches, which are controlled by the inverse dimensionality of the lattice model. On the other hand, this model can be efficiently treated using matrix product state (MPS) techniques. In Sec. IV A, we use MPS techniques to compute and investigate the full frequency *and* momentum dependence of its single-particle spectral function and self-energy. These results are numerically (almost) exact, and we will view them as “ground truth” for this model. We use our MPS results (i) to show that $\mathcal{L}$ is indeed more short-ranged than Σ or M ; and (ii) as benchmark data against which we subsequently, in Sec. IV B, compare interpolated CDMFT results obtained using several different schemes: G -, Σ -, M - and $\mathcal{L}$ -interpolation.

A. MPS analysis

For our MPS-based analysis, we compute the ground state of Hubbard chain of $L = 50$ sites with $U = 5$ and $\mu = -U/2$ (half-filling) using the density matrix renormalization group (DMRG). We then compute the single-particle spectral function $A_k(\omega)$ associated with the retarded correlator

$$\tilde{G}_k^R(t) = -i\theta(t)\langle\{c_k(0), c_k^\dagger(-t)\}\rangle, \quad (73)$$

where $c_k = \frac{1}{\sqrt{L}} \sum_{\ell=1}^L e^{-ik\ell} c_{\ell\sigma}$, using the tangent-space Krylov (TaSK) approach [64]. TaSK yields the spectral function in the form of a discrete Lehmann representation, $A_k^{\text{disc}}(\omega)$. The eigenstates and eigenenergies involved therein are computed via a Lanczos scheme that constructs a Krylov basis within the 1-site tangent space of the ground state. $A_k^{\text{disc}}(\omega)$ is a discrete function of ω (since the chain has finite length). We broaden it to obtain $A_k(\omega)$ as a smooth function of ω . For details see App. H and Ref. 64.

From $A_k(\omega)$ we compute $G_k(\omega)$ (8a), and then $\Sigma_k(\omega)$ and $M_k(\omega)$ via Eqs. (1). The resulting spectral function $A_k(\omega)$, self-energy $\Sigma_k(\omega)$ and cumulant $M_k(\omega)$ are

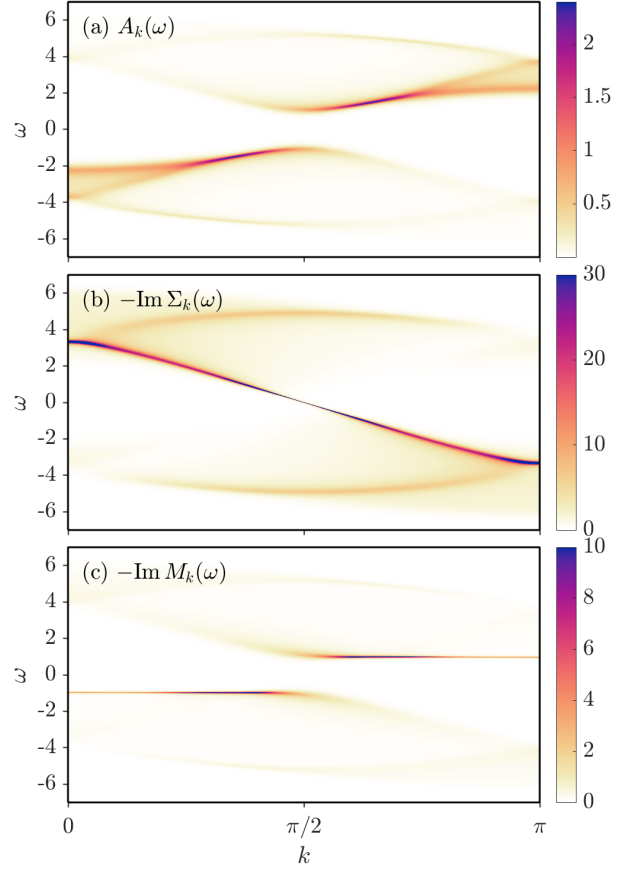


FIG. 1. (a) Spectral function, (b) self-energy and (c) cumulant computed with the TaSK method for a $L = 50$ Hubbard model.

shown in Figs. 1(a), (b) and (c), respectively. As expected, $A_k(\omega)$ exhibits a Mott gap while $\Sigma_k(\omega)$ has a dispersive pole. The main feature of $M_k(\omega)$, on the other hand, is a k -independent peak at negative frequencies for $0 \leq k \leq \pi/2$ and another flat peak at positive frequencies at $\pi/2 \leq k \leq \pi$. Thus, the features of $M_k(\omega)$ are significantly less dispersive than those of both $A_k(\omega)$ and $\Sigma_k(\omega)$. As a result, M -interpolation is expected to yield better results than Σ -interpolation for the present parameters where the model is in a Mott phase. This aligns with findings in the literature [11].

In order to test more quantitatively which interpolation scheme may yield the best outcomes, we Fourier-transform to position space and compute the Fourier coefficients

$$\tilde{\Sigma}_r(\omega) = \frac{1}{L} \sum_k e^{ikr} \Sigma_k(\omega), \quad \tilde{M}_r(\omega) = \frac{1}{L} \sum_k e^{ikr} M_k(\omega). \quad (74)$$

For $r \leq 5$, the Fourier coefficients $\tilde{\Sigma}_r(\omega)$ and $\tilde{M}_r(\omega)$ are shown in Fig. 3(a) and (b), respectively. The maximal

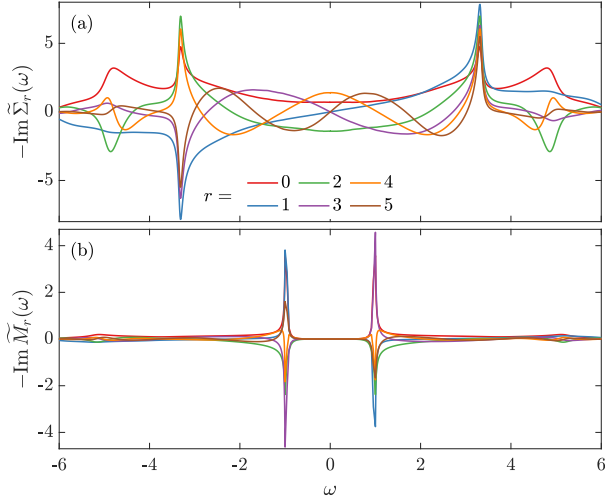


FIG. 2. The first six Fourier coefficients of the imaginary part of (a) the self-energy of Fig. 1(b) and (b) the cumulant of Fig. 1(c).

absolute amplitude of $\tilde{M}_r(\omega)$ clearly decays faster with increasing r than that of $\tilde{\Sigma}_r(\omega)$. This suggests that here M -interpolation will outperform Σ -interpolation. Indeed, we confirm this explicitly below.

Now consider the truncated Fourier series,

$$\Sigma_k^{[R]}(\omega) = \sum_{r=0}^R \tilde{\Sigma}_r(\omega) \cos(kr), \quad (75a)$$

$$M_k^{[R]}(\omega) = \sum_{r=0}^R \tilde{M}_r(\omega) \cos(kr). \quad (75b)$$

Here, r plays the role of δ from Sec. III. (Compared

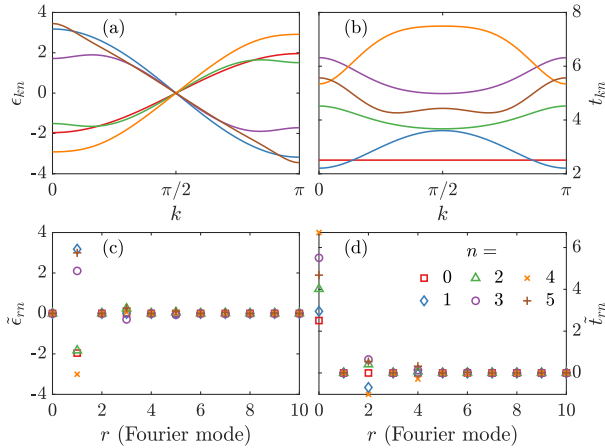


FIG. 3. (a,b) Matrix elements ϵ_{kn} and t_{kn} of $\mathcal{L}$, extracted via CFE from the spectral data in Fig. 1. (c,d) The corresponding Fourier coefficients $\tilde{\epsilon}_{rn}$ and $\tilde{t}_{rn}$ up to order $r = 10$. The color scheme of panel (d) applies to all panels.

to Eq. (53), we combined terms with $e^{\pm ikr}$ in the sum above, so that the magnitude of the non-local coefficients $\tilde{\Sigma}_r(\omega)$ with $r > 0$ is directly comparable to the local coefficient $\tilde{\Sigma}_0(\omega)$, and similarly for M .) Such truncated Fourier series will generically lead to non-causal features (positive imaginary parts for $\Sigma_k(\omega)$ or $M_k(\omega)$) due to ringing [63] because the truncation discards ω -dependent terms. Consider, for instance, approximating $\Sigma_k(\omega)$ by the first two terms of its Fourier expansion,

$$\Sigma_k^{[1]}(\omega) = \tilde{\Sigma}_0(\omega) + \cos(k) \tilde{\Sigma}_1(\omega). \quad (76)$$

As shown in Fig. 2, there exist frequencies where $-\text{Im}\tilde{\Sigma}_0(\omega) < -\text{Im}\tilde{\Sigma}_1(\omega)$. At these frequencies, the approximation $\Sigma_k^{[1]}(\omega)$ will be non-causal at $k = \pi$, because $-\text{Im}\Sigma_{k=\pi}^{[1]}(\omega) = -\text{Im}[\tilde{\Sigma}_0(\omega) - \tilde{\Sigma}_1(\omega)] < 0$. In general, $\Sigma_k^{[1]}(\omega)$ will have non-causal features whenever $|\text{Im}\tilde{\Sigma}_0(\omega)| < |\text{Im}\tilde{\Sigma}_1(\omega)|$, and likewise for $M_k^{[1]}(\omega)$. Less severe truncation by keeping more Fourier coefficients (thus considering longer-ranged terms) gradually reduces non-causal features. We discuss this in more detail below, together with Fig. 4.

As just discussed, non-causal behavior can arise when truncating Fourier series with ω -dependent coefficients. This problem can be avoided by adopting a strategy in which all Fourier series to be truncated involve only ω -independent coefficients. To this end, we consider the CFE representation of $G_k(\omega^+)$, which amounts to a change of variables from ω to n : it encodes the ω dependence explicitly in a continued fraction involving ω -independent CFE coefficients ϵ_{kn} and t_{kn} . Fourier representations of the k dependence of ϵ_{kn} and t_{kn} can then be safely truncated without yielding non-causal behavior.

To illustrate this, we have computed a CFE for $G_{\mathbf{k}}(\omega^+)$ starting from our TaSK result for the discrete spectral function $A_k^{\text{disc}}(\omega)$, using the strategy discussed after Eq. (46). Figures 3(a) and 3(b) show the resulting Liouvillian matrix elements ϵ_{kn} and t_{kn} , respectively, for $n \leq 5$. For fixed n they are smooth functions of k . Their Fourier coefficients,

$$\tilde{\epsilon}_{rn} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} (2 - \delta_{r,0}) \cos(kr) \epsilon_{kn}, \quad (77a)$$

$$\tilde{t}_{rn} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} (2 - \delta_{r,0}) \cos(kr) t_{kn} \quad (77b)$$

turn out to decay quickly with r . This can be seen from Figs. 3(c) and 3(d), showing the Fourier coefficients $\tilde{\epsilon}_{rn}$ and $\tilde{t}_{rn}$, respectively. We find that $\tilde{\epsilon}_{rn} = 0$ for even r while $\tilde{t}_{rn} = 0$ for odd m (because particle-hole symmetry implies $\epsilon_{k,n} = -\epsilon_{k+\pi,n}$ and $t_{k,n} = t_{k+\pi,n}$). We find that the magnitude of the Fourier coefficients decays monotonically with r , $|\tilde{\epsilon}_{1,n}| > |\tilde{\epsilon}_{3,n}| > \dots$ and $|\tilde{t}_{0,n}| > |\tilde{t}_{2,n}| > \dots$. This suggests that the Fourier series, defined as

$$\epsilon_k^{[R]} = \sum_{r=0}^R \tilde{\epsilon}_{rn} \cos(kr), \quad t_k^{[R]} = \sum_{r=0}^R \tilde{t}_{rn} \cos(kr), \quad (78)$$

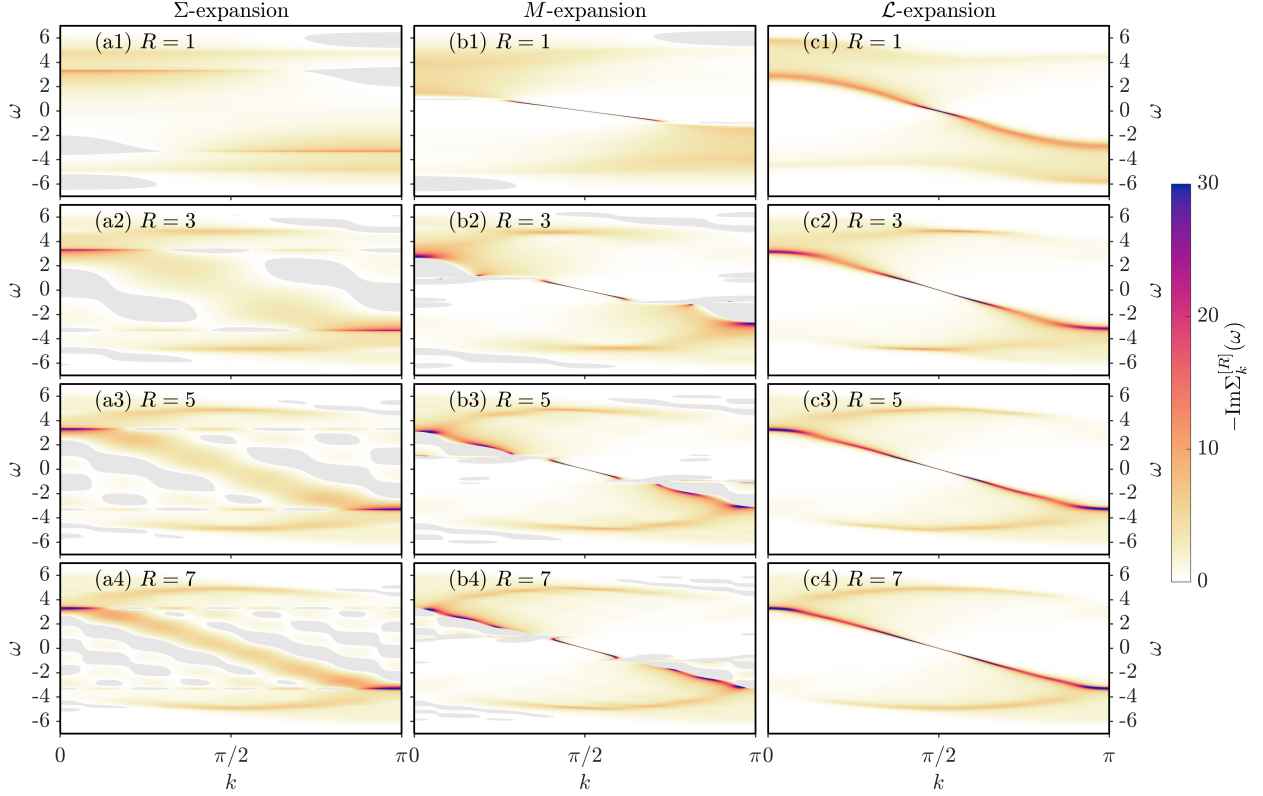


FIG. 4. Self-energy $\Sigma_k^{[R]}(\omega)$ obtained from truncating the Fourier series of Σ -, M - or $\mathcal{L}$ -expansions at $r \leq R$ as described in the text. Regions where $-\text{Im}\Sigma_k^{[R]}(\omega) < 0$ (non-causal behavior) are depicted gray.

converge smoothly, and that truncating them will not cause significant ringing artifacts. Note that even if ringing does occur, the resulting spectral functions and self-energies are still guaranteed to be causal, in stark contrast to the truncated Fourier series of $\Sigma_k(\omega)$ or $M_k(\omega)$. The reason is that *any* approximation of ϵ_{kn} or t_{kn} that leaves ϵ_{kn} real leads to a hermitian $\mathcal{L}$ and therefore to causal spectra.

Our discussion so far suggests that a truncated Fourier expansion of $\mathcal{L}$ has much more favorable convergence properties than a truncated expansion of Σ or M . We verify this explicitly in Fig. 4, where we investigate how $\Sigma_k^{[R]}(\omega)$, obtained via Σ , M or $\mathcal{L}$ expansions involving truncated ($r \leq R$) summations, evolves when the expansion order R is increased.

The first column, Figs. 4(a1-a4), shows the evolution with R of the self-energy $\Sigma_k^{[R]}(\omega)$, represented by the truncated Fourier series Eq. (75a). In Fig. 4(a1) with $R = 1$, only the first two coefficients are retained, i.e. Eq. (76). This corresponds to neglecting any contributions to the self-energy beyond nearest neighbors, similar to 2-site CDMFT/DCA. Clearly, the approximated self-energy in Fig. 4(a1) does not capture the main features of the actual self-energy shown in Fig. 1(b). The disper-

sive Mott pole, the most distinctive feature of the self-energy in Fig. 1(b), is not captured at all by the truncated Fourier expansion of $\Sigma_k(\omega)$. Further, as discussed earlier, the truncated Fourier expansion yields non-causal artifacts (positive imaginary part) due to ringing, shown as gray areas. With increasing expansion order [Fig. 4(a2-a4)], the correct features are better captured, but convergence is very slow in the expansion order. Even for $R = 7$, which corresponds to considering up to 7 nearest-neighbors (as one would do for 8-site CDMFT/DCA), the self-energy is not fully converged and still shows non-causal features due to ringing.

The second column, Fig. 4(b1-b4), shows the evolution with R of the self-energy $\Sigma_k^{[R]}(\omega) = \omega + \mu - [M_k^{[R]}(\omega)]^{-1}$ when $M_k^{[R]}(\omega)$ is represented by the Fourier expansion (75b) truncated at $r \leq R$. In contrast to the truncated Σ expansion, the truncated M expansion captures the dispersive pole of the self-energy already at the lowest order shown, $R = 1$. However, a low-order truncation also leads to significant non-causal ringing artifacts, appearing prominently in the vicinity of the dispersive pole. Further, the shape of the pole dispersion is not very well captured at low orders. Even at the highest order shown, $R = 7$ in Fig. 4(b4), the self-energy is not captured very

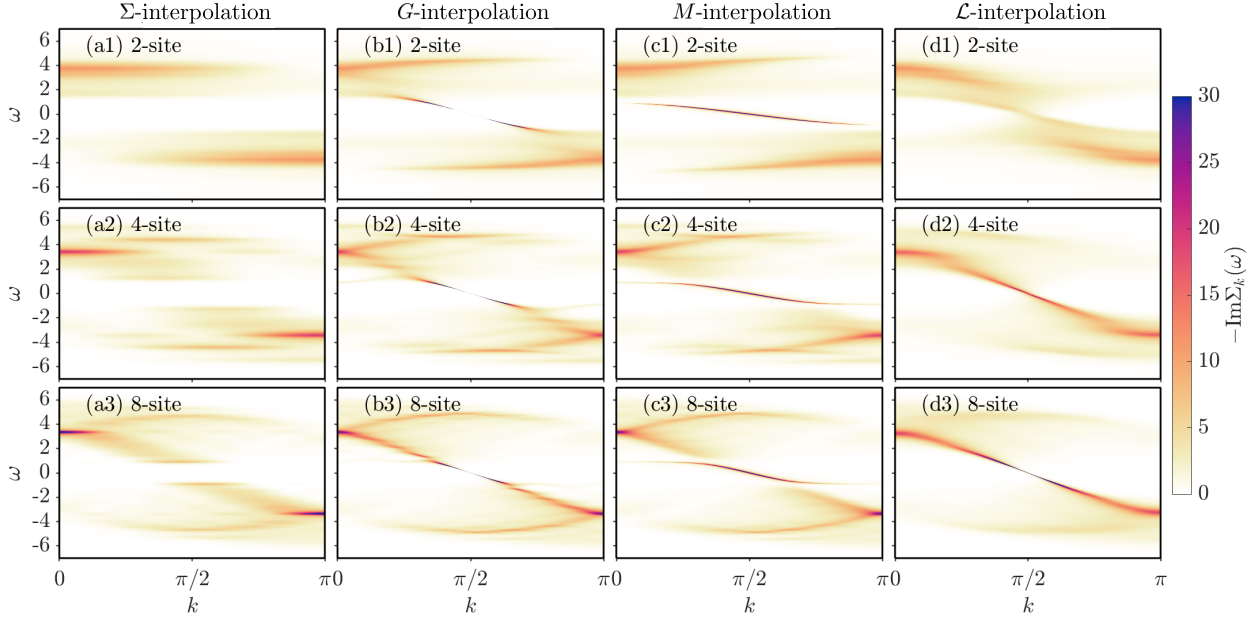


FIG. 5. Interpolated CDMFT self-energies for different cluster sizes N_c , obtained using four different interpolation schemes.

well, and there are still non-causal ringing artifacts left (though to a lesser extent than for the Σ expansion). Overall, truncating the Fourier expansion of M leads to somewhat better results than truncating that of Σ .

The third column, Fig. 4(c1-c4), shows a self-energy $\Sigma_k^{[R]}(\omega)$ obtained as follows: using $A_k^{\text{disc}}(\omega)$ as input, we performed a finite-depth CFE expansion of $G_k(\omega)$ to obtain the Liouvillian matrix elements ϵ_{kn} and t_{kn} ; these were Fourier transformed via Eq. (77) to obtain $\tilde{\epsilon}_{rn}$ and $\tilde{t}_{rn}$, from which we constructed R -truncated Fourier expansions $\epsilon_{kn}^{[R]}$ and $t_{kn}^{[R]}$ [Eq. (78)]. We used these to compute $\Sigma_k^{[R]}(\omega)$ via the CFE (41) while using the broadening scheme of Ref. 64, Sec. S-2.2, henceforth to be called “CFE+Gaussian broadening”.

As can be seen from Fig. 4(c1-c4), non-causal features are absent at any truncation order, in stark contrast to the truncated Σ or M expansion. Further, the correct dispersion of the self-energy pole is already captured at the lowest order, $R = 1$, with higher orders revealing more and more details. Qualitative convergence is reached at $R = 3$ (as one would use for 4-site CDMFT/DCA). At order $R = 5$ and beyond, the self-energy appears to be quite well converged, changes beyond this order are only minor.

To summarize, our analysis of numerically (almost) exact MPS data reveals that truncating the Fourier expansion of $\mathcal{L}$ matrix elements leads to faster and more controlled convergence than truncating that of Σ or M . Additionally, truncating the $\mathcal{L}$ expansion leads to causal spectra at all expansion orders, in stark contrast to truncating the Σ or M expansion where non-causal features

appear at low orders. Therefore, we can expect $\mathcal{L}$ -interpolation to outperform Σ or M -interpolation. We explicitly explore this in Sec. IV B.

B. Cellular DMFT

To illustrate how $\mathcal{L}$ -interpolation performs compared to M or Σ interpolation when applied to cDMFT data, we perform CDMFT calculations for the 1d Hubbard model analyzed in the previous section. The cluster impurity model that we solve with CDMFT contains as impurity an open-boundary Hubbard chain of N_c sites (thus N_c is the cell size); its two outermost sites on the left and right hybridize with two self-consistent baths with continuous spectra [2]. We discretize each bath using the “mean method” from Ref. 65 and map the discretized impurity model to a chain geometry, with each bath represented by 64 spinful orbitals. For the chain so obtained we use DMRG to compute the ground state. Then, we combine TaSK with a discrete version [60] of the equations of motion approach of Ref. 66 to compute a *discrete* version of the impurity self-energy, a $N_c \times N_c$ matrix-valued function with elements $[\tilde{\Sigma}_{\text{imp}}^{\text{disc}}(\omega)]_{\ell, \ell'}$, whose ω -dependence is represented by a sum of δ -peaks. (Due to CDMFT self-consistency, this also corresponds to the discrete lattice self-energy, $\tilde{\Sigma}_{\text{lattice}}^{\text{disc}}(\omega)$.) We then use $\tilde{\Sigma}_{\text{imp}}^{\text{disc}}(\omega)$ for two purposes. On the one hand, we use CFE+Gaussian broadening to obtain a smooth version of the impurity self-energy, $\tilde{\Sigma}_{\text{imp}}(\omega)$. We then take the latter as input for traditional Σ -, G -, M -interpolation employing super-

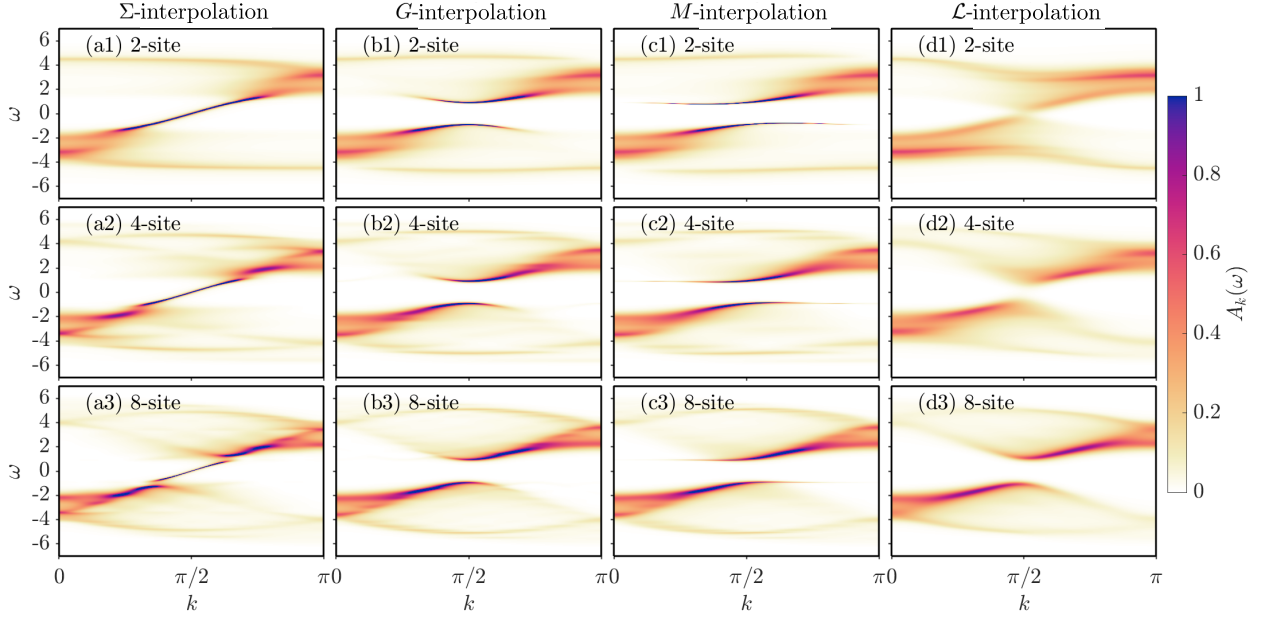


FIG. 6. Spectral function from different interpolation schemes for different cluster sizes.

lattice averaging [Eqs. (55), (56)], using for $\tilde{\mathbf{Q}}(\omega)$ either the broadened $\tilde{\Sigma}(\omega)$, or corresponding functions $\tilde{\mathbf{G}}(\omega)$ or $\tilde{\mathbf{M}}(\omega)$ obtained from the former in standard manner (Eqs. (7) and (6) of Ref. 33). On the other hand, for $\mathcal{L}$ -interpolation, we compute the CFE of the discrete $\tilde{\Sigma}_{\text{imp}}^{\text{disc}}(\omega)$ to obtain the single-particle irreducible Liouvillian matrix elements $\tilde{\epsilon}_n$ and $\tilde{\mathbf{t}}_n$. Next, we $\mathcal{L}$ -interpolate them, using the superlattice average (66) to obtain $\bar{\epsilon}_{rn}$, $\bar{\mathbf{t}}_{rn}$, and Eq. (67) to obtain ϵ_{kn} and $\mathbf{t}_{kn}$. We use these in Eq. (69) to construct an $\mathcal{L}$ -interpolated self-energy $\Sigma_k(\omega)$ while using CFE+Gaussian broadening (see App. H for details). This, finally, is the estimate produced by $\mathcal{L}$ -interpolated CDMFT for the lattice self-energy, to be compared to the self-energy computed in Sec. IV A.

In the following, we compare lattice self-energies (Fig. 5), spectral functions (Fig. 7) and cumulants (Fig. 7), for three different cluster sizes, $N_c \in \{2, 4, 8\}$, in each case obtained in four different ways, via Σ , G , M and $\mathcal{L}$ -interpolation. The self-energies are shown in Fig. 5(a1-a3). Even at the largest cluster size, the Σ -interpolation fails to reproduce the dispersive pole of the self-energy, i.e. it fails to correctly capture the Mott physics in this model. This behavior is in line with the analysis of the truncated Fourier series in Fig. 4, where we have seen that a large number of Fourier coefficients are required to capture the dispersive pole. Σ -interpolation is based on the assumption that the self-energy is weakly k -dependent, and for the 1d Hubbard model, this is simply not the case.

Figures 5(b1-b3) and (c1-c3) show the self-energy resulting from G - and M -interpolation, respectively. Both interpolation schemes work very well in producing the

dispersive Mott pole, even for the small 2-site cluster. However, for the larger clusters (4-site and 8-site), stripy structures show up which are artifacts of the interpolation. These stripy structures are more pronounced for G -interpolation than for M -interpolation. For the 2-site cluster, G -interpolation seems to perform better than M -interpolation in reproducing the features of the self-energy, in particular the slope of the dispersive pole. The reason for that exceptional performance of the G and M schemes at small N_c is the very weak k -dependence of the cumulant in this model. However, if the cumulant would be strongly k -dependent (for instance, if it had a dispersive pole), then G and M -interpolation are expected to encounter issues similar to Σ -interpolation in the present case. The 1d Mott insulator is therefore a case where the G and M -interpolation performs very well, but there is no guarantee that this is generically the case.

Figures 5(d1-d3) show the self-energy resulting from $\mathcal{L}$ -interpolation. The dispersive pole of the self-energy, which is one of its main features, is captured for all cluster sizes. However, the pole strength is not correctly captured for the small clusters, which results in an incorrect size of the Mott gap. The information on the correct self-energy pole weight therefore seems to reside in longer-ranged matrix elements of $\mathcal{L}$, a conclusion which can also be drawn from Fig. 4.

Figures 6 and 7 show the spectral functions and cumulants corresponding to the self-energies in Fig. 5. The Σ -interpolated spectral functions and cumulants display a dispersive pole even for the largest cluster size, a result that is evidently incorrect. The G and M schemes both produce the correct Mott gap in G and M , even for the

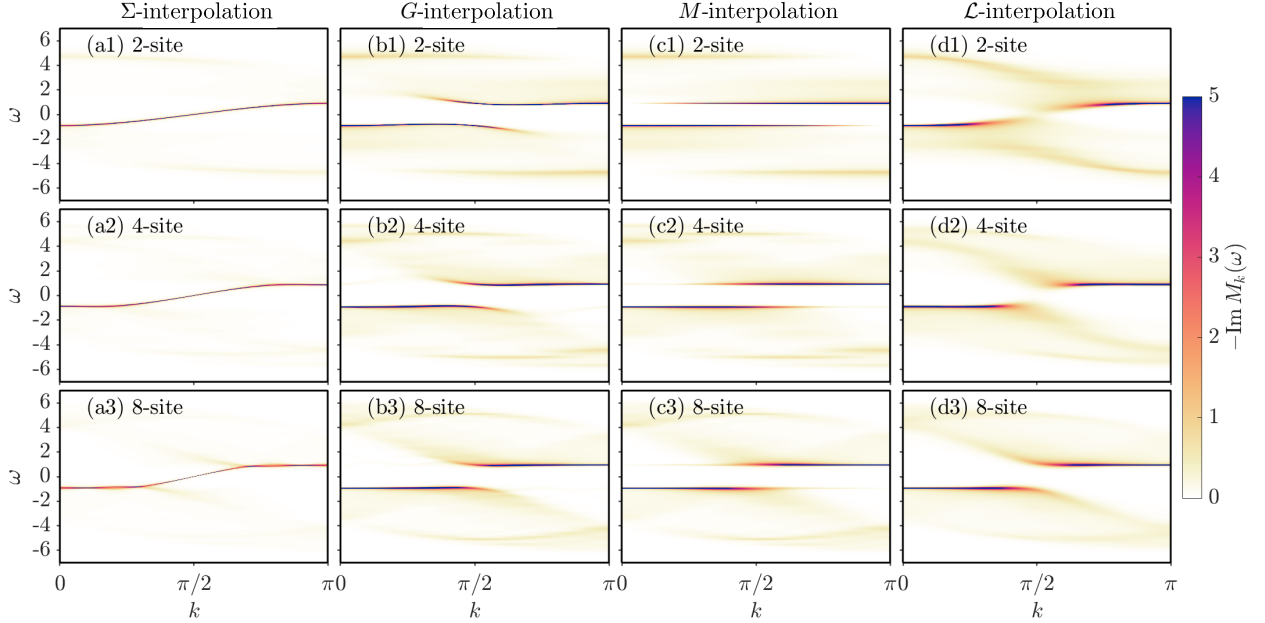


FIG. 7. Cumulant from different interpolation schemes for different cluster sizes.

smallest cluster size. Further, when using these interpolation schemes, the qualitative features of G and M compare quite well with the DMRG result for the 1d Mott insulator. $\mathcal{L}$ -interpolation, on the other hand, has trouble reproducing the correct size of the Mott gap at small cluster sizes, which is due to the incorrect weight of the self-energy pole. For the largest $N_c = 8$ cluster, however, $\mathcal{L}$ -interpolation reproduces the correct Mott gap and the qualitative features of both M and G compare very well with the DMRG result. For $N_c = 8$, $\mathcal{L}$ interpolation further provides smoother spectral features than the G or M schemes, with fewer interpolation artifacts.

To summarize, the Fourier series of matrix elements ϵ_{kn} and t_{kn} , of a numerically (almost) exact model, decay more rapidly than the Σ and M expansion of the same data. The conservation of causality of the $\mathcal{L}$ -interpolation becomes also evident within these examples. Our $\mathcal{L}$ -interpolation yields a fully causal interpolation that converges faster with cDMFT cluster size, which is confirmed by a benchmark test of the 1d Hubbard model using CDMFT+TaSK with several cluster sizes N_c .

V. DCA OF THE 2D HUBBARD MODEL

This section deals focuses on the interpolation of DCA results (i.e. in this section, “interpolation” means $\mathbf{k}$ -space interpolation). We obtain the input data for our interpolations from a 4-patch DCA+NRG treatment of the two-dimensional Hubbard model for three choices of doping, corresponding to Fermi-liquid, pseudo-gap and Mott insulator regimes. A thorough analysis of our DCA+NRG

results for this model will be published separately [67]. Here, we focus on interpolation rather than physical implications. We compare the non-interpolated discontinuous DCA results to smooth interpolated versions obtained from M -, Σ - and $\mathcal{L}$ -interpolations, focusing on data sets for which different interpolation schemes turn out to yield strikingly different results. Our analysis contains a striking physical result: $\mathcal{L}$ -interpolation can (depending on doping) resolve Fermi and Luttinger arcs which together form a closed surface, with a smooth crossover between Fermi and Luttinger arcs.

A. Model and periodization

We study the two-dimensional Hubbard model,

$$H = - \sum_{\mathbf{r}\mathbf{r}'} t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} - \mu \sum_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \quad (79)$$

where $t_{\mathbf{r}\mathbf{r}'}$ contains nearest- and next-nearest-neighbor hopping t and t' , respectively. The terms in the Hamiltonian are illustrated in Fig. 8(a). For the results presented below, we use $t = 1$ as our energy unit, set $t' = -0.3t$, $U = 7t$, use temperature $T = 10^{-10}t$, and adjust μ to vary the doping δ , which is our tuning parameter.

We obtain approximate solutions using 4-patch DCA, using the “star patching” scheme of Ref. 68, as illustrated in Fig. 8(b). To solve the cluster impurity model, we use the MuNRG implementation [69, 70] of the numerical renormalization group (NRG) [66, 71–74], which is based on the QSpace tensor library [75–79]. We exploit $U(1)$ charge and $SU(2)$ spin rotation symmetry, use a

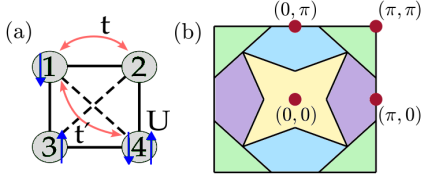


FIG. 8. (a) Illustration of hopping and interaction terms in the 2d Hubbard model. (b) Star patching geometry with patch momenta $\mathbf{K} \in \{(0,0), (0,\pi), (\pi,0), (\pi,\pi)\}$.

discretization parameter of $\Lambda_{\text{NRG}} = 8$, no z -shifting, and keep up to $N_{\text{keep}} = 10^5$ $U(1) \times \text{SU}(2)$ multiplets. Further, we use an interleaved Wilson chain geometry [80, 81], fully interleaving the bath modes associated with the different patches (labeled by their patch momenta) in the following order: $\mathbf{K}_1 = (0,0)$, $\mathbf{K}_2 = (\pi,0)$, $\mathbf{K}_3 = (0,\pi)$, $\mathbf{K}_4 = (\pi,\pi)$. We broaden discrete NRG data using a log-Gaussian broadening scheme [69] with broadening parameter $\sigma = 0.7$ there, and use Kugler's symmetric estimator approach [66] to compute the self-energies $\Sigma_{\mathbf{K}}(\omega)$.

Although interleaving breaks the expected symmetry between the $(\pi,0)$ and $(0,\pi)$ patches, the resulting broadened self-energy functions $\Sigma_{(\pi,0)}(\omega)$ and $\Sigma_{(0,\pi)}(\omega)$ are essentially identical, differing by less than 10^{-3} . Therefore, we enforced the symmetry between them in the DMFT loop, setting $\Sigma_{(0,\pi)}(\omega) \leftarrow \Sigma_{(\pi,0)}(\omega)$ before proceeding to the next DMFT iteration.

To extract the Liouvillian matrix elements $\epsilon_{\mathbf{K}n}$ and $t_{\mathbf{K}n}$ associated with each patch, we use the log-CFE described in Sec. II H. We set $\Lambda = 1.2$ and $\tau = 5$ for the splitting function $w_n^S(\omega)$, see Eq. (52). Further, we set $\Omega_{\min} = 10^{-9}$ (smaller values of $\Omega_{\min}$ lead to low-frequency inaccuracies due to double precision), and choose $\Omega_{\max}$ such that $\mathbf{A}_{\text{disc}}(\omega)$, the discrete spectral function output of our NRG impurity solver, satisfies its spectral sum rule to within 10^{-5} , i.e. $1 - \sum_{|\omega_i| < \Omega_{\max}} \mathbf{A}_{\text{disc}}(\omega_i) < 1 \cdot 10^{-5}$. This ensures that we capture essentially the entire support of the spectral function $\mathbf{A}(\omega)$; note that this choice amounts to cutting off over-broadened self-energy tails. For numerical details, and a discussion on how the interpolated results depend on τ and Λ , see App. E 3.

Figure 9 shows exemplary DCA patch self-energies (dashed lines) and their CFE representations (solid lines), confirming that our log-CFE accurately represents the cluster self-energies. Figures 10(a,b) show the corresponding Liouvillian matrix elements $\epsilon_{\mathbf{K}n}$ and $t_{\mathbf{K}n}$, demonstrating that they decrease exponentially with n . Figure 10(c) shows the imaginary part of the fast modes, $R_{\mathbf{K}n}^{\text{F}''}(\omega) = -\frac{1}{\pi} \text{Im} R_{\mathbf{K}n}^{\text{F}}(\omega)$, for several choices of n , with individual patch momenta distinguished by line color. The lines for the different patches show some slight differences for $n = 1$ but overlap increasingly well with decreasing n . This implies that the $\mathbf{K}$ -dependence of $R_{\mathbf{K}n}^{\text{F}''}(\omega)$ is weak and becomes ever weaker with increasing n . This property, which appears to arise generically for log-CFEs, is important for reducing the likelihood of

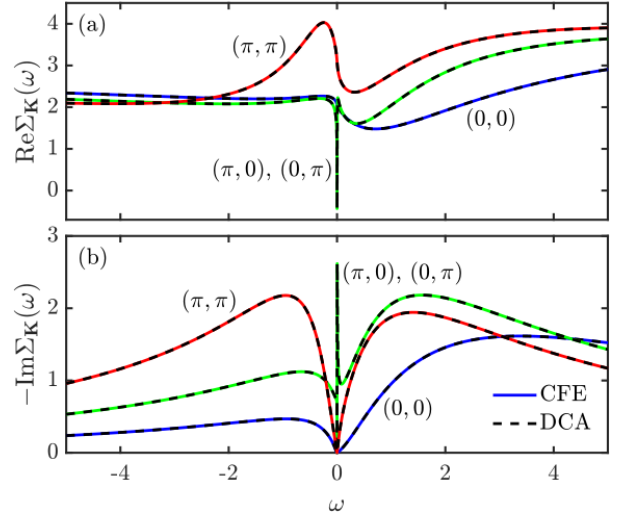


FIG. 9. (a) Real and (b) imaginary parts of the original DCA patch self-energy $\Sigma_{\mathbf{K}}(\omega)$ (dashed lines) and its log-CFE representation (51) (colored lines), for the patch momenta $\mathbf{K}_1 = (0,0)$ (blue), $\mathbf{K}_2 = (\pi,0)$ and $\mathbf{K}_3 = (0,\pi)$ (green), and $\mathbf{K}_4 = (\pi,\pi)$ (red). The excellent agreement between colored and dashed curves demonstrates that the log-CFE accurately represents the DCA results.

causality problems to arise when interpolating fast-mode functions, as will be elaborated below.

Our choice of $\tau = 5$ results in a rather sharp split between fast and slow modes. The dependence on τ is discussed in detail in App. E 3. The fact that $|\epsilon_{\mathbf{K}n}|$ shows a very much stronger patch dependence than $R_{\mathbf{K}n}^{\text{F}''}(\omega)$ means that most of the $\mathbf{k}$ -dependence of the interpolation will enter through the Liouvillian matrix elements.

Having obtained the Liouvillian matrix elements, our next step is to interpolate them using canonical DCA interpolation, as described in Sec. III B. For the star patching illustrated in Fig. 8, the $N_p = 4$ patches are invariant under x - and y -reflections, but not under $\pi/2$ rotations about the origin. The lowest few lattice harmonics that are invariant under these symmetry operations are constructed explicitly in App. F. They have the form

$$\begin{aligned} \phi_{\mathbf{k},1} &= 1, & \phi_{\mathbf{k},3} &= \cos k_x - \cos k_y, \\ \phi_{\mathbf{k},2} &= \cos k_x + \cos k_y, & \phi_{\mathbf{k},4} &= \cos k_x \cos k_y. \end{aligned} \quad (80)$$

leading to

$$\Psi_{j,\mathbf{K}} \simeq \begin{pmatrix} 0.2500 & 0.2500 & 0.2500 & 0.2500 \\ 0.4010 & 0.0092 & 0.0092 & -0.4194 \\ 0.0000 & 0.4050 & -0.4050 & 0.0000 \\ 0.7591 & -0.6645 & -0.6645 & 0.5698 \end{pmatrix} \quad (81)$$

for the coefficients appearing in Eq. (59) for the canonical DCA interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}$. The latter are then used to interpolate $\epsilon_{\mathbf{K}n}$, $t_{\mathbf{K}n}$, and $R_{\mathbf{K}n}^{\text{F}}(z)$ via Eq. (58).

The interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}$ are depicted in the first row of Fig. 11. They exhibit large positive weights in

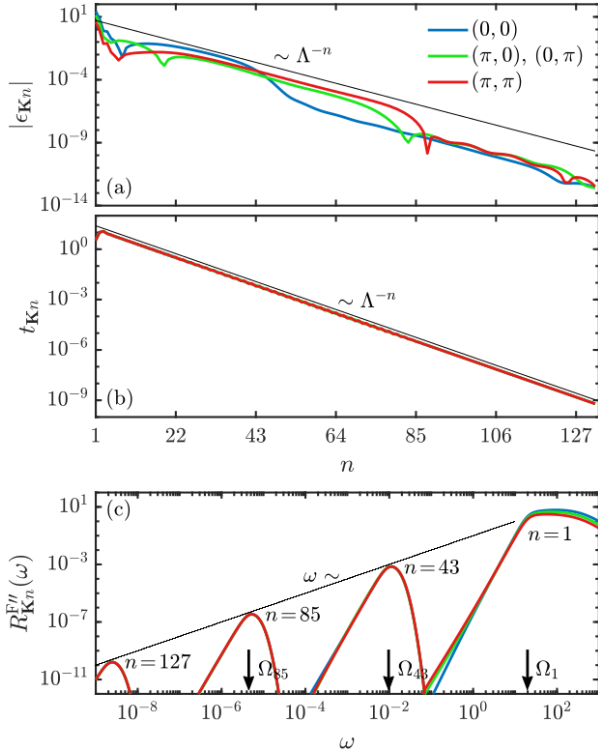


FIG. 10. (a,b) The Liouvillian matrix elements $|\epsilon_{\mathbf{K}n}|$ and $t_{\mathbf{K}n}$ obtained from a log-CFE with $\Lambda = 1.2$ and $\tau = 5$. (c) The spectral part of four fast modes $R_{\mathbf{K}n}^{\prime\prime}(\omega)$ with $n \in \{1, 43, 85, 127\}$; arrows indicate the corresponding energy scales Ω_n (cf. Eq. (52)). Thin black lines indicate the scaling behavior. As in Fig. 9, colors distinguish patch momenta.

the centers of their respective patches and fall off towards the other patches. Importantly, to fulfill the patch average condition (60), they become negative in the centers of some other patches. As an aside, we note that this can cause $\mathbf{Q}_{\mathbf{k}}(\omega) = \sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} \mathbf{Q}_{\mathbf{K}}(\omega)$ to be negative for some combinations of $\mathbf{k}$ and ω even if all $\mathbf{Q}_{\mathbf{K}}(\omega)$ are strictly positive functions of ω . This may lead to causality violations in some situations, e.g. when used for Σ - or M -interpolation. In sections VB and VC below, where we compare $\mathcal{L}$ -, Σ - and M -interpolation, we sidestep the potential causality issues of Σ - and M -interpolation by implementing the latter two schemes using the modified interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ of Eq. (65) (instead of $\alpha_{\mathbf{k},\mathbf{K}}$). There, the non-local Fourier modes $\phi_{\mathbf{k},j>1}$ are rescaled by a factor $1/N_j$ (defined in App. F), which counteracts their causality-violating tendencies. The resulting functions $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ are shown in the second row of Fig. 11. They are positive everywhere, as desired; however, they also exhibit a much weaker momentum dependence compared to $\alpha_{\mathbf{k},\mathbf{K}}$, and they do not preserve the patch average since Eq. (60) is not fulfilled. (We have also explored using other interpolation function for Σ - and M -interpolation, e.g. ones satisfying $\alpha_{\mathbf{K},\mathbf{K}} = 1$, so that setting $\mathbf{k} = \mathbf{K}$

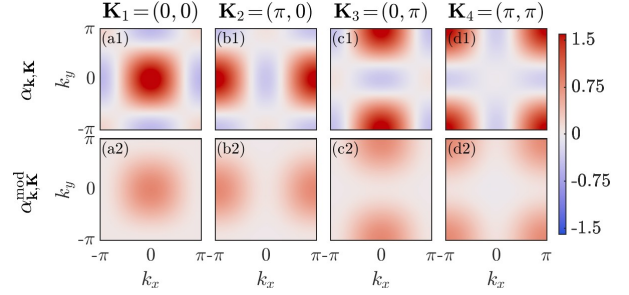


FIG. 11. (a1-d1) The canonical DCA interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}$ of Eq. (59), and (a2-d2) the modified interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ of Eq. (65), for the star patching geometry of Fig. 8(b). All plots employ the same diverging color scale. The $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ functions are strictly positive due to the reduced non-local contributions.

in the interpolated $Q_{\mathbf{k}}(z)$ reproduces the original patch function $Q_{\mathbf{K}}(z)$. These yielded minor quantitative but no qualitative differences from the results shown below, obtained using $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$.)

Returning to $\mathcal{L}$ -interpolation, we reiterate that we used the canonical DCA interpolation functions $\alpha_{\mathbf{k},\mathbf{K}}$ not only for obtaining $\epsilon_{\mathbf{K}n}$ and $t_{\mathbf{K}n}$, but also for $R_{\mathbf{K}n}^{\text{F}}(z)$. This did not lead to any causality problems, since the $\mathbf{K}$ -dependence of the $R_{\mathbf{K}n}^{\text{F}}(z)$ functions obtained from our log-CFE is so weak (cf. Fig. 10(c)).

B. Interpolated Spectra

In this section, we compare results for spectral functions $A_{\mathbf{k}}(\omega)$ and imaginary parts of the self-energy $\Sigma_{\mathbf{k}}(\omega)$ obtained from different interpolation schemes. We consider results at three values of doping, corresponding to a Fermi liquid (FL) at doping $\delta = 0.25$, the pseudogap phase (PG) at $\delta = 0.21$, and a Mott insulator (MI) at $\delta = 0.00$. We plot both $\Sigma_{\mathbf{k}}(\omega)$ and $A_{\mathbf{k}}(\omega)$ along the path $\Gamma = (0,0) \rightarrow X = (0,\pi) \rightarrow M = (\pi,\pi) \rightarrow \Pi = (\pi/2,\pi/2) \rightarrow \Gamma = (0,0)$ in the Brillouin zone ($\Gamma\text{XMI}\Pi\Gamma$), with momentum $\mathbf{k}$ on the abscissa and frequency ω on the ordinate. The corresponding Fermi surfaces (FS) are presented in the next section.

The spectral functions $A_{\mathbf{k}}(\omega)$ are presented in Fig. 12, where we compare the non-interpolated “raw” DCA data in column (a) with that obtained after Σ , M and $\mathcal{L}$ -interpolation in columns (b), (c) and (d), respectively. The rows correspond to the different regimes, with the Fermi liquid ($\delta = 0.25$) in the top row, pseudogap ($\delta = 0.21$) in the middle row, and Mott insulator ($\delta = 0.00$) in the bottom row. We checked that the filling is preserved by all three interpolation schemes.

In the Fermi liquid, the self-energy is only weakly $\mathbf{K}$ -dependent. interpolation therefore does not strongly depend on the method, and interpolated results closely match the non-interpolated data.

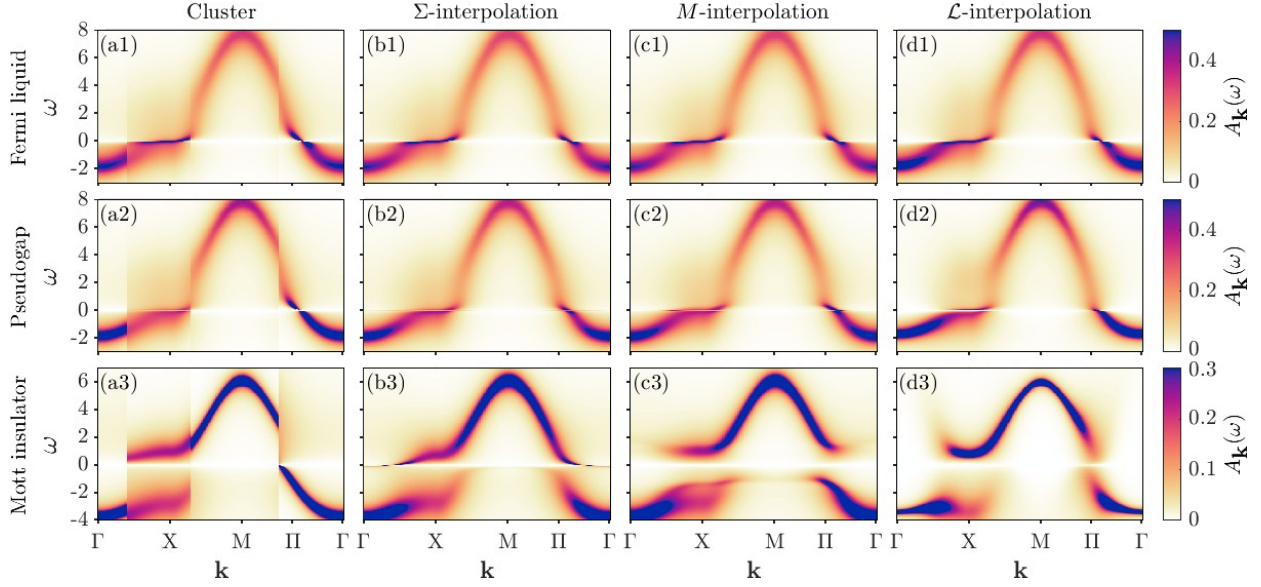


FIG. 12. Spectral function $A_{\mathbf{k}}(\omega)$ of DCA+NRG computations performed using the 4-patch star geometry of Fig. 9, for $t = 1$, $t' = -0.3t$, $T = 10^{-10}t$, and $U = 7t$. $A_{\mathbf{k}}(\omega)$ is plotted as functions of frequency ω and momentum $\mathbf{k}$ along the path $\Gamma = (0,0) \rightarrow X = (0,\pi) \rightarrow M = (\pi,\pi) \rightarrow \Pi = (\pi/2,\pi/2) \rightarrow \Gamma = (0,0)$ in the Brillouin zone. For column (a) no interpolation was used, for (b-d) Σ -, M - and $\mathcal{L}$ -interpolation are used, respectively. The first, second and third row depict a Fermi liquid, pseudogap and Mott insulator, respectively, for doping $\delta = 0.25$, $\delta = 0.21$ and $\delta = 0.00$.

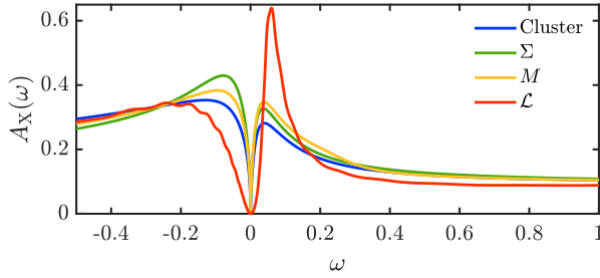


FIG. 13. Spectral function $A_{\mathbf{k}}(\omega)$ at $\mathbf{k} = X$ corresponding to $\delta = 0.21$ emphasizing the gap opening at X for the different interpolation depicted by colors.

In the pseudogap regime, by contrast, the self-energy exhibits strong $\mathbf{K}$ -dependence, and interpolation results depend significantly on the employed method. In this regime, a small gap opens in the vicinity of momentum X which is more pronounced when using $\mathcal{L}$ -interpolation compared to the Σ -, and M -interpolation. To make this more apparent, we show $A_{\mathbf{k}=X}(\omega)$ in Fig. 13. The reason why the Σ - and M -interpolated spectral functions are closer to the non-interpolated one is because the functions $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ resemble smeared-out step functions that never become negative. By contrast, the functions $\alpha_{\mathbf{k},\mathbf{K}}$, have a much stronger $\mathbf{k}$ -dependence and do become negative, a property needed to preserve patch averages (cf. property (ii) on p. 11).

We elaborate this in Fig. 13, where we show a slice

of the spectral functions in Fig. 12 at momentum X , $A_X(\omega)$. There, Σ - and M -interpolation yield curves qualitatively similar to the non-interpolated one. The reason is that in the interpolation formula (58), $\mathbf{Q}_{\mathbf{k}}(\omega) = \sum_{\mathbf{K}} \alpha_{\mathbf{k},\mathbf{K}} \mathbf{Q}_{\mathbf{K}}(\omega)$, the ω -dependence on the left is linearly inherited from that on the right. By contrast, the $\mathcal{L}$ -interpolated result differs from that of the other three significantly, because its ω -dependence is inherited non-linearly, via the different levels of the CFE.

Reducing the doping from the pseudogap phase to $\delta = 0.00$ yields the Mott phase. This case is the strong suit of the M -scheme, since the interpolation of the cumulant, which is inversely proportional to the self-energy, facilitates a reliable reconstruction of self-energy poles [38]. Specifically, the M -interpolation yields a clear gap along the path $\Gamma X M \Pi \Gamma$, while the Σ -interpolation struggles to fully extend the gap throughout $\mathbf{k}$ -space, due to band tails reaching into the $\omega \sim 0$ regime. On the other hand, the $\mathcal{L}$ -interpolation, similar to the M -scheme, shows a fully gapped Brillouin zone, with gap sizes comparable to the cluster result.

Note that M -interpolation yields a rather large gap throughout the path $\Gamma X M \Pi \Gamma$. This suggests that it may overestimate the gap at Π . For Σ -interpolation and M -interpolation the distribution of poles in the self-energy within the $\mathbf{k}$ -space depends solely on the interpolation function $\alpha_{\mathbf{k},\mathbf{K}}$. By contrast, the $\mathcal{L}$ -scheme resolves the self-energy poles in terms of multiple Liouvillian matrix elements, allowing the weight to accumulate in a more flexible distribution throughout $\mathbf{k}$ -space—resulting

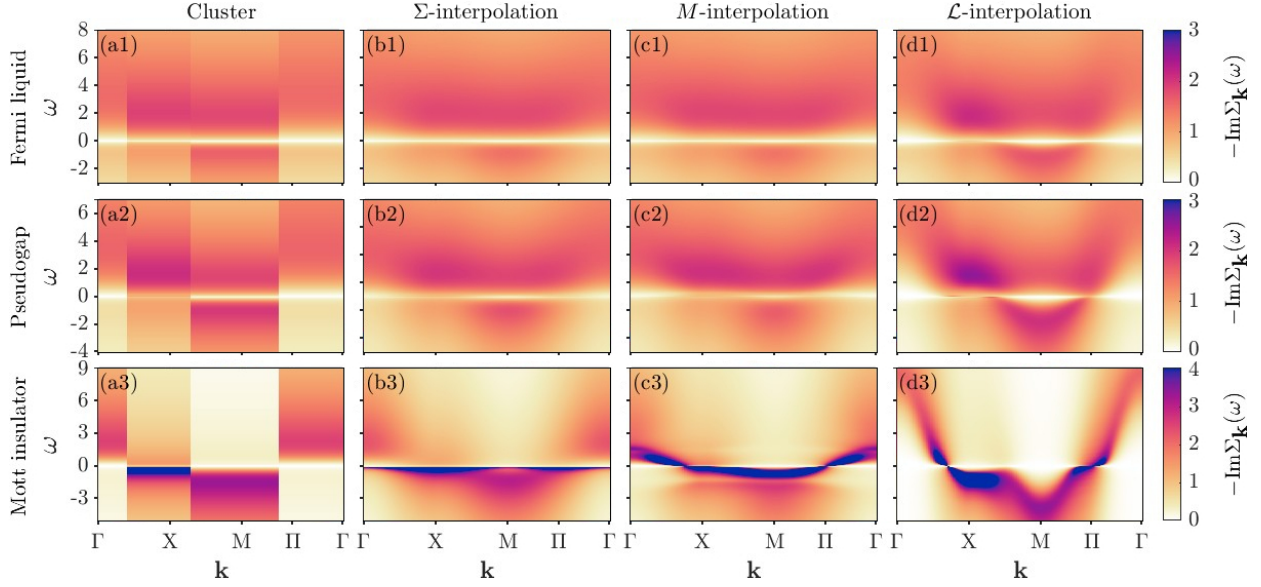


FIG. 14. Same as Fig. 12, but for the imaginary part of the self-energy $-\text{Im}\Sigma_{\mathbf{k}}(\omega)$.

in two differently sized gaps near X and II.

Figure 14 shows the spectral part of the self-energy, $-\text{Im}\Sigma_{\mathbf{k}}(\omega)$, in the same manner as Fig. 12. All periodizations mimic the non-interpolated case, with the $\mathcal{L}$ -scheme exhibiting a more structured intensity profile.

The Fermi liquid at $\delta = 0.25$ is already close to the pseudogap transition; hence, non-local (i.e. $\mathbf{k}$ -dependent) effects are slightly enhanced compared to a FL at $\delta \gg 0.25$. Due to the faster-converging Fourier coefficients in the $\mathcal{L}$ -scheme, we argue that these non-local contributions are better captured in this scheme—leading to the large self-energy at momentum X, where the pseudogap opens.

In the pseudogap phase, $-\text{Im}\Sigma_{\mathbf{k}}(\omega)$ exhibits a narrow peak near $\omega \sim 0$ in the anti-nodal patches (see Fig. 9). All interpolation schemes are able to resolve this peak. In the Σ - and M -interpolation, however, it is resolved in broad and flat structures around X and along $M\Gamma$ (these are not prominently visible in the second row of Fig. 14, due to the linear ω -scale.) By contrast, the $\mathcal{L}$ -scheme connects these broad and flat structures to high-energy structures, resulting in a more prominently structured profile for $\Sigma_{\mathbf{k}}(\omega)$, i.e. more clearly defined bands. The appearance of such clearly defined bands suggests that $\mathcal{L}$ -interpolation yields a more plausible representation of the pseudogap phase.

For the Mott insulator, Σ -interpolation fails to capture the self-energy divergence across (i.e. on both sides of) $\omega = 0$, resulting erroneously in some finite spectral weight of $A_{\mathbf{k}}(\omega)$ [Fig. 12(b3)] at $\omega = 0$ throughout the path $\Gamma X M \Pi \Gamma$. By contrast, M -interpolation yields a narrow self-energy band that lies close to $\omega = 0$ and crosses $\omega = 0$ two times, visible in Fig. 14(c3). This explains the large gaps in the corresponding spectral function of

Fig. 12(c3). $\mathcal{L}$ -interpolation yields a similar self-energy band, however, it is much more dispersive [Fig. 12(d3)] due to the non-linear ω -dependence of the CFE. As mentioned above, this causes the weight of the self-energy around $\omega = 0$ to have a much stronger momentum dependence along $\Gamma X M \Pi \Gamma$, which yields a correspondingly strong variation for the gap size of the spectral function [Fig. 12(d3)]. This further demonstrates the advantage of its flexible weight distribution among multiple Liouvillian matrix elements.

We conclude this discussion with some remarks regarding the band-width of the self-energy pole. In a 2-dimensional Mott insulator, a dispersive self-energy pole, with a dispersion roughly proportional to $-\epsilon_{\mathbf{k}}$, is expected on general grounds [82]. Qualitatively, this hallmark feature is captured by both M and $\mathcal{L}$ -interpolation, albeit with very different bandwidths. At intermediate coupling, as studied here ($U = 7t$), the bandwidth of the self-energy pole is usually somewhat larger than the electronic bandwidth, see for instance Fig. 5 of Ref. [83] ($U = 4t$) or Fig. 3 of Ref. [64] ($U = 7.5t$). Our electronic bandwidth is $8t$, and we find a self-energy pole bandwidth of $\simeq 11t$ with $\mathcal{L}$ -interpolation, but only $\simeq 2t$ with M -interpolation. Thus $\mathcal{L}$ -interpolation yields a self-energy pole bandwidth consistent with expectations, whereas M -interpolation severely underestimates it.

C. interpolation results at $\omega = 0$

An examination of the Fermi surface (FS) provides additional insight into the performance of the $\mathcal{L}$ -scheme compared to other interpolation methods. Fig. 15

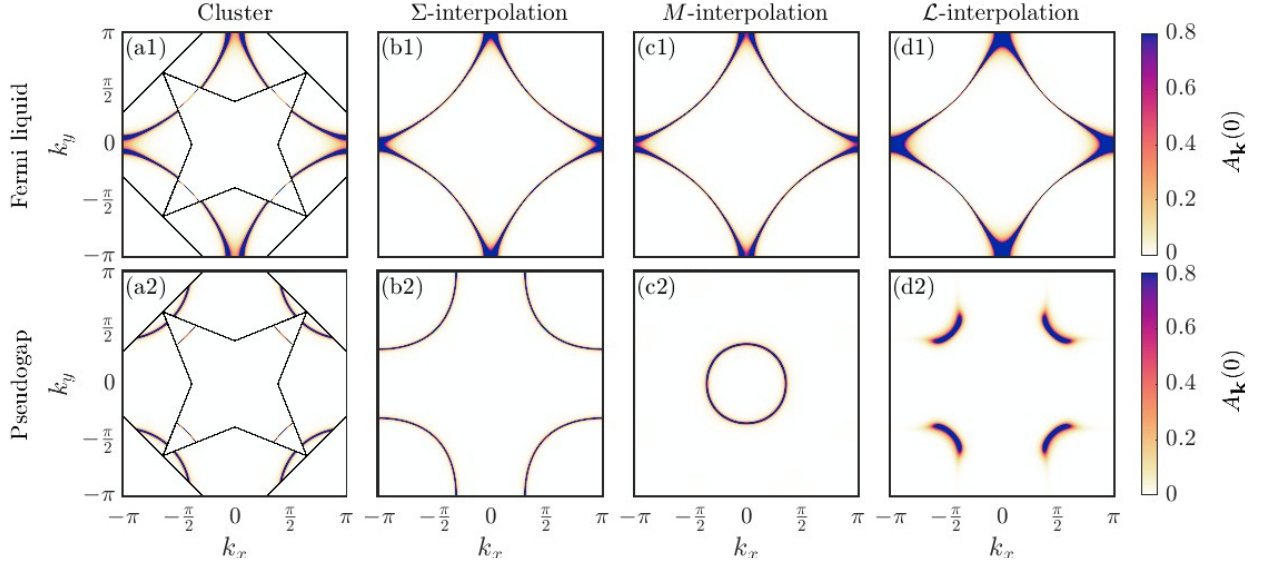


FIG. 15. Spectral function at zero frequency, $A_{\mathbf{k}}(0)$, for the same settings as in Fig. 12. Column (a): (non-periodized) cluster results, featuring discontinuities at the patch borders (straight black lines). Columns (b-d): results from Σ -, M -, and $\mathcal{L}$ -interpolation. Rows 1 and 2 show results for doping $\delta = 0.25$ and $\delta = 0.21$, yielding a Fermi liquid and pseudogap, respectively.

presents a comparison of the Fermi surfaces via plots of the spectral function at zero frequency, $A_{\mathbf{k}}(0)$ for both the Fermi liquid and pseudogap phases. (The Mott insulator is not shown, as $A_{\mathbf{k}}(0) < 10^{-5}$, except for Σ -interpolation, which erroneously does not show a true Mott insulator.) Panels (a1–d1) display the FS of the Fermi liquid, while panels (a2–d2) show the FS in the pseudogap phase. In column (a), the straight black lines indicate the DCA patch boundaries.

The FS for the Fermi liquid is essentially identical across all scheme and mimics the non-interpolated result well. However, the $\mathcal{L}$ -scheme has enhanced intensity at the anti-nodal points. Apparently, any interpolation works well for a simple Fermi liquid.

In the pseudogap phase, the cluster result [Fig. 15(a2)] features hole-like arcs cut off by the patch boundaries, without extending to the Brillouin zone (BZ) edge, leading to gaps around the four “antinodal” points $(\pm\pi, 0)$ and $(0, \pm\pi)$. This is because the $\mathbf{K} = (\pi, \pi)$ cluster patch carries no spectral weight. The traditional Σ - and M -schemes are unable to reproduce key aspects of the cluster result: the Σ -interpolated FS is hole-like but extends all the way to the opposite BZ edges without showing gaps near the edges, while the M -interpolated FS is electron-like.

The $\mathcal{L}$ -scheme is the only interpolation that qualitatively captures all aspects of the cluster computation in the pseudogap phase. First, it preserves the hole-like characteristics; second it also accumulates spectral weight around the four “nodal” points at $(\pm\pi/2, \pm\pi/2)$ and $(\pm\pi/2, \mp\pi/2)$, similar to the cluster result but distributed more smoothly in the shape of Fermi arcs. These

are similar to those observed in photoemission spectra measured by ARPES experiments [37]. Third, $\mathcal{L}$ -interpolation captures the spectral weight distribution along the Fermi surface far better than the other schemes, as discussed in more detail below (see Fig. 18).

At first glance, the Fermi-arc structures seem to imply a non-closed FS. However, additional details become apparent when using a logarithmic color scale, as done in the first row of Fig. 16: The M -scheme yields a slightly enhanced intensity near the BZ edge, in the regions where the Σ -scheme FS is located. The hole-like FS of the $\mathcal{L}$ -scheme actually does close across the BZ edges, albeit with very small spectral weight there, while an electron-like ring with even less weight is also present. On a logarithmic color scale the $\mathcal{L}$ -scheme thus displays structural features from both the Σ - and M -schemes.

The second row of Fig. 16 shows the imaginary part of the self-energy at zero frequency, $-\text{Im}\Sigma_{\mathbf{k}}(0)$, corresponding to the FS data in the first row. The Σ -interpolation closely resembles the nearly constant self-energy of the non-interpolated DCA calculation, showing no enhanced structures. The M -scheme produces Σ -pole rings around the nodal points; these are strongly modified in the $\mathcal{L}$ -interpolation. The $\mathcal{L}$ -scheme displays sharp pocket structures around X that suppress the FS near the BZ boundary. These pockets are connected by a less intense arc close to the FS intensity maximum. Note that for $\mathcal{L}$ -interpolation, the peaks of the self-energy and the Green’s function occur very close to each other.

The last row in Fig. 16 presents the real part of the Green’s function at zero frequency, $\text{Re}G_{\mathbf{k}}(0)$. Here, a sudden blue-to-red change indicates a sign change of

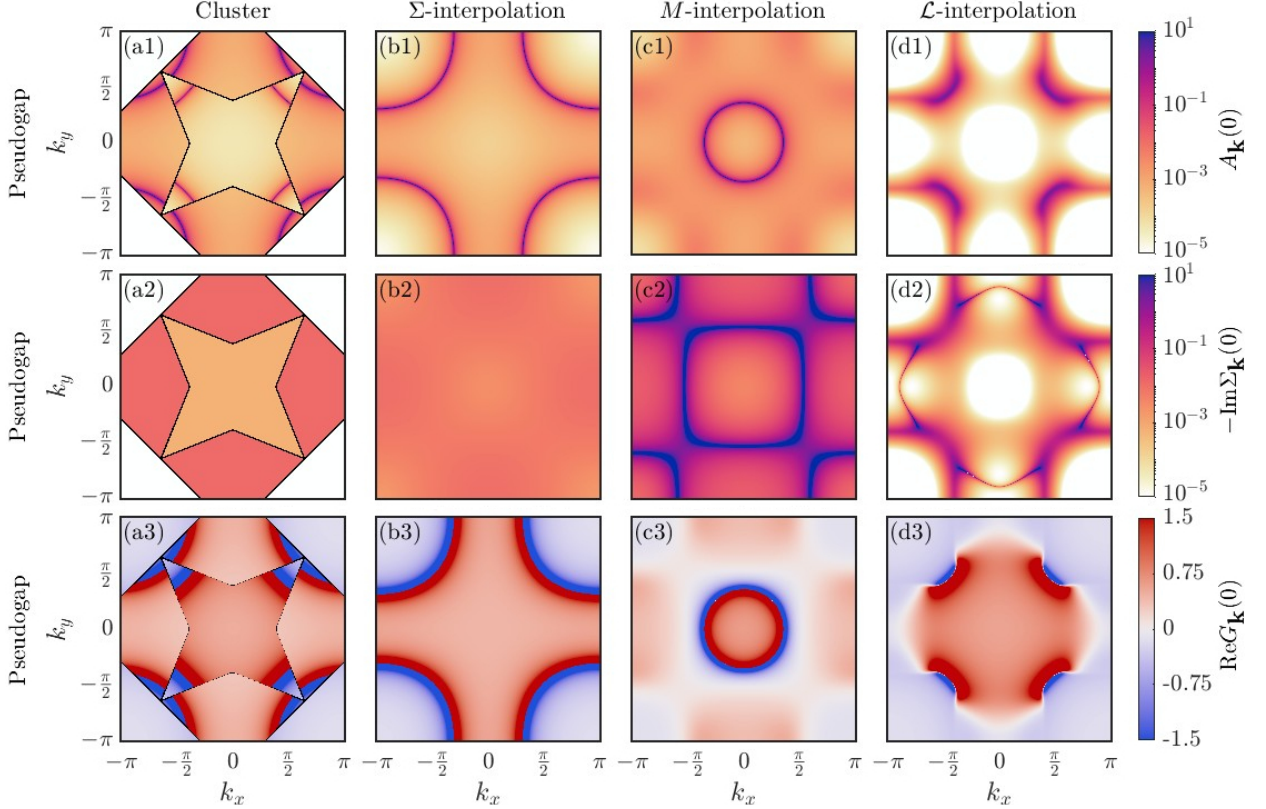


FIG. 16. DCA computation of the pseudogap phase at $\delta = 0.21$. Columns correspond to the same interpolation methods as in Fig. 15. The rows (1-3) depict, respectively, $A_{\mathbf{k}}(\omega = 0)$, $-\text{Im}\Sigma_{\mathbf{k}}(\omega = 0)$ and $\text{Re}G_{\mathbf{k}}(\omega = 0)$. Here row (1) shows the same data as row 2 of Fig. 15 but on a logarithmic color-scale.

$\text{Re}G_{\mathbf{k}}(0)$ via a divergence, i.e. a Fermi surface. By contrast, a gradual blue-to-white-to-red evolution, as seen in parts of panels (c3) and (d3), indicates a smooth evolution through zero, i.e. a Luttinger surface (LS).

The cluster result shows no true LS; instead, it shows small discontinuities at some patch edges. The Σ -scheme interpolates these to yield a hole-like FS. The M -scheme yields a closed, electron-like FS and a closed LS around the anti-nodal points. These are well separated and don't form arcs. The $\mathcal{L}$ -scheme, which most faithfully captures the characteristic structures of the cluster result, yields Fermi and Luttinger arcs. Remarkably, these *smoothly* evolve into each other. We describe this evolution in more detail via the next three figures by showing how three key quantities, $\text{Re}G_{\mathbf{k}}(0)$, $A_{\mathbf{k}}(0)$ and $Z_{\mathbf{k}}$, evolve along the Fermi and Luttinger surfaces.

Figure 17 shows a series of slices of $\text{Re}G_{\mathbf{k}}(0)$, taken for panel (a) from non-interpolated cluster results, and for panel (b) from the corresponding $\mathcal{L}$ -interpolations. Each slice follows a “ $\mathbf{k}$ -ray” (straight-line $\mathbf{k}$ -trajectory through the BZ) emanating from (π, π) at a fixed angle, $0 \leq \theta \leq \frac{\pi}{4}$, as indicated in the top-left insets of Figs. 17(a,b). The curves are plotted vs. $|\mathbf{k} - \mathbf{k}_0|$, where

$\mathbf{k}_0$ is the momentum where $\text{Re}G_{\mathbf{k}}(0)$ changes sign. For small θ , the non-interpolated curves in (a) change sign at the patch boundaries via small discontinuities. With increasing θ , the sign change shifts to within one of the patches and occurs via a divergence. The pole weight of the divergences is largest at $\theta = \pi/4$, when the $\mathbf{k}$ -ray cuts the nodal point. The $\mathcal{L}$ -scheme interpolates the small patch-boundary discontinuity to a flat zero crossing, i.e. a LS. With increasing θ , the curve crosses zero with increasing slope, *smoothly* evolving into a shape resembling a regularized divergence which is most prominent for $\theta = \pi/4$. The regularization arises through a small (non-divergent) imaginary part of the self-energy.

Figure 18 shows $\max[A_{\mathbf{k}(\theta)}(0)]$, the maximum value assumed by the zero-frequency spectral function along a $\mathbf{k}$ -ray at fixed angle θ , plotted as a function of θ . This quantity corresponds to that measured in ARPES studies aiming to analyse the quasi-particle weight (see, e.g., Fig. 4 of [37]). The cluster result shows a step function profile (blue). The $\mathcal{L}$ -scheme smooths out this step into a broader but still well-defined peak (red) whose flanks smoothly approach zero for $|\theta - \pi/4| \gtrsim \pi/8$. By contrast, the Σ - and M -profiles (green, yellow) show only a very

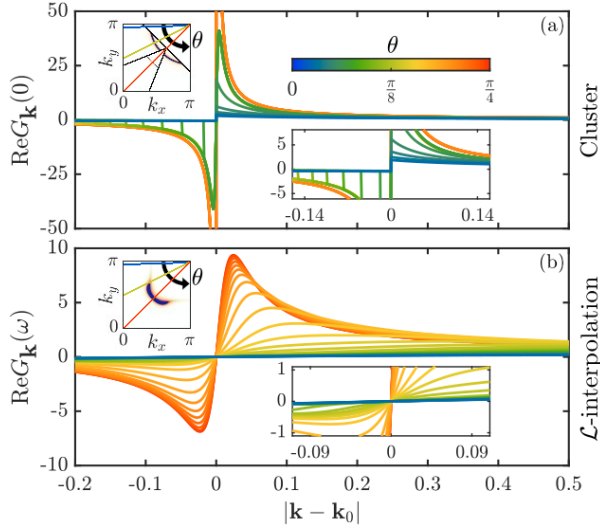


FIG. 17. Real part of the Green's function at zero frequency, $\text{Re}G_{\mathbf{k}}(0)$, computed (a) without interpolation and (b) with $\mathcal{L}$ -interpolation. They are plotted along several $\mathbf{k}$ -rays emanating from (π, π) at angles $0 \leq \theta \leq \frac{\pi}{4}$ (indicated by the color bar and defined in the top-left insets), as functions of $|\mathbf{k} - \mathbf{k}_0|$, where $\mathbf{k}_0$ is the momentum where $\text{Re}G_{\mathbf{k}}(0)$ changes sign. Bottom-right insets zoom in to small values of $|\mathbf{k} - \mathbf{k}_0|$.

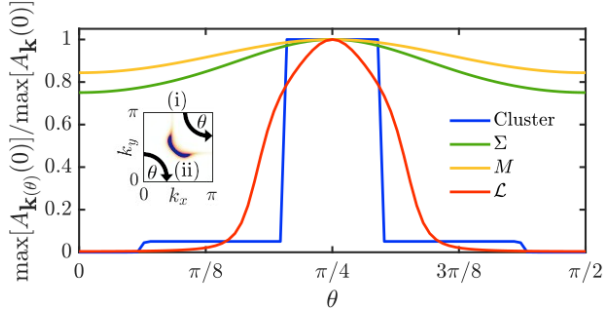


FIG. 18. Maximum of the zero-frequency spectral function along a $\mathbf{k}$ -ray at angle θ , $\max[A_{\mathbf{k}(\theta)}(0)]$, plotted as function of θ and normalized, for ease of comparison, by its peak value at $\theta = \pi/4$. The angle θ , defined in the inset, characterizes $\mathbf{k}$ -rays emanating (i) from (π, π) for Σ -, $\mathcal{L}$ - and no interpolation, and (ii) from $(0, 0)$ for M -interpolation.

broad, weak maximum.

Finally, Fig. 19 shows the quasi-particle weight $Z_{\mathbf{k}_0} = (1 - \partial_{\omega} \text{Re}\Sigma_{\mathbf{k}_0}(0))^{-1}$ along the “sign-change trajectory” through the BZ (the $\mathbf{k}_0$ -points where $\text{Re}G_{\mathbf{k}}(0)$ changes sign), i.e. along the trajectory that defines the Fermi and Luttinger surfaces. We compute the slope $\partial_{\omega} \text{Re}\Sigma_{\mathbf{k}_0}(0)$ via a linear fit, adjusting the fitting range along the sign-change trajectory to match appropriate fitting ranges found for our cluster data ($\omega_{\text{fit}} \sim \pm 10^{-6}$ for $\mathbf{k}_0 \sim (0, \pi)$ and $\omega_{\text{fit}} \sim \pm 10^{-4}$ for $\mathbf{k}_0 \sim (\pi/2, \pi/2)$). The resulting $Z_{\mathbf{k}_0}$ is depicted along the sign-change trajectory using a

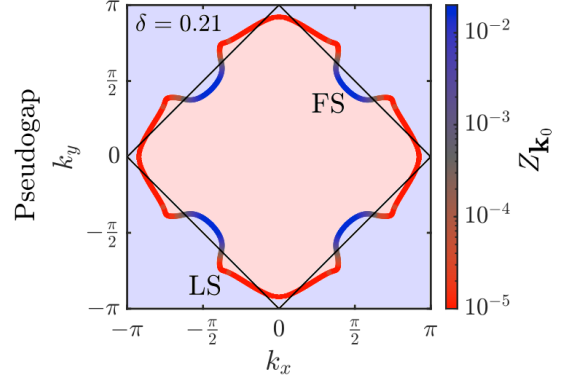


FIG. 19. Quasi-particle weight, $Z_{\mathbf{k}_0} = (1 - \partial_{\omega} \text{Re}\Sigma_{\mathbf{k}_0}(0))^{-1}$, for the pseudogap phase at $\delta = 0.21$, plotted along the “sign-change trajectory” in the BZ, i.e. along the locus of points $\mathbf{k}_0$ where $\text{Re}G_{\mathbf{k}}(0)$ changes sign. The color-scale shows the evolution from Fermi arcs (blue) to Luttinger arcs (red) and vice version when crossing the antiferromagnetic zone boundary (black lines). The light blue or red background shading indicates regions of the BZ with filling 1 or 0, respectively.

logarithmic red-to-blue color-scale. The blue portions of the trajectory correspond to a sign change via a divergence, i.e. a FS; the red portions correspond to a sign change via a smooth zero crossing, i.e. a LS. The evolution from Fermi arcs to Luttinger arcs and back occurs *smoothly*, in regions (shown in grey), that intersect the antiferromagnetic zone boundaries (straight black lines). (The reason why the quasi-particle weight is very small, $Z_{\mathbf{k}_0} \lesssim 0.02$, also along the FS parts of the sign-change trajectory is that $\delta = 0.21$ lies is very close to a quantum phase transition, which will be the subject of a separate publication [67].)

To summarize: In the pseudogap regime, $\mathcal{L}$ -interpolation, in contrast to Σ - and M -interpolation, yields a smooth evolution between hole-like Fermi arcs and Luttinger arcs, realizing these two concepts on one surface. The Fermi arcs lie within the AF zone boundaries, and the change to Luttinger arcs occurs while crossing these boundaries. In the literature, such a smooth FS-to-LS evolution has previously been found in a numerically demanding DfA study requiring the computation of two-particle quantities [84]. That this behavior can be obtained via $\mathcal{L}$ -interpolation of computationally much cheaper DCA+NRG data constitutes a major result of our work. It illustrates that $\mathcal{L}$ -interpolation is able to generate more intricate features than Σ - or M -interpolation, while preserving key qualitative properties of the cluster result, such as the hole-like character of the FS.

VI. SUMMARY AND OUTLOOK

In this paper, we introduced a scheme for interpolating CDMFT and DCA results through a suitable interpolation of single-particle irreducible Liouvillian matrix elements ϵ_n and $\mathbf{t}_n$. We showed (Sec. II) that these Liouvillian matrix elements are in fact coefficients of a continued fraction expansion of the dynamical part of the self-energy, $\Sigma^{\text{dyn}}(z)$ [Eq. (31)]. They can be obtained from the spectrum $\mathbf{W}(\omega)$ of the self-energy via a Lanczos scheme. The resulting matrix elements ϵ_n and $\mathbf{t}_n$ are then interpolated (Sec. III) using a truncated Fourier ansatz to obtain $\epsilon_{\mathbf{k}n}$ and $\mathbf{t}_{\mathbf{k}n}$, which are inserted back to the CFE to obtain an interpolated self-energy, $\Sigma_{\mathbf{k}}(z)$.

Since the Liouvillian is independent of frequency, the same is true for its matrix elements ϵ_n and $\mathbf{t}_n$. Consequently, the interpolated version of the Liouvillian remains hermitian, which ensures causality. This poses an inherent advantage of our $\mathcal{L}$ -scheme compared to traditional schemes, like Σ -, M -, and G -periodization.

To benchmark our $\mathcal{L}$ -interpolation scheme (Sec. IV A), we considered the one-dimensional Hubbard model and computed its spectral function using TaSK [64], a numerically (almost) exact MPS method. We Fourier-transformed the TaSK results for G , Σ , M , and $\mathcal{L}$ to position space and found that $\mathcal{L}$ shows the most local behavior (its matrix elements decay most quickly with distance). Consequently, truncating the Fourier coefficients of $\mathcal{L}$ by range yields a much more faithful representation of the true spectral function and self-energy than a corresponding truncation of Σ or M .

Next, we considered the same one-dimensional Hubbard model, but now treated with CDMFT for various cluster sizes, using TaSK [64] as an impurity solver (Sec. IV B). We compared the results obtained by interpolating its self-energy using the G -, Σ -, M -, and $\mathcal{L}$ -schemes. We studied the convergence with cluster size of the interpolated CDMFT results to the benchmark TaSK results of Sec. IV A. For the 2-site cluster, $\mathcal{L}$ -periodization arguably performed somewhat worse than G -periodization; but for 4- and 8-site clusters, $\mathcal{L}$ -interpolation yielded smoother spectra that resembled the benchmark TaSK result much better.

Finally, we presented an example of DCA interpolation for the doped, two-dimensional t - t' Hubbard model, studied using four-patch DCA and an NRG impurity solver (Sec. V). We considered three choices of doping, yielding three distinct phases: a Fermi liquid, a pseudogap phase, and a Mott insulator. For each, we compared non-interpolated cluster result for the spectral function $A_{\mathbf{k}}(\omega)$ and self-energy $\Sigma_{\mathbf{k}}(\omega)$ to interpolated versions obtained via Σ -, M - and $\mathcal{L}$ -interpolation.

We performed the CFE expansion of the DCA+NRG self-energy $\Sigma_{\mathbf{K}}(z)$ using a fast-slow splitting scheme (Sec. II H), implemented in such a manner that the resulting coefficients $\epsilon_{\mathbf{K}n}$, $\mathbf{t}_{\mathbf{K}n}$ and the fast-mode contributions $\mathbf{R}_{\mathbf{K}n}^{\text{F}}(z)$ decay exponentially with CFE depth n . The dependence of $\Sigma_{\mathbf{K}}(z)$ on the patch index $\mathbf{K}$ is then mainly

encoded in the matrix elements $\epsilon_{\mathbf{K}n}$, $\mathbf{t}_{\mathbf{K}n}$, while the functions $\mathbf{R}_{\mathbf{K}n}^{\text{F}}(z)$ depend only weakly on $\mathbf{K}$ and hence are easy to interpolate. Consequently, $\mathcal{L}$ -interpolation yields better results than Σ - or M -interpolation: it produces more detailed structures with higher $\mathbf{k}$ -space resolution, that better mimic key intrinsic features of the non-interpolated cluster results.

This is especially pronounced for Fermi surface properties (Sec. V C). Comparing the spectral functions $A_{\mathbf{k}}(\omega)$ obtained from the various interpolation schemes, we find that $\mathcal{L}$ -interpolation resolves its structures most sharply. While all interpolations perform well for the Fermi liquid, the differences become strikingly apparent in the pseudogap phase. The $\mathcal{L}$ -scheme interpolates the FS of the pseudogap phase to Fermi arcs, qualitatively similar to those observed in ARPES experiments. The $\mathcal{L}$ -scheme also is the one that best mimics the non-interpolated cluster results, not only for the Fermi surface but also for the quasi-particle weight, as illustrated by tracking $\max[A_{\mathbf{k}}(0)]$ along the Fermi surface. Perhaps most remarkably, $\mathcal{L}$ -interpolation yields a smooth evolution between Fermi and Luttinger surfaces, similar to that found previously using computationally much more costly DGA computations [84].

In summary, we presented a Liouvillian interpolation scheme for cluster DMFT data. Exploiting the fact that the spectral function and self-energy can be fully expressed through matrix elements of the Liouvillian, our key idea is to interpolate the latter. This yields causal results, because these matrix elements are independent of frequency. We interpolate them using a real-space-truncated Fourier expansion, exploiting the fact that the real-space matrix elements of the Liouvillian $\mathcal{L}$ are more local than those of Green's function G , self-energy Σ or cumulant M . Liouvillian periodization yields results with better $\mathbf{k}$ -space resolution than traditional periodization schemes, because it distributes $\mathbf{k}$ -space information among a large number of Liouvillian matrix elements.

In this paper, we discussed interpolation as a post-processing tool, to be used after DMFT self-consistency has been achieved. This is to be distinguished from interpolation *within* cDMFT loops. The latter can yield non-causal hybridization functions if the standard self-consistency equations are used, but this causality issue has recently been solved with the generalized cavity construction of Ref. [85]. In future work, it would be interesting to set up within-cDMFT-interpolations that combine the generalized cavity construction with $\mathcal{L}$ -interpolation.

Final remarks: Liouvillian interpolation can be used in any context requiring the interpolation of frequency-dependent dynamical response functions, making it relevant also for other quantum many-body embedding methods beyond cDMFT. Even more generally, the CFE representation of the Green's function or the self-energy through *Liouvillian* matrix elements, as described in Sec. II, constitutes a versatile tool that promises to be useful also in contexts other than interpolation.

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Appendix A: Operator inner product for $T = 0$

This appendix discusses subtleties arising in the definition of operator inner products at zero temperature.

The operator inner product $(|)$ of Eq. (5) is well-defined only if ρ has full rank, i.e. if $\langle \Psi | \rho | \Psi \rangle \neq 0$ for every state $|\Psi\rangle \in \mathbb{V}$; otherwise $|\Psi\rangle\langle\Psi|$ would have zero norm w.r.t $(|)$ despite being a nonzero operator. The thermal density matrix ρ does have full rank for $T \neq 0$. However, the zero-temperature density matrix, $\rho_G = \rho(T=0)$, does not have full rank, since $\langle \Psi | \rho_G | \Psi \rangle \neq 0$ only if $|\Psi\rangle \in \mathbb{V}_G$, the ground state subspace of $\mathbb{V}$. In this case, we restrict attention to $\mathbb{W}_G = \{O_G\}$, the space of all operators with the property that either O_G or $O_G^\dagger$ does not annihilate all ground states. For any $|O\rangle \in \mathbb{W}$, its projection into $\mathbb{W}_G$ is defined as $|O_G\rangle = \mathcal{P}_G|O\rangle = |O - \bar{P}_G O \bar{P}_G\rangle$. Here $\bar{P}_G = 1 - P_G$, where P_G and $\bar{P}_G$ respectively are projectors onto the ground state subspace $\mathbb{V}_G$ and its complement, $\bar{\mathbb{V}}_G$, the space of excited states, defined such that $\mathbb{V} = \mathbb{V}_G \oplus \bar{\mathbb{V}}_G$. The projector property $\mathcal{P}_G^2 = \mathcal{P}_G$ is readily verified. For $T = 0$, the inner product is well-defined on $\mathbb{W}_G$: indeed, it yields

$$(O_G|O_G) = \text{Tr}[\rho_G\{O_G^\dagger, O_G\}] = \text{Tr}[\rho_G\{O^\dagger, O\}], \quad (\text{A1})$$

since $\rho_G \bar{P}_G = \bar{P}_G \rho_G = 0$. If $|O_G\rangle \neq 0$, then $O \neq \bar{P}_G O \bar{P}_G$, hence O or $O^\dagger$ does not annihilate $\mathbb{V}_G$; thus the right side of Eq. (A1), and hence also $(O_G|O_G)$, is nonzero.

Appendix B: Measures, the moment problem, and orthogonal polynomials

In this Appendix, we provide some background material on moment problems, measures, and their relation to orthogonal polynomials. This material is used implicitly in Sec. II on CFE representations of Liouvillian dynamics: it forms the basis for our statement there that the CFE coefficients for a Green's function $\mathbf{G}(z)$ or its self-energy $\Sigma(z)$ are the same, although their spectral functions, $\mathbf{A}(\omega)$ or $\mathbf{W}(\omega)$, generate two different sets of orthogonal polynomials. All the information presented below is well-established and can be found in numerous textbooks [86–92] and articles [93–98].

Let μ be a positive semidefinite, hermitian $M \times M$ matrix-valued Borel measure on $\mathbb{R}$; that is, $\mu : \mathcal{B}(\mathbb{R}) \rightarrow \mathbb{C}^{M \times M}$ is countably additive and $\mu(B)$ is positive semidefinite for all Borel sets B . We write, distributionally,

$$\mu(d\omega) = \mathbf{A}(\omega)d\omega, \quad (\text{B1})$$

with a spectral function $\mathbf{A}(\omega) = \mathbf{A}_c(\omega) + \sum_\alpha \mathbf{A}_\alpha \delta(\omega - \omega_\alpha)$ that exhibits both a continuous part $\mathbf{A}_c(\omega)$ and point masses with weights $\mathbf{A}_\alpha$, encoded by the δ -terms. We further assume the normalization

$$\mu(\mathbb{R}) = \int_{-\infty}^{\infty} d\omega \mathbf{A}(\omega) = \mathbf{1}, \quad (\text{B2})$$

where $\mathbf{1}$ is the $M \times M$ unit matrix.

The Stieltjes transform of μ is defined as

$$\mathbf{G}(z) = \int_{\mathbb{R}} \frac{\mu(d\omega)}{z - \omega}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \quad (\text{B3})$$

The spectral function can be recovered from $\mathbf{G}(z)$ via

$$\mathbf{A}(\omega) = \frac{i}{2\pi} [\mathbf{G}(\omega^+) - [\mathbf{G}(\omega^+)]^\dagger], \quad (\text{B4})$$

with $\omega^+ = \omega + i0^+$.

The (equivalence classes of) square-integrable vector fields $f : \mathbb{R} \rightarrow \mathbb{C}^M$ with respect to μ form the Hilbert space $L^2(\mu)$, with inner product

$$\langle g, f \rangle = \int_{\mathbb{R}} g^\dagger(\omega) \mu(d\omega) f(\omega) \in \mathbb{C}. \quad (\text{B5})$$

In the following, we write $|f\rangle \in L^2(\mu)$ for the vector which is represented by the vector field $f(\omega)$. For later usage, we further define blocks of M vectors by a bold symbol $|\mathbf{f}\rangle = (|f_1\rangle, \dots, |f_M\rangle)$. Similarly, $\mathbf{f}(\omega) = (f_1(\omega), \dots, f_M(\omega)) \in \mathbb{C}^{M \times M}$ denotes the block of representing vector fields. Furthermore, $\langle \mathbf{g}, \mathbf{f} \rangle$ denotes a column vector with α -th entry $\langle g_\alpha, f \rangle$, $\langle f, \mathbf{g} \rangle = \langle \mathbf{g}, \mathbf{f} \rangle^\dagger$ a corresponding row vector, and $\langle \mathbf{g}, \mathbf{f} \rangle$ a matrix with entries $\langle g_\alpha, f_\beta \rangle$. For a more formal treatment of matrix-valued measures and their L^2 spaces, see Ref. 92, pages 1337 and onward.

The (matrix) moments of μ are

$$\mathbf{m}_n = \int_{\mathbb{R}} \mu(d\omega) \omega^n, \quad (\text{B6})$$

with $n = 0, 1, 2, \dots$ and hermitian $\mathbf{m}_n$. Throughout, we assume that all moments in (B6) are finite.

The (matrix-valued) *moment problem* asks: given a sequence of hermitian matrices $\{\mathbf{m}_n\}_{n \geq 0}$, (i) does there exist a positive semidefinite, hermitian matrix-valued Borel measure μ on $\mathbb{R}$ with moments (B6); and (ii) if so, is it unique? In our setting we start from μ (equivalently, from the spectral function $\mathbf{A}(\omega)$) and compute $\{\mathbf{m}_n\}$, so existence is automatic. Uniqueness, however, is not guaranteed: if exactly one representing measure has the moments (B6), the problem is determinate; otherwise, it is indeterminate.

A sufficient condition for a unique measure (determinate moment problem) is either a compact support of the spectral function $\mathbf{A}(\omega)$, or an exponential decay at large $|\omega|$. Spectral functions of finite-size fermionic systems, even if macroscopically large, fulfill these conditions. We therefore assume that the moment problem is determinate in our work, i.e., the spectral function $\mathbf{A}(\omega)$ having these moments is unique.

In the determinate case, Eq. (B6) can be used to generate a set of orthonormal polynomials that form a complete orthonormal basis of $L^2(\mu)$ (c.f. Eq. (B7) below): every $|f\rangle \in L^2(\mu)$ admits a unique L^2 -expansion in these polynomials. By contrast, in the indeterminate case, there exist representing measures μ for which the orthonormal polynomials are *not* a complete basis of $L^2(\mu)$. For example, this is the case for a log-Gaussian spectral function. Nevertheless, the same moment sequence admits a family of representing measures (the Nevanlinna-extremal measures) for which the corresponding orthonormal block polynomials *are* a complete orthonormal basis of $L^2(\mu)$, see, for instance, Refs. 97 and 99.

We caution that some popular broadening kernels used in DMFT computations spoil determinacy or even moment existence. The log-Gaussian kernel, a standard kernel used to broaden discrete NRG spectra, has indeterminate moments, see Sec. 11.2 of Ref. 91. The Lorentzian kernel, a common choice for broadening discrete finite-size spectra, has no finite moments of order > 1 . In such cases, one should either work with the underlying discrete data when possible, or use the slow-fast mode splitting described in Sec. E2. In these cases, the loss of determinacy is an artifact of the long high-frequency tails of the broadening kernel and is unrelated to the underlying physics.

The block Lanczos algorithm described in Eq. (38) can be used to construct an orthonormal polynomial basis,

$$\langle \mathbf{p}_n, \mathbf{p}_{n'} \rangle = \int_{\mathbb{R}} d\omega \mathbf{p}_n^\dagger(\omega) \mathbf{A}(\omega) \mathbf{p}_{n'}(\omega) = \delta_{nn'} \mathbf{1}. \quad (\text{B7})$$

Here, every column of $\mathbf{p}_n(\omega)$ is a degree n polynomial $\mathbb{C}^M$ vector field. The Lanczos algorithm also generates

the hermitian matrices ϵ_n and positive semidefinite hermitian matrices $\mathbf{t}_n$. The polynomials $\mathbf{p}_n(\omega)$ obey a three-term recursion relation

$$\omega \mathbf{p}_n(\omega) = \mathbf{p}_n(\omega) \epsilon_n + \mathbf{p}_{n+1}(\omega) \mathbf{t}_{n+1} + \mathbf{p}_{n-1}(\omega) \mathbf{t}_n, \quad (\text{B8})$$

with initial conditions $\mathbf{p}_{-1}(\omega) = \mathbf{0}$ and $\mathbf{p}_0(\omega) = \mathbf{1}$.

While the Lanczos procedure takes a given measure μ as input to generate polynomials satisfying the recursion relation (B8), one may ask, conversely: given such a recursion relation, are the polynomials generated from it orthonormal w.r.t. some measure? The answer is yes: Favard's theorem guarantees that polynomials that obey the three-term recursion (B8), with initial condition $\mathbf{p}_{-1}(\omega) = \mathbf{0}$ and $\mathbf{p}_0(\omega) = \mathbf{1}$, are orthogonal w.r.t. at least one measure μ . The measure is unique if its moment problem is determinate, a property that can also be determined from the coefficients ϵ_n and $\mathbf{t}_n$ [94–96].

The three-term recursion can be used to generate an infinite-depth CFE for $\mathbf{G}(z)$, the Stieltjes transform of $\mathbf{A}(\omega)$, of the form (with $\mathbf{z}_n = \mathbf{z} - \epsilon_n$)

$$\mathbf{G}(z) = \frac{1}{\mathbf{z}_0 - \mathbf{t}_1 \frac{1}{\mathbf{z}_1 - \mathbf{t}_2 \frac{1}{\mathbf{z}_2 - \dots}}}. \quad (\text{B9})$$

Another set of matrix polynomials, called *associated polynomials of the first kind* and denoted $\mathbf{p}_n^{(1)}(\omega)$, is obtained if the recursion relation Eq. (B8) (with the same coefficients ϵ_n and $\mathbf{t}_n$) is initialized with the initial conditions $\mathbf{p}_{-1}^{(1)}(\omega) = \mathbf{0}$, $\mathbf{p}_0^{(1)}(\omega) = \mathbf{0}$ and $\mathbf{p}_1^{(1)}(\omega) = \mathbf{1}$. Then, $\mathbf{p}_n^{(1)}(\omega)$ is a polynomial of degree $n - 1$. The $\mathbf{p}_n^{(1)}(\omega)$ and $\mathbf{p}_n(\omega)$ polynomials are related via the integral

$$\mathbf{p}_n^{(1)}(\omega) = \int_{\mathbb{R}} d\omega' \mathbf{t}_1 \mathbf{A}(\omega') \frac{\mathbf{p}_n(\omega) - \mathbf{p}_n(\omega')}{\omega - \omega'}, \quad (\text{B10})$$

as follows readily by induction using Eq. (B8). Now, Favard's theorem tells us that there is at least one measure w.r.t. which these polynomials are orthonormal, say $\mu^{(1)}$, with $\mu^{(1)}(d\omega) = \mathbf{A}^{(1)}(\omega) d\omega$. Moreover, since we have assumed that the moment problem of μ is determinate, the same is true for the measure $\mu^{(1)}$, which therefore is unique.

The three-term recursion relation also tells us that the Stieltjes transform of $\mu^{(1)}$, say $\mathbf{G}^{(1)}(z)$, has the infinite-depth CFE

$$\mathbf{G}^{(1)}(z) = \frac{1}{\mathbf{z}_1 - \mathbf{t}_2 \frac{1}{\mathbf{z}_2 - \mathbf{t}_3 \frac{1}{\mathbf{z}_3 - \dots}}}, \quad (\text{B11})$$

involving the *same* CFE coefficients $\epsilon_{n \geq 1}$, $\mathbf{t}_{n \geq 2}$ as $\mathbf{G}(z)$ of Eq. (B9). Therefore, $\mathbf{G}^{(1)}(z)$ and $\mathbf{G}(z)$ are related by

$$\mathbf{G}(z) = \frac{1}{\mathbf{z}_0 - \mathbf{t}_1 \mathbf{G}^{(1)}(z) \mathbf{t}_1}, \quad (\text{B12a})$$

$$\mathbf{G}^{(1)}(z) = \mathbf{t}_1^{-1} [\mathbf{z}_0 - \mathbf{G}^{-1}(z)] \mathbf{t}_1^{-1}. \quad (\text{B12b})$$

The spectral density $\mathbf{A}^{(1)}(\omega)$ of $\mathbf{G}^{(1)}(z)$ can be obtained explicitly, if needed, by inserting Eq. (B12b) into a relation analogous to Eq. (B4).

The above framework is directly relevant for our discussion in Sec. IID. Identifying the functions $\mathbf{G}(z)$ and $\mathbf{A}(\omega)$ discussed above with the epimous Green's function and spectral function there, and Eq. (B12a) with the Dyson equation (9), we note that $\mathbf{G}^{(1)}(z)$ and $\mathbf{A}^{(1)}(\omega)$ correspond to the functions $\mathbf{S}(z)$ and $\mathbf{W}(\omega)$ characterizing the dynamical part of the self-energy, $\Sigma^{\text{dyn}}(z) = \mathbf{t}_1 \mathbf{S}(z) \mathbf{t}_1^\dagger$. Thus, the two sets of orthogonal block polynomials generated from measures involving the spectral functions $\mathbf{A}(\omega)$ or $\mathbf{W}(\omega)$ of the Green's function or its self-energy, respectively, are related; the polynomials generated from $\mathbf{W}(\omega)$ are associated polynomials of the first kind w.r.t. to the polynomials generated from $\mathbf{A}(\omega)$. (That is why we put the superscript on $\mathbf{p}_n^{(1)}$ in Sec. IID.) Moreover, the coefficients $\epsilon_{n \geq 1}$ and $\mathbf{t}_{n \geq 2}$ generated using either $\mathbf{W}(\omega)$ or $\mathbf{A}(\omega)$ are identical. We also note that the computational steps involved in obtaining the CFE (B9) for $\mathbf{G}(z)$ are entirely analogous to those presented in Sec. IIE for obtaining the CFE (31) for $\mathbf{S}(z)$, with $\mathbf{W}(\omega)$ there now replaced by $\mathbf{A}(\omega)$.

Appendix C: Matrix elements of inverse matrices

This appendix collects elementary identities, needed in the main text, expressing the 11-blocks of inverses of block matrices through Schur complements. All (block) matrix inverses appearing below are assumed to exist.

Let $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$ be an invertible 2×2 block matrix, then the 11-block of its inverse is given by

$$(A^{-1})_{11} = [A/A_{22}]^{-1}, \quad (\text{C1a})$$

$$[A/A_{22}] = A_{11} - A_{12}(A_{22})^{-1}A_{21}. \quad (\text{C1b})$$

$[A/A_{22}]$ is known as the Schur complement of A w.r.t. block A_{22} . Equations (C1) can be used to obtain similar expressions for the 11-blocks of larger block matrices. Let A be a 3×3 block matrix and B a 2×2 submatrix,

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}, \quad B = \begin{pmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{pmatrix}, \quad (\text{C2})$$

then the 11-block of A^{-1} , found using Eq. (C1) with A_{22} replaced by B and A_{12} by (A_{12}, A_{13}) , etc., is given by

$$(A^{-1})_{11} = [A/B]^{-1}, \quad (\text{C3a})$$

$$[A/B] = A_{11} - (A_{12}, A_{13}) (B)^{-1} \begin{pmatrix} A_{21} \\ A_{31} \end{pmatrix}. \quad (\text{C3b})$$

If $A_{23} = A_{32} = 0$, the Schur complement $[A/B]$ becomes

$$[A/B] = A_{11} - A_{12}(A_{22})^{-1}A_{21} - A_{13}(A_{33})^{-1}A_{31}. \quad (\text{C4})$$

If instead $A_{13} = A_{31} = 0$, we have

$$[A/B] = A_{11} - A_{12}(B^{-1})_{22}A_{21}. \quad (\text{C5})$$

Finally, let A be an invertible $N \times N$ tridiagonal block matrix, defined recursively, with $n = 1, \dots, N-1$:

$$A = (\bar{A}_{11}), \quad \bar{A}_{nn} = \left(\begin{array}{c|ccc} A_{nn} & A_{n,n+1} & 0 & \dots & 0 \\ \hline A_{n+1,n} & & & & \\ 0 & & \bar{A}_{n+1,n+1} & & \\ \vdots & & & & \\ 0 & & & & \end{array} \right). \quad (\text{C6})$$

Then, recursive use of Eq. (C5) yields (with $n' = n+1$):

$$(A^{-1})_{11} = [\bar{A}_{11}/\bar{A}_{22}]^{-1}, \quad (\text{C7a})$$

$$[\bar{A}_{nn}/\bar{A}_{n'n'}]^{-1} = A_{nn} - A_{nn'}(\bar{A}_{n'n'})_{11}^{-1}A_{n'n}, \quad (\text{C7b})$$

This leads to a CFE for the 11-block of A^{-1} :

$$\left(\frac{1}{A} \right)_{11} = \frac{1}{A_{11} - A_{12} \frac{1}{A_{22} - \dots - A_{N-1,N} \frac{1}{A_{NN}}} A_{21}}. \quad (\text{C8})$$

Appendix D: Finding the residual function $\mathbf{R}_N(z)$

In this appendix, we provide technical details underlying two results stated in the main text, for (i) the CFE representations of $\mathbf{G}(z)$ (see Eq. (46)), and (ii) the residual functions terminating these CFEs (see Eqs. (43)).

We consider the space, $L^2(\mu)$, of functions that are square integrable against a measure μ , that is such that $L^2(\mu)$ contains block polynomials of arbitrary degree. For definiteness, we consider the case $\mu^{(1)}(d\omega) = \mathbf{W}(\omega)d\omega$, where $\mathbf{W}(\omega)$, the normalized spectral function of the dynamical part of the self-energy $\Sigma^{\text{dyn}}(z)$, is assumed to be known analytically or numerically. (An analogous discussion applies for $\mu(d\omega) = \mathbf{A}(\omega)d\omega$, where $\mathbf{A}(\omega)$ is the spectral function of $\mathbf{G}(\omega)$.) In this space, the Liouvillian $\hat{\mathcal{L}}$ acts on functions $\mathbf{f} \in L^2(\mu)$ according to $\hat{\mathcal{L}}\mathbf{f}(\omega) = \omega \mathbf{f}(\omega)$ (cf. Eq. (14b)). Since $\hat{\mathcal{L}}$ is self-adjoint and therefore has a real spectrum, $(z - \hat{\mathcal{L}})$ with $\text{Im } z \neq 0$ is a normal operator that is invertible.

In Sec. IIE, a Lanczos scheme is used to generate blocks of vector-valued polynomials, $\{\mathbf{p}_n^{(1)}(\omega), n = 1, \dots, N\}$, that are orthogonal w.r.t. $\mu^{(1)}$ (cf. Eq. (37a)). These polynomials span an NM -dimensional subspace of $L^2(\mu)$, the space of vector-valued polynomials with degree $\leq N-1$. We call the projector onto this space $\mathcal{P}_N$, while $\bar{\mathcal{P}}_N$ projects onto its orthonormal complement (such that $\mathcal{P}_N + \bar{\mathcal{P}}_N = \mathbb{1}$). In the polynomial basis, the single-particle irreducible Liouvillian $\hat{\mathcal{L}}_{\bar{\mathcal{P}}_N}$ is represented by an $N \times N$ block-tridiagonal matrix (cf. Eq. (37b)). This block-tridiagonal structure implies a block-CFE for $\mathbf{S}(z) = \langle \mathbf{p}_1^{(1)}, (z - \hat{\mathcal{L}}_{\bar{\mathcal{P}}_N})^{-1} \mathbf{p}_1^{(1)} \rangle$, which is terminated by a residual function, $\mathbf{R}_N(z)$, that ensures the representation is exact (cf. Eq. (42)). With Eqs. (43), we provided a formula for this residual function. Below, we derive this

formula. The explicit construction of $\mathbf{R}_N(z)$ (i) shows its existence, and (ii) will also show that there exists a measure μ_N such that

$$\mathbf{R}_N(z) = \int \frac{\mu_N(d\omega)}{z - \omega}. \quad (\text{D1})$$

Following the notation of Sec. II, we denote projections to $\mathcal{P}_N$ and $\bar{\mathcal{P}}_N$ by indices p and $\bar{p}$, and blocks of matrix representations by square brackets with indices $\mathbf{p}$ and $\bar{\mathbf{p}}$, respectively. By applying formula (C1), we find

$$\begin{aligned} [(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}} &= \\ (z - [\hat{\mathcal{L}}]_{\mathbf{p}\mathbf{p}} - [\hat{\mathcal{L}}_{\bar{p}\bar{p}}(z - \hat{\mathcal{L}}_{\bar{p}\bar{p}})^{-1}\hat{\mathcal{L}}_{\bar{p}p}]_{\mathbf{p}\mathbf{p}})^{-1}. \end{aligned} \quad (\text{D2})$$

Here, $[\hat{\mathcal{L}}]_{\mathbf{p}\mathbf{p}}$, represented in the polynomial basis $\mathbf{p}_n$, is the tridiagonal matrix Eq. (37b). From the three-term recursion for the polynomials $\mathbf{p}_n$ [Eq. (39)], it follows that

$$\bar{\mathcal{P}}_N \hat{\mathcal{L}} \mathbf{p}_n^{(1)}(\omega) = \delta_{nN} \mathbf{p}_{N+1}^{(1)}(\omega) \mathbf{t}_{N+1}. \quad (\text{D3})$$

For $[\hat{\mathcal{L}}_{\bar{p}\bar{p}}(z - \hat{\mathcal{L}}_{\bar{p}\bar{p}})^{-1}\hat{\mathcal{L}}_{\bar{p}p}]_{nn'}$, with $n, n' \leq N$, this implies

$$\langle \mathbf{p}_n^{(1)}, \hat{\mathcal{L}}_{\bar{p}\bar{p}}(z - \hat{\mathcal{L}}_{\bar{p}\bar{p}})^{-1}\hat{\mathcal{L}}_{\bar{p}p} \mathbf{p}_{n'}^{(1)} \rangle = \delta_{nN} \delta_{n'N} \mathbf{R}_N(z), \quad (\text{D4a})$$

$$\mathbf{R}_N(z) = \mathbf{t}_{N+1} \langle \mathbf{p}_{N+1}^{(1)}, (z - \hat{\mathcal{L}}_{\bar{p}\bar{p}})^{-1} \mathbf{p}_{N+1}^{(1)} \rangle \mathbf{t}_{N+1}. \quad (\text{D4b})$$

Equation (D4a) shows by explicit construction that the only nonzero block of $\hat{\mathcal{L}}_{\bar{p}\bar{p}}(z - \hat{\mathcal{L}}_{\bar{p}\bar{p}})^{-1}\hat{\mathcal{L}}_{\bar{p}p}$ is its NN block; we denote it by $\mathbf{R}_N(z)$. Equation (D4b) expresses it through the $N+1, N+1$ block of $(z - \hat{\mathcal{L}}_{\bar{p}\bar{p}})^{-1}$, exploiting Eq. (D3), whose left side provides a link (the only one available!) between the $\bar{\mathcal{P}}_N$ and $\mathcal{P}_N$ sectors. Further, Eq. (D1) immediately follows from an explicit construction of the measure,

$$\mu_N(d\omega) = \mathbf{t}_{N+1} \langle \mathbf{p}_{N+1}, \delta(\omega - \hat{\mathcal{L}}_{\bar{p}\bar{p}}) \mathbf{p}_{N+1} \rangle \mathbf{t}_{N+1} d\omega. \quad (\text{D5})$$

To arrive at Eq. (43) for the residual function, we consider the inverse of the matrix in Eq. (D2), which is a block-tridiagonal matrix:

$$[(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}}^{-1} = \begin{pmatrix} \mathbf{z}_1 & \mathbf{t}_2 & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{t}_2 & \mathbf{z}_2 & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{z}_{N-2} & \mathbf{t}_{N-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{t}_{N-1} & \mathbf{z}_{N-1} & \mathbf{t}_N \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{t}_N & \tilde{\mathbf{z}}_N \end{pmatrix}. \quad (\text{D6})$$

Here, $\mathbf{z}_n(z) = \mathbf{z} - \epsilon_n$ and $\tilde{\mathbf{z}}_N(z) = \mathbf{z}_N - \mathbf{R}_N(z)$. The NN block contains an extra term, the residual function $\mathbf{R}_N(z)$ of Eqs. (D4).

Using $[(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}}^{-1}[(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}} = \mathbb{1}_{\mathbf{p}\mathbf{p}}$, where $\mathbb{1}_{\mathbf{p}\mathbf{p}}$ is the identity in the pp block, and exploiting the tridiagonal form of $[(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}}^{-1}$ (cf. Eq. (D6)),

we arrive at the equations

$$\begin{aligned} \left([(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}}^{-1} [(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}} \right)_{NN-1} &= \\ \mathbf{t}_N \mathbf{G}_N(z) + \tilde{\mathbf{z}}_N \tilde{\mathbf{F}}_N^L(z) &= \mathbf{0}, \end{aligned} \quad (\text{D7a})$$

$$\begin{aligned} \left([(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}}^{-1} [(z - \hat{\mathcal{L}}_{\bar{c}\bar{c}})^{-1}]_{\mathbf{p}\mathbf{p}} \right)_{NN} &= \\ \tilde{\mathbf{F}}_N^R(z) + \tilde{\mathbf{z}}_N \tilde{\mathbf{I}}_N(z) &= \mathbf{1}. \end{aligned} \quad (\text{D7b})$$

Here, we have used the definitions

$$\mathbf{G}_N(z) = [(z - \hat{\mathcal{L}})^{-1}]_{N-1N-1} \quad (\text{D8a})$$

$$\tilde{\mathbf{F}}_N^L(z) = [(z - \hat{\mathcal{L}})^{-1}]_{NN-1} \quad (\text{D8b})$$

$$\tilde{\mathbf{F}}_N^R(z) = [(z - \hat{\mathcal{L}})^{-1}]_{N-1N} \quad (\text{D8c})$$

$$\tilde{\mathbf{I}}_N(z) = [(z - \hat{\mathcal{L}})^{-1}]_{NN}. \quad (\text{D8d})$$

By rearranging Eq. (D7), we arrive at the relation

$$\tilde{\mathbf{z}}_N^{-1} = \tilde{\mathbf{I}}_N - \tilde{\mathbf{F}}_N^L \mathbf{G}_N^{-1} \tilde{\mathbf{F}}_N^R. \quad (\text{D9})$$

Now, the 00-element of the inverse of Eq. (D6) is explicitly presented by a CFE that is terminated at level $N-1$ by $\mathbf{z}_{N-1} - \mathbf{t}_N \tilde{\mathbf{z}}_N^{-1} \mathbf{t}_N$. Equating this to $\mathbf{z}_{N-1} - \mathbf{R}_{N-1}$ and using (D9) yields

$$\mathbf{R}_{N-1} = \mathbf{t}_N (\tilde{\mathbf{I}}_N - \tilde{\mathbf{F}}_N^L \mathbf{G}_N^{-1} \tilde{\mathbf{F}}_N^R) \mathbf{t}_N. \quad (\text{D10})$$

Defining $\mathbf{I}_N = \mathbf{t}_N \tilde{\mathbf{I}}_N \mathbf{t}_N$, $\mathbf{F}_N^L = \mathbf{t}_N \tilde{\mathbf{F}}_N^L$, $\mathbf{F}_N^R = \tilde{\mathbf{F}}_N^R \mathbf{t}_N$, and using $\mathbf{p}_N^{(1)} \mathbf{t}_N = \mathbf{p}_N^{(1)\perp}$, we get Eq. (43) of the main text.

To conclude this appendix, we note that the residual functions can also be computed recursively: By equating two exact CFEs for $\Sigma^{\text{dyn}}(z)$ of the form (42), having depth $N-1$ or N , we obtain a recursion relation for the residual functions:

$$\mathbf{R}_N(z) = \mathbf{z}_N - \mathbf{t}_N \mathbf{R}_{N-1}^{-1}(z) \mathbf{t}_N. \quad (\text{D11})$$

Starting from $\mathbf{R}_0(z) = \Sigma^{\text{dyn}}(z)$, this equation can in principle be used recursively to compute the residual functions to any required depth. However, using Eq. (D11) turns out to be numerically less stable than using Eq. (D10). Though both involve a difference between two terms, one of which involves a matrix inversion, the quotient of z -dependent functions $\mathbf{F}_N(z) \mathbf{G}_N^{-1}(z) \mathbf{F}_N(z)$ turns out to have better numerical stability than $\mathbf{t}_N \mathbf{R}_{N-1}^{-1}(z) \mathbf{t}_N$, involving just one z -dependent function in the denominator. One reason for the improved stability of Eq. (D10) is that its right side falls off with z^{-1} at large $|z|$ by construction, while Eq. (D11) relies on precise cancelations at high frequencies to produce z^{-1} behavior.

Finally, we note that an equation structurally similar to Eq. (D10) was obtained by Kugler [66] (see his Eq. (12)) in the context of computing self-energies via symmetric improved estimators. He gives a detailed discussion of the numerical stability of this construction.

Appendix E: Numerical computation of the continued fraction expansion

We compute single-particle irreducible Liouvillian matrix elements by constructing a continued fraction expansion of the self-energy through iterative application of the Liouvillian to the initial state, as described in Sec. II. This section outlines our numerical implementation, designed to construct the CFE of any function of form (22).

1. Liouvillian matrix elements

Our numerical implementation constructs the orthonormal polynomial basis $\{\mathbf{p}(\omega)\}_{1,\dots,N}$ of Sec. II E, using the spectrum of the self-energy as input. A pseudocode for our algorithm is presented in Alg. 1.

Note that a discrete system yields polynomials of discrete frequencies. Due to the discrete nature of the spectrum, the dimension of the Liouvillian and corresponding Krylov space, N , equals the number of discrete energies. As a result, the Lanczos procedure terminates after N steps exactly representing the discrete self-energy without any rest function $\mathbf{R}_N(z)$.

If the spectrum is not discrete, the rest function $\mathbf{R}_N(z)$ can be computed using Eqs. (43). Note that this requires first computing the polynomial $\mathbf{p}_{N+1}^{(1)}(\omega)$.

2. Rest function and F/S-modes

After terminating the Lancos scheme at step N and evaluating the rest function, it has to be interpolated together with the matrix elements ϵ_N and $\mathbf{t}_N$. However, to gain an advantage compared to standard interpolation schemes, the rest function must have a much weaker $\mathbf{k}$ -dependence than the Liouvillian matrix elements. A weak $\mathbf{k}$ -dependence is not guaranteed *a priori* for any termination point N . Additionally, the broadening of the CFE to obtain a smooth function of frequency is entirely governed by the rest function (unless poles at individual CFE steps are broadened by hand, which we prefer to avoid). A strategy addressing these issues is to split the rest function into slow and fast modes, as described next.

Our solution is based on the open Wilson chain approach of Ref. 61, as mentioned in the main text (Sec. II H). For convenience, we repeat here our choice for the splitting function $w_n^{S/F}(\omega)$, that fulfill $w_n^F(\omega) + w_n^S(\omega) = 1$. Our choice is a box function,

$$w_n^S(\omega) = \frac{1}{1 + |\omega/\Omega_n|^\tau}, \quad (\text{E1})$$

with half-bandwidth $\Omega_n = \Omega_{\max}\Lambda^{1-n}$ (where $\Lambda > 1$) that ranges between a minimal and maximal frequency, respectively, $\Omega_{\min}$ and $\Omega_{\max}$. The parameter $\tau > 2$ is adjustable and controls the sharpness of the defined box functions. How to choose these parameters is explained

Algorithm 1: CFE coefficients

Input: Self-energy $\Sigma(z)$

Output: Matrix elements $\epsilon_n, \mathbf{t}_n$

Computation: We use the same subscripts as in main text, but in code, only ϵ_n and $\mathbf{t}_n$ are saved as vectors.

Initialization:

Compute $\Sigma''(\omega) \leftarrow \frac{i}{2\pi} [\Sigma(z) - \Sigma^\dagger(z)]$ and set up $\mathbf{W}(\omega) = \mathbf{t}_1^{-1} \Sigma''(\omega) \mathbf{t}_1^{-1}$, where

$$\mathbf{t}_1 \mathbf{t}_1 = \int d\omega \Sigma''(\omega)$$

Iteration: Perform a N -step Lanczos scheme to set up an orthonormal polynomial basis $\{\mathbf{p}_n^{(1)}(\omega)\}_{n=1,\dots,N}$ with starting polynomial $\mathbf{p}_1^{(1)}(\omega) = \mathbf{1}$:

for $n = 1, \dots, N$

(a) Set $\tilde{\mathbf{p}}_{n+1}^{(1)}(\omega) \leftarrow \omega \mathbf{p}_n^{(1)}(\omega)$

(b) Compute

$$\epsilon_n = \int d\omega \mathbf{p}_n^{(1)\dagger}(\omega) \mathbf{W}(\omega) \tilde{\mathbf{p}}_{n+1}^{(1)}(\omega)$$

(c) Orthogonalize by

$$\mathbf{p}_{n+1}^{(1)\perp}(\omega) \leftarrow \tilde{\mathbf{p}}_{n+1}^{(1)}(\omega) - \sum_i \mathbf{p}_i^{(1)}(\omega) \int d\omega \mathbf{p}_i^{(1)\dagger}(\omega) \mathbf{W}(\omega) \tilde{\mathbf{p}}_{n+1}^{(1)}(\omega)$$

(d) Normalize $\mathbf{p}_{n+1}^{(1)}(\omega) = \mathbf{p}_{n+1}^{(1)\perp}(\omega) \mathbf{t}_{n+1}^{-1}$, where

$$\mathbf{t}_{n+1} \mathbf{t}_{n+1} = \int d\omega [\mathbf{p}_{n+1}^{(1)\perp}(\omega)]^\dagger \mathbf{W}(\omega) \mathbf{p}_{n+1}^{(1)\perp}(\omega)$$

Here, steps (c) and (d) should be repeated for improved numerical stability.

end

in detail in App. E3. Figure 20 depicts $w_n^S(\omega)$ for ten values of n , yielding logarithmically spaced values of Ω_n . The slow/fast splitting strategy yields an exponential decay with n of the modes $\mathbf{R}_n^F(z) \sim \Lambda^{-n}$ and the matrix elements $\epsilon_n \sim \Lambda^{-n}$ and $\mathbf{t}_n \sim \Lambda^{-n}$, as discussed in the main text (cf. Fig. 10).

A pseudocode for our computation of CFE coefficients is given in Alg. 2. At each iteration n the spectral part of the slow modes $\mathbf{R}_n^{S''}(\omega)$ serves as new input function, while the fast modes $\mathbf{R}_n^F(z)$ are kept in the respective CFE step, where their imaginary parts in effect act as scale-dependent broadening functions. The starting point of fast and slow mode splitting can be set at arbitrary n , yielding a general expression for a CFE of the self-energy, where the exponential decay sets in at the corresponding n .

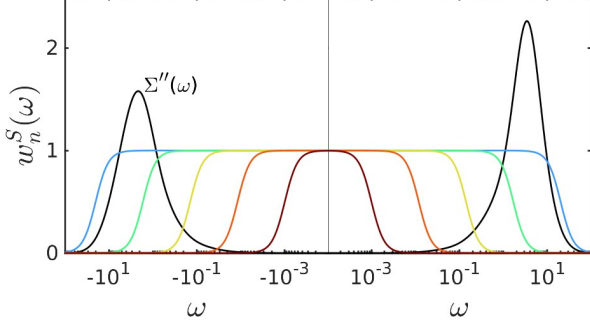


FIG. 20. Exemplary splitting functions $w_n^S(\omega)$ [Eq. (E1)], plotted for $\tau = 3$ and 5 values of n , resulting in logarithmically spaced box widths Ω_n . The black line shows a spectral part of an arbitrary self-energy.

3. Dependency on splitting function $w_n^{S/F}(\omega)$ and CFE length N

The shape of the splitting function $w_n^S(\omega)$ of Eq. (E1) is governed by the two numerical parameters τ and Λ . We now illustrate how the choice of these parameters affects the results obtained from $\mathcal{L}$ -interpolation of DCA data.

a. Sharpness of splitting function

The frequency values of the turning point of the distribution for each CFE step, $\Omega_n \sim \Lambda^{-n}$, are logarithmically spaced between a minimal and a maximal frequency, $\Omega_{\min}$ and $\Omega_{\max}$. We set the minimal frequency $\Omega_{\min} = 10^{-9}$ to capture the numerical accuracy of the NRG impurity solver. (For smaller values $\Omega_{\min} \lesssim 10^{-9}$ numerical errors appear at scales below $\Omega_{\min}$, due to reaching machine precision within the computation.) The parameter $\Omega_{\max}$ is chosen large enough to capture the full spectral weight of the cluster Green's function $\mathbf{A}(\omega)$:

$$1 - \sum_{|\omega_i| < \Omega_{\max}} \mathbf{A}_{\text{disc}}(\omega_i) < \delta \mathbf{1}, \quad (\text{E2})$$

Here, $\mathbf{A}_{\text{disc}}(\omega_i)$ is the discrete spectral function output of our NRG impurity solver and δ is an accuracy tolerance. We set it to $\delta = 10^{-5}$ for our DCA examples. We cut off over-broadened tails of $w_1^F(\omega)$, thereby regularizing the spectral part of the self-energy, to ensure that the measure $\mathbf{W}(\omega)d\omega$ is not indeterminate.

The parameter $\tau > 2$ controls the sharpness of $w_n^S(\omega)$. It tunes the overlap between successive fast modes and determines the smoothness of the continuous spectrum represented by the resulting CFE. The top row of Fig. 21 illustrates this effect by showing $A_{\mathbf{k}}(0)$ in the pseudogap regime for four values of τ . Correspondingly, Fig. 22(a) displays a frequency slice at momentum $\mathbf{X} = (0, \pi)$ for the same values.

Algorithm 2: CFE with F/S splitting

Input: Self-energy $\Sigma(z)$ and splitting function parameters $\Omega_{\min}$, $\Omega_{\max}$, Λ and τ .

Output: CFE coefficients ϵ_n , $\mathbf{t}_n$, fast modes $\mathbf{R}_n^F(z)$.

Computation: We use the same subscripts as in main text, but in the code, only ϵ_n , $\mathbf{t}_n$ and $\mathbf{R}_n^F$ are saved as vectors.

Initialization:

CFE length $N = 1 + \ln(\Omega_{\max}/\Omega_{\min})/\ln \Lambda$ and the self-energy spectrum $\Sigma''(\omega) \leftarrow \frac{i}{2\pi} [\Sigma(z) - \Sigma^\dagger(z)]$.

Iteration: Perform N one-step Lanczos schemes:

for $n = 1, \dots, N$

(a) Normalize $\Sigma''(\omega)$ to obtain $\mathbf{t}_n$ and $\mathbf{W}_{n-1}$:

$$\mathbf{t}_n \mathbf{t}_n = \int d\omega \Sigma''(\omega),$$

$$\mathbf{W}_{n-1}(\omega) \leftarrow \mathbf{t}_n^{-1} \Sigma''(\omega) \mathbf{t}_n^{-1}.$$

(b) Compute $\epsilon_n = \int d\omega \mathbf{W}_{n-1}(\omega) \omega$

(c) Compute $\mathbf{R}_n(\omega)$ via Eqs. (43):

$$\mathbf{G}_2(z) \leftarrow \int d\omega \frac{\mathbf{W}_{n-1}(\omega)}{z - \omega}$$

$$\tilde{\mathbf{F}}_2^L(z) \leftarrow \int d\omega (\omega \mathbf{1} - \epsilon_n) \frac{\mathbf{W}_{n-1}(\omega)}{z - \omega}$$

$$\tilde{\mathbf{F}}_2^R(z) \leftarrow \int d\omega \frac{\mathbf{W}_{n-1}(\omega)}{z - \omega} (\omega \mathbf{1} - \epsilon_n)$$

$$\tilde{\mathbf{I}}_2(z) \leftarrow \int d\omega (\omega \mathbf{1} - \epsilon_n) \frac{\mathbf{W}_{n-1}(\omega)}{z - \omega} (\omega \mathbf{1} - \epsilon_n)$$

$$\mathbf{R}_n(z) \leftarrow \tilde{\mathbf{I}}_2(z) - \tilde{\mathbf{F}}_2^L(z) [\mathbf{G}_2(z)]^{-1} \tilde{\mathbf{F}}_2^R(z)$$

(d) Define splitting functions: $\Omega_n = \Omega_{\max} \Lambda^{1-n}$, $w_n^S(\omega) \leftarrow (1 + |\omega/\Omega_n|^\tau)^{-1}$, $w_n^F(\omega) \leftarrow 1 - w_n^S(\omega)$.

Split $\mathbf{R}_n(z)$, reset $\Sigma''(\omega)$ for next iteration:

$$\mathbf{R}_n''(\omega) \leftarrow \frac{i}{2\pi} [\mathbf{R}_n(z) - \mathbf{R}_n^\dagger(z)]$$

$$\mathbf{R}_n^F(z) = \int d\omega \frac{w_n^F(\omega) \mathbf{R}_n''(\omega)}{z - \omega}$$

$$\Sigma''(\omega) \leftarrow w_n^S(\omega) \mathbf{R}_n''(\omega)$$

For the last step N , don't split $\mathbf{R}_n(z)$.

end

The impact of decreasing τ is clearly visible: while $\tau = 10$ yields a slightly underbroadened interpolation, reducing τ gradually removes the wiggles and, at the same time, sharpens the main features. However, for τ too small (e.g. $\tau \simeq 2$), the fast modes retain significant weight at low frequencies and the slow modes retain substantial high-frequency tails, i.e. $\mathbf{R}_n^F(\omega)$ and $\mathbf{R}_n^{S''}(\omega)$ overlap significantly and don't achieve a clean scale separation between fast and slow modes. We find that this causes them to also retain a strong $\mathbf{k}$ -dependence. This is undesirable, since Liouvillian interpolation works best if the $\mathbf{k}$ -dependence is encoded entirely (or as much as possible) in the Liouvillian matrix elements ϵ_n and $\mathbf{t}_n$. For

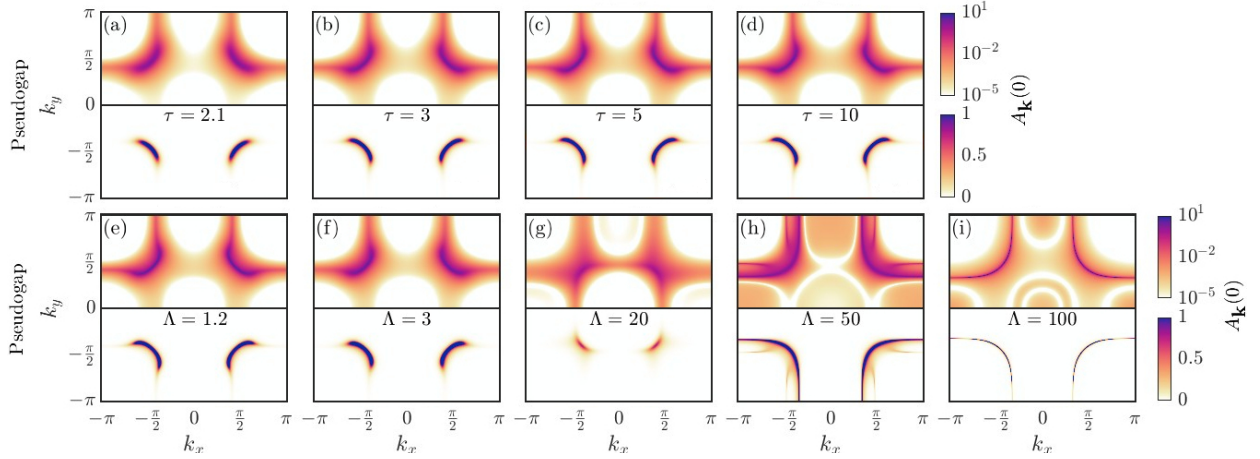


FIG. 21. $\mathcal{L}$ -interpolated DCA results for $A_{\mathbf{k}}(0)$ in the pseudogap phase, computed for the same model parameters as in Fig. 12, shown (a-d) for four values of the parameter τ in Eq. (E1), with $\Lambda = 1.2$ throughout, and (e-i) for five values of the parameter Λ in Eq. (E1), with $\tau = 5$ throughout. The top and bottom rows of each panel show the upper and lower halves of the BZ using logarithmic and linear color scales, respectively.

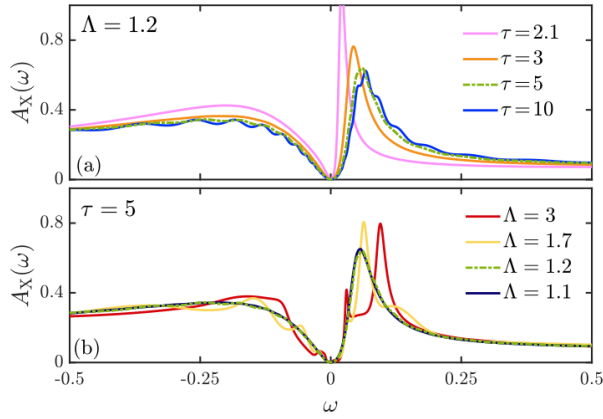


FIG. 22. Spectral function as function of ω at $\mathbf{k} = \mathbf{X} = (0, \pi)$, (a) for the four values of τ used for Figs. 21(a-d), and (b) for four values of Λ in the range used for Figs. 21(e-f) or smaller.

$\tau \leq 2$, we even observe a breakdown of tail regularization: sufficient weight remains in the tails after splitting such that $\epsilon_n \sim \Lambda^{-n}$, $\mathbf{t}_n \sim \Lambda^{-n}$, and $\mathbf{R}_n^F(z) \sim \Lambda^{-n}$.

Conversely, increasing τ reduces the fast-mode overlap, yielding cleaner scale separation and a more stable interpolation. However, a too large τ leads to underbroadening, exemplified by the wiggles in the $\tau = 10$ curve of Fig. 22(a). The optimal choice of τ is therefore the largest value at which, upon decreasing τ , these wiggles have just disappeared. We therefore choose $\tau = 5$.

b. CFE length with rest function

Due to the exponential decrease $\Omega_n \sim \Lambda^{-n}$ with n , the quantities ϵ_n , $\mathbf{t}_n$, and $\mathbf{R}_n^F(z)$ also decay exponentially and eventually reach the scale of numerical floating-point errors. As a result, the CFE exhibits artificial convergence. Increasing the CFE length N , or equivalently decreasing the logarithmic discretization factor Λ (while keeping $\Lambda > 1$), increases the number of matrix elements in the CFE representation.

The second row of Fig. 21 shows $\mathcal{L}$ -interpolated results for $A_{\mathbf{k}}(0)$ in the pseudogap regime for several values of Λ , where panels (e)–(i) correspond to a progressively shorter CFE. Figure Fig. 22(b) presents a frequency slice at momentum $\mathbf{X} = (0, \pi)$ for four values with $\Lambda \leq 3$. Smaller Λ increases the number of Liouvillian matrix elements and thus the number of bands contributing to the interpolated spectrum. Encoding the $\mathbf{k}$ -dependence through more matrix elements improves the interpolation of a continuous spectrum.

Comparing the lower row of Fig. 21 with Fig. 22(b) shows that the low-energy regime converges more rapidly ($\Lambda \lesssim 3$) than the high-energy regime as Λ decreases, reflecting the logarithmic discretization. Accurately resolving high-energy features requires a higher matrix element density, i.e., even smaller Λ . In our calculations, convergence at high energies is achieved for $\Lambda \lesssim 1.2$, as shown in Fig. 22(b).

Since we interpolate the fast modes using $\alpha_{\mathbf{k}, \mathbf{K}}$ (not $\alpha_{\mathbf{k}, \mathbf{K}}^{\text{mod}}$), causality issues begin to arise for $\Lambda \gtrsim 3$, foreshadowing the fact that in the limit $\Lambda \gg 1$, $\mathbf{R}_n^F$ -interpolation has similar issues as Σ -interpolation. This behavior originates from the enhanced $\mathbf{k}$ -dependence of the fast modes when fewer matrix elements are retained. We therefore choose $\Lambda = 1.2$ as a good compromise between a man-

ageable log-CFE depth and an accurate representation of the $\Lambda \rightarrow 1$ limit. Note that decreasing Λ allows for larger values of τ while maintaining numerical stability.

Appendix F: Lattice harmonics

This appendix gives some background on lattice harmonics and their symmetry properties [100, 101], evoked in Sec. III B on canonical DCA interpolation.

Lattice harmonics are functions of $\mathbf{k}$ that transform according to irreducible representations (irreps) of the symmetry point group, say G , of the model's real-space Bravais lattice and its BZ. (For a symmetry-broken phase, let G describe the remaining symmetry.) Let Γ be an irrep of G , with dimension d_Γ and matrix representation D^Γ . Lattice harmonics forming a $\mathbf{k}$ -space basis for Γ can be constructed by projecting the plane wave function $e^{-i\mathbf{k}\cdot\mathbf{r}}$, for some fixed seed vector $\mathbf{r}$ from the real-space lattice, onto Γ using the standard group-theory projector:

$$[\phi_\Gamma]_\alpha = \frac{d_\Gamma}{|G|} \sum_{g \in G} [D^\Gamma(g)]_{\alpha 1} e^{-i\mathbf{k}\cdot g(\mathbf{r})}. \quad (\text{F1})$$

The D^Γ matrices can always be chosen such that the resulting functions $[\phi_\Gamma]_\alpha$ are real, and we assume this to be the case in this work. For $\mathbf{r} = \mathbf{0}$, Eq. (F1) yields a $\mathbf{k}$ -independent function; for seed vectors of increasing length $|\mathbf{r}|$, it yields lattice harmonics with an increasingly complex dependence on $\mathbf{k}$.

Consider, for example, a 2-dimensional square lattice, invariant under $G = C_{4v}$, the group of reflections about the x - and y -axes and of multiples-of- $\pi/2$ rotations about the origin. Then, the lattice harmonics obtained for seed vectors with $|\mathbf{r}| = 1$ are linear combinations of cosine and sine functions, and those obtained for $|\mathbf{r}| > 1$ can include nonlinear combinations of cosine and sine functions.

For a given DCA patching scheme, let G_p be that subgroup of G which leaves every patch individually invariant, i.e. for every patch $V_{\mathbf{k}}$, if $\mathbf{k} \in V_{\mathbf{k}}$ then $g(\mathbf{k}) \in V_{\mathbf{k}}$ for all $g \in G_p$. A subset of all lattice harmonics of G are invariant under G_p (i.e. transform trivially under G_p). In the main text (Sec. III B), we denote them by $\phi_{\mathbf{k},j}$, where $j = 1, 2, 3, \dots$ enumerates them in order of increasing complexity, with $\phi_{\mathbf{k},1} = 1$. By definition, these functions obey $\phi_{g(\mathbf{k}),j} = \phi_{\mathbf{k},j}$ for all $g \in G_p$.

In Sec. V of the main text, we consider a 2-dimensional square lattice with point group symmetry C_{4v} , and a DCA scheme with $N_p = 4$ patches arranged in a star geometry, see Fig. 8. These patches are invariant under $G_p = C_{2v}$, the group of reflections about the x - and y -axes (but not under $\pi/2$ rotations about the origin). Since C_{4v} contains C_{2v} as a subgroup, all C_{4v} irreps are also C_{2v} irreps, and since C_{2v} is abelian, all its irreps are one-dimensional. This means that all C_{4v} irreps transform trivially under C_{2v} . We therefore simply choose the $\phi_{\mathbf{k},j}$ functions to be the first N_p irreps of C_{4v} , enumerated

in order of increasing complexity:

$$\begin{aligned} \phi_{\mathbf{k},1} &= 1, & \phi_{\mathbf{k},3} &= \cos k_x - \cos k_y, \\ \phi_{\mathbf{k},2} &= \cos k_x + \cos k_y, & \phi_{\mathbf{k},4} &= \cos k_x \cos k_y. \end{aligned} \quad (\text{F2})$$

Remark: These functions are linearly related to the lattice harmonics of the patch-symmetry group $G_p = C_{2v}$,

$$\begin{aligned} \phi'_{\mathbf{k},1} &= 1, & \phi'_{\mathbf{k},3} &= \cos k_y, \\ \phi'_{\mathbf{k},2} &= \cos k_x, & \phi'_{\mathbf{k},4} &= \cos k_x \cos k_y. \end{aligned} \quad (\text{F3})$$

These follow from a version of Eq. (F1) appropriate for abelian groups,

$$\phi'_{\mathbf{k},j} = \frac{1}{|G_p|} \sum_{g \in G_p} e^{-i\mathbf{k}\cdot g(\mathbf{r}_j)} = \frac{1}{N_j} \sum_{\mathbf{r} \in O_j} e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad (\text{F4})$$

seeded by $\mathbf{r}_1 = (0, 0)$, $\mathbf{r}_2 = (1, 0)$, $\mathbf{r}_3 = (0, 1)$, $\mathbf{r}_4 = (1, 1)$. On the right, the sum is over all points in the orbit O_j seeded by $\mathbf{r}_j$, i.e. the set of distinct points obtained by acting with all elements of G_p on $\mathbf{r}_j$, and N_j is the number of points in orbit O_j (here: $N_1 = 1$, $N_2 = N_3 = 2$, $N_4 = 4$). We regard N_j as a measure of the non-locality of the Fourier modes contributing to $\phi'_{\mathbf{k},j}$ and $\phi_{\mathbf{k},j}$. The modified form factors $\alpha_{\mathbf{k},\mathbf{K}}^{\text{mod}}$ of Eq. (65) aim to ameliorate non-causality issues by reducing the weight of these non-local Fourier modes by an extra factor $1/N_j$.

To conclude this appendix, we remark that the interpolation Ansatz of Eqs. (58) and (59) for $\mathbf{Q}_{\mathbf{k}}(z)$ and $\alpha_{\mathbf{k},\mathbf{K}}$ can be expressed as a truncated Fourier expansion of the form of Eq. (2): by Eq. (F1), lattice harmonics are symmetry projections of Fourier factors $e^{-i\mathbf{k}\cdot\mathbf{r}}$, and those used for $\phi_{\mathbf{k},j \leq N_p}$ are lattice harmonics of low complexity, for which $|\mathbf{r}|$ is of limited range, say $|\mathbf{r}| \leq R$.

Appendix G: Pseudogap of cellular DMFT+ED

In this appendix we perform another test of $\mathcal{L}$ -interpolation, based on CDMFT+ED results for the pseudogap phase in the 2D Hubbard model. These results were kindly provided to us by the authors of Ref. 33. Their results were computed for $t = 1$, $t' = -0.3t$, $t'' = 0.2t$, $U = 8t$ and a doping level of $x = 0.065$, and include broadening with $\eta = 0.1$. For further details regarding the numerical methodology, we refer the reader to Refs. [33, 102].

The rationale for testing the $\mathcal{L}$ -scheme with an exact diagonalization (ED) impurity solver stems from the discrete nature of the pole spectrum produced by this method. Since the spectrum is both finite and discrete, the continued fraction expansion (CFE) is likewise finite, with its length dictated by the number of poles, thereby eliminating the necessity for a rest function.

We start from CDMFT+ED results for the discrete spectrum of the impurity Green's function $\mathbf{G}_{\text{dd}}(z)$, computed for a given hybridization function $\Delta(z)$ having a discrete spectrum of $\Delta(z)$ of the form

$$\Delta''(\omega) = \sum_{\ell} \Delta_{\ell} \delta(\omega - \xi_{\ell}). \quad (\text{G1})$$

To we extract the discrete spectrum of the self-energy $\Sigma(z)$ we first invert the Dyson equation (cf. Eq. (48)),

$$\mathbf{G}_{\text{dd}}(z) = \frac{1}{z - \epsilon - \Delta(z) - \Sigma(z)}, \quad (\text{G2})$$

using a strategy explained in Ref. 60. This provides us with the spectrum of $\Delta(z) + \Sigma(z)$, obtained in the form

$$\Delta''(\omega) + \Sigma''(\omega) = \sum_i [\Delta + \Sigma]_i \delta(\omega - \tilde{\omega}_i). \quad (\text{G3})$$

We then extract $\Sigma''(\omega)$ from Eq. (G3) by subtracting $\Delta''(z)$ via the pole-subtraction strategy of Ref. 103: we identify matching energies ξ_ℓ and $\tilde{\omega}_\ell$ (for every ξ_ℓ , we always found a unique $\tilde{\omega}_\ell$ with $|\xi_\ell - \tilde{\omega}_\ell| < 10^{-8}$), and subtract the corresponding Δ_ℓ to obtain

$$\Sigma_\ell = \begin{cases} [\Delta + \Sigma]_\ell - \Delta_\ell & \text{if } \exists \xi_\ell : |\xi_\ell - \tilde{\omega}_\ell| < \varepsilon \\ [\Delta + \Sigma]_\ell & \text{otherwise.} \end{cases} \quad (\text{G4})$$

We found $\Sigma_\ell \simeq 0$ whenever $|\xi_\ell - \tilde{\omega}_\ell| < \varepsilon$, signifying a clean subtraction of the hybridization function poles.

Let us now compare the results of applying M - and $\mathcal{L}$ -interpolation to this data. For M -interpolation we broaden the self-energy using Gaussian broadening (with standard deviation $\sigma = 0.15$) and compute the cumulant from the Gaussian broadened self-energy spectrum. For $\mathcal{L}$ -interpolation we construct the CFE (41) of the discrete self-energy represented by $\{\Sigma_\ell, \omega_\ell\}$, periodize the resulting ω -independent Liouvillian matrix elements, and broaden the reconstructed $\Sigma_{\mathbf{k}}(\omega_\ell)$ for individual $\mathbf{k}$ -points using CFE+Gaussian broadening (following Ref. 64, Sec. S-2.2).

In Figure 23, we present the comparison between the $\mathcal{L}$ -scheme and the M -scheme for the spectral function $A_{\mathbf{k}}(\omega = 0)$. The left panel corresponds to the M -scheme, while the right panel shows the $\mathcal{L}$ -scheme results.

The M -interpolation produces a hole-like Fermi surface, however, the spectral weight decays strongly towards the BZ boundary. In contrast, the $\mathcal{L}$ -scheme unveils a more refined structure: rather than arcs, it reveals an intersected arc suggestive of a hole pocket. This result highlights the $\mathcal{L}$ -scheme's ability to capture finer details of the Fermi surface, including potential hole pockets that may be overlooked by other interpolation methods.

The second row of Fig. 23 shows the spectral function $A_{\mathbf{k}}(\omega)$ along the path $\Gamma\text{XMI}\Gamma$ in the BZ, corresponding to the first row. The $\mathcal{L}$ -interpolation produces a clear gap at X and $\omega = 0$ compared to M -interpolation. These plots highlight how the individual CFE bands accumulate, ultimately approximating the full spectral band. The cuts in band structure are attributed to finite size effects of the ED impurity solver and missing poles. This results in a resolution of the jagged ED structure within the interpolation even with a relatively large broadening. Even though we are able to resolve hole pockets, the finite size effects of make it hard to decipher if this structure is the correct one.

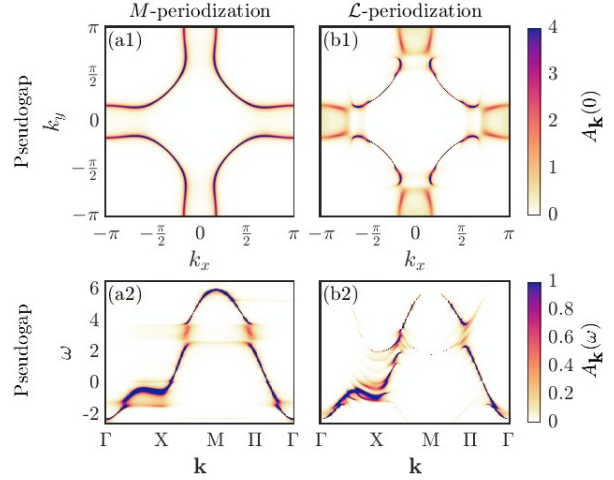


FIG. 23. Interpolated CDMFT+ED results for a 4-site cluster impurity with $t = 1$, $t' = -0.3t$, $t'' = 0.2t$, and $U = 8t$, in the pseudogap phase at doping $\delta = 0.065$. (a1,b1) The spectral function at the Fermi surface, $A_{\mathbf{k}}(\omega = 0)$, and (a2,b2) the spectral function along the path $\Gamma\text{XMI}\Gamma$, $A_{\mathbf{k}}(\omega)$ obtained via (a) M - and (b) $\mathcal{L}$ -periodization.

Although the $\mathcal{L}$ -scheme successfully resolves the hole pocket-like structure, it remains uncertain whether this feature is fully accurate due to the finite size effects inherent in ED. Nevertheless, these results suggest that the $\mathcal{L}$ -scheme provides a more detailed and potentially more accurate interpolation of the spectral function compared to the M -scheme.

Appendix H: Details on TaSK calculations

The MPS results on the 1D Hubbard model presented in Sec. IV A were obtained using the tangent space Krylov (TaSK) scheme recently proposed in Ref. 64. The CDMFT results of Sec. IV B were obtained by applying TaSK to impurity models, following Ref. 104. Here, we discuss some aspects specific to our present TaSK computations that are not discussed those two references.

1. Hubbard chain

We consider a 1D Hubbard chain of $L = 50$ sites, with $U = 5$ and $\mu = -U/2$ (half-filling). To compute the spectral function $A_k(\omega)$ of the correlator $G_k(t)$ of Eq. (73), we use the k -dependent single-particle operator

$$c_k = \frac{1}{\sqrt{L}} \sum_{\ell=1}^L e^{-ik\ell} c_\ell, \quad (\text{H1})$$

where we treat k as a continuous variable to achieve finer k resolution. We exploit $U(1) \times SU(2)$ charge and spin

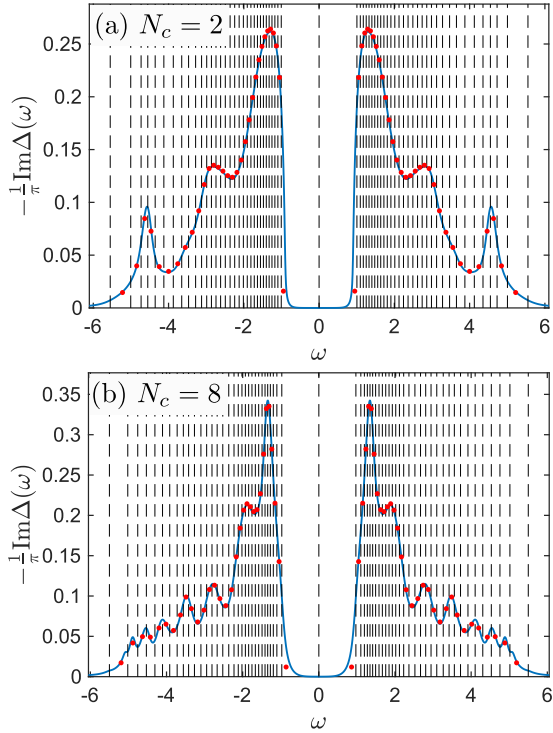


FIG. 24. Hybridization functions (blue lines) at self-consistency for (a) $N_c = 2$ and (b) $N_c = 8$. The black dashed lines mark the boundaries between the 64 frequency intervals used for discretization. The discretized hybridization function is plotted as red dots. Their ω positions are the frequency of the delta peaks, their height is the weight of the delta peak normalized by the size of the corresponding frequency interval.

symmetries. We compute the ground state using state-of-the-art single-site DMRG [105, 106] with bond expansion [107–109]. The bond dimension of our ground state is $D^* = 500$ SU(2) multiplets.

We choose 51 equally spaced values for k between 0 and π , and for each momentum point use TaSK to compute a discrete version, $A_k^{\text{disc}}(\omega)$, of the spectral function, comprising 204 discrete δ -peaks. We then compute the CFE coefficients ϵ_{kn} and t_{kn} (shown in Fig. 3) from $A_k^{\text{disc}}(\omega)$ (known at 51 k -values). To obtain a spectrum for arbitrary k , we interpolate $A_k^{\text{disc}}(\omega)$ for k -values between our chosen 51 ones by linear interpolation of the CFE coefficients ϵ_{kn} and t_{kn} . To obtain the continuous-in-frequency spectra shown in Fig. 1(a), we use the CFE+Gaussian broadening scheme of Sec. S-2 of Ref. [64], with broadening parameter $\sigma = 0.3$ and $N_{\text{CFE}} = 2$ there. For the lattice model, this is equivalent to broadening the discrete self-energy with $\sigma = 0.3$ and $N_{\text{CFE}} = 1$.

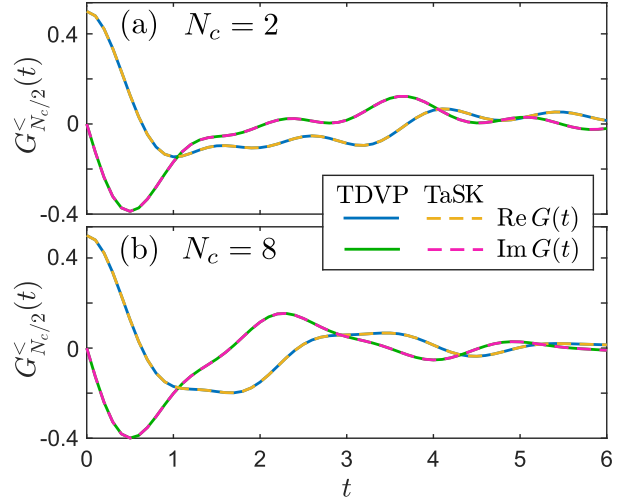


FIG. 25. Lesser Green's function $G_{N_c/2}^<(t)$ computed via TDVP (solid lines) and TaSK (dashed lines) for (a) $N_c = 2$ and (b) $N_c = 8$. For TDVP, we have used a time step $\delta t = 0.1$ and a third-order integrator; the bond dimension is allowed to grow to ensure a numerically exact result. With TaSK, we compute the spectrum of $G_{N_c/2}^<(t)$ and Fourier transform to the time domain.

2. Impurity solver for cellular DMFT

In Sec. IV B, we presented CDMFT results for the 1d Hubbard model. (For details on CDMFT for the 1d Hubbard model, see for instance Ref. [110].) The impurity solver we employ for this purpose closely follows the implementation presented in Ref. 104. The impurity model consists of an N_c -site Hubbard chain, whose outermost sites hybridize with left and right spinful baths described by two identical hybridization functions $\Delta_L(\omega) = \Delta_R(\omega)$. In contrast to Ref. 104, we discretize our baths using a linear grid generated via the mean method of Ref. 65. For the data shown in this manuscript, we use 64 spinful orbitals per bath. The discretization intervals, level positions and hybridization weights at self-consistency are illustrated in Fig. 24 for $N_c = 2$ and $N_c = 8$. Each of the discretized baths is mapped to the chain geometry depicted in Fig. 2 (b) of Ref. [111]. Since only the boundary sites of the cluster couple to the bath, we arrange our system such that the 64 left-most sites belong to the bath coupling to the left-most cluster orbital, followed by the N_c cluster sites and finally the 64 bath sites that belong to the bath hybridizing with the right-most cluster site. Again, we compute the ground state using single-site DMRG with bond expansion [108]. For the impurity solver, we truncate by singular values, using a truncation threshold of 2×10^{-8} . We then compute the discrete self-energy ($N_c \times N_c$ matrix valued) of this impurity model using a strategy described in Ref. [60]. The spectral functions necessary for that are calculated using TaSK, see Ref. 104 for specifics about using TaSK for

impurity models. Within the self-consistency cycle, the self-energy is then broadened using the CFE+Gaussian scheme of Ref. [64], using $\sigma = 0.3$ and $\mathcal{N}_{\text{CFE}} = 1$.

To gauge whether TaSK provides accurate impurity spectral functions for the impurity model at hand we also conduct an independent benchmark test, formulated in the time domain. We use the single-site time-dependent variational principle (TDVP) [112] with bond expansion [113] to compute the lesser Green's function,

$$G_{N_c/2}^<(t) = \langle \Psi_0 | c_{N_c/2\sigma}^\dagger e^{i(H-E_0)t} c_{N_c/2\sigma} | \Psi \rangle \quad (\text{H2})$$

for short times. Here, $c_{N_c/2\sigma}$ is the spin- σ annihilation operator at cluster site $N_c/2$, $|\Psi_0\rangle$ the ground state and E_0 its energy. We then compare the TDVP result for $G_{N_c/2}^<(t)$ with the TaSK result, which can be easily computed from the discrete spectra. The result of this comparison is shown in Fig. 25, for $N_c = 4, 8$. The time-dependent data obtained from both methods agree very well, which shows that our TaSK spectra are reliable.

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Symmetric estimator for discrete self-energy of discrete many-body systems

by

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We derive a discrete spectral representation of the single-particle self-energy using a discrete evaluation of Kugler’s symmetric improved estimator. Our construction can be used on both the real and the complex (Matsubara) frequency axis. It is guaranteed to remain causal at the numerical level, in contrast to standard approaches that may generate unphysical negative spectral weight or require additional broadening. Our representation can be used for any Hamiltonian; here we apply it to quantum impurity models and in dynamical mean-field theory. The latter is formulated with a discrete hybridization function throughout its self-consistency loop. In both cases and across various numerical methods, we obtain significantly improved accuracy for a range of impurity properties.

I. INTRODUCTION

Quantum impurity models, introduced by Anderson in 1961 [1], feature a small number of interacting spin-orbitals that hybridize with a large set of non-interacting bath modes. Originally devised to explain the Kondo effect [2], they also –among others– model quantum dots [3] and are employed in dynamical mean-field theory (DMFT) [4] which maps an interacting lattice problem onto a self-consistently determined impurity model. Closely related, in quantum chemistry, impurity models emerge in quantum embedding approaches [5–9].

To calculate impurity observables and spectral functions, different impurity solvers have been devised, ranging from perturbative and semi-analytical approaches [10–14] to quantum Monte Carlo (QMC) algorithms [15–18] to Hamiltonian-based methods with a discretized bath. In the latter class, one approximates the bath spectral function by a finite set of poles and solves the resulting finite Anderson impurity Hamiltonian. This is done, e.g., in exact diagonalization and Lanczos/Krylov approaches [19–21], restricted active space solvers [22–28], numerical renormalization group (NRG) [29–32], and tensor-network approaches [33–39].

In many cases, most notably DMFT, it is further important to reliably extract the single-particle self-energy. A direct evaluation via the Dyson equation

$$\Sigma(z) = G_0^{-1}(z) - G^{-1}(z), \quad (1)$$

where $G_0(z)$ and $G(z)$ are the Green functions of two different Hamiltonians, the non-interacting and the interacting one, is ill-conditioned. For a discretized bath, this is exacerbated as the poles of $G_0(z)$ and $G(z)$ will be at different energies z . Even with a tiny numerical offset in the poles of $G(z)$ or numerical limitations in the number of poles, delicate cancellations are not perfect, and the self-energy becomes non-causal.

This can be avoided by an explicit broadening of the Green’s functions or spectra [40–42], which can be further stabilized by imposing exact high-frequency moments or asymptotic limits [43, 44] or by schemes that explicitly enforce analyticity and causality [45, 46]. Alternatively, one can work with a discrete pole representation [26] and merge unphysical negative spectral weight of $\Sigma(z)$ with positive weight so that causality is eventually achieved.

The numerical instabilities inherent to the subtraction $G_0^{-1}(z) - G^{-1}(z)$ can be fully avoided by using the equations of motion for the Green’s function. This substantially more stable extraction scheme was introduced by Bulla, Hewson, and Pruschke [47] for NRG, and later transferred to QMC [48] and improved to a symmetric variant by Werner and Millis [49] and Kaufmann *et al.* [50]. This, in turn, inspired the largely improved symmetric self-energy estimator by Kugler [51]. For real-frequency calculations, however, again an artificial broadening is applied.

As a consequence, a discrete spectral representation (DSR), i.e., a pole expansion for the self-energy, is not yet available. Access to such a DSR is desirable when computing quantities that are sensitive to broadening artifacts; e.g., the asymptotic low-energy behavior of the self-energy or the DMFT self-consistency loop.

In this paper, we show how to compute the discrete self-energy of discrete many-body systems in a manner that avoids delicate cancellations and involves no broadening. The key idea is to use Kugler’s symmetric improved estimator for self-energies [51], recognize that it corresponds to the Schur complement of a sub-block of an augmented Green’s function, and compute the latter directly in a fully discrete manner.

This idea is both general and elementary, derivable in just a few lines of algebra. It can be implemented easily and used in conjunction with any computational tool capable of computing unbroadened Green’s functions

for any discrete many-body system. In this paper, we illustrate it for quantum impurity models; its transcription to other contexts should be self-evident. In the DMFT context, our DSR approach allows us to carry out the self-consistency loop entirely in terms of DSRs of the hybridization function and self-energy, without the need to remove unphysical negative spectral weight.

In Sec. II, we define the general Anderson impurity model, as well as its local Green's function $G(z)$ and the non-interacting Green's function $G_0(z)$, which define the self-energy we aim to compute. In Sec. III, we present our method to compute causal and numerically stable self-energies for DSRs, based on Kugler's symmetric improved estimator [51]. Sec. IV presents numerical examples that demonstrate the performance of the method for an impurity model and for DMFT.

Depending on the impurity solver employed, correlation functions may be given in different discrete representations. Based in part on previous literature [25, 26, 52–59], Appendix A summarizes several of these representations together with the transformations between them. In Appendix B, we discuss representation-specific algorithms for the calculation of DSR of the self-energy. In Appendix C, we show how the impurity problem can be updated using the discrete representation of self-energy $\Sigma(z)$ required for the implementation of the discrete DMFT self-consistency cycle. Finally, in Appendix D, we discuss how the calculation of the quasiparticle weight Z can be regularized in the presence of spurious poles at low energies.

For readability and connection to previous literature, we will use matrix powers for matrix inverses and symmetric matrix square roots, but fractions for matrix resolvents; e.g., $G^{-1}(z)$, and $S^{1/2}$ but $1/(z - H)$.

II. MODEL HAMILTONIAN

The formulation for obtaining the discrete self-energy, as derived in Eq. (13) below, is in principle valid for any Hamiltonian $H = H_0 + H_1$, acting on a set of fermionic single-particle states and downfolded onto a subset of these states. For concreteness, and to obtain numerical models that can be solved with the techniques currently available to us, we focus on its application to an Anderson impurity model. In particular, we consider a fermionic multi-orbital quantum impurity model with N local degrees of freedom, labelled by $\mathbf{m} \in \{1, \dots, N\}$. The local degrees of freedom may correspond to atomic-like states $\mathbf{m} = (n, l, m, \sigma)$ or to different cluster sites in extended impurity models. We label the impurity site by $i = 0$ and the M discrete bath sites by $i \in \{1, \dots, M\}$. Particles in these states are created and annihilated by the operators $a_{i,\mathbf{m}}^\dagger$ and $a_{i,\mathbf{m}}$, respectively. To suppress the spin-orbital index $\mathbf{m}$ as much as possible, we introduce row-vectors $a_i^\dagger$ containing the operators $a_{i,\mathbf{m}}^\dagger$ for all values

N of $\mathbf{m}$,

$$a_i^\dagger = \left(a_{i,\mathbf{m}=1}^\dagger a_{i,\mathbf{m}=2}^\dagger \dots a_{i,\mathbf{m}=N}^\dagger \right), \quad (2)$$

and the column vector $a_i = \left(a_i^\dagger \right)^\dagger$.

The Hamiltonian for our model consists of two parts. The term H_0 contains contributions quadratic in the creation and annihilation operators and acts non-trivially both on the bath and on the impurity, while H_1 is an arbitrary interacting part that only acts non-trivially on the impurity. The full Hamiltonian is given by

$$H = H_0 + H_1, \quad (3)$$

with

$$H_0 = \sum_{i=0}^M a_i^\dagger E_i a_i + \sum_{i=1}^M a_0^\dagger V_i^\dagger a_i + a_i^\dagger V_i a_0, \quad (4)$$

where E_i and V_i are $N \times N$ matrices describing the on-site energies (including the chemical potential) and the hybridization between impurity and bath sites, respectively. While H_1 is in principle an arbitrary interacting term which acts non-trivially only on the impurity, it usually exhibits a bilinear and a quartic term,

$$H_1 = \sum_{\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3, \mathbf{m}_4} U_{\mathbf{m}_1 \mathbf{m}_2 \mathbf{m}_3 \mathbf{m}_4} a_{0,\mathbf{m}_1}^\dagger a_{0,\mathbf{m}_2}^\dagger a_{0,\mathbf{m}_3} a_{0,\mathbf{m}_4} \quad (5) \\ - \sum_{\mathbf{m}_1, \mathbf{m}_2} U_{\mathbf{m}_1 \mathbf{m}_2}^{\text{MF}} a_{0,\mathbf{m}_1}^\dagger a_{0,\mathbf{m}_2}.$$

Here, the tensor $U_{\mathbf{m}_1 \mathbf{m}_2 \mathbf{m}_3 \mathbf{m}_4}$ defines the local interaction on the impurity and $U_{\mathbf{m}_1 \mathbf{m}_2}^{\text{MF}}$ can be used to subtract the mean-field contributions of the interaction, which in some approaches are already included in H_0 .

The influence of the bath on impurity dynamics is completely encoded in the hybridization function,

$$\Delta(z) = \sum_{i=1}^M V_i^\dagger \frac{1}{z - E_i} V_i, \quad (6)$$

with $z \in \mathbb{C}$. For real-frequency calculations, we take $z = \omega + i0^+$. There is an inherent freedom in the choice of E_i and V_i for $i \geq 1$, since any bath representation that results in the same $\Delta(z)$ leads to the same impurity dynamics. From a numerical point of view, it is often advantageous to exploit this freedom. For example, by applying a unitary transformation in the bath subspace, one can obtain a representation in which the bath Hamiltonian is diagonal, i.e. with diagonal E_i for $i \geq 1$. Moreover, by ordering the bath sites by energy and grouping degenerate bath states, one can construct a symmetry-preserving [25, 52–54] representation in which $E_i = \epsilon_i I_N$ and V_i is Hermitian. (Here, and in the following we will denote the $N \times N$ identity matrix as I_N .) An explicit algorithm for constructing such a representation is given in Appendix A 1.

The calculation of the self-energy of an impurity model via its definition of Eq. (1) requires the knowledge of the single-particle Green's functions $G(z)$ and $G_0(z)$. For an Anderson impurity model, the fermionic impurity Green's function $G(z)$ is defined as an $N \times N$ matrix in spin-orbital space ($\mathbf{m}$) with elements

$$G(z)_{\mathbf{m},\mathbf{m}'} = \sum_s \rho_s \left(\left\langle \Psi_s \left| a_{0,\mathbf{m}} \frac{1}{z - H + \mathcal{E}_s} a_{0,\mathbf{m}'}^\dagger \right| \Psi_s \right\rangle + \left\langle \Psi_s \left| a_{0,\mathbf{m}'}^\dagger \frac{1}{z + H - \mathcal{E}_s} a_{0,\mathbf{m}} \right| \Psi_s \right\rangle \right). \quad (7)$$

Here, $|\Psi_s\rangle$ are the eigenstates of H with eigenenergies $\mathcal{E}_s$, and $H = H_0 + H_1$ is the full Hamiltonian and the Boltzmann weight $\rho_s = \frac{e^{-\mathcal{E}_s/(k_B T)}}{\sum_{s'} e^{-\mathcal{E}_{s'}/(k_B T)}}$, with T the temperature of the system. $G_0(z)$ is obtained analogously from Eq. (7) by replacing H with H_0 , and $|\Psi_s\rangle$ and $\mathcal{E}_s$ by the eigenstates $|\Psi_{0s}\rangle$ and eigenenergies $\mathcal{E}_{0s}$ of H_0 . For the Anderson impurity model, it can be written as

$$G_0(z) = \frac{1}{z - E_0 - \Delta(z)}, \quad (8)$$

with E_0 and $\Delta(z)$ defined in Eqs. (4) and (6).

As outlined in the introduction, calculating $\Sigma(z)$ from $G_0(z)$ and $G(z)$ can be numerically challenging. The next section presents a solution that works for discrete representations of Green's functions and guarantees the causality of $\Sigma(z)$ even in the presence of numerical inaccuracies.

III. DISCRETE REALIZATION OF THE SYMMETRIC IMPROVED SELF-ENERGY ESTIMATOR

In Ref. [51], Kugler showed how the self-energy can be obtained from a combination of two equations of motion. The construction involves an $\tilde{N} \times \tilde{N}$ matrix-valued propagator $\tilde{G}(z)$, defined analogously to Eq. (7), with $\tilde{N} = 2N$. Here, the N impurity operators $a_{0,\mathbf{m}}$ appearing in Eq. (7) are augmented by N additional auxiliary operators $q_{\mathbf{m}}$, defined as

$$q_{\mathbf{m}} = [a_{0,\mathbf{m}}, H_1]. \quad (9)$$

The propagator $\tilde{G}(z) = \begin{pmatrix} \tilde{G}_{11} & \tilde{G}_{12} \\ \tilde{G}_{21} & \tilde{G}_{22} \end{pmatrix}$ therefore has a 2×2 block structure. Index 1 refers to the states where one acts with the operators $a_{0,\mathbf{m}}$ and $a_{0,\mathbf{m}}^\dagger$ on $|\Psi_s\rangle$, index 2 refers to the states where one acts with the operators $q_{\mathbf{m}}$ and $q_{\mathbf{m}}^\dagger$ on $|\Psi_s\rangle$. As a result, $\tilde{G}_{11}(z) = G(z)$ is the conventional impurity propagator defined above.

Kugler showed [51] that the self-energy, defined in Eq. (1), can be obtained from elements of $\tilde{G}(z)$ via [60]

$$\Sigma(z) - \Sigma^{\text{HF}} = \tilde{G}_{22}(z) - \tilde{G}_{21}(z) \frac{1}{\tilde{G}_{11}(z)} \tilde{G}_{12}(z). \quad (10)$$

Here, Σ^{HF} is the Hartree-Fock contribution to the self-energy. It can be calculated with [51]

$$(\Sigma^{\text{HF}})_{\mathbf{m},\mathbf{m}'} = \langle \{q_{\mathbf{m}}, a_{0,\mathbf{m}'}^\dagger\} \rangle = \langle \{a_{0,\mathbf{m}}, q_{\mathbf{m}'}^\dagger\} \rangle, \quad (11)$$

where $\langle \bullet \rangle$ denotes the thermal expectation value.

Now recall the Schur complement formula,

$$\left(\left[\begin{pmatrix} \tilde{G}_{11} & \tilde{G}_{12} \\ \tilde{G}_{21} & \tilde{G}_{22} \end{pmatrix} \right]_{22}^{-1} \right)^{-1} = \tilde{G}_{22} - \tilde{G}_{21} \frac{1}{\tilde{G}_{11}} \tilde{G}_{12}, \quad (12)$$

a block matrix identity that holds provided the inverses involved in it exist. (Its name reflects the fact that its right side is known as the Schur complement of $\tilde{G}$ w.r.t. $\tilde{G}_{11}$.) We can thus express the self-energy as the inverse of the 22-block of the inverse of $\tilde{G}$:

$$\Sigma(z) - \Sigma^{\text{HF}} = \left([\tilde{G}^{-1}(z)]_{22} \right)^{-1}. \quad (13)$$

This is the central equation of this paper. If the impurity solver yields a causal $\tilde{G}(z)$, Eq. (13) is guaranteed to result in a causal self-energy. This is because causality of $\tilde{G}(z)$ implies causality of $\tilde{G}^{-1}(z)$. The subsequent projection to the 22 sector also preserves causality, and so does the final inversion.

Obtaining a causal $\tilde{G}(z)$ is much easier to achieve than highly accurate pole energies and weights. While high accuracy of individual pole energies and weights is usually not guaranteed as soon as approximations are involved, causality is baked into the design of most Hamiltonian-based impurity solvers. Indeed, except for full density-matrix NRG [61, 62], where minor causality violations can occur, all impurity solvers used in this work are guaranteed to yield a causal $\tilde{G}(z)$ and therefore a causal self-energy estimate via Eq. (13).

The reformulation (13) avoids subtracting two nearly canceling quantities, instead expressing the self-energy directly through a sub-block of the inverse propagator $\tilde{G}^{-1}(z)$. It thus offers a straightforward strategy for computing the self-energy: compute the full $\tilde{G}(z)$ as a 2×2 block matrix, then (i) invert it, (ii) project to the 22 block, and (iii) invert again. The three steps (i)-(iii), described in detail in Appendix B, can be performed using matrix manipulations not involving z .

When inverting $\tilde{G}(z)$, it is important to realize that the operators $a_{0,\mathbf{m}}$ and $q_{\mathbf{m}}$ do not satisfy the canonical fermionic anticommutation relations. Consequently, $\tilde{G}(z)$ is not canonically normalized, in the sense that

$$-\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \text{Im} \tilde{G}(\omega + i0^+) = \tilde{S}, \quad (14)$$

where the weight matrix $\tilde{S}$ is a positive semi-definite Hermitian matrix instead of the identity matrix with blocks given by

$$(\tilde{S}_{11})_{\mathbf{m}\mathbf{m}'} = \delta_{\mathbf{m}\mathbf{m}'} \quad (\tilde{S}_{12})_{\mathbf{m}\mathbf{m}'} = (\Sigma^{\text{HF}})_{\mathbf{m}\mathbf{m}'} \quad (15a)$$

$$(\tilde{S}_{21})_{\mathbf{m}\mathbf{m}'} = (\Sigma^{\text{HF}})_{\mathbf{m}\mathbf{m}'} \quad (\tilde{S}_{22})_{\mathbf{m}\mathbf{m}'} = \langle \{q_{\mathbf{m}}, q_{\mathbf{m}'}^\dagger\} \rangle. \quad (15b)$$

The block $\tilde{S}_{12}$ can be made to vanish by absorbing the Hartree–Fock mean-field part of H_1 , evaluated from the ground-state one-particle density matrix, into H_0 , and correspondingly removing it from H_1 , i.e., setting $U_{\text{mm}'}^{\text{MF}} = (\Sigma^{\text{HF}})_{\text{mm}'}$ in Eq. (5).

To invert $\tilde{G}(z)$, we express it in terms of an effective energy dependent matrix-valued effective Hamiltonian $\tilde{H}_{\text{eff}}(z) \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$ (see [26, 52, 57, 59]) as

$$\tilde{G}(z) = \tilde{S}^{1/2} \frac{1}{z - \tilde{H}_{\text{eff}}(z)} \tilde{S}^{1/2}, \quad (16)$$

with $\tilde{S}^{1/2}$ the Hermitian principle square root of $\tilde{S}$. The inverse of $\tilde{G}(z)$ then becomes

$$\tilde{G}^{-1}(z) = \tilde{S}^{-1/2} (z - \tilde{H}_{\text{eff}}(z)) \tilde{S}^{-1/2}, \quad (17)$$

and the lower-right block becomes

$$[\tilde{G}^{-1}(z)]_{22} = [\tilde{S}^{-1}]_{22} z - [\tilde{S}^{-1/2} \tilde{H}_{\text{eff}}(z) \tilde{S}^{-1/2}]_{22}. \quad (18)$$

Inverting the matrices on both sides yields

$$\begin{aligned} ([\tilde{G}^{-1}(z)]_{22})^{-1} &= \frac{1}{[\tilde{S}^{-1}]_{22} z - [\tilde{S}^{-1/2} \tilde{H}_{\text{eff}}(z) \tilde{S}^{-1/2}]_{22}} \\ &= S^{1/2} \frac{1}{z - S^{1/2} [\tilde{S}^{-1/2} \tilde{H}_{\text{eff}}(z) \tilde{S}^{-1/2}]_{22} S^{1/2}} S^{1/2}. \end{aligned} \quad (19)$$

Here, $S^{1/2}$ is the Hermitian principle square root of $S = ([\tilde{S}^{-1}]_{22})^{-1}$, which constitutes the weight matrix of $\Sigma(z) - \Sigma^{\text{HF}}$. Explicit expressions for $\Sigma(z)$ when $\tilde{G}(z)$ is known in various representations are given in the Appendix B.

Although shown here for Anderson impurity models, the above construction is more general and applicable to interacting fermionic problems downfolded onto a chosen subspace. This makes it particularly useful for applications that are highly sensitive to causality and moment conservation, such as the extraction of low-energy Fermi-liquid parameters and realization of a fully discrete real-frequency DMFT self-consistency loop, as discussed in the following two benchmark applications.

IV. APPLICATIONS

We now apply our discrete self-energy scheme to two challenging problems, employing various zero-temperature impurity solvers. First, Sec. IV A gives an overview of the impurity solvers used, and Sec. IV B provides details of our benchmark method. In Sec. IV C, we consider the single-impurity Anderson model (SIAM) and compute the low-frequency expansion coefficients of the self-energy. Then, in Sec. IV D, we treat the Hubbard model on the $d \rightarrow \infty$ Bethe lattice using discrete DMFT and compute the U -dependent double occupancy, low-order moments, and quasiparticle weight.

A. Overview of impurity solvers

In the following, we employ four different impurity solvers: (i) the tangent-space Krylov (TaSK) [63, 64] approach; (ii)–(iii) natural-impurity-orbital solvers [26–28] in two independent implementations, (ii) QUANTY [65] and (iii) RAS_DMFT.jl [66]; and (iv) the numerical renormalization group (NRG) [29, 31]. All four solvers discretize the bath, making them amenable to our DSR of the self-energy. Below, we show that the DSR yields highly accurate self-energies for all of these solvers, demonstrating the generality and versatility of our scheme.

The TaSK method used in solver (i) is a generic approach to compute spectral functions on top of ground states that are represented as a matrix product state (MPS) [63]. It approximates excitations within the tangent space of the ground state MPS using an otherwise standard Krylov scheme. In this work, we use TaSK as an impurity solver to determine low-frequency Fermi-liquid coefficients of a SIAM. We therefore employ a logarithmic discretization as in NRG to obtain high resolution at the Fermi level (though TaSK does not rely on energy-scale separation). To resolve spectra with contributions extending over several decades with a Krylov scheme, TaSK is initialized with a block of states across all energy scales, as explained in Ref. [64].

The natural-impurity-orbital solver used both in (ii) and (iii) is an exact diagonalization (ED)-based approach that employs a truncated configuration space. The truncation is performed by restricting the occupation of bath orbitals in the natural-impurity-orbital basis [26], thereby selecting the most relevant configurations [28].

The NRG approach [solver (iv)] relies on logarithmic discretization and an ensuing energy-scale separation along the Wilson chain [29, 31]. By iterative diagonalization, it generates a complete but approximate many-body basis [67]. Correlation functions can then be computed in textbook fashion [61, 62]. Our DSR for the self-energy can also be used in NRG, see Fig. 1(b). In all other cases, however, we choose to employ NRG in the conventional way with a continuous self-energy for benchmarking purposes. Since this NRG benchmark is used in both Sec. IV C and IV D, we summarize its computational details in the following subsection.

B. Details of NRG benchmark

Within NRG, quasiparticle parameters such as the quasiparticle weight Z and the scattering-rate coefficient C can be extracted from the finite-size many-body spectra obtained from iterative diagonalization using Hewson’s renormalized perturbation theory (RPT) [68–71]. In short, Z is readily determined from the lowest-energy single-particle excitation. For C , the quasiparticle interaction is first deduced from two-particle excitations, and a second-order renormalized expansion of the self-

energy in terms of quasiparticle propagators provides the ω^2 coefficient [72].

Applied to a SIAM as in Sec. IV C, this NRG+RPT approach does not involve any dynamical correlation functions and is thus extremely accurate. We also use NRG+RPT to determine the quasiparticle weight for the DMFT solution of the Hubbard model in Sec. IV D. However, in this setting, the hybridization function is determined self-consistently involving NRG continuous self-energies that are obtained via a logarithmic broadening. Through the DMFT self-consistency the self-energy develops non-trivial features at high energies, which are poorly resolved on a logarithmic grid. Both aspects lead to a small but finite error in the final results.

The NRG results were obtained with the MuNRG package [42, 73, 74], built on top of the QSpace tensor library [75–78], allowing us to exploit SU(2) charge and SU(2) spin symmetry. For the results in Sec. IV C, we keep up to 4000 low-energy multiplets during the iterative diagonalization, which provides highly accurate finite-size spectra, and consider different discretization parameters Λ . For the results in Sec. IV D, involving continuous self-energies, we used $\Lambda = 1.7$ and kept $N_{\text{keep}} = 5000$ multiplets during the iterative diagonalization. We averaged results over $n_z = 4$ shifted discretization grids [79] and used an adaptive broadening parameter [42] $\alpha_z = \alpha/n_z$ with $\alpha = 1$.

C. Low-energy Fermi-liquid behavior in the SIAM

In this section, we apply our method for extracting the discrete spectrum of the self-energy to the SIAM. Our goal is to obtain low-frequency expansion parameters of the self-energy in the limit of a continuous bath, in order to illustrate the ability of our approach to yield high-quality numerical data for the self-energy.

We focus on the particle-hole symmetric, spin-degenerate case (i.e. $N = 2$), with $E_0 = 0$ and

$$H_1 = U \left(n_{\uparrow} - \frac{1}{2} \right) \left(n_{\downarrow} - \frac{1}{2} \right), \quad (20)$$

where $n_{\sigma} = a_{0\sigma}^{\dagger} a_{0\sigma}$ is the spin- σ density at the impurity and we set $U = 2$. Further, we choose a hybridization function with a semicircular density of states with half-bandwidth $D = 1$ (our unit of energy),

$$-\frac{1}{\pi} \text{Im} \Delta(\omega) = \Delta''(\omega) = \frac{1}{2\pi} \sqrt{1 - \omega^2}. \quad (21)$$

With decreasing energies, this model flows to a local Fermi-liquid fixed point.

At $T = 0$ and given particle-hole symmetry, the impurity self-energy has the low-frequency expansion

$$\text{Re} \Sigma(\omega^+) = \Sigma(0) + (1 - Z^{-1})\omega + O(\omega^3), \quad (22a)$$

$$-\text{Im} \Sigma(\omega^+) = C\omega^2 + O(\omega^4), \quad (22b)$$

where $\Sigma(0) = 0$, consistent with $E_0 = 0$ set above, and

$$Z = [1 - \partial_{\omega} \text{Re} \Sigma(\omega^+)|_{\omega=0}]^{-1} \quad (23)$$

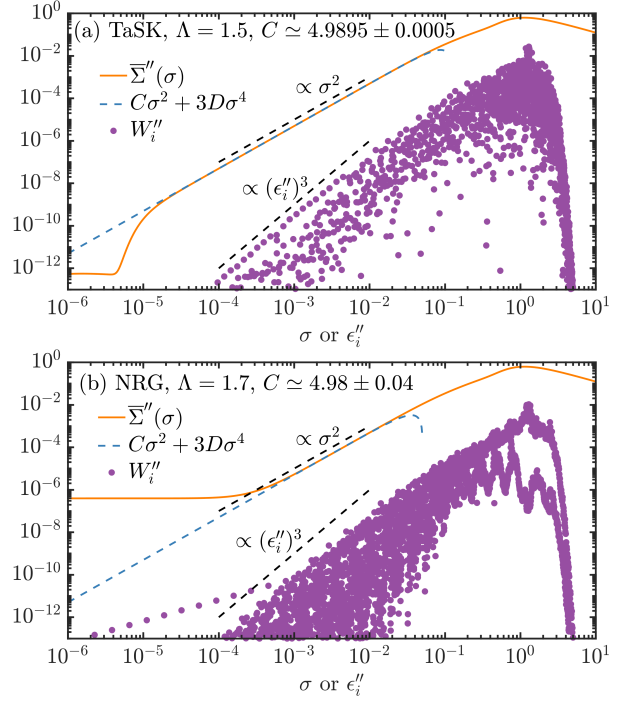


FIG. 1. Discrete self-energy spectrum $\{\epsilon''_i, W''_i\}$ (purple dots) computed for a particle-hole symmetric SIAM with $U = 2$ and logarithmically discretized semicircular hybridization density of states [see Eq. (21)], using (a) TaSK with logarithmic discretization parameter $\Lambda = 1.5$ and (b) NRG with $\Lambda = 1.7$. At small discrete frequencies ϵ''_i , we find $W''_i \propto (\epsilon''_i)^3$. Due to the logarithmic spacing of ϵ''_i , the number of weights in an interval $[\omega - \delta\omega, \omega + \delta\omega]$ (with constant $\delta\omega > 0$) around a small frequency ω is $\propto 1/\omega$. Hence, the total spectral weight in such an interval is $\propto \omega^2$, consistent with Fermi-liquid behavior. The orange line shows $\bar{\Sigma}''(\sigma)$ [see Eq. (25)], the Gaussian-weighted average of the discrete spectrum with varying kernel width σ , and the dashed blue line is a fit to $\bar{\Sigma}''(\sigma)$. For panel (a), the fitting range is $\sigma \in [10^{-4}, 10^{-2}]$, while for panel (b) it is $\sigma \in [10^{-3}, 10^{-2}]$. The coefficient C and its uncertainty are estimated from independent fits of $\bar{\Sigma}''(\sigma)$ over multiple subintervals $\mathcal{I}_n$ of the corresponding fitting range; the quoted values reflect the fit uncertainty together with the spread among these subinterval fits.

is the quasiparticle weight.

Determining the parameters Z and C accurately in the continuum limit is challenging. A well-established method to access low-energy behavior is to logarithmically discretize the bath spectrum with a discretization parameter $\Lambda > 1$ and subsequently map the model to a Wilson chain, see Ref. [31] for details. The discretized impurity model has discrete spectral properties, from which Λ -dependent expansion coefficients Z_{Λ} and C_{Λ} can be extracted with high accuracy. Importantly, this can be done without ever broadening spectral functions, a procedure that

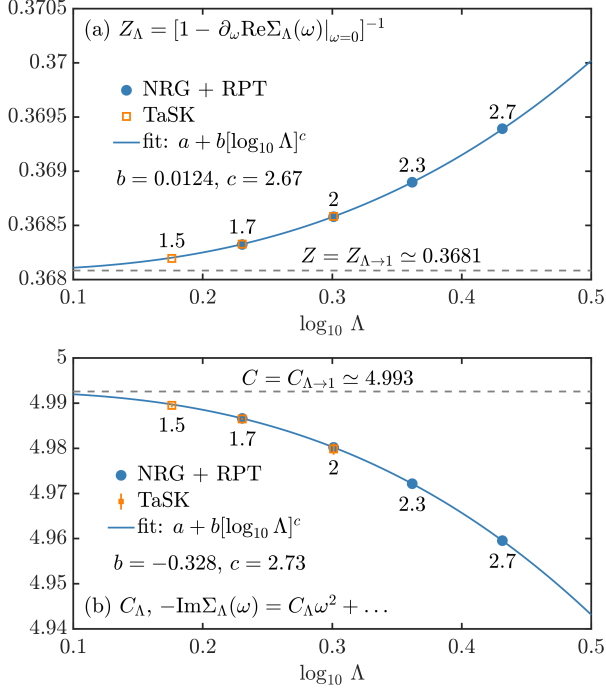


FIG. 2. (a) Quasiparticle weight Z and (b) ω^2 coefficient C of the spectral part of the self-energy for the same SIAM as in Fig. 1. We obtain Z and C either from NRG combined with RPT, or from TaSK via the discrete self-energy spectrum. The hybridization function is logarithmically discretized with discretization parameter $\Lambda > 1$ (indicated next to the symbols), and the true continuous hybridization function is recovered in the $\Lambda \rightarrow 1$ limit. Both Z and C depend on Λ ; their true values are obtained by extrapolating to $\Lambda = 1$. The solid lines show fits to the NRG+RPT data only, while the TaSK data serves as a consistency check at $\Lambda = 2$ and $\Lambda = 1.7$, and as validation of the fit at $\Lambda = 1.5$. TaSK does not rely on energy scale separation and can therefore access lower values of Λ . The error bars of the TaSK results in (b) are estimated from the fitting uncertainty (see text), and are smaller than the symbol size for $\Lambda = 1.7$ and $\Lambda = 1.5$.

introduces additional, somewhat uncontrolled errors. Finally, Z_Λ and C_Λ can be extrapolated to the continuum limit ($\Lambda \rightarrow 1$) in which the discretization error vanishes.

Now, NRG is reliable only for $\Lambda \geq 1.7$, since it relies on energy-scale separation. TaSK, by contrast, does not and hence is reliable also for $\Lambda < 1.7$. However, TaSK only computes states relevant for specific dynamical correlation functions and does not have access to an entire approximate many-body spectrum, as needed for the current formulation of RPT. Therefore, within TaSK, Z and C have to be extracted from explicit dynamical calculations of the self-energy; the details of this extraction are explained below. (That can also be done for NRG self-energies, but the results turn out to be significantly less accurate than those from TaSK.)

Our strategy, therefore, is to compute the Λ -dependent

coefficients C_Λ and Z_Λ for $\Lambda \in \{1.7, 2, 2.3, 2.7\}$ using NRG+RPT, and for $\Lambda \in \{1.5, 1.7, 2\}$ using TaSK with an explicit discrete self-energy calculation. The TaSK results at $\Lambda = 1.7$ and $\Lambda = 2$ serve as a consistency check against NRG+RPT, while $\Lambda = 1.5$ provides us with a new data point that cannot be accessed reliably with NRG. We then extrapolate the Λ -dependent expansion parameters obtained from NRG+RPT to the continuum limit at $\Lambda = 1$ and use the TaSK data at $\Lambda = 1.5$ for validation. This yields a highly accurate estimate for the true parameters in the presence of a continuous bath.

Computational details. Our TaSK code also uses the QSpace tensor library [75–78], allowing us to exploit both SU(2) spin and charge symmetries. Within TaSK, we first compute the ground state of the discretized impurity model using the density matrix renormalization group (DMRG) [80–82] with controlled bond expansion (CBE) [83–85] and mixing [86, 87]. To control the bond dimension, we set a singular-value truncation threshold of $\epsilon_{\text{SVD}} = 10^{-8}$, which results in a numerically exact ground state. At $\Lambda = 1.5$, this leads to a bond dimension of at most $D^* = 198$ multiplets. TaSK then uses the tangent space of this ground state MPS to approximate excited states relevant for dynamical correlation functions [63]. In contrast to NRG, this tangent space approximation does not discard shell-off-diagonal matrix elements, which is why energy-scale separation is not required for TaSK. As explained in Ref. [64], TaSK is initialized with a block of initial states across all energy scales, and 20 block Krylov steps are subsequently performed to compute spectral functions. The resulting discrete self-energy at $\Lambda = 1.5$ is shown in Fig. 1(a); Fig. 1(b) shows a discrete self-energy spectrum computed with NRG at $\Lambda = 1.7$ for comparison.

The quasiparticle weight in Eq. (23) can be readily evaluated for a discrete self-energy,

$$\Sigma(\omega + i0^+) = \Sigma^{\text{HF}} + \sum_i \frac{W_i''}{\omega + i0^+ - \epsilon_i''}, \quad (24a)$$

$$\partial_\omega \text{Re} \Sigma(\omega + i0^+)|_{\omega=0} = - \sum_{\epsilon_i'' \neq 0} \frac{W_i''}{(\epsilon_i'')^2} + \sum_{\epsilon_i''=0} \frac{W_i''}{(0^+)^2}. \quad (24b)$$

If $\sum_{\epsilon_i''=0} W_i'' \neq 0$, the second term in Eq. (24b) diverges, and the quasiparticle weight is zero. To avoid artifacts from tiny spectral weights at small frequencies in our TaSK calculations, we omit spectral weights where both $W_i'' \leq 10^{-14}$ and $|\epsilon_i''| \leq 10^{-14}$. Appendix D discusses an alternative regularization scheme.

To obtain the ω^2 coefficient, we average the self-energy spectrum over a Gaussian kernel of varying width, similar

to the scheme used in Sec. IV.C of Ref. 88,

$$\bar{\Sigma}''(\sigma) = \int_{-\infty}^{\infty} d\omega \pi \Sigma''(\omega) g_{\sigma}(\omega), \quad (25)$$

$$g_{\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}}. \quad (26)$$

At small frequencies, $\pi \Sigma''(\omega) = C\omega^2 + D\omega^4 + \dots$, and, for small width $\sigma \ll 1$, Eq. (25) becomes

$$\bar{\Sigma}''(\sigma) = C\sigma^2 + 3D\sigma^4 + \dots \quad (27)$$

From that, we extract C via a log-scale fit. For this purpose, we choose a fitting interval $\sigma \in \mathcal{I}$ and perform log-scale fits on multiple subintervals $\mathcal{I}_n \subset \mathcal{I}$. We then discard outlying fits based on the resulting values of C and the fit quality, take C to be the median of the remaining fit values, and estimate its uncertainty by combining the individual fit uncertainties with the spread across subintervals.

Figure 1(a), computed for $\Lambda = 1.5$, shows TaSK data for the self-energy spectrum (purple dots), the resulting curve $\bar{\Sigma}''(\sigma)$ (orange), and a fit to it (blue dashed), using the fitting interval $\mathcal{I} = [10^{-4}, 10^{-2}]$. Figure 1(b) shows analogous data, obtained for $\Lambda = 1.7$ using NRG. We use a smaller fit interval $\mathcal{I} = [10^{-3}, 10^{-2}]$ here, since the dynamical data provided by NRG is not as clean as that obtained from TaSK. For TaSK at $\Lambda = 1.5$, we estimate a relative uncertainty of 0.01%, while the fit to the NRG data has a much larger uncertainty of 0.9%. We have checked that the result obtained from fitting dynamical NRG data differs by 0.14% from the corresponding RPT result, confirming a reasonable albeit possibly somewhat conservative error estimate. An error of 0.9% is more than an order of magnitude too large for the accuracy requirements of our extraction of Z_{Λ} and C_{Λ} [the error bars would exceed the axis limits of Fig. 2(b)]; the dynamical data used for that purpose was therefore based only on TaSK, not on NRG.

The Λ -dependent quasiparticle weight and ω^2 coefficients, fitted either from dynamical TaSK data or obtained through NRG+RPT, are shown in Fig. 2(a) and (b), respectively. For $\Lambda = 1.7$ and $\Lambda = 2$, we performed both NRG+RPT and TaSK computations and find excellent agreement. We empirically find that both Z_{Λ} and C_{Λ} follow a power law in terms of $\log \Lambda$, which we use to extrapolate to $\Lambda \rightarrow 1$ (continuum limit) by fitting the NRG+RPT data. We then validate the extrapolation using the $\Lambda = 1.5$ TaSK result and find excellent agreement: the relative difference between the extrapolated and TaSK results at $\Lambda = 1.5$ is 0.002% for Z and 0.004% for C . The resulting extrapolated quasiparticle weight Z and ω^2 coefficient C are highly accurate estimates.

D. Discrete dynamical mean-field theory

In this section, we take our scheme a step further and employ the discrete representation of self-energy Eq. (10) to construct a fully discrete DMFT self-consistency cycle, i.e., without introducing any artificial broadening. Two slightly different implementations of a DMFT(ED) code with restricted Hilbert space, QUANTY and RAS_DMFT.jl, are employed, see Sec. IV D 2 for computational details.

We validate this approach on the half-filled Hubbard model on the infinite-dimensional Bethe lattice with nearest-neighbor hopping. This model has a semicircular density of states,

$$\rho(\epsilon) = \theta(D - |\epsilon|) \frac{2}{\pi D^2} \sqrt{D^2 - \epsilon^2}, \quad (28)$$

where D is the half bandwidth. We choose H_0 to contain only the hopping terms (no chemical potential or on-site energies) and

$$H_1 = U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}). \quad (29)$$

The effective impurity model that arises when solving this model with DMFT is a SIAM with a self-consistently adjusted hybridization function and an interaction as in Eq. (20). With this choice of H_1 ,

$$q_{\sigma} = U a_{0\sigma}(n_{\bar{\sigma}} - \frac{1}{2}), \quad (30a)$$

$$\tilde{S}_{\sigma} = \text{diag}(1, \langle \{q_{\sigma}^{\dagger}, q_{\sigma}\} \rangle) = \text{diag}(1, U^2/4), \quad (30b)$$

where $\bar{\sigma}$ is the spin projection opposite to σ and $n_{\sigma} = a_{0\sigma}^{\dagger} a_{0\sigma}$.

We first confirm that the self-consistency cycle converges to the correct fixed-point solution by comparing the double occupation $\langle n_{\uparrow} n_{\downarrow} \rangle$ against reference conventional NRG data with a continuous (broadened) DMFT self-energy. We then test the accuracy of $\Sigma(z)$ directly through the quasiparticle weight Z . We proceed to examine the pole structure of $\Sigma(z)$ in the metallic and insulating phases, where an isolated pole in the insulating gap provides a stringent check via its analytically constrained residue [4]. Finally, we verify that the discrete representation satisfies known sum rules for the moments of $\Sigma(z)$, improving on earlier work [26] by several orders of magnitude.

For the implementation of discrete DMFT, the impurity problem needs to be updated using the discrete self-energy $\Sigma(z)$, either via the bath Green's function $\mathcal{G}(z)$ or the hybridization function $\Delta(z)$. In this work, we employ the procedure proposed in Ref. [26]. The hybridization function is updated as

$$\Delta^{\text{eff}}(z) = \Delta(z I_N - \Sigma(z)) = \sum_{i=1}^M V_i^{\dagger} \frac{1}{z - E_i - \Sigma(z)} V_i. \quad (31)$$

The resulting $\Delta^{\text{eff}}(z)$ is then transformed to the form of Eq. (6) with a subsequent reduction of the number of

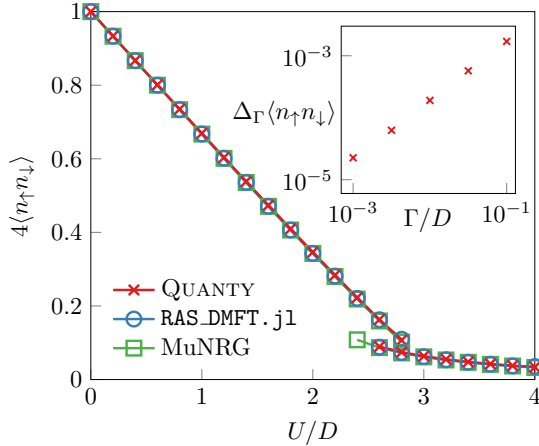


FIG. 3. Double occupation $\langle n_{\uparrow}n_{\downarrow} \rangle$ as a function of interaction strength U/D for the half-filled Hubbard model on the Bethe lattice. Results obtained using discrete DMFT with QUANTY and RAS_DMFT.jl are compared to conventional NRG data calculated with MuNRG. The inset shows the absolute deviation $\Delta_{\Gamma}\langle n_{\uparrow}n_{\downarrow} \rangle = |\langle n_{\uparrow}n_{\downarrow} \rangle(\Gamma) - \langle n_{\uparrow}n_{\downarrow} \rangle(\text{discrete})|$ at $U/D = 2$ as a function of the Lorentzian broadening Γ (full width at half maximum) calculated with QUANTY.

poles. For completeness, we discuss this construction in more detail in Appendix C.

1. Numerical results

We begin by asking whether the discrete self-consistency cycle converges to the same fixed point solution as conventional NRG. To test this, in Fig. 3 we show the double occupation $\langle n_{\uparrow}n_{\downarrow} \rangle$ as a function of U/D . The good agreement between QUANTY, RAS_DMFT.jl, and reference NRG data in Fig. 3 indicates that all approaches converge to similar fixed-point solutions of the DMFT self-consistency cycle. This supports the reliability of the discrete DMFT approach based on a discrete self-energy $\Sigma(z)$ introduced in Sec. III. We note that with the present parameter set, QUANTY and RAS_DMFT.jl could not converge to the metastable insulating solution at $U/D = 2.4$, in contrast to MuNRG.

The inset of Fig. 3 shows the effect of spectral broadening on the double occupation $\langle n_{\uparrow}n_{\downarrow} \rangle$. For $\Gamma > 0$, the self-energy is computed using Eq. (10) with $z = \omega + i\Gamma/2$, corresponding to Lorentzian broadening with full width at half maximum Γ . The broadening enters only through the calculation of $\Sigma(z)$, and thus affects the DMFT self-consistency, but does not enter the evaluation of $\langle n_{\uparrow}n_{\downarrow} \rangle$ directly. As Γ decreases, the double occupation converges to the discrete DMFT result, which validates our scheme as a proper $\Gamma \rightarrow 0$ limit.

Next, in Fig. 4, we show the quasiparticle weight Z calculated from Eq. (23). For QUANTY and

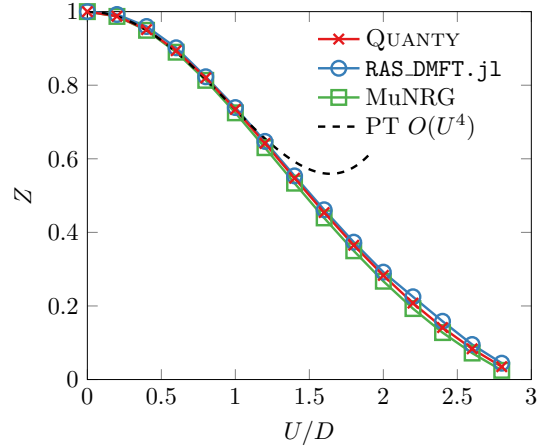


FIG. 4. Quasiparticle weight Z as a function of interaction strength U/D . Results from discrete DMFT (QUANTY and RAS_DMFT.jl) are compared with conventional NRG reference data. For small values of U , we also compare against fourth-order perturbation theory (PT) (Eq. (113) of Ref. [89]).

RAS_DMFT.jl the quasiparticle weight Z was extracted from the discrete representation of the self-energy using Eq. (24b). To deal with spurious poles at low energies, a regularization parameter $\lambda/D = 10^{-2}$ was used (See Appendix D for details). For MuNRG, Z was obtained with NRG+RPT, as described in Sec. IV B, after DMFT self-consistency was reached.

A minor discrepancy between the discrete DMFT solvers (QUANTY and RAS_DMFT.jl) and the MuNRG data in Fig. 4 may be attributed to finite discretization and truncated Hilbert space used in the former. Let us emphasize that this is a limitation of the impurity solver, rather than the approach of discrete DMFT or discrete self-energy. Systematic error introduced by finite broadening [90] in MuNRG calculations may be another source of discrepancy. However, note the excellent agreement between MuNRG and fourth-order perturbation theory at low interaction strengths U . An implementation of a similar discrete DMFT scheme in MuNRG is planned for the future.

In Fig. 5, we show the discrete residues of the self-energy for the metallic (a) and insulating (b) solutions. Small discrepancies in the positions or residues of individual self-energy poles between the two codes are not problematic. Since the total spectral weight $\sum_i W_i^{\Sigma} = S_0^{\Sigma}$ is fixed, the individual residues depend on the number of poles in the discrete representation: fewer poles necessarily imply larger residues. Consequently, multiple discrete representations can correspond to the same continuous self-energy once an appropriate broadening is applied. To illustrate this, the insets show the broadened self-energy, obtained by convolving the discrete poles with a Gaussian. After broadening, the overall shape of the self-energy $\Sigma(z)$ from the two codes is in very good

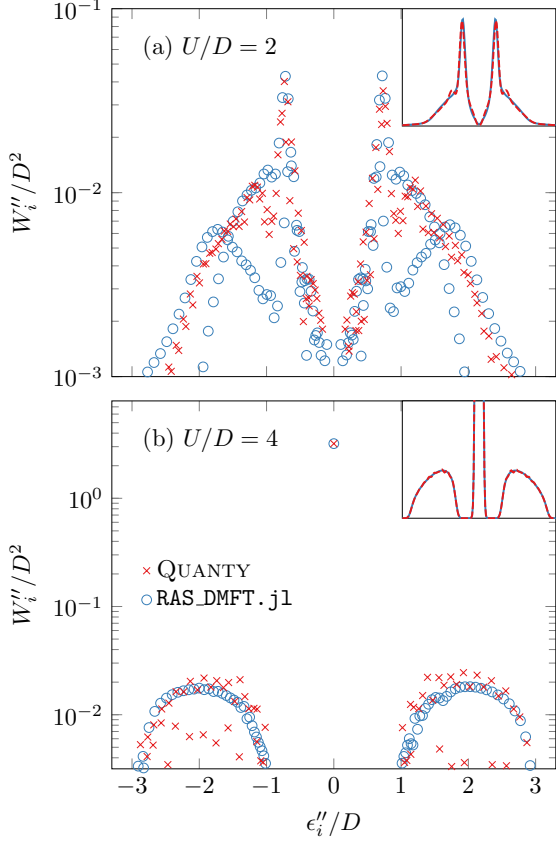


FIG. 5. Discrete self-energy spectrum $\{\epsilon''_i, W''_i\}$ for (a) a metallic solution ($U/D = 2$) and (b) an insulating solution ($U/D = 4$). In the metallic case, $\Sigma(\omega)$ exhibits no poles at $\omega = 0$, keeping the height of the Kondo peak unchanged at zero temperature, while in the insulating case, the self-energy exhibits a single pole inside the insulating gap, located at $\omega = 0$. The residue of this pole is related to the negative second moment of the Green's function [see Eq. (32)] and shows excellent agreement between the two codes. Particle-hole symmetry was not enforced, demonstrating the numerical stability of the solution. The insets show the respective self-energy convolved with a Gaussian with standard deviation $\sigma/D = 0.08$.

agreement. Minor discrepancies at high energies in the insets can be attributed to differences in computational parameters.

For the metallic case [Fig. 5(a)], the self-energy is expected to follow a Fermi-liquid behavior in the continuous limit, $-\text{Im} \Sigma(\omega) \propto \omega^2$. The discrete residues, however, need not reflect this behavior directly: several nearly degenerate poles may be represented by a single pole with larger residue. There is, however, one special pole whose residue is constrained: the isolated pole within the insulating gap in Fig. 5(b). Its residue w_0

satisfies the relation (see Eq. (237) of Ref. [4])

$$w_0^{-1} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\text{Im} G(\omega + i0^+)}{\omega^2}. \quad (32)$$

We find excellent agreement for the residue of this pole between the two implementations. Apart from this pole, the self-energy is purely real within the insulating gap.

To demonstrate numerical stability, particle-hole symmetry was not enforced, i.e. $G^>(\omega)$ and $G^<(\omega)$ were computed independently. Although the resulting pole structure is only approximately symmetric, these small asymmetries are not significant. Upon broadening, the self-energy becomes clearly particle-hole symmetric, as evident from the insets of Fig. 5 and Table I.

Finally, in Table I, we compare numerical and analytical moments of the Green's function and the self-energy. We define the n -th moment $S_n^{(C)}$ of a generic correlation function $C(z)$ as

$$S_n^{(C)} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \omega^n \text{Im} C(\omega + i0^+). \quad (33)$$

For the half-filled Bethe lattice, the first moments of the Green's function and the self-energy are [91]

$$S_0^{(G)} = 1, \quad S_2^{(G)} = \frac{U^2}{4} + \frac{D^2}{4}, \quad (34a)$$

$$\Sigma^{\text{HF}} = 0, \quad S_0^{(\Sigma)} = \frac{U^2}{4}, \quad (34b)$$

with every odd moment vanishing due to particle-hole symmetry. The Hartree-Fock term Σ^{HF} is zero with H_1 defined in Eq. (29).

Compared to Ref. [26], where the self-energy was calculated using Eq. (1) (instead of Eq. (13), which is used in this work), we observe an improvement of several orders of magnitude in the accuracy of the zeroth moment of the self-energy $S_0^{(\Sigma)}$, reaching near machine precision. This improvement can be understood from the fact that $S_0^{(\Sigma)}$ is directly given by $\tilde{S}$, the zeroth moment of the matrix-valued propagator $\tilde{G}(z)$ [see Eq. (14)]. The norm of self-energy $S_0^{(\Sigma)}$ is therefore expected to be extremely accurate in sum-rule conserving impurity solvers.

2. Computational Details

For calculations performed with RAS_DMFT.jl, the first two conduction and valence bath sites are kept fully unrestricted. In the remaining conduction and valence chains, up to either a single valence-conduction excitation or up to two of valence-impurity or conduction-impurity excitations are allowed. This corresponds to $L = 2$, $p = 2$ in notation used in Ref. [28]. The hybridization function was discretized on a linear grid, resulting in around $N_b = 300$ bath sites. The electron addition and removal Green's function $G^<(z)$ and $G^>(z)$ were

TABLE I. Moments of the Green's function and self-energy for the half-filled Bethe lattice. For non-zero analytical moments we report the relative error $\delta S = |S - S_{\text{analytical}}|/S_{\text{analytical}}$, while for moments that vanish due to particle-hole symmetry the numerical value is shown directly.

U/D	Code	$\delta S_0^{(G)}$	$\delta S_2^{(G)}$	$\delta S_0^{(\Sigma)}$
2	QUANTY	2.2×10^{-16}	2.7×10^{-7}	6.6×10^{-14}
2	RAS_DMFT.jl	1.1×10^{-15}	1.2×10^{-8}	1.3×10^{-14}
4	QUANTY	4.4×10^{-16}	1.5×10^{-7}	4.2×10^{-15}
4	RAS_DMFT.jl	6.7×10^{-16}	1.4×10^{-10}	3.2×10^{-15}
Vanishing moments (analytical value = 0)				
U/D	Code	Σ^{HF}/D	$S_1^{(G)}/D$	$S_1^{(\Sigma)}/D^3$
2	QUANTY	2.4×10^{-7}	2.4×10^{-7}	-9.2×10^{-7}
2	RAS_DMFT.jl	5.3×10^{-8}	5.3×10^{-8}	-1.8×10^{-7}
4	QUANTY	-3.7×10^{-9}	-3.7×10^{-9}	1.3×10^{-8}
4	RAS_DMFT.jl	1.0×10^{-8}	-2.0×10^{-8}	6.5×10^{-8}

calculated independently (i.e. particle-hole symmetry was not enforced), with 200 Krylov states calculated at each DMFT iteration.

For calculations using QUANTY, two different parameter sets were employed: For Figs. 3 and 4, the bath was discretized on a logarithmic grid, resulting in around $N_b = 40$ bath sites. Only the first sites of valence and conduction chains are kept unrestricted ($L = 1$), while allowing for up to two of any: valence-impurity, conduction-impurity, valence-conduction excitations. This is a larger subspace than $p = 2$ used in RAS_DMFT.jl, since $p = 2$ allows only a single valence-conduction excitation. $G^>(z)$ was calculated using 50 states in the Krylov subspace and $G^<(z)$ was set equal to $G^>(z)$, enforcing particle-hole symmetry.

For Fig. 5 and Table I, the bath was discretized on a linear grid, resulting in around $N_b = 250$ bath sites. The configuration space was reduced, allowing for only one of the valence-impurity, conduction-impurity or valence-conduction excitations. $G^>(z)$ and $G^<(z)$ were computed independently, with 150 states in the Krylov subspace. This set of parameters provides improved high-energy resolution and greater number of poles in the self-energy, which is beneficial for visualization in Fig. 5.

The data for $\Gamma > 0$ shown in the inset of Fig. 3 were obtained by broadening the four components of $\tilde{G}(z)$ with a Lorentzian kernel on a linear frequency grid of 50001 points. The continuous self-energy is calculated via Eq. (10) and discretized afterward. The hybridization function is then updated via Eq. (31).

V. CONCLUSION

We showed that Kugler's symmetric self-energy estimator [51] $\Sigma(z)$, can be computed by downfolding an augmented matrix-valued propagator $\tilde{G}(z)$, i.e., by inverting, projecting, and re-inverting it. These operations can be carried out using numerically stable matrix manipulations on a discrete spectral representation of $\tilde{G}(z)$, yielding a discrete spectral representation of $\Sigma(z)$. This construction avoids the systematic errors that arise in direct Dyson subtraction. In contrast to the Dyson equation, whose formal correctness does not prevent numerical loss of accuracy in floating-point arithmetic, the present method preserves causality and proper normalization also at the numerical level. Further, Kugler's symmetric self-energy estimator can be extended to irreducible cumulants of Hubbard operators, as explained in Sec. IX A of the Supplemental Material of Ref. [92]. Our results also apply to this case.

We discussed two prominent zero-temperature applications of the discrete self-energy: the determination of low-energy properties of the single-impurity Anderson model and the implementation of the DMFT self-consistency cycle using only DSRs. In the former case, we accurately determine the ω^2 coefficient C of $\text{Im}\Sigma(\omega^+)$ and the quasiparticle weight Z for the continuous-bath limit. In the latter, we demonstrate the reliability of the discrete DMFT approach by computing the double occupancy $\langle n_{\uparrow}n_{\downarrow} \rangle$, the quasiparticle weight Z , and the first moments of the self-energy on the $d \rightarrow \infty$ Bethe lattice, all of which are in very good agreement with reference NRG data and analytical results.

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Appendix A: Discrete representations of response functions as implemented in `Quanty` and `RAS_DMFT.jl`

When manipulating response functions (e.g. Green's function $G(z)$, hybridization function $\Delta(z)$, or self-energy $\Sigma(z)$) it is often convenient to switch between different discrete representations. In this appendix we summarize the relevant transformations as implemented in `QUANTY` and `RAS_DMFT.jl` below, following the work of Löwdin and others [25, 26, 52–59].

In the following, we assume that response functions are represented by $N \times N$ matrices as functions of the complex variable z . There are several ways to represent these functions on a discrete grid. One common method, which is also used throughout the manuscript, is the pole expansion, which we refer to as the list-of-poles representation (Appendix A 1):

$$G(z) = A_0 + \sum_{i=1}^M B_i \frac{1}{z - \alpha_i} B_i,$$

Besides a pole expansion, other possible discrete representations of response function include a tridiagonal (continued fraction or chain) representation (Appendix A 2)

$$G(z) = \mathcal{A}_0 + \mathcal{B}_0 \frac{1}{z - \mathcal{A}_1 - \mathcal{B}_1 \frac{1}{z - \mathcal{A}_2 - \dots} \mathcal{B}_1} \mathcal{B}_0,$$

Anderson (star) representation (Appendix A 3)

$$G(z) = \mathbf{A}_0 + \mathbf{B}_0 \frac{1}{z - \mathbf{A}_1 - \sum_{i=1}^{M'} \mathbf{B}_i \frac{1}{z - \mathbf{a}_{i+1}} \mathbf{B}_i} \mathbf{B}_0,$$

as well as a mix of chain and star representations, such as the natural-impurity-orbital representation [26], which is central to the natural-orbital impurity solver [28].

To limit the number of symbols with similar roles, we distinguish the different submatrices $\mathcal{A}_i$ and B_i by font style; in particular, $\mathcal{A}_i$ and $\mathcal{B}_i$ denote submatrices used in tridiagonal representations, whereas $\mathbf{A}_i$ and $\mathbf{B}_i$ denote submatrices used in Anderson representations.

For brevity, we write the formulas in terms of Green's functions $G(z)$, but the same notation also applies to generic response functions, including effective Hamiltonians $H_{\text{eff}}(z)$ and self-energies $\Sigma(z)$. For this reason, we also explicitly include $A_0 = \mathcal{A}_0 = \mathbf{A}_0$, which is zero for physical Green's functions, but may be non-zero for the self-energy $\Sigma(z)$.

1. List-of-poles representation

We can represent response functions on a discrete set of energies $\alpha_i \in \mathbb{R}$, with $i \in \{1, \dots, M\}$, which may be viewed both as pole positions and as points of an energy mesh:

$$G(z) = A_0 + \sum_{i=1}^M \frac{W_i}{z - \alpha_i}, \quad (\text{A1})$$

with positive semidefinite, Hermitian spectral weight matrices W_i . Those may be decomposed as

$$W_i = B_i B_i, \quad (\text{A2})$$

where we choose B_i to be the Hermitian principal square root of W_i , i.e., $B_i = B_i^\dagger$. This yields a unique factorization that preserves, when present, the symmetry-imposed block structure of W_i . Moreover, storing and manipulating B_i instead of W_i ensures that $W_i = B_i^\dagger B_i$ remains Hermitian and positive semidefinite by construction, even in the presence of numerical noise.

a. Symmetric eigenbasis representation

Throughout this work, we represent pole expansions of response functions in a symmetric form, i.e. with Hermitian couplings $B_i = B_i^\dagger$, and in the eigenbasis of each pole term, i.e. such that the pole energy is the same for all spin-orbitals within a given term of the pole expansion. In other words, we use Eq. (A1) rather than the seemingly more general form

$$G(z) = A'_0 + \sum_{j=1}^{M'} B_j'^\dagger \frac{1}{z - A'_j} B'_j, \quad (\text{A3})$$

where A'_j is a general Hermitian matrix and B'_j is a general complex matrix. The pole expansion in Eq. (A3) can always be rewritten in the more symmetric form of Eq. (A1), which is advantageous for numerical stability with guaranteed causality and for the construction of discretization.

To transform Eq. (A3) into the symmetric eigenbasis representation of Eq. (A1), we first diagonalize the matrix A'_j . Let U_j contain the eigenvectors of A'_j in its columns, and let α_{jm} denote the corresponding m -th eigenvalue, such that

$$U_j^\dagger A'_j U_j = \text{diag}(\alpha_{j1}, \dots, \alpha_{jN}). \quad (\text{A4})$$

We then insert the identity, $U_j U_j^\dagger$ twice, into Eq. (A3), which yields

$$\begin{aligned} G(z) &= A'_0 + \sum_{j=1}^{M'} B_j'^\dagger \frac{1}{z - U_j U_j^\dagger A'_j U_j U_j^\dagger} B'_j \\ &= A'_0 + \sum_{j=1}^{M'} B_j'^\dagger \frac{1}{U_j (z - \text{diag}(\alpha_{j1}, \dots, \alpha_{jN})) U_j^\dagger} B'_j. \end{aligned} \quad (\text{A5})$$

We now use that $(U(z - H)U^\dagger)^{-1} = (U^\dagger)^{-1} (z - H)^{-1} \times U^{-1} = U(z - H)^{-1}U^\dagger$ and find

$$G(z) = A'_0 + \sum_{j=1}^{M'} B_j'^\dagger U_j \frac{1}{z - \text{diag}(\alpha_{j1}, \dots, \alpha_{jN})} U_j^\dagger B'_j. \quad (\text{A6})$$

We can split the single term for each j into N terms, corresponding to poles at the eigenvalues $\alpha_{j\mathbf{m}}$. The spectral weight at the pole $z = \alpha_{j\mathbf{m}}$ is then the outer product of the row vectors

$$W_{j\mathbf{m}} = \left(\left(U_j^\dagger B_j' \right)_{\mathbf{m}} \right)^\dagger \left(\left(U_j^\dagger B_j' \right)_{\mathbf{m}} \right), \quad (\text{A7})$$

and the corresponding coupling matrix is

$$B_{j\mathbf{m}} = W_{j\mathbf{m}}^{1/2}. \quad (\text{A8})$$

Thus, the symmetric pole expansion of $G(z)$ in its eigenbasis becomes

$$G(z) = A'_0 + \sum_{j=1}^{M'} \sum_{\mathbf{m}=1}^N B_{j\mathbf{m}} \frac{1}{z - \alpha_{j\mathbf{m}}} B_{j\mathbf{m}}. \quad (\text{A9})$$

Finally, one may combine the sums over j and $\mathbf{m}$ into a single sum over i , with $i = 1, \dots, M = M'N$, to recover the form of Eq. (A1). Note that one can combine two poles at the same energy $\alpha_i = \alpha_j$ by summing their spectral weights W_i and W_j . A general method to reduce the number of poles can be found in Appendix F of Ref. [26].

2. Tridiagonal (chain-impurity) representation

Instead of representing a discretized Green's function as a sum over poles and residues, we may represent it as the Green's function of a local site coupled to a one-dimensional chain of bath sites. This yields a matrix-valued continued-fraction representation,

$$G(z) = \mathcal{A}_0 + \mathcal{B}_0 \frac{1}{z - \mathcal{A}_1 - \mathcal{B}_1 \frac{1}{z - \mathcal{A}_2 - \dots}} \mathcal{B}_1, \quad (\text{A10})$$

where $\mathcal{A}_i, \mathcal{B}_i \in \mathbb{C}^{N \times N}$ are Hermitian matrices, and the chain has length M .

Equivalently, $G(z)$ can be written as the upper-left $N \times N$ block of the resolvent of a block-tridiagonal Hamiltonian $H_t \in \mathbb{C}^{NM \times NM}$,

$$G(z) = \mathcal{A}_0 + \mathcal{B}_0 \left(\frac{1}{z - H_t} \right)_{1:N, 1:N} \mathcal{B}_0, \quad (\text{A11})$$

with

$$H_t = \begin{pmatrix} \mathcal{A}_1 & \mathcal{B}_1 & 0 & \cdots & 0 \\ \mathcal{B}_1 & \mathcal{A}_2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \mathcal{A}_{M-1} & \mathcal{B}_{M-1} \\ 0 & \cdots & 0 & \mathcal{B}_{M-1} & \mathcal{A}_M \end{pmatrix}. \quad (\text{A12})$$

This representation has a natural interpretation as a non-interacting tight-binding chain. Writing the corresponding second-quantized Hamiltonian as

$$H_t = \sum_{i=1}^M a_i^\dagger \mathcal{A}_i a_i + \sum_{i=1}^{M-1} a_i^\dagger \mathcal{B}_i a_{i+1} + a_{i+1}^\dagger \mathcal{B}_i a_i, \quad (\text{A13})$$

using the compact vector notation from Eq. (2) to suppress the summation over the local spin-orbital indices $\mathbf{m}$, we can express $G(z)$ as the local Green's function at the endpoint ($i = 1$) of the one-dimensional chain,

$$G(z)_{\mathbf{m}, \mathbf{m}'} = \left\langle 0 \left| a_{\mathbf{m}, i=1} \frac{1}{z - H_t} a_{\mathbf{m}', i=1}^\dagger \right| 0 \right\rangle. \quad (\text{A14})$$

The tridiagonal representation of $G(z)$ therefore maps the original problem onto a non-interacting one-dimensional tight-binding chain of length M , with the probed site located at one end.

a. Construction from the list-of-poles representation. The matrices $\mathcal{A}_i$ and $\mathcal{B}_i$ can be obtained from the list-of-poles representation. For the constant term, we have

$$\mathcal{A}_0 = A_0. \quad (\text{A15})$$

In order to find the other block matrices we define the block-vector $V \in \mathbb{C}^{NM \times N}$ as

$$V = \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_M \end{pmatrix}, \quad (\text{A16})$$

where the $B_i \in \mathbb{C}^{N \times N}$ are the principal square roots of the residues in Eq. (A1). As the column vectors of V are not orthonormal for general response functions, we define the overlap matrix $S \in \mathbb{C}^{N \times N}$

$$S = V^\dagger V = \sum_{i=1}^M B_i B_i = \sum_{i=1}^M W_i, \quad (\text{A17})$$

with W_i defined in Eq. (A2). This allows us to write

$$\begin{aligned} R_a &= V S^{-1/2}, \\ \mathcal{B}_0 &= S^{1/2}, \end{aligned} \quad (\text{A18})$$

with $R_a^\dagger R_a = I_N$.

We further define the diagonal matrix

$$H_{\text{LP}} = \text{diag}(\alpha_1 I_N, \alpha_2 I_N, \dots, \alpha_M I_N) \in \mathbb{R}^{NM \times NM}, \quad (\text{A19})$$

where α_i are the pole energies from Eq. (A1).

Applying a block-Lanczos tridiagonalization to H_{LP} with starting block $V_0 = R_a$ yields the block-tridiagonal

matrix H_t of Eq. (A12), from which the matrices $\mathcal{A}_i$ and $\mathcal{B}_i$ can be read off. Standard block- or band-Lanczos implementations often produce a banded form with minimal bandwidth, in which $\mathcal{B}_i$ is block upper or lower triangular and therefore not Hermitian. It is important to keep $\mathcal{B}_i$ Hermitian in order to preserve symmetric couplings between the bath sites. In the next paragraph we discuss Löwdin symmetric tridiagonalization, which can be used to ensure Hermiticity of $\mathcal{B}_i$.

b. Löwdin symmetric tridiagonalization using block Lanczos. We can determine H_t using a block-Lanczos algorithm. Given an effective Hamiltonian $H_{\text{eff}} \in \mathbb{C}^{NM \times NM}$ and an orthonormal block vector $V_i \in \mathbb{C}^{NM \times N}$, whose columns contain the N orthonormal Krylov states of block i , we construct the Hermitian matrices $\mathcal{A}_i, \mathcal{B}_i \in \mathbb{C}^{N \times N}$, as well as the next set of Krylov states $V_{i+1} \in \mathbb{C}^{NM \times N}$, as follows.

We first define the block vector

$$\bar{V}_{i+1} = H_{\text{eff}} V_i. \quad (\text{A20})$$

From $\bar{V}_{i+1}$, we obtain $\mathcal{A}_i$ as

$$\mathcal{A}_i = V_i^\dagger \bar{V}_{i+1}. \quad (\text{A21})$$

Next, we orthogonalize the N vectors in $\bar{V}_{i+1}$ against all previously determined Krylov states,

$$\bar{\bar{V}}_{i+1} = \bar{V}_{i+1} - V_i(V_i^\dagger \bar{V}_{i+1}) - V_{i-1}(V_{i-1}^\dagger \bar{V}_{i+1}). \quad (\text{A22})$$

The orthogonalization against V_{i-2} , V_{i-3} , and earlier states is not necessary, as $\bar{V}_{i+1}$ is already orthogonal against those states by construction.

At this point the N column vectors inside $\bar{\bar{V}}_{i+1}$ are orthogonal to all column vectors inside V_j of blocks $j \in \{1, 2, \dots, i\}$: $V_j^\dagger \bar{\bar{V}}_{i+1} = 0_N$, but not necessarily to each other: $\bar{\bar{V}}_{i+1}^\dagger \bar{\bar{V}}_{i+1} \neq I_N$.

We now need to orthonormalize $\bar{\bar{V}}_{i+1}$ symmetrically. To this end, we define the overlap matrix.

$$\bar{\bar{S}}_{i+1} = \bar{\bar{V}}_{i+1}^\dagger \bar{\bar{V}}_{i+1}, \quad (\text{A23})$$

and obtain the orthonormal Krylov states as

$$V_{i+1} = \bar{\bar{V}}_{i+1} \bar{\bar{S}}_{i+1}^{-1/2}. \quad (\text{A24})$$

Finally, we compute $\mathcal{B}_i$ as

$$\mathcal{B}_i = \bar{\bar{S}}_{i+1}^{-1/2}. \quad (\text{A25})$$

Note that Eq. (A24) requires the inverse square root of the overlap matrix. This is not possible if $\bar{\bar{S}}_{i+1}$ is singular. In that case, some form of deflation [93] must be implemented. One may obtain V_{i+1} from $\bar{\bar{V}}_{i+1}$ by performing a singular value decomposition of the column matrix $\bar{\bar{V}}_{i+1}$ and discarding states whose singular values fall below a chosen numerical threshold.

3. Anderson (star-impurity) representation

In the Anderson (or star) representation, the bath degrees of freedom are diagonalized. The Green's function then takes the form

$$G(z) = \mathbf{A}_0 + \mathbf{B}_0 \frac{1}{z - \mathbf{A}_1 - \sum_{i=1}^{M'} \mathbf{B}_i \frac{1}{z - \mathbf{a}_{i+1}} \mathbf{B}_i} \mathbf{B}_0, \quad (\text{A26})$$

with the impurity at site index 1 and the bath sites at indices 2 to $M' + 1$.

Note that the number of bath sites and their internal dimensions are, to some extent, a matter of representation. We allow bath sites that do not couple to the impurity in order to keep the internal dimension of each bath site equal to N . This increases the number of bath sites to at most $M' = N(M - 1)$ for a $N \times N$ matrix valued Green's function with M poles. Keeping the bath dimension fixed can be useful in multi-spin-orbital situations with symmetry. By representing $\mathbf{B}_i$ as a Hermitian matrix, different spin-orbital states that belong to the same multidimensional irreducible representation have no coupling between them. This is important to conserve numerically the symmetry of the system. At the same time spin-orbitals belonging to different irreducible representations may couple to bath states at different energies, thereby making the rank of $\mathbf{B}_i$ smaller than N . If the numerical storage of the additional zeros is a concern one can transform the spin-orbital basis of the Green's function to symmetric states, e.g., using a spherical tensor coupling and only store the irreducible elements [94]. The symmetric representation on the eigenbasis of the bath is also useful when one wants to reduce the number of bath sites. Since the denominator in the Anderson representation is itself a Green's function represented as a list of poles, one may reduce the number of poles by discretizing this function on a newly chosen grid, as described in Appendix F of Ref. [26].

We choose the hybridization between the impurity and the bath level at energy $\mathbf{a}_{i+1}$ to be described by a Hermitian matrix $\mathbf{B}_i$. Since each bath site of dimension N has all spin-orbitals at the same energy, we may apply a unitary rotation within that bath site, which allows us to choose $\mathbf{B}_i$ Hermitian. See Appendix A 1 a for how the symmetric eigenbasis representation of the bath hybridization can be obtained from a general non-symmetric representation.

a. Resolvent form. We can write $G(z)$ in Anderson form as the upper-left $N \times N$ block of the resolvent of a matrix $H_A \in \mathbb{C}^{N(M'+1) \times N(M'+1)}$,

$$G(z) = \mathbf{A}_0 + \mathbf{B}_0 \left(\frac{1}{z - H_A} \right)_{1:N, 1:N} \mathbf{B}_0, \quad (\text{A27})$$

where H_A is a sparse matrix with the following block structure,

$$H_A = \begin{pmatrix} \mathbf{A}_1 & \mathbf{B}_1 & \cdots & \mathbf{B}_{M'} \\ \mathbf{B}_1 & \mathbf{a}_2 I_N & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{B}_{M'} & 0 & \cdots & \mathbf{a}_{M'+1} I_N \end{pmatrix}. \quad (\text{A28})$$

b. Tight-binding interpretation. The matrix H_A in Eq. (A28) can be interpreted as the one-particle representation of a non-interacting tight-binding Hamiltonian with one impurity site and M' bath sites. A convenient second-quantized form is

$$H_A = a_{i=1}^\dagger \mathbf{A}_1 a_{i=1} + \sum_{i=2}^{M'+1} \mathbf{a}_i a_i^\dagger a_i \quad (\text{A29})$$

$$+ \sum_{i=2}^{M'+1} a_{i=1}^\dagger \mathbf{B}_{i-1} a_i + a_i^\dagger \mathbf{B}_{i-1} a_{i=1},$$

using the compact vector notation from Eq. (2) to suppress the summation over the local spin-orbital indices $\mathbf{m}$. The impurity Green's function for this Hamiltonian is

$$G(z)_{\mathbf{m},\mathbf{m}'} = \left\langle 0 \left| a_{\mathbf{m},i=1} \frac{1}{z - H_A} a_{\mathbf{m}',i=1}^\dagger \right| 0 \right\rangle. \quad (\text{A30})$$

c. Construction from the tridiagonal representation. We can construct an Anderson block representation from a tridiagonal block representation. The blocks $\mathbf{A}_0$ and $\mathbf{B}_0$ are the same in the Anderson representation as in the tridiagonal representation,

$$\mathbf{A}_0 = \mathcal{A}_0, \quad \mathbf{B}_0 = \mathcal{B}_0. \quad (\text{A31})$$

To obtain the remaining bath parameters, we start from the tridiagonal representation, i.e. from H_t [Eq. (A12)]. We construct a unitary matrix $U \in \mathbb{C}^{NM \times NM}$ such that its upper-left $N \times N$ block is equal to I_N , while the remaining $N(M-1) \times N(M-1)$ block consists of the eigenvectors, written in column order, of the lower $N(M-1) \times N(M-1)$ block of H_t . This transformation diagonalizes the bath subspace and yields

$$U^\dagger H_t U = \begin{pmatrix} \mathbf{A}_1 & \mathbf{b}_1 & \cdots & \mathbf{b}_{N(M-1)} \\ (\mathbf{b}_1)^\dagger & \mathbf{a}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ (\mathbf{b}_{N(M-1)})^\dagger & 0 & \cdots & \mathbf{a}_{N(M-1)+1} \end{pmatrix}, \quad (\text{A32})$$

where each $\mathbf{b}_i \in \mathbb{C}^{N \times 1}$ is a column vector. In this form, the impurity couples to $N(M-1)$ bath levels, each with a single internal degree of freedom. To restore bath sites with internal dimension N , we define the Hermitian weight matrices as the outer product

$$\mathbf{W}_i = \mathbf{b}_i (\mathbf{b}_i)^\dagger, \quad (\text{A33})$$

and their Hermitian principal square roots

$$\mathbf{B}_i = (\mathbf{W}_i)^{1/2}. \quad (\text{A34})$$

With these blocks, we construct H_A as in Eq. (A28): the eigenvalues $\mathbf{a}_i$ of the bath subspace define the diagonal blocks $\mathbf{a}_i I_N$, and the coupling between the impurity and bath site i is given by $\mathbf{B}_i$ from Eqs. (A33) and (A34).

Since $\mathbf{b}_i$ is a column vector, $\mathbf{W}_i = \mathbf{b}_i (\mathbf{b}_i)^\dagger$ is an outer product and therefore has $\text{rank}(\mathbf{W}_i) \leq 1$ (rank 0 if the coupling vanishes). If several bath eigenvalues $\mathbf{a}_i$ are degenerate, one should recombine the corresponding couplings within the degenerate subspace. In that case, one may sum the weights $\mathbf{W}_j$ for all states with the same eigenvalue $\mathbf{a}_j$, $\mathbf{W} = \sum_j \mathbf{W}_j$, and obtain the impurity-bath coupling from the principal square root of this sum, $\mathbf{B} = \mathbf{W}^{1/2}$. This ensures a symmetry-conserving representation of the impurity-bath hybridization function.

d. Construction from the list-of-poles representation. To obtain an Anderson representation of $G(z)$ from its list-of-poles representation, we first-of-all find for the constant term

$$\mathbf{A}_0 = A_0. \quad (\text{A35})$$

In order to determine the other block elements we start with the pole energies a_i and block matrices B_i that define the list-of-pole representation Eq. (A1) and define the block-vector

$$V = \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_M \end{pmatrix} \in \mathbb{C}^{NM \times N}, \quad (\text{A36})$$

and diagonal matrix

$$H_{LP} = \text{diag}(\alpha_1 I_N, \alpha_2 I_N, \dots, \alpha_M I_N) \in \mathbb{R}^{NM \times NM}. \quad (\text{A37})$$

This allows us to rewrite our Green's function as

$$G(z) = \mathbf{A}_0 + V^\dagger \frac{1}{z - H_{LP}} V. \quad (\text{A38})$$

As the column vectors in V are not orthonormal for general response functions, (they are for Green's functions), we use the same symmetric orthonormalization as in Appendix A 2 a by using the overlap matrix

$$S = V^\dagger V = \sum_{i=1}^M B_i B_i = \sum_{i=1}^M \mathbf{W}_i, \quad (\text{A39})$$

to create the matrices

$$R_a = V S^{-1/2} \in \mathbb{C}^{NM \times N}, \quad (\text{A40})$$

$$\mathbf{B}_0 = S^{1/2},$$

with $R_a^\dagger R_a = I_N$. We then find the orthogonal complement $R_{\bar{a}} \in \mathbb{C}^{NM \times N(M-1)}$ and collect the column vectors to generate the unitary matrix $U = R_a \oplus R_{\bar{a}} \in \mathbb{C}^{NM \times NM}$.

We then insert the identity, $UU^\dagger$ twice, into Eq. (A38), which yields

$$\begin{aligned} G(z) &= \mathbf{A}_0 + \mathbf{B}_0 R_a^\dagger \frac{1}{z - UU^\dagger H_{\text{LP}} UU^\dagger} R_a \mathbf{B}_0 \\ &= \mathbf{A}_0 + \mathbf{B}_0 R_a^\dagger U \frac{1}{z - U^\dagger H_{\text{LP}} U} U^\dagger R_a \mathbf{B}_0. \end{aligned} \quad (\text{A41})$$

We now use the property

$$U^\dagger R_a = \begin{pmatrix} R_a^\dagger \\ R_{\bar{a}}^\dagger \end{pmatrix} R_a = \begin{pmatrix} I_{N \times N} \\ 0_{N(M-1) \times N} \end{pmatrix}, \quad (\text{A42})$$

which can be interpreted as taking the upper left $N \times N$ block of the resolvent of $U^\dagger H_{\text{LP}} U$

$$G(z) = \mathbf{A}_0 + \mathbf{B}_0 \left[\frac{1}{z - U^\dagger H_{\text{LP}} U} \right]_{1:N, 1:N} \mathbf{B}_0. \quad (\text{A43})$$

In the next step, we want to bring the matrix $U^\dagger H_{\text{LP}} U$ into the form of Eq. (A32). The derivation for the Green's function in Anderson representation is then analogous to the second step in transforming $G(z)$ from tridiagonal form to Anderson form. After diagonalizing the lower right $N(M-1) \times N(M-1)$ block, the Anderson matrix associated with $G(z)$ takes the form of Eq. (A32). To obtain the symmetric coupling matrices $\mathbf{B}_i$, we follow the procedure of Appendix A 3 c starting from Eq. (A32).

Appendix B: Discrete self-energy starting from different representations.

In the main text, we have found for the self-energy:

$$\begin{aligned} \Sigma(z) - \Sigma^{\text{HF}} &= \left([\tilde{G}^{-1}(z)]_{22} \right)^{-1} \\ &= S^{1/2} \frac{1}{z - S^{1/2} \left[\tilde{S}^{-1/2} \tilde{H}_{\text{eff}}(z) \tilde{S}^{-1/2} \right]_{22} S^{1/2}} S^{1/2}, \end{aligned} \quad (\text{B1})$$

where $\tilde{G}(z)$ is a $\tilde{N} \times \tilde{N}$ matrix-valued propagator with $\tilde{N} = 2N$. The matrix $\tilde{S}$ is the norm of $\tilde{G}(z)$ and $S = ([\tilde{S}^{-1}]_{22})^{-1}$ is the norm of $\Sigma(z) - \Sigma^{\text{HF}}$. Eq. (B1) can be evaluated by applying three steps to $\tilde{G}(z)$: (i) inversion, (ii) projection to the 22 block, and (iii) reinversion. In the following three subsections, we show, using equations from the literature [25, 26, 52–59], how these steps can be implemented explicitly, starting from any one of three different representations of $\tilde{G}(z)$, namely a tridiagonal, Anderson or list-of-pole representation.

1. Starting from tridiagonal representation of $\tilde{G}(z)$

We start from

$$\tilde{G}(z) = \tilde{\mathbf{B}}_0^{1/2} \frac{1}{z - \tilde{\mathcal{A}}_1 - \tilde{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \tilde{\mathbf{B}}_1} \tilde{\mathbf{B}}_0^{1/2}. \quad (\text{B2})$$

Comparing this expression to Eq. (16) gives

$$\tilde{S}^{1/2} = \tilde{\mathbf{B}}^{1/2}, \quad (\text{B3})$$

$$\tilde{H}_{\text{eff}}(z) = \tilde{\mathcal{A}}_1 + \tilde{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \tilde{\mathbf{B}}_1, \quad (\text{B4})$$

with $\tilde{H}_{\text{eff}}(z)$ also given in tridiagonal representation.

(i) *Inversion.* The inverse of $\tilde{G}(z)$ is written as

$$\tilde{G}^{-1}(z) = \tilde{S}^{-1/2} \left(z - \tilde{\mathcal{A}}_1 - \tilde{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \tilde{\mathbf{B}}_1 \right) \tilde{S}^{-1/2}. \quad (\text{B5})$$

(ii) *Projection.* To project to the lower-right block, we need to calculate

$$\begin{aligned} \left[\tilde{S}^{-1/2} \tilde{H}_{\text{eff}}(z) \tilde{S}^{-1/2} \right]_{22} &= \left[\tilde{S}^{-1/2} \tilde{\mathcal{A}}_1 \tilde{S}^{-1/2} \right]_{22} \\ &+ \left[\tilde{S}^{-1/2} \tilde{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \tilde{\mathbf{B}}_1 \tilde{S}^{-1/2} \right]_{22}. \end{aligned} \quad (\text{B6})$$

To bring the full result into a tridiagonal form with block dimension N , rather than retaining intermediate blocks of dimension $\tilde{N}$, one may apply a block-Lanczos procedure to

$$\tilde{S}^{-1/2} \tilde{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \tilde{\mathbf{B}}_1 \tilde{S}^{-1/2}, \quad (\text{B7})$$

using as starting block-vector the projection onto the subspace 2 at block $i = 1$. With

$$\begin{aligned} S &= ([\tilde{S}^{-1}]_{22})^{-1}, \\ \bar{\mathcal{A}}_1 &= [\tilde{S}^{-1/2} \tilde{\mathcal{A}}_1 \tilde{S}^{-1/2}]_{22}, \end{aligned}$$

$$\begin{aligned} \bar{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \bar{\mathbf{B}}_1 &= \left[\tilde{S}^{-1/2} \tilde{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \tilde{\mathbf{B}}_1 \tilde{S}^{-1/2} \right]_{22}, \end{aligned} \quad (\text{B8})$$

the projection of $\tilde{G}^{-1}(z)$ is written as

$$[\tilde{G}^{-1}(z)]_{22} = S^{-1} z - \bar{\mathcal{A}}_1 - \bar{\mathbf{B}}_1 \frac{1}{z - \tilde{\mathcal{A}}_2 - \dots} \bar{\mathbf{B}}_1. \quad (\text{B9})$$

(iii) *Reinversion.* To invert the previous expression, we first define

$$\begin{aligned} \mathcal{A}_1 &= S^{1/2} \bar{\mathcal{A}}_1 S^{1/2}, \\ \mathcal{B}_1 &= S^{1/2} \bar{\mathbf{B}}_1, \end{aligned} \quad (\text{B10})$$

to rewrite Eq. (B9) as

$$[\tilde{G}^{-1}(z)]_{22} = S^{-1/2} \left(z - \mathcal{A}_1 - \mathcal{B}_1 \frac{1}{z - \mathcal{A}_2 - \dots} \mathcal{B}_1 \right) S^{-1/2}. \quad (\text{B11})$$

Inverting this gives us the self-energy in tridiagonal form

$$\Sigma(z) = \Sigma^{\text{HF}} + S^{1/2} \frac{1}{z - \mathcal{A}_1 - \mathcal{B}_1 \frac{1}{z - \mathcal{A}_2 - \dots} \mathcal{B}_1} S^{1/2}. \quad (\text{B12})$$

2. Starting from Anderson representation of $\tilde{G}(z)$

For a response function $\tilde{G}(z)$ in Anderson representation

$$\tilde{G}(z) = \tilde{S}^{1/2} \frac{1}{z - \tilde{\mathbf{A}}_1 - \sum_i \tilde{\mathbf{B}}_i \frac{1}{z - \tilde{\mathbf{a}}_{i+1}} \tilde{\mathbf{B}}_i} \tilde{S}^{1/2}, \quad (\text{B13})$$

$\tilde{H}_{\text{eff}}(z)$ is given in a list-of-poles representation:

$$\tilde{H}_{\text{eff}}(z) = \tilde{\mathbf{A}}_1 + \sum_i \tilde{\mathbf{B}}_i \frac{1}{z - \tilde{\mathbf{a}}_{i+1}} \tilde{\mathbf{B}}_i. \quad (\text{B14})$$

(i) *Inversion.* The inverse of $\tilde{G}(z)$ is given as

$$\tilde{G}^{-1}(z) = \tilde{S}^{-1/2} \left(z - \tilde{\mathbf{A}}_1 - \sum_i \tilde{\mathbf{B}}_i \frac{1}{z - \tilde{\mathbf{a}}_{i+1}} \tilde{\mathbf{B}}_i \right) \tilde{S}^{-1/2}. \quad (\text{B15})$$

(ii) *Projection.* To project to the lower right block, we define

$$\begin{aligned} S &= ([\tilde{S}^{-1}]_{22})^{-1}, \\ \bar{\mathbf{A}}_1 &= [\tilde{S}^{-1/2} \tilde{\mathbf{A}}_1 \tilde{S}^{-1/2}]_{22}, \\ \bar{\mathbf{B}}_i &= \left([\tilde{S}^{-1/2} \tilde{\mathbf{B}}_i \tilde{S}^{-1/2}]_{22} \right)^{1/2}, \\ \mathbf{a}_i &= \tilde{\mathbf{a}}_i, \end{aligned} \quad (\text{B16})$$

and express the projection of $\tilde{G}^{-1}(z)$ as

$$[\tilde{G}^{-1}(z)]_{22} = S^{-1} z - \bar{\mathbf{A}} - \sum_i \bar{\mathbf{B}}_i \frac{1}{z - \mathbf{a}_{i+1}} \bar{\mathbf{B}}_i. \quad (\text{B17})$$

(iii) *Reinversion.* To invert the previous expression, we first define

$$\begin{aligned} \mathbf{A}_1 &= S^{1/2} \bar{\mathbf{A}}_1 S^{1/2}, \\ \mathbf{B}_i &= \left(S^{1/2} \bar{\mathbf{B}}_i \bar{\mathbf{B}}_i S^{1/2} \right)^{1/2}, \end{aligned} \quad (\text{B18})$$

to rewrite Eq. (B17) as

$$[\tilde{G}^{-1}(z)]_{22} = S^{-1/2} \left(z - \mathbf{A}_1 - \sum_i \mathbf{B}_i \frac{1}{z - \mathbf{a}_{i+1}} \mathbf{B}_i \right) S^{-1/2}. \quad (\text{B19})$$

Inverting this gives us the self-energy in Anderson form

$$\Sigma(z) = \Sigma^{\text{HF}} + S^{1/2} \frac{1}{z - \mathbf{A}_1 - \sum_i \mathbf{B}_i \frac{1}{z - \mathbf{a}_{i+1}} \mathbf{B}_i} S^{1/2}. \quad (\text{B20})$$

3. Starting from list-of-poles representation of $\tilde{G}(z)$

If the transformations between different types of response functions (Appendices A 2 a, A 3 d) are available, one could first transform $\tilde{G}(z)$ to tridiagonal or Anderson representation and continue as described in Appendices B 1 or B 2, respectively.

Here, we describe an alternative approach that obtains the pole expansion of $\Sigma(z)$ directly from the pole expansion of $\tilde{G}(z)$ using standard linear algebra techniques. This is the approach used to obtain the TaskK and NRG results shown in Figs. 1 and 2.

We consider a matrix-valued function $\tilde{G}(z) \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$ with elements $[\tilde{G}(z)]_{\alpha\alpha'}$ and $\alpha = 1, \dots, \tilde{N} = 2N$, as defined in Sec. III of the main text: $\alpha = 1, \dots, N$ enumerates $a_{0,\mathbf{m}}, a_{0,\mathbf{m}}^\dagger$ operators, $\alpha = N + 1, \dots, 2N$ enumerates the corresponding $q_{\mathbf{m}}, q_{\mathbf{m}}^\dagger$ operators. We assume $\tilde{G}(z)$ to be given as a list-of-pole representation,

$$\tilde{G}(z) = \sum_{i=1}^M \frac{\tilde{W}_i}{z - \tilde{a}_i}, \quad (\text{B21})$$

having three key properties, all of which are used below: (i) The M poles are real, $\tilde{a}_i \in \mathbb{R}$; (ii) the M matrices $\tilde{W}_i \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$ are Hermitian and positive semidefinite; and (iii) each $\tilde{W}_i$ matrix has rank one (this does not imply loss of generality, see Appendix A 1 a.). Then, each $\tilde{W}_i$ can be written as the outer product, $\tilde{W}_i = \tilde{v}_i^\dagger \tilde{v}_i$, of a row vector $\tilde{v}_i \in \mathbb{C}^{1 \times \tilde{N}}$ and its Hermitian conjugate column vector $\tilde{v}_i^\dagger \in \mathbb{C}^{\tilde{N} \times 1}$, with elements $[\tilde{W}_i]_{\alpha\alpha'} = [\tilde{v}_i^\dagger]_\alpha [\tilde{v}_i]_{\alpha'}$.

We will call the collection of data $\{\tilde{a}_i, \tilde{W}_i\}$ the spectrum of $\tilde{G}(z)$; it describes the positions and matrix-valued weights of the discrete δ -peaks of $-\frac{1}{\pi} \text{Im} \tilde{G}(\omega + i0^+)$. The spectrum is fully encoded in the two matrices $\{\tilde{\Omega}, \tilde{V}\}$, where $\tilde{\Omega} = \text{diag}(\tilde{a}_1, \dots, \tilde{a}_M) \in \mathbb{R}^{M \times M}$ is diagonal and $\tilde{V} \in \mathbb{C}^{M \times \tilde{N}}$ has elements $\tilde{V}_{i\alpha} = [\tilde{v}_i]_\alpha$. Indeed,

$$\tilde{G}(z) = \tilde{V}^\dagger \frac{1}{z - \tilde{\Omega}} \tilde{V}. \quad (\text{B22})$$

The integrated weight matrix $\tilde{S}$ of Eq. (14) is given by

$$\tilde{S} = \tilde{V}^\dagger \tilde{V} \in \mathbb{C}^{\tilde{N} \times \tilde{N}}. \quad (\text{B23})$$

We can further perform the polar decomposition [95]

$$\tilde{V} = \tilde{R}_a \tilde{S}^{1/2}, \quad \tilde{R}_a^\dagger \tilde{R}_a = I_{\tilde{N}}, \quad (\text{B24})$$

where $\tilde{R}_a \in \mathbb{C}^{M \times \tilde{N}}$ is an isometry and $\tilde{S}^{1/2} \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$ is Hermitian and positive semidefinite. Then, the latter is the principal square root of $\tilde{S}$, justifying the notation $\tilde{S}^{1/2}$. (Note: the subscript on $\tilde{R}_a$ is a single-valued label, not an index, used to distinguish $\tilde{R}_a$ from $\tilde{R}_{\tilde{a}}$, defined

below.) Furthermore, the propagator $\tilde{G}(z)$ takes the form

$$\tilde{G}(z) = \tilde{S}^{1/2} \tilde{R}_a^\dagger \frac{1}{z - \tilde{\Omega}} \tilde{R}_a \tilde{S}^{1/2}, \quad (\text{B25})$$

with the norm factors $\tilde{S}^{1/2}$ split from the dynamical part.

(i) *Inversion.* To obtain a DSR for $G^{-1}(z)$, we seek to transcribe $G(z)$ to the form

$$\tilde{G}(z) = \tilde{S}^{1/2} \frac{1}{z - \tilde{H}_{\text{eff}}(z)} \tilde{S}^{1/2} \quad (\text{B26})$$

and find the DSR of $\tilde{H}_{\text{eff}}(z) \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$. To this end, our strategy will be to express $\tilde{G}(z)$ as the projection of the $M \times M$ matrix $(z - \tilde{\Omega})^{-1}$ to an $\tilde{N} \times \tilde{N}$ block submatrix, and then to invert the latter using the Schur complement formula, which involves other blocks of $\tilde{\Omega}$.

For that, we define an orthogonal complement to $\tilde{R}_a$, the isometry $\tilde{R}_{\bar{a}} \in \mathbb{C}^{M \times \tilde{N}}$, with $\tilde{N} = M - \tilde{N}$, such that $\tilde{R}_a^\dagger \tilde{R}_{\bar{a}} = 0$ and $\tilde{R}_a^\dagger \tilde{R}_a = I_{\tilde{N}}$ [96]. Then, $\tilde{U} = \tilde{R}_a \oplus \tilde{R}_{\bar{a}} \in \mathbb{C}^{M \times M}$, built from the columns of $\tilde{R}_a$ and $\tilde{R}_{\bar{a}}$, is unitary. Next, we define the blocks $\tilde{\Omega}_{x\tilde{x}} = \tilde{R}_x^\dagger \tilde{\Omega} \tilde{R}_{\tilde{x}}$, for $x, \tilde{x} \in \{a, \bar{a}\}$, and write

$$\tilde{\Omega} = (\tilde{R}_a, \tilde{R}_{\bar{a}}) \begin{pmatrix} \tilde{\Omega}_{aa} & \tilde{\Omega}_{a\bar{a}} \\ \tilde{\Omega}_{\bar{a}a} & \tilde{\Omega}_{\bar{a}\bar{a}} \end{pmatrix} \begin{pmatrix} \tilde{R}_a^\dagger \\ \tilde{R}_{\bar{a}}^\dagger \end{pmatrix} = \tilde{U} \begin{pmatrix} \tilde{\Omega}_{aa} & \tilde{\Omega}_{a\bar{a}} \\ \tilde{\Omega}_{\bar{a}a} & \tilde{\Omega}_{\bar{a}\bar{a}} \end{pmatrix} \tilde{U}^\dagger, \quad (\text{B27})$$

obtaining a block decomposition of $\tilde{\Omega}$ in the basis of the columns of $\tilde{U}^\dagger$. With this notation, Eq. (B25) yields

$$\tilde{G}(z) = \tilde{S}^{1/2} \left(\frac{1}{z - \tilde{\Omega}} \right)_{aa} \tilde{S}^{1/2}. \quad (\text{B28})$$

$\tilde{G}(z)$ thus involves the projection of the inverse of a 2×2 block matrix to its aa block. This calls for use of the Schur complement formula for block matrix inversion,

$$\left(\begin{pmatrix} M_{aa} & M_{a\bar{a}} \\ M_{\bar{a}a} & M_{\bar{a}\bar{a}} \end{pmatrix}^{-1} \right)_{aa} = \left(M_{aa} - M_{a\bar{a}} \frac{1}{M_{\bar{a}\bar{a}}} M_{\bar{a}a} \right)^{-1}, \quad (\text{B29})$$

which yields

$$\left(\frac{1}{z - \tilde{\Omega}} \right)_{aa} = \left(z - \tilde{\Omega}_{aa} - \tilde{\Omega}_{a\bar{a}} \frac{1}{z - \tilde{\Omega}_{\bar{a}\bar{a}}} \tilde{\Omega}_{\bar{a}a} \right)^{-1}. \quad (\text{B30})$$

By comparing Eq. (B26) to Eqs. (B28) and (B30), we find

$$\tilde{H}_{\text{eff}}(z) = \tilde{\Omega}_{aa} + \tilde{\Omega}_{a\bar{a}} \frac{1}{z - \tilde{\Omega}_{\bar{a}\bar{a}}} \tilde{\Omega}_{\bar{a}a}. \quad (\text{B31})$$

Now we diagonalize the block $\tilde{\Omega}_{\bar{a}\bar{a}}$ as $\bar{U}^\dagger \tilde{\Omega}_{\bar{a}\bar{a}} \bar{U} = \bar{\Omega}$, where $\bar{\Omega} = \text{diag}(\bar{\omega}_1, \dots, \bar{\omega}_{\tilde{N}}) \in \mathbb{R}^{\tilde{N} \times \tilde{N}}$ is diagonal and $\bar{U} \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$ is unitary, and define $\bar{V} = \bar{U}^\dagger \tilde{\Omega}_{\bar{a}\bar{a}} \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$. Then, Eq. (B31) leads to the desired DSR for $\tilde{H}_{\text{eff}}(z)$,

$$\tilde{H}_{\text{eff}}(z) = \tilde{\Omega}_{aa} + \sum_{i=1}^{\tilde{N}} \frac{\bar{W}_i}{z - \bar{\omega}_i}, \quad (\text{B32})$$

where each $\bar{W}_i \in \mathbb{C}^{\tilde{N} \times \tilde{N}}$ is a rank-1 matrix with elements given by $[\bar{W}_i]_{\alpha\alpha'} = [\bar{V}^\dagger]_{\alpha i} [\bar{V}]_{i\alpha'}$. Moreover, we have

$$\tilde{G}^{-1}(z) = \tilde{S}^{-1/2} \left[z - \tilde{\Omega}_{aa} + \sum_{i=1}^{\tilde{N}} \frac{\bar{W}_i}{z - \bar{\omega}_i} \right] \tilde{S}^{-1/2}. \quad (\text{B33})$$

(ii) *Projection.* The self-energy formula Eq. (B1) involves $[\tilde{G}^{-1}(z)]_{22} \in \mathbb{C}^{N \times N}$, with $N = \tilde{N}/2$. This is the projection of $\tilde{G}^{-1}(z)$, viewed as a 2×2 block matrix of four blocks $\in \mathbb{C}^{N \times N}$, to its 22 block. We express it as

$$[\tilde{G}^{-1}(z)]_{22} = S^{-1/2} \left[z - \Omega_{aa} + \sum_{i=1}^{\tilde{N}} \frac{W_i}{z - \bar{\omega}_i} \right] S^{-1/2}, \quad (\text{B34})$$

where we defined $S = ([\tilde{S}^{-1}]_{22})^{-1} \in \mathbb{C}^{N \times N}$, denoted its principal square root by $S^{1/2}$, and defined the matrices

$$\Omega_{aa} = S^{1/2} [\tilde{S}^{-1/2} \tilde{\Omega}_{aa} \tilde{S}^{-1/2}]_{22} S^{1/2} \in \mathbb{C}^{N \times N}, \quad (\text{B35a})$$

$$W_i = S^{1/2} [\tilde{S}^{-1/2} \bar{W}_i \tilde{S}^{-1/2}]_{22} S^{1/2} \in \mathbb{C}^{N \times N}.$$

Since all $\bar{W}_i$ are Hermitian rank-1 matrices, the same is true for all W_i , hence their matrix elements can be expressed as $[W_i]_{\alpha\alpha'} = [V^\dagger]_{\alpha i} [V]_{i\alpha'}$, with $V \in \mathbb{C}^{\tilde{N} \times N}$. By Eq. (B1), the self-energy can thus be expressed as

$$\Sigma(z) - \Sigma^{\text{HF}} = S^{1/2} \left(z - \Omega_{aa} - V^\dagger \frac{1}{z - \bar{\Omega}} V \right)^{-1} S^{1/2}. \quad (\text{B36})$$

(iii) *Reinversion.* Our final goal is to obtain a list-of-poles representation for the self-energy from Eq. (B36). To this end, we use the Schur complement formula (B29) to express the central factor of (B36) as [see Eq. (B30)]

$$\left(z - \Omega_{aa} - V^\dagger \frac{1}{z - \bar{\Omega}} V \right)^{-1} = \left(\frac{1}{z - \Omega'} \right)_{aa}, \quad (\text{B37})$$

where we defined the matrix

$$\Omega' = \begin{pmatrix} \Omega_{aa} & V^\dagger \\ V & \bar{\Omega} \end{pmatrix} \in \mathbb{C}^{\bar{M} \times \bar{M}}, \quad (\text{B38})$$

with $\bar{M} = N + \tilde{N} = M - N$. We diagonalize it as $U'^\dagger \Omega' U' = \Omega''$, where $\Omega'' = \text{diag}(\epsilon''_1, \dots, \epsilon''_{\bar{M}}) \in \mathbb{R}^{\bar{M} \times \bar{M}}$. Then

$$\left(\frac{1}{z - \Omega'} \right)_{aa} = \left(U' \frac{1}{z - \Omega''} U'^\dagger \right)_{aa} = R_a'^\dagger \frac{1}{z - \Omega''} R_a', \quad (\text{B39})$$

where we collected the first N columns of $U'^\dagger$ to construct the isometry $R_a' \in \mathbb{C}^{\bar{M} \times N}$, with $R_a'^\dagger R_a' = I_N$. Equations (B36), (B37) and (B39) yield the desired DSR for $\Sigma(z)$,

$$\Sigma(z) - \Sigma^{\text{HF}} = V''^\dagger \frac{1}{z - \Omega''} V'' = \sum_{i=1}^{\bar{M}} \frac{W_i''}{z - \epsilon''_i}, \quad (\text{B40a})$$

where $V'' = R_a' S^{1/2} \in \mathbb{C}^{\bar{M} \times N}$, and each $W_i'' \in \mathbb{C}^{N \times N}$ is a rank-1 matrix with elements $[W_i'']_{\alpha\alpha'} = [V''^\dagger]_{i\alpha} [V'']_{i\alpha'}$. Note that the norm of $\Sigma(z) - \Sigma^{\text{HF}}$ is given by $V''^\dagger V'' = S$.

Appendix C: Update of the hybridization function using a discrete self-energy

In the DMFT self-consistency loop, the hybridization function of the impurity model is updated using the impurity self-energy. In `RAS_DMFT.jl` and `QUANTY` this update is performed directly at the level of the discrete pole representation of $\Delta(z)$ and $\Sigma(z)$. The effective hybridization function is obtained from [26]

$$\Delta^{\text{eff}}(z) = \Delta(zI_N - \Sigma(z)), \quad (\text{C1})$$

whereby the matrix valued arguments of Δ should be interpreted using the discrete representation of the hybridization function [Eq. (6)] as

$$\Delta^{\text{eff}}(z) = \sum_{i=1}^M V_i^\dagger \frac{1}{z - E_i - \Sigma(z)} V_i. \quad (\text{C2})$$

Note that this equation requires the spin-orbital basis of $\Delta(z)$ and $\Sigma(z)$ to be the same and independent of z , which for the examples in the current paper is trivially fulfilled.

For a self-energy in the list-of-poles representation, one obtains $\Delta^{\text{eff}}(z)$ as a sum over M Anderson-type response functions:

$$\Delta^{\text{eff}}(z) = \sum_{i=1}^M V_i^\dagger \frac{1}{z - E_i - \Sigma^{\text{HF}} - \sum_{j=1}^{M^\Sigma} W_j'' \frac{1}{z - \epsilon_j'}} V_i. \quad (\text{C3})$$

To bring $\Delta^{\text{eff}}(z)$ to the list-of-poles representation, we transform each summand in Eq. (C3) from Anderson-type into the list-of-poles representation.

$$\Delta^{\text{eff}}(z) = \sum_{i=1}^M \left[\sum_{j=1}^{M^\Sigma+1} V_j'^\dagger \frac{1}{z - E_j'} V_j' \right]_i. \quad (\text{C4})$$

The double sum can be combined into a single sum over $M(M^\Sigma + 1)$ poles:

$$\Delta^{\text{eff}}(z) = \sum_{i=1}^{M(M^\Sigma+1)} V_i^{\text{eff}\dagger} \frac{1}{z - E_i^{\text{eff}}} V_i^{\text{eff}}. \quad (\text{C5})$$

The number of poles can then be reduced to keep the computational cost moderate.

Appendix D: Regularization of the quasiparticle weight from a discrete spectral representation

In the main text we have shown how the quasiparticle weight Z can be obtained from the DSR of the self-energy $\Sigma(z)$:

$$\Sigma(\omega + i0^+) = \Sigma^{\text{HF}} + \sum_i \frac{W_i''}{\omega + i0^+ - \epsilon_i''}, \quad (\text{D1a})$$

$$\partial_\omega \text{Re} \Sigma(\omega + i0^+) |_{\omega=0} = - \sum_{\epsilon_i'' \neq 0} \frac{W_i''}{(\epsilon_i'')^2} + \sum_{\epsilon_i''=0} \frac{W_i''}{(0^+)^2}, \quad (\text{D1b})$$

$$Z = [I_N - \partial_\omega \text{Re} \Sigma(\omega + i0^+) |_{\omega=0}]^{-1}. \quad (\text{D1c})$$

Numerical algorithms might yield spurious poles with small ($\text{Tr}(W_i'') \ll 1$) residue. When such a pole occurs at small energies ($|\epsilon_i''| \sim \text{Tr}(W_i'')$), these spurious poles will dominate the calculation of the quasiparticle weight and may lead to $Z = 0$ even for a metallic solution. In this appendix we discuss strategies to regularize the calculation of Z in the presence of such spurious poles.

A first approach is to remove poles whose spectral weight falls below a chosen threshold. If the spurious poles are close to machine precision ($\text{Tr}(W_i'') < 10^{-14}$), which is the case for the application in Sec. IV C of the main text, spurious and physical poles are well separated. In this case, Z can be straightforwardly regularized by removing these poles.

A second approach becomes necessary when the spurious poles have larger spectral weight ($\text{Tr}(W_i'') \approx 10^{-7}$), which happens for the application in Sec. IV D of the main text. By choosing larger threshold values, one might risk removing poles that are physically relevant. A more systematic way to regularize the calculation of Z is to modify the expression for Z in Eq. (D1) by introducing a regularization parameter λ :

$$Z_\lambda = \left(I_N + \sum_i W_i'' \frac{1}{\epsilon_i''^2 + \lambda^2} \right)^{-1}. \quad (\text{D2})$$

In the absence of spurious poles at the Fermi level Z_λ will approach Z when $\lambda \rightarrow 0$. When spurious poles are present, too small λ will lead to numerical instabilities, while too large λ will modify the results. Instead, one needs to find a range of λ where Z_λ is approximately constant with respect to λ .

In Fig. 6 we show the effect of such a regularization on the self-energy represented by different number of poles. If no spurious poles are present ($K = 40$ and $K = 80$), one can take the limit $\lambda \rightarrow 0$ without problems. For $K = 160$ however, one needs to find a range where Z_λ is approximately constant. In this case, it happens around $\lambda/D \approx 10^{-2}$, where Z_λ has an inflection point. For intermediate values of λ , the quasiparticle weight is the same between the different Krylov sizes K , which determine the number of poles in $\Sigma(z)$.

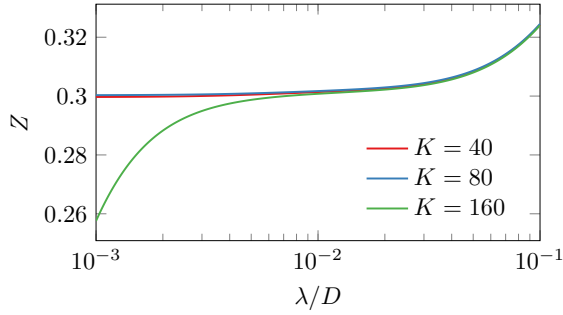


FIG. 6. Quasiparticle weight Z as a function of the regularization parameter λ at an interaction $U/D = 2$. The parameter K is the size of the Krylov space of the propagator $\bar{G}$ and indirectly determines the number of poles of the self-energy.

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 - [96] To find $\tilde{R}_a$, we construct $P_a = \tilde{R}_a \tilde{R}_a^\dagger$ the projector leaving $\tilde{R}_a$ invariant, QR-decompose its complement, $QR = P_a = I_M - P_a$, and set $\tilde{R}_a = Q$.

3 Quantum criticality in the Hubbard model

In this chapter, we present our findings on the two-dimensional Hubbard model and quantum criticality at finite hole doping p . In Sec. 3.1, we provide a brief overview, including benchmark results and a short discussion of cluster size dependence in cDMFT for the Hubbard model, with a comparison to the Emery model.

3.1 Benchmark & Cluster size dependence

We begin our investigation of the Hubbard model by setting up a two-site DCA+NRG implementation to reproduce the established results of Ref. [Fer+09]. Our DCA+NRG approach enables the direct computation of real frequency spectral functions for the individual momentum patches, which we compare to the spectral functions reported in Ref. [Fer+09], obtained via analytical continuation.

Subsequently, we increased the cluster size to four sites arranged in a 2×2 geometry. Ref. [Gul+10] serves as a reference for further benchmarking and for motivating the use of the so-called “star patching” geometry. As a second benchmark, we compute the patch dependent filling

$$n_{\mathbf{K}} = 2 \int d\omega f_{\text{FD}}(\omega) A_{\mathbf{K}}(\omega) \quad \text{and} \quad n = \frac{1}{N_c} \sum_{\mathbf{K}} n_{\mathbf{K}}, \quad (3.1)$$

where $f_{\text{FD}}(\omega)$ denotes the Fermi–Dirac distribution and $A_{\mathbf{K}}(\omega)$ are the patch resolved spectral functions at fixed chemical potential μ . The hole doping is defined as $p = 1 - n$. We emphasize that a further increase in cluster size enhances spatial resolution and improves the description of pseudogap physics in the hole doped Hubbard model. However, since NRG is a tensor network based impurity solver that explicitly tracks excitations of the local cluster Hamiltonian, the corresponding Hilbert space grows exponentially with each additional cluster site. Consequently, the numerical effort required to solve the impurity problem also increases exponentially with cluster size. In practice, a four-site impurity already approaches the numerical limits of NRG. Due to these numerical limitations imposed by NRG, we initiated a systematic investigation of the cluster size dependence of pseudogap formation in both the Hubbard and Emery models. This project resulted in a supervised Master’s thesis [Niu24].

Since our two-site computations, which are expanded on in this thesis, are not able to capture quantum criticality due to insufficient spatial resolution, whereas the four-site calculations do, the question arose whether a two-site DCA+NRG computation of the Emery model, solved with NRG, is capable of capturing the quantum critical transition. We find that DCA+NRG of a two-site Emery model, where each cluster site includes two non-interacting oxygen orbital within the lattice integration, enhances the pseudogap physics compared to the Hubbard model counterpart. However, the inclusion of additional orbital degrees of freedom is not enough to yield a quantum critical transition. In conclusion, we argue that resolving a quantum critical transition requires a clear momentum separation between the antinodal points $\mathbf{k} = (0, \pi)$, $\mathbf{k} = (\pi, 0)$, and the nodal

point $\mathbf{k} = (\pi, \pi)$. Scattering processes between these three momenta enables the onset of antiferromagnetic correlations already at relatively high doping levels ($p \sim 15\%$). From our analysis, orbital degrees of freedom appear to be less relevant for pseudogap physics than non-local spatial correlations.

Building on the insights gained from the four-site calculations, a natural next step is to improve the numerical treatment by performing a refined four-site DCA+NRG study in which the (π, π) patch is treated as a Hubbard atom without an attached bath. This effectively reduces the numerical effort to that of a three-site impurity problem while retaining the essential momentum differentiation.

Quantum criticality in the two-dimensional Hubbard model

by

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Quantum criticality in the two-dimensional Hubbard model

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We study the normal-state, doping-driven phase diagram of the square-lattice Hubbard model using the dynamical cluster approximation combined with the numerical renormalization group as a cluster solver, which gives direct access to real-frequency dynamics at essentially zero temperature. In a parameter regime relevant for cuprates, $U = 7t$ and $t' = -0.3t$, we find a critical doping p^* that marks a continuous quantum phase transition between a pseudogap metal and a normal Fermi liquid. The transition is identified by a continuous collapse, from both sides, of the Fermi-liquid scale extracted from charge, spin, and $d_{x^2-y^2}$ -wave pairing susceptibilities. This collapse produces a non-Fermi-liquid regime at intermediate energy scales, which appears to extend to arbitrarily low scales at p^* . As p^* is crossed from the normal Fermi liquid at $p > p^*$ into the pseudogap metal at $p < p^*$, the coherent low-energy spectral weight in the antinodal region is lost and replaced by a narrow, metallic pseudogap, while the nodal region evolves smoothly and remains comparatively coherent. This gives rise to Fermi arcs in the pseudogap metal at $p < p^*$, since the zero-frequency spectral weight remains large in the nodal region but is strongly suppressed in the antinodal region.

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Due to its relevance to high- T_c cuprates, the problem of doping a Mott insulator [1] has been a topic of intense discussion in the past three decades. A major mystery is the normal state that emerges upon hole doping in cuprates [2]. On the overdoped side, transport, thermodynamics, and spectroscopy are broadly consistent with a correlated normal Fermi liquid (FL). By contrast, on the underdoped side, a pseudogap (PG) metal emerges, featuring a loss of electronic spectral weight predominantly in the antinodal region and a reconstructed Fermi surface incompatible with Luttinger's sum rule. A central question, raised very early on [3–6], is whether the PG metal and the overdoped FL are separated by a quantum critical point (QCP) at some critical doping p^* [7–13].

Evidence for quantum criticality at the pseudogap endpoint at p^* has accumulated in several cuprate families. The Hall number, angle-dependent magnetoresistance, and quantum oscillations indicate a transformation of the Fermi surface across p^* , while thermodynamic measurements find a strong enhancement of the specific-heat coefficient near the same regime [14–19]. Further, the strange-metal region of the phase diagram features several aspects associated with quantum criticality, such as ω/T scaling and anomalous metallic behavior inconsistent with coherent quasiparticles, both within a fan-like shape that appears to emanate from p^* . Some experimental data also suggests an extended quantum critical region [12, 20], which has been argued to be a result of disorder [21].

The description of such a PG-QCP poses a major challenge. This is because on the one hand, the PG metal itself is still mysterious and not completely understood, while on the other hand, this QCP, if present, does not seem to be a conventional order-parameter driven QCP describable by Hertz–Millis–Moriya theory [22–24]. Several routes to describe the PG metal and the PG-QCP have been explored, such as the idea of a fractionalized Fermi liquid with topological order that is separated from the normal FL by a deconfined QCP [25–34]; fluctuating conventional order [35–46]; or non-local extensions of dynamical mean-field theory (DMFT) [47–50].

In particular, cluster DMFT approaches to the Hubbard model have been very successful in capturing PG metal physics [28, 29, 50–72]. For instance, these have successfully captured the depression of spectral weight at the Fermi level [49], the reconstructed Fermi surface due to the presence of Luttinger surfaces [55], and the momentum-dependence of spectral weight along the Fermi surface that leads to Fermi arcs and to the nodal–antinodal dichotomy [52].

Interestingly, it seems that all of this physics can be captured with relatively small four-site clusters, and the qualitative results do not strongly depend on the type of cluster scheme or periodization used. However, the precise nature of the PG metal, in particular the nature and structure of its low-energy excitations, has not been established so far. Furthermore, the existence of a QCP separating the PG metal from the normal FL within cluster DMFT is controversial. While some work found apparent evidence for a QCP, Sordi *et al.* [68] established that within a certain parameter region ($t'/t = 0$, $U/t \leq 6$) criticality is associated with the finite-temperature endpoint of a first-order transition.

The main limitation in establishing the existence or

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not of a PG-QCP in a relevant parameter regime of the Hubbard model within cluster DMFT has been insufficient low-energy and low-temperature resolution, and the inability to access the relevant parameters directly. In this work, we overcome this limitation by using four-patch DCA together with the numerical renormalization group (NRG) as a cluster impurity solver. NRG can resolve exponentially low energy and temperature scales and can access arbitrary parameters, though NRG is limited by Hilbert space size. We therefore deliberately restrict calculations to the normal state and do not consider symmetry-broken solutions. For details on the methods see Sec. III and Supplemental Material S-I.

To describe cuprate physics, we use the square lattice Hubbard model with Hamiltonian

$$H = \sum_{\mathbf{r}\mathbf{r}'} -t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} - \mu \sum_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} \\ = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \quad (1)$$

where $c_{\mathbf{r}\sigma}$ annihilates a spin- σ electron at site $\mathbf{r}$, $n_{\mathbf{r}\sigma} = c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma}$. For the hopping matrix elements $t_{\mathbf{r}\mathbf{r}'}$, we consider nearest and next-nearest neighbor terms, denoted t and t' . We set $t = 1$ as our unit of energy and choose $t'/t = -0.3$ and $U/t = 7$, suitable for describing cuprate physics. We tune μ to adjust the hole-doping p (filling $n = 1 - p$). We study this model using four-patch DCA+NRG (see Sec. S-I of the supplemental material (SM) [73]) and analyze its physics by computing several real-frequency correlators involving local or short-ranged operators defined on the cluster, see Sec. III on Methods.

I. RESULTS

A. Phase diagram

Figure 1(a) shows the doping-driven, zero-temperature normal-state phase diagram obtained from DCA+NRG. Since symmetry breaking is excluded, all regimes shown are normal-state solutions. For $p > 0$, we find two metallic phases: a normal FL for $p > p^*$ and a PG metal for $p < p^*$. The critical doping $p^* = 0.14$ is the only point in this part of the phase diagram where we find a genuine quantum phase transition. Its central signatures are (i) the continuous suppression of the FL coherence scale as p^* is approached from either side, and (ii) the abrupt change of the low-frequency cluster spectral functions in the antinodal patches, $\mathbf{K} = (0, \pi)$ and $\mathbf{K} = (\pi, 0)$, from exhibiting a narrow metallic pseudogap for $p < p^*$ to a sharp resonance for $p > p^*$ [cf. Fig. 3, discussed later].

The markers p_{LS} and p_{Σ} at lower doping in Fig. 1 have a different status: rather than additional quantum phase transitions, they denote crossovers within the PG metal, associated with changes in the Luttinger-surface and self-energy-pole structure familiar from cluster studies of the pseudogap [55, 57, 58, 63]. Upon increasing p

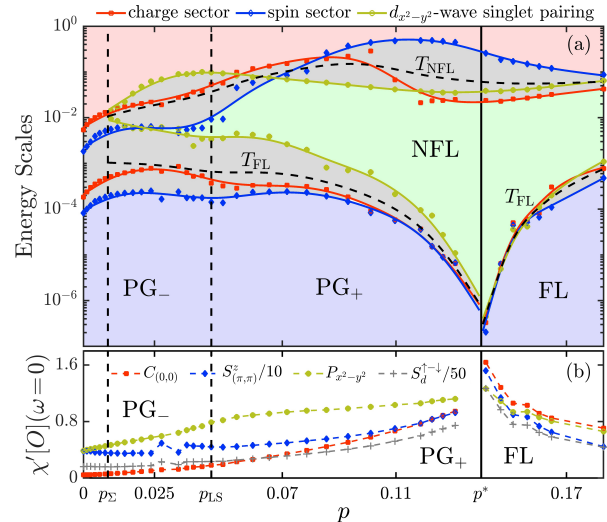


FIG. 1. Doping-driven, zero-temperature normal-state phase diagram and static susceptibilities of the square lattice Hubbard model with $U = 7t$ and $t' = -0.3t$, obtained with DCA+NRG. (a) Crossover energy scales (dots) extracted from the frequency dependence of dynamical cluster susceptibilities $\chi[O](\omega)$ for operators O describing charge (red), spin (blue) and d -wave pairing (green) [see Eqs. (3)]. Colored lines are guides-to-the-eye. The geometric averages of the lower-lying or upper-lying three crossover scales are indicated by black curves marked T_{FL} or T_{NFL} , respectively. For $p > 0$, we find FL behavior for energies below T_{FL} , and non-Fermi-liquid (NFL) behavior for energies between T_{FL} and T_{NFL} . There are several low-energy FL phases: a normal FL for $p > p^*$ and a PG metal for $p < p^*$, separated by a QCP at $p^* = 0.14$ (vertical solid line) where T_{FL} is suppressed to zero. The PG metal comprises two sub-regimes, PG₋ and PG₊, which are not separated by a phase transition (see the text for definitions of p_{LS} and p_{Σ} , vertical dashed lines). (b) Selected static susceptibilities $-\chi'[O](\omega = 0)$ as functions of doping p .

from the Mott-insulating side, the antinodal gap starts to fill when p rises above p_{LS} ; equivalently, upon decreasing p from within the PG₊ regime, the partially filled antinodal pseudogap becomes fully gapped when p drops below p_{LS} . The doping p_{Σ} denotes the point where the antinodal self-energy pole crosses the Fermi level. Neither p_{LS} nor p_{Σ} is accompanied by a suppression of the FL scale. In the discussion below, we therefore first focus on the PG₊ and normal FL regimes ($p > p_{LS}$), in particular the vicinity of p^* , before briefly returning to these two crossovers at lower doping.

To identify the quantum phase transition at p^* , we track energy scales extracted from dynamical susceptibilities of local charge, spin and d -wave pairing operators. The corresponding operators and computational details are discussed in Sec. III. As a representative example, Fig. 2 shows the doping dependence of $\chi''[P_{x^2-y^2}](\omega)$, the spectral part of the local d -wave pair susceptibility. At frequencies below a crossover scale T_{FL} , $\chi''(\omega)$ shows

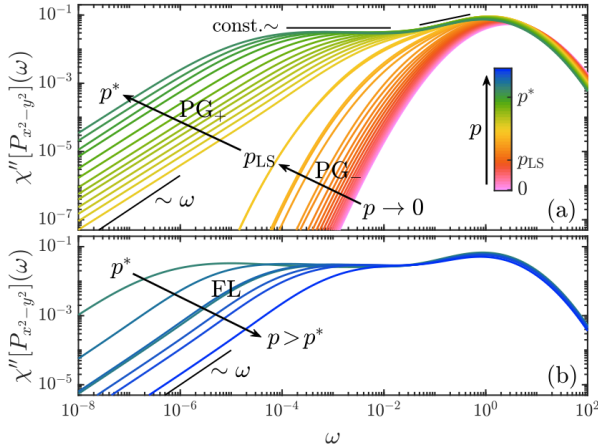


FIG. 2. Doping evolution of the local $d_{x^2-y^2}$ -wave singlet-pair spectrum $\chi''[P_{x^2-y^2}](\omega)$ on a log-log scale. (a) Evolution from small doping in the PG_- regime (pink), through p_{LS} , and toward p^* (green). (b) Evolution from p^* into the overdoped FL regime (blue). Arrows indicate increasing p . The guide-to-the-eye lines mark the low-frequency FL behavior, $\chi'' \propto \omega$, and the intermediate-frequency NFL plateau $\chi'' \propto \text{const.}$; the crossover between them defines the FL scale T_{FL} . Approaching p^* from either side, this scale is suppressed, and the plateau extends to ever lower frequencies. The upper end of the plateau defines the NFL scale T_{NFL} .

linear-in- ω behavior typical of a FL. We have checked that the NRG finite-size many-body are indeed Fermi liquid spectra for both $p > p^*$ and $p < p^*$. The FL scale is continuously suppressed to zero at p^* , signaling a QCP governed by a non-Fermi liquid fixed point. Figure 1(b) shows $\chi'(\omega = 0)$, the real part of the static charge, spin and pairing susceptibilities; all exhibit a pronounced peak and possibly a divergence at p^* .

Returning to Fig. 2 for $\chi''[P_{x^2-y^2}](\omega)$ as a representative example, we next describe how we identified the various crossover energy scales and regimes. Starting from high frequencies, χ'' exhibits a broad maximum around $\omega \simeq 1$ and decreases toward lower frequencies. Near p^* , an intermediate-frequency plateau emerges, $\chi''(\omega) \propto \text{const.}$, reminiscent of bosonic spectra in the non-Fermi-liquid regimes of, for instance, the two-channel and two-impurity Kondo models. At even lower frequencies, this plateau crosses over to FL behavior, with $\chi''(\omega) \propto \omega$. As p^* is approached from either side, the FL crossover scale is pushed to ever lower frequencies and the plateau correspondingly extends downward. At the QCP, our data suggest that the plateau persists to $\omega \rightarrow 0$, which would imply a logarithmical divergence for $\chi'(\omega = 0)$, the real part of the static susceptibility. The evolution with doping of $\chi''[P_{x^2-y^2}](\omega)$ across p^* is otherwise smooth, consistent with a continuous quantum phase transition.

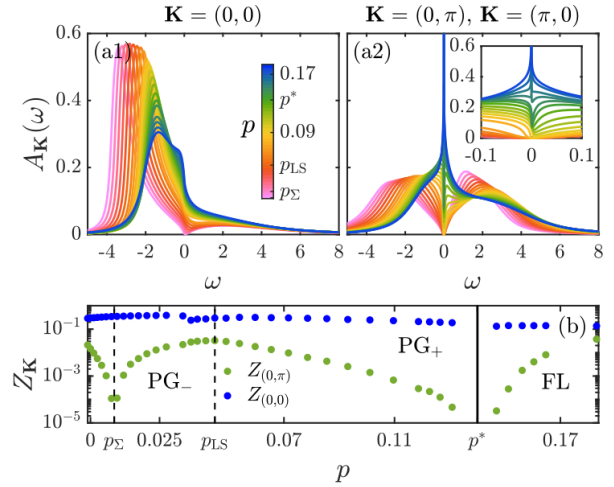


FIG. 3. Patch spectral functions and quasiparticle weights. (a1,a2) Cluster spectral functions $A_{\mathbf{K}}(\omega)$ of the nodal patch $\mathbf{K} = (0,0)$ and the antinodal patches $\mathbf{K} = (0,\pi)$, equivalently $\mathbf{K} = (\pi,0)$. The inset shows details of the low-frequency region around $\omega = 0$; colors indicate doping. Across p^* , the antinodal spectrum changes from a resonance for $p > p^*$ to a pseudogap for $p < p^*$, whereas the nodal spectrum evolves smoothly. (b) Corresponding quasiparticle weights $Z_{\mathbf{K}} = [1 - \partial_\omega \text{Re} \Sigma_{\mathbf{K}}(\omega)|_{\omega=0}]^{-1}$ versus doping for the same patches. Vertical lines mark p^* , p_{LS} , and p_Σ . The antinodal $Z_{(0,\pi)}$ is suppressed to zero at p^* and again at p_Σ ; the latter occurs because the antinodal self-energy pole crosses $\omega = 0$. The nodal $Z_{(0,0)}$ remains finite within numerical resolution. The $\mathbf{K} = (\pi,\pi)$ patch is omitted because it remains gapped.

B. Single-particle spectra

The same transition is visible in the single-particle spectra. Figures 3(a1) and 3(a2) show the cluster spectral functions $A_{\mathbf{K}}(\omega)$ of the patches $\mathbf{K} = (0,0)$ [or equivalently $\mathbf{K} = (\pi,0)$], respectively. These correspond to the momentum-averages of the lattice spectral functions in the nodal and antinodal regions, respectively. For $p > p_{\text{LS}}$, the Fermi surface is located within in these patches, and the corresponding patch spectral functions are therefore metallic, i.e. $A_{\mathbf{K}}(\omega = 0) > 0$. The $\mathbf{K} = (\pi,\pi)$ patch is not shown, since it remains gapped for all dopings considered.

While $A_{(0,0)}$ [Fig. 3(a1)] evolves smoothly with doping through the transition, $A_{(0,\pi)}$ [Fig. 3(a2)] changes sharply at the Fermi level. For $p > p^*$, in the normal FL, $A_{(0,\pi)}$ contains a narrow resonance at $\omega = 0$ [inset of Fig. 3(a2)], which sharpens as p is lowered toward p^* . For $p < p^*$, this resonance gives way to narrow PG. This PG arises due to a pole in the antinodal self-energy that emerges at $p < p^*$, see Fig. S5(b2) of the SM [73]. In the PG_+ regime ($p_{\text{LS}} < p < p^*$), the PG is still partially filled, $A_{(0,\pi)}(\omega = 0) > 0$, so the antinodal patches still contribute quasiparticle excitations and a Fermi-surface segment.

Figure 3(b) shows the corresponding quasiparticle

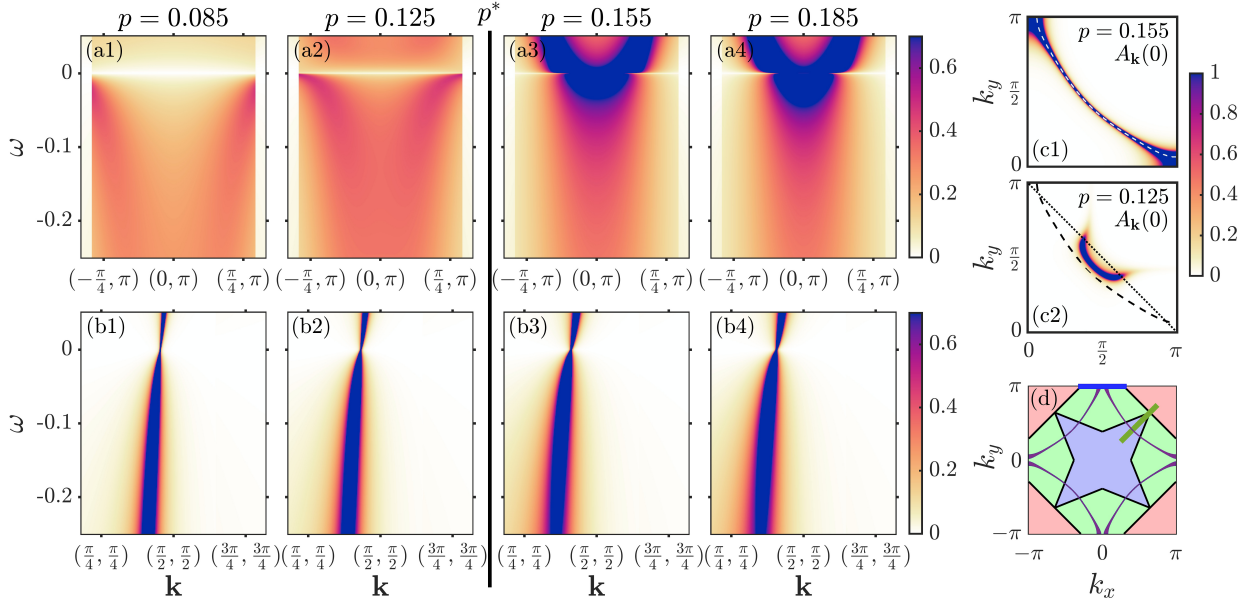


FIG. 4. Momentum-resolved spectral functions on both sides of the pseudogap QCP at p^* . (a,b) Non-interpolated DCA spectra $A_{\mathbf{k}}(\omega)$ along antinodal and nodal cuts [indicated in (d)], respectively. Columns show dopings below and above $p^* \simeq 0.14$; the black vertical separator marks p^* . For the antinodal cut (a), the low-energy spectral weight present on the FL side ($p > p^*$) is strongly depleted on the PG side ($p < p^*$), whereas for the nodal cut (b) the low-energy spectrum evolves smoothly. (c1,c2) $\mathcal{L}$ -interpolated zero-frequency spectral function $A_{\mathbf{k}}(0)$ in the FL at $p = 0.155 > p^*$ and in the PG₊ regime at $p = 0.125 < p^*$, respectively. In (c1), the curved dashed line denotes the locus of maximal $A_{\mathbf{k}}(0)$; it is shown in (c2), too, as a reference for the unreconstructed Fermi surface; the straight dashed line in (c2) marks the antiferromagnetic zone boundary. (d) DCA patch geometry, showing the antinodal (thick blue) and nodal (thick green) momentum cuts used for (a) and (b), respectively, and the Fermi surface (purple) depicted in (c1).

weights, $Z_{\mathbf{K}} = [1 - \partial_{\omega} \text{Re} \Sigma_{\mathbf{K}}(\omega)|_{\omega=0}]^{-1}$, obtained from a numerical derivative of the corresponding real part of the patch self-energy. On approaching the QCP from either side, $Z_{(0,\pi)}$ is suppressed to zero. This is consistent both with the change of the low-frequency structure of $A_{(0,\pi)}(\omega)$ and with the collapse of the FL scale in the cluster susceptibilities.

By contrast, $Z_{(0,0)}$ appears to remain finite across the transition. Taken at face value, this would suggest a momentum-selective NFL at the QCP. However, this apparent patch selectivity should not be overinterpreted: it is difficult to reconcile a non-zero nodal quasiparticle weight with the vanishing FL scale that we observe for several cluster susceptibilities at the QCP [cf. Fig. 1(a)]. Following arguments from marginal FL (MFL) phenomenology [74], scattering of the $\mathbf{K} = (0,0)$ electrons off short-ranged critical bosonic fluctuations as found, for instance, in Fig. 2 should generate at least a logarithmically weak suppression of $Z_{(0,0)}$, with $Z_{(0,0)}^{-1}$ growing as $\ln(1/T_{\text{FL}})$ close to the QCP. However, resolving such a logarithmic dependence requires highly accurate numerics extremely close to p^* . In a follow-up paper [75], where we examine quantum critical scaling in the finite-temperature NFL region, we find evidence for MFL physics in the $\mathbf{K} = (0,0)$ patch from an ω/T

scaling analysis. A definitive zero-temperature statement on the nodal quasiparticle weight will require additional methodological improvements and is left for future work.

The PG metal below p^* is further subdivided into PG₊ for $p^* > p > p_{\text{LS}}$ and PG₋ for $p < p_{\text{LS}}$. This subdivision reflects changes in the antinodal spectral weight that occur smoothly, not an additional quantum phase transition. In PG₊ the antinodal pseudogap is partially filled, whereas at p_{LS} it becomes fully gapped upon lowering p , see Fig. 3(a2) and its inset. Equivalently, upon increasing the doping from the Mott insulator at $p = 0$, p_{LS} is the point where antinodal spectral weight at the Fermi level first appears. Thus, in PG₋ only the $\mathbf{K} = (0,0)$ patch remains metallic; the state is a patch-selective metal with insulating antinodal patches. Because the full gap in $A_{(0,\pi)}(\omega)$ opens smoothly and the FL scale is not suppressed at p_{LS} , this crossover is distinct from the QCP at p^* . The mechanism for the full antinodal gap is analogous to that of Ref. [58] and is discussed further in Fig. S6 of the SM [73].

The full antinodal gap for $p < p_{\text{LS}}$ leads to a suppression of the low-frequency spectral weight of bosonic dynamical susceptibilities. In particular, the local d -wave pair spectrum decreases faster than linear-in- ω at low frequencies [Fig. 2(a)], reflecting the absence of antinodal

quasiparticle excitations. Other susceptibilities, such as the uniform charge susceptibility on the cluster (see Fig. S3 of the SM [73]), remain linear in ω , but with a much smaller slope than for $p > p_{LS}$.

As the doping is reduced further, a more subtle crossover occurs at p_{Σ} . There, the antinodal self-energy pole that suppresses $A_{(0,\pi)}(\omega)$ near $\omega = 0$ crosses from positive to negative frequency. This crossing produces a zero of $Z_{(0,\pi)}$ [Fig. 3(b)], because $\Sigma_{(0,\pi)}(0)$ diverges at p_{Σ} . It does not produce a new feature in the spectral function, though, since $A_{(0,\pi)}(\omega)$ is already fully gapped at this point. Thus, in stark contrast to the collapse $Z_{(0,\pi)} \rightarrow 0$ at p^* , the zero of $Z_{(0,\pi)}$ at p_{Σ} does not signal the destruction of existing QPs.

For completeness, we have mapped out the phase diagram for several values of the next-nearest-neighbor hopping, $t'/t \leq 0$, at fixed $U = 7t$; the resulting characteristic dopings are summarized in Fig. S8 of the SM [73]. The dopings p^* , p_{LS} , and p_{Σ} all shift quantitatively with t' , but the overall physical picture remains qualitatively unchanged. This indicates that the discussion above is not special to the representative choice $t' = -0.3t$, but is a robust feature of the square-lattice Hubbard model within the parameter range studied.

C. Fermi surface reconstruction

As discussed above, the QCP is marked by a sharp change in the single-particle spectra of the antinodal patches: the $\mathbf{K} = (0, \pi)$ and $\mathbf{K} = (\pi, 0)$ spectra lose their low-energy FL resonance and develop a narrow pseudogap, while the $\mathbf{K} = (0, 0)$ spectrum evolves smoothly across p^* . This is the cluster analogue of the ARPES phenomenology of the cuprate PG, where low-energy spectral weight is strongly depleted near the antinode when entering the PG regime, while Fermi arcs survive around the node [8–12, 76].

These signatures of cluster spectra have a direct momentum-resolved manifestation. Figure 4 shows how the momentum-resolved spectral functions, $A_{\mathbf{k}}(\omega)$, evolve with doping across the QCP. Rows (a) and (b) show non-interpolated DCA spectra along antinodal and nodal cuts [indicated in panel (d)], respectively. Along the antinodal cut, the coherent low-energy weight present for $p > p^*$ is strongly depleted once $p < p^*$, consistent with the pseudogap in the antinodal patch spectral function of Fig. 3(a2) and with the suppression of $Z_{(0,\pi)}$ in Fig. 3(b). Along the nodal cut, by contrast, the dispersive low-energy feature changes only weakly with doping, in line with the smooth evolution of $A_{(0,0)}(\omega)$. A phenomenologically similar doping-driven evolution of spectral weight is found experimentally in Bi2212 [12, 76].

The spectral functions at the Fermi level at $p = 0.125 < p^*$ (PG₊) and $p = 0.155 > p^*$ (FL) are shown in Figs. 4(c1,c2). They are computed using an interpolated self-energy $\Sigma_{\mathbf{k}}(\omega)$ obtained using Liouvillian ($\mathcal{L}$) interpolation [77]. At $p = 0.155 > p^*$ in the normal FL,

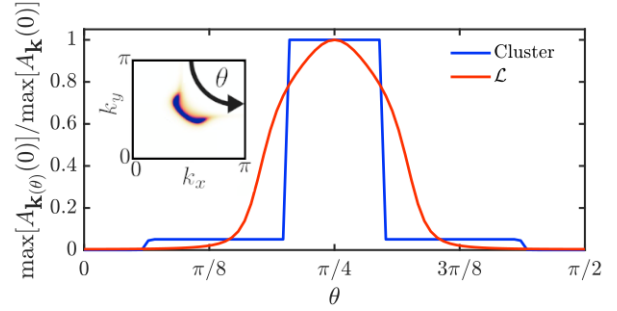


FIG. 5. Angular distribution of the zero-frequency spectral weight along the Fermi surface in the PG₊ regime at $p = 0.125$. For each ray ℓ_{θ} emanating from (π, π) at a specified angle θ as indicated in the inset, we plot $\max_{\mathbf{k} \in \ell_{\theta}} A_{\mathbf{k}}(\omega = 0)$, normalized by its maximum value. Blue: the direct DCA cluster result, with abrupt steps at the patch boundaries; red: Liouvillian ($\mathcal{L}$) interpolation smooths out the steps.

the spectral weight is distributed evenly along the Fermi surface [dashed line in Fig. 4(c1)]. Further, the Fermi surface volume is consistent with the Luttinger sum rule. Its shape roughly resembles that of the free system, since the self-energy is only weakly momentum dependent. By contrast, at $p = 0.125 < p^*$ in the PG₊ region, the spectral weight depends strongly on the position along the Fermi surface: it exhibits prominent spectral weight in the nodal region and vanishingly small spectral weight in the antinodal region, leading to Fermi arcs which seem to terminate at the antiferromagnetic zone boundary.

Figure 5 quantifies this by showing the distribution of the zero-frequency spectral weight along the Fermi surface in the PG₊ regime. This quantity corresponds to that measured in ARPES studies aimed at analyzing the quasiparticle weight (see, e.g. Refs. [78, 79]). The cluster result (blue) exhibits a step-like profile, while Liouvillian interpolation (red) provides a smooth interpolation. Similar to experimental findings [78, 79], we find a maximum around $\theta = \pi/4$ (nodal region), with strongly decaying flanks approaching zero around $|\theta - \pi/4| \gtrsim \pi/8$ (antinodal region).

II. CONCLUSION

Using DCA+NRG, we have mapped out the doping-driven, zero-temperature normal-state phase diagram of the square-lattice Hubbard model at $U = 7t$, focusing on $t' = -0.3t$ (for other values of $t'/t \leq 0$, see the SM [73]). For hole doping $p > 0$, we find two distinct metallic phases: a PG metal for $p < p^*$ and a normal FL for $p > p^*$. These are separated by a QCP at the critical doping p^* , where the FL scale T_{FL} is suppressed to zero. At intermediate energy scales in the vicinity of the QCP, various dynamical susceptibilities display NFL behavior. We thus settle a long-standing open question: the NFL behavior observed in DMFT treatments of this

model indeed does stem from a QCP. We provide a detailed finite-temperature analysis of the NFL regime in Ref. [75].

In future work, it would be interesting to make a more detailed connection with previous cluster DMFT studies of the doped Hubbard model [52, 55, 57, 58, 63, 68], in particular with the work of Sordi *et al.* [68]. That work showed that for $t' = 0$ and $U/t \leq 6$, the PG-to-normal FL transition is first-order, and criticality is associated with a finite-temperature critical endpoint. In the parameter regime studied here, we do not find evidence for a first-order transition; instead, the FL scale appears to vanish continuously at p^* and physical observables evolve smoothly across p^* . Nevertheless, we cannot exclude a very narrow coexistence region, or a critical endpoint at exponentially low temperatures. It would therefore be useful to use cluster DMFT+NRG to bridge the gap between the regime studied here and that of Sordi *et al.* [68].

III. METHODS

To obtain approximate normal-state solutions of the doped square-lattice Hubbard model, we employ a four-patch DCA scheme, which approximates the momentum dependence of the self-energy as piecewise constant within patches. These are labeled by the momenta at the center of the patch, $\mathbf{K}_1 = (0, 0)$, $\mathbf{K}_2 = (0, \pi)$, $\mathbf{K}_3 = (\pi, 0)$ and $\mathbf{K}_4 = (\pi, \pi)$. We use the “star patching geometry” of Ref. [63] (see Fig. 4(d), and Sec. S-I of the SM [73] for details), which includes the nodal points $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ in the patch centered around $\mathbf{K}_1$. For details on the numerical evaluations of local lattice Green’s functions and hybridization functions, see Sec. S-I A of the SM [73].

The cluster impurity model is solved using the MuNRG implementation [80, 81] of NRG [82–86], based on the QSpace tensor library [87–91]. We exploit U(1) charge and SU(2) spin symmetry, use a discretization parameter $\Lambda = 8$ without z -shifting. We retain up to $N_{\text{keep}} = 3 \cdot 10^4$ U(1)×SU(2) multiplets, which results in truncation energies $E_{\text{trunc}} \geq 5$. We further employ a fully interleaved Wilson chain geometry [92, 93] with bath modes ordered as $\mathbf{K}_1 = (0, 0)$, $\mathbf{K}_2 = (\pi, 0)$, $\mathbf{K}_3 = (0, \pi)$, and $\mathbf{K}_4 = (\pi, \pi)$. Discrete NRG data are broadened using a log-Gaussian scheme [80] with broadening parameter $\sigma = 0.7$, and self-energies $\Sigma_{\mathbf{K}}(\omega)$ are computed using Kugler’s symmetric estimator approach [86]. Although interleaving formally breaks the symmetry between the $(\pi, 0)$ and $(0, \pi)$ patches, the resulting self-energies differ by less than 10^{-3} . We therefore enforce the symmetry in the DMFT loop by setting $\Sigma_{(0,\pi)}(\omega) \leftarrow \Sigma_{(\pi,0)}(\omega)$ in each iteration.

We analyze the physics of this model both through electronic spectral functions and by computing real-frequency dynamical susceptibilities for several local or short-ranged operators defined on the cluster. Suscepti-

bilities are defined by

$$\chi[O](\omega) = -i \int_0^\infty dt e^{i(\omega+i0^+)t} \langle [O(t), O^\dagger(0)] \rangle, \quad (2)$$

where O is some bosonic operator acting non-trivially only on the cluster, and $\langle \cdot \rangle$ denotes the thermal expectation value. We compose them as $\chi = \chi' - i\pi\chi''$ into a real part χ' and a spectral part χ'' . Within NRG, we compute discrete spectral functions, broaden them with a log-Gaussian, and then compute χ' via Kramers-Kronig. In the vicinity of fixed points, spectral functions of dynamical susceptibilities usually exhibit power-law behavior, i.e. straight lines on a log-log scale. We infer crossover energy scales by inflection points of the spectra on the log-log scale (see Fig. S4 of Ref. [73]).

The operators discussed in the main text, whose energy scales are presented in Fig. 1, are defined as:

$$C_{\mathbf{Q}} = \sum_{\mathbf{K}, \sigma\sigma'} c_{\mathbf{K}+\mathbf{Q}, \sigma}^\dagger \delta_{\sigma\sigma'} c_{\mathbf{K}, \sigma'}, \quad (3a)$$

$$S_{\mathbf{Q}}^z = \sum_{\mathbf{K}, \sigma\sigma'} c_{\mathbf{K}+\mathbf{Q}, \sigma}^\dagger \sigma_{\sigma\sigma'}^z c_{\mathbf{K}, \sigma'}, \quad (3b)$$

$$P_{x^2-y^2} = \sum_{\sigma\sigma'} (c_{\delta\mathbf{X}, \sigma} - c_{\delta\mathbf{Y}, \sigma}) i\sigma_{\sigma\sigma'}^y c_{\mathbf{0}, \sigma'}, \quad (3c)$$

$$S_d^{\uparrow\downarrow} = \sum_{\sigma\sigma'} (c_{\delta\mathbf{D}, \sigma}^\dagger - c_{\mathbf{0}, \sigma}^\dagger) \sigma_{\sigma\sigma'}^z (c_{\delta\mathbf{D}, \sigma'} - c_{\mathbf{0}, \sigma'}) \quad (3d)$$

Here, σ^z and σ^y are Pauli matrices in the spin sector, $\mathbf{K}$, $\mathbf{Q}$ are DCA patch momenta, and $\delta\mathbf{X}$, $\delta\mathbf{Y}$, $\delta\mathbf{D} = \delta\mathbf{X} + \delta\mathbf{Y}$ denote real-space displacements on the cluster relative to its site $\mathbf{0}$. For Fig. 1(a), the crossover scales in the charge and spin sectors were extracted from susceptibilities $\chi''[C_{\text{loc}}]$ and $\chi''[S_{\text{loc}}^z]$ involving the local charge and spin operators,

$$C_{\text{loc}} = \frac{1}{\sqrt{4}} \sum_{\mathbf{Q}} C_{\mathbf{Q}}, \quad S_{\text{loc}}^z = \frac{1}{\sqrt{4}} \sum_{\mathbf{Q}} S_{\mathbf{Q}}^z. \quad (4)$$

Further operators for which we computed susceptibilities [Figs. S2, S4] and details on the extraction of energy scales [Fig. S3] are provided in Supplement S-II [73].

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Supplemental Material for “Quantum criticality in the two-dimensional Hubbard model”

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S-I. MODEL AND METHOD

The model we use to describe the cuprate physics is the Hubbard model [94, 95]. Its lattice Hamiltonian reads

$$\begin{aligned} H &= \sum_{\mathbf{r}\mathbf{r}'\sigma} -t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} - \mu \sum_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} \\ &= \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \end{aligned} \quad (\text{S1})$$

where $c_{\mathbf{r}\sigma}^{(\dagger)}$ are creation and annihilation operators in real space, and $n_{\mathbf{r}\sigma} = c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}\sigma}$ denotes the number operator. Indices $\mathbf{k}$ refer to momentum space. The first, second and third terms represent the kinetic energy with hopping matrix elements $t_{\mathbf{r}\mathbf{r}'}$, the energy shift due to the chemical potential μ , and the local on-site Coulomb interaction U , respectively. The kinetic energy contains only nearest-neighbor (t) and next-nearest-neighbor (t') hopping terms, leading to the band dispersion $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$ and μ is used to control the doping p . Throughout, we use the parameters $t = 1$, $U = 7t$, focusing on $t'/t = -0.3$ in the main text and exploring $t'/t = \{0, -0.15, -0.2, -0.25, -0.3\}$ in Fig. S8. The temperature is set to $T = 10^{-10}t$.

We solve the model by means of DCA [48–50, 63, 96], due to mapping on a 2×2 cluster impurity

$$\begin{aligned} H_{\text{imp}} &= \sum_{\mathbf{R}\mathbf{R}'\sigma} -\bar{t}_{\mathbf{R}\mathbf{R}'} c_{\mathbf{R}\sigma}^\dagger c_{\mathbf{R}'\sigma} - \mu \sum_{\mathbf{R}\sigma} n_{\mathbf{R}\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow} \\ &= \sum_{\mathbf{K}\sigma} (\epsilon_{\mathbf{K}} - \mu) n_{\mathbf{K}\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow}, \end{aligned} \quad (\text{S2})$$

where $\mathbf{R}$ denotes cluster impurity sites and $\mathbf{K}$ the momentum averaged patches of the Brillouin zone (BZ) of the lattice model. On the impurity level the diagonal representation of the annihilation/creation operators $c_{\mathbf{K}\sigma}^{(\dagger)} = \sum_{\mathbf{R}} V_{\mathbf{K}\mathbf{R}} c_{\mathbf{R}\sigma}^{(\dagger)}$ are found by diagonalization $V_{\mathbf{K}\mathbf{R}} \bar{t}_{\mathbf{R}\mathbf{R}'} = \lambda_{\mathbf{K}\mathbf{K}'} V_{\mathbf{K}'\mathbf{R}'}$. The energies

$$\epsilon_{\mathbf{K}} = \int d\epsilon \rho_{\mathbf{K}}(\epsilon) \epsilon, \quad \rho_{\mathbf{K}}(\epsilon) = \int_{V_{\mathbf{K}}} \frac{d\mathbf{k}}{V_{\mathbf{K}}} \delta(\epsilon - \epsilon_{\mathbf{k}}), \quad (\text{S3})$$

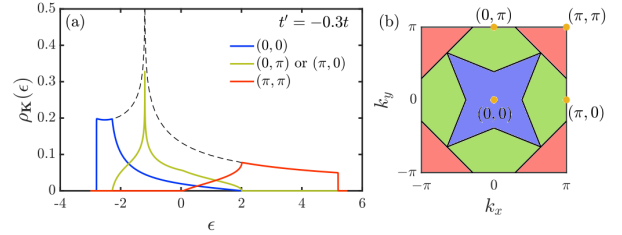


FIG. S1. (a) Patch resolved density of states (DoS) $\rho_{\mathbf{K}}(\epsilon)$ for $t' = -0.3t$. The dashed line indicates the sum of the four patches. (b) Corresponding patch geometry, referred to as “star geometry”.

where we integrate over momentum patches $V_{\mathbf{K}}$ specified by the “star patching” geometry of [63] and replotted in Fig. S1(b). Note that nodal point $\mathbf{k} = (\pi/2, \pi/2)$ is included in patch $\mathbf{K} = (0,0)$. The corresponding patch density of states, $\rho_{\mathbf{K}}(\epsilon)$, for $t' = -0.3t$ are shown in Fig. S1(a). The dashed line indicates the sum of the four patches.

A NRG impurity solver [80, 82–85] is employed to evaluate the self-energy $\Sigma_{\mathbf{K}}(z)$ by the means of the improved estimator approach [86]. Within NRG we interleave all four cluster momenta [92, 93], where the antinodal patches are symmetric. Therefore, references to patch $(0, \pi)$ also refer implicitly to $(\pi, 0)$. We use the QSpace library [87–91] to keep track of symmetries. An $U(1)$ charge and $SU(2)$ spin symmetry is enforced on the system prohibiting symmetry-breaking and the emergence of superconductivity. Within the computation we use a discretization $\Lambda = 8$, no z -shifting, and kept multiplets of $N_{\text{keep}} \leq 3 \cdot 10^4$. We double-checked the convergence in N_{keep} via $N_{\text{keep}} \leq 10^5$ computations observing essentially no change in the spectral behavior of the correlators.

We use a density of states (DoS) integration for a stable computation of the local Green’s function

$$G_{\mathbf{K}}(z) = \int \frac{d\epsilon \rho_{\mathbf{K}}(\epsilon)}{z + \mu - \epsilon - \Sigma_{\mathbf{K}}(z)}, \quad (\text{S4})$$

where $z = \omega + i0^+$. To update the hybridization $\Delta_{\mathbf{K}}(z)$ for the next DCA iteration we use an asymmetric esti-

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mator approach (Sup. S-1A),

$$\Delta_{\mathbf{K}}(z) = \frac{F_{\mathbf{K}}(z)}{G_{\mathbf{K}}(z)} - \epsilon_{\mathbf{K}}, \quad F_{\mathbf{K}}(z) = \int \frac{d\epsilon \rho_{\mathbf{K}}(\epsilon) \epsilon}{z + \mu - \epsilon - \Sigma_{\mathbf{K}}(z)}. \quad (\text{S5})$$

A. Asymmetric estimator for lattice integration

In this section we discuss the computation of the hybridization, analogous to an asymmetric estimator approach within the DMFT context [86, 97]. The DCA approximation of the local lattice Green's function is

$$G_{\mathbf{K}}(\mathbf{k}, z) = \frac{1}{z + \mu - \epsilon(\mathbf{k}) - \Sigma_{\mathbf{K}}(z)}. \quad (\text{S6})$$

Rewriting and averaging over the patch volume $V_{\mathbf{K}}$ gives

$$[z + \mu - \Sigma_{\mathbf{K}}(z)]G_{\mathbf{K}}(z) - F_{\mathbf{K}}(z) = 1, \quad (\text{S7})$$

where

$$G_{\mathbf{K}}(z) = \int_{V_{\mathbf{K}}} \frac{d\mathbf{k}}{V_{\mathbf{K}}} G_{\mathbf{K}}(\mathbf{k}, z), \quad (\text{S8a})$$

$$F_{\mathbf{K}}(z) = \int_{V_{\mathbf{K}}} \frac{d\mathbf{k}}{V_{\mathbf{K}}} \epsilon(\mathbf{k}) G_{\mathbf{K}}(\mathbf{k}, z). \quad (\text{S8b})$$

Expressing these integrals as density-of-states (DoS) integrations yields Eqs. (S4) and (S5).

Adding the identity $0 = \epsilon_{\mathbf{K}} + \Delta_{\mathbf{K}}(z) - \epsilon_{\mathbf{K}} - \Delta_{\mathbf{K}}(z)$ to the first term of Eq. (S7) gives

$$[G_{\mathbf{K}}^{-1}(z) + \epsilon_{\mathbf{K}} + \Delta_{\mathbf{K}}(z)]G_{\mathbf{K}}(z) - F_{\mathbf{K}}(z) = 1, \quad (\text{S9})$$

where $G_{\mathbf{K}}^{-1}(z) = z + \mu - \epsilon_{\mathbf{K}} - \Delta_{\mathbf{K}}(z) - \Sigma_{\mathbf{K}}(z)$. Rearranging this expression leads to the asymmetric estimator for the hybridization, Eq. (S5).

Eq. (S5) provides a more stable computation of the hybridization than the Dyson equation

$$\Delta_{\mathbf{K}}(z) = z + \mu - \epsilon_{\mathbf{K}} - \Sigma_{\mathbf{K}}(z) - G_{\mathbf{K}}^{-1}(z). \quad (\text{S10})$$

Inverting numerical zeros of $G_{\mathbf{K}}(z)$ and subtracting these from $\Sigma_{\mathbf{K}}(z)$ in Eq. (S10) leads to large peak heights, that scale with numerical errors. Consequently, this approach can produce large errors near the poles of $\Sigma_{\mathbf{K}}(z)$. In contrast, these errors cancel in the quotient form of Eq. (S5), keeping numerical errors small.

S-II. SUSCEPTIBILITIES

Here, we discuss the computation and behavior of various susceptibilities $\chi''[O](\omega)$ computed on the cluster level using our NRG impurity solver. Further, we provide an example of the energy scale extraction from $\chi''[O](\omega)$.

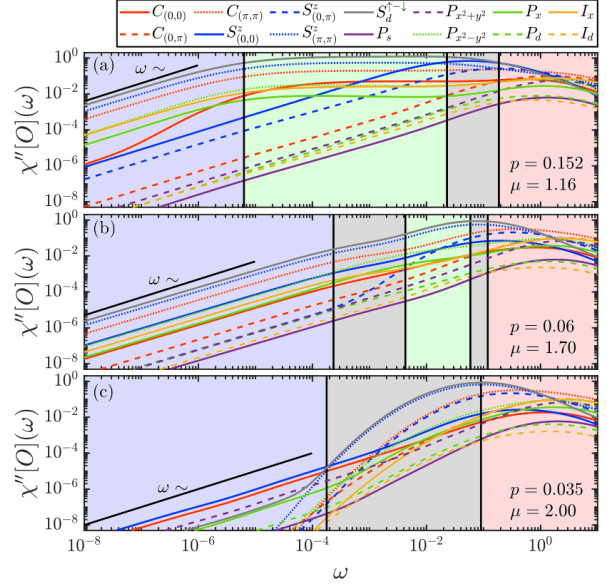


FIG. S2. Spectral parts $\chi''[O](\omega)$ of the susceptibilities of various operators O with phase regimes corresponding to Fig. 1 for (a) $p \gtrsim p^*$, (b) $p_{\text{LS}} \lesssim p \lesssim p^*$, and (c) $p_S < p < p_{\text{LS}}$. Color shadings correspond to the respective areas in Fig. 1(a).

A. Computed susceptibilities

We have computed dynamical susceptibilities $\chi[O](\omega)$, defined via Eq. (2), for the following operators:

$$C_{\mathbf{Q}} = c_{\mathbf{K}+\mathbf{Q},\sigma}^\dagger \delta_{\sigma\sigma'} c_{\mathbf{K},\sigma'} \quad (\text{momentum charge})$$

$$S_{\mathbf{Q}}^z = c_{\mathbf{K}+\mathbf{Q},\sigma}^\dagger \sigma_{\sigma\sigma'}^z c_{\mathbf{K},\sigma'} \quad (\text{momentum spin})$$

where $\mathbf{K}$ and $\mathbf{Q}$ are cluster momenta, and

$$S_d^{\pm\pm} = (c_{\delta\mathbf{D},\sigma}^\dagger \pm c_{\mathbf{0},\sigma}^\dagger) \sigma_{\sigma\sigma'}^z (c_{\delta\mathbf{D},\sigma'} \pm c_{\mathbf{0},\sigma'}) \quad (\text{stag. spin})$$

$$P_s = c_{\mathbf{0},\sigma}^\dagger i \sigma_{\sigma\sigma'}^y c_{\mathbf{0},\sigma'} \quad (s\text{-wave})$$

$$P_x = c_{\delta\mathbf{X},\sigma}^\dagger i \sigma_{\sigma\sigma'}^y c_{\mathbf{0},\sigma'} \quad (\text{NN singlet})$$

$$P_d = c_{\delta\mathbf{D},\sigma}^\dagger i \sigma_{\sigma\sigma'}^y c_{\mathbf{0},\sigma'} \quad (\text{NNN singlet})$$

$$P_{x^2 \pm y^2} = (c_{\delta\mathbf{X},\sigma}^\dagger \pm c_{\delta\mathbf{Y},\sigma}^\dagger) i \sigma_{\sigma\sigma'}^y c_{\mathbf{0},\sigma'} \quad (\text{singlet})$$

$$I_x = -it e (c_{\delta\mathbf{X},\sigma}^\dagger c_{\mathbf{0},\sigma} - \text{h.c.}) \quad (x\text{-current})$$

$$I_d = -it' e (c_{\delta\mathbf{D},\sigma}^\dagger c_{\mathbf{0},\sigma} - \text{h.c.}) \quad (\text{diagonal current})$$

where $\delta\mathbf{X}$, $\delta\mathbf{Y}$ and $\delta\mathbf{D} = \delta\mathbf{X} + \delta\mathbf{Y}$ denote real-space displacements relative to cluster site $\mathbf{0}$. Throughout, sums over repeated spin indices are implied, and σ^z and σ^y are Pauli matrices.

Figure S2 presents the spectral parts $\chi''[O](\omega)$ of various such correlators for three values of doping. Several of them, such as $\chi''[S_d^{\pm\pm}]$, exhibit plateaus that widen for $p \rightarrow p^*$, similar to those seen in Fig. 2 of the main text. Others, such as $\chi''[S_{(0,0)}^z]$, show no plateau at all; for

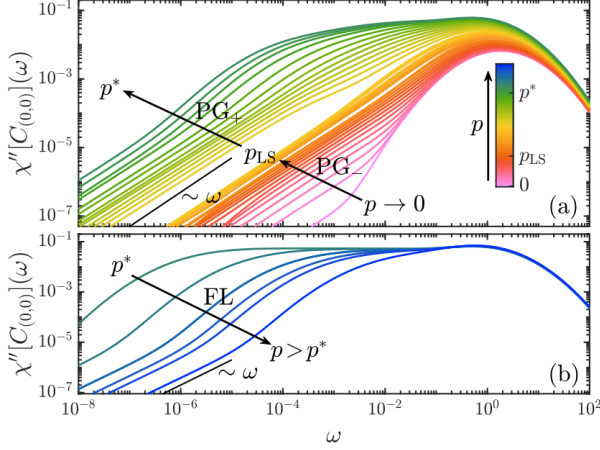


FIG. S3. Spectral part of $\chi[C_{(0,0)}](\omega)$ shown on a log-log scale. Doping evolution from (a) $p \rightarrow 0$ (pink) to p^* (green), and (b) from p^* (green) to $p > p^*$ (blue). Arrows indicate increasing p , tracing the progression through the corresponding phases.

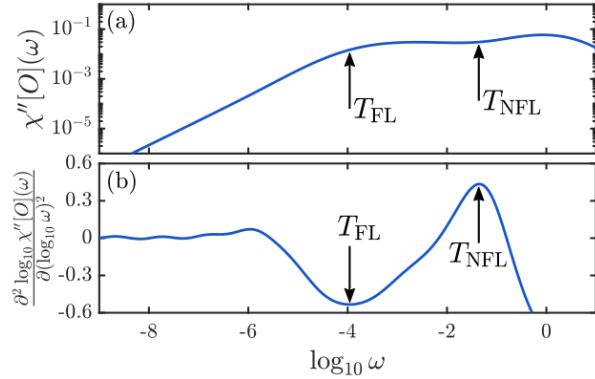


FIG. S4. (a) A spectral function $\chi''[O](\omega)$ showing a plateau. (b) Its second logarithmic derivative; we identify T_{FL} and T_{NFL} with its extrema, which align with the plateau's ends.

$p \rightarrow 0$ [Fig. S2(c)] they show faster-than-power-law decay for $\omega \rightarrow 0$, and with increasing p evolve directly to linear-in- ω behavior all the way up to $\omega \simeq T_{NFL}$ [Figs. S2(a,b)]. We have not found any obvious connection between operators whose spectra exhibit plateaus. A detailed understanding of why the spectra of so many seemingly unrelated operators exhibit this feature is left for future work.

Figure S3 displays the evolution with doping of the correlator $\chi''[C_{(0,0)}](\omega)$ in a manner similar to Fig. 2. The doping increases from $p \rightarrow 0$ to $p > p^*$, as indicated by the color gradient from pink to blue and the accompanying arrows. The positions of p_{LS} and p^* are marked accordingly.

B. Extraction of energy scales

For spectral functions that exhibit a plateau, we identify the crossover scales T_{FL} and T_{NFL} with the left and right “ends” of the plateau. There, the function

$$\frac{\partial^2 \log_{10} \chi''[O](\omega)}{\partial(\log_{10} \omega)^2} \quad (S13)$$

takes on extremal values, signifying curvature changes in $\chi''[O](\omega)$ [Fig. S4]. We identify the location of the first and second extremum with T_{FL} and T_{NFL} , respectively, a robust and reliable manner for extracting these scales.

C. Static susceptibilities

In Fig. 1(b) we present four static susceptibilities $\chi'(\omega = 0)$ that diverge for p approaching p^* , implying a divergent *local* response of the corresponding observable at p^* . This occurs for susceptibilities whose spectral parts $\chi''(\omega)$ exhibit a plateau whose extent increases towards $\omega \rightarrow 0$ for p approaching p^* .

We use Kramers-Kronig to compute $\chi'(0)$ from the corresponding spectral function $\chi''(\omega)$ obtained from NRG,

$$\chi'[O](\omega = 0) = - \int d\omega \frac{\chi''[O](\omega)}{\omega}. \quad (S14)$$

In the charge sector, the static susceptibility is directly related to the compressibility [98],

$$\kappa_T = (\partial n / \partial \mu)_T = - \lim_{\mathbf{q} \rightarrow 0} \chi'[C_{\mathbf{q}}](0), \quad (S15)$$

where $C_{\mathbf{q}} = \sum_{\mathbf{k}, \sigma} c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma}$ involves operators defined on the lattice, not the cluster. Viewing the cluster operator $C_{\mathbf{Q}=(0,0)}$ as a proxy for $C_{\mathbf{q} \rightarrow 0}$, we may expect $\chi'[C_{\mathbf{Q}=(0,0)}](0)$ to mimic the behavior of κ_T . In this regard, its discontinuous behavior seen in Fig. 1(b) is suggestive of a divergence for κ_T . We expect that increased momentum resolution and closer proximity to p^* would reveal a clear divergence, defining a second-order phase transition at the quantum critical point, since κ_T is defined as second derivative of the free energy.

S-III. PATCH GREEN'S FUNCTION, SELF-ENERGY AND HYBRIDIZATION

In this appendix, we present and discuss the spectral behavior of Green's function, self-energy and hybridization for individual patch momenta, and how the extracted critical dopings depend on t' .

A. Spectral behavior

Here, we discuss the spectral behavior of the Green's function $G_{\mathbf{K}}$, self-energy $\Sigma_{\mathbf{K}}$ and hybridization $\Delta_{\mathbf{K}}$ of

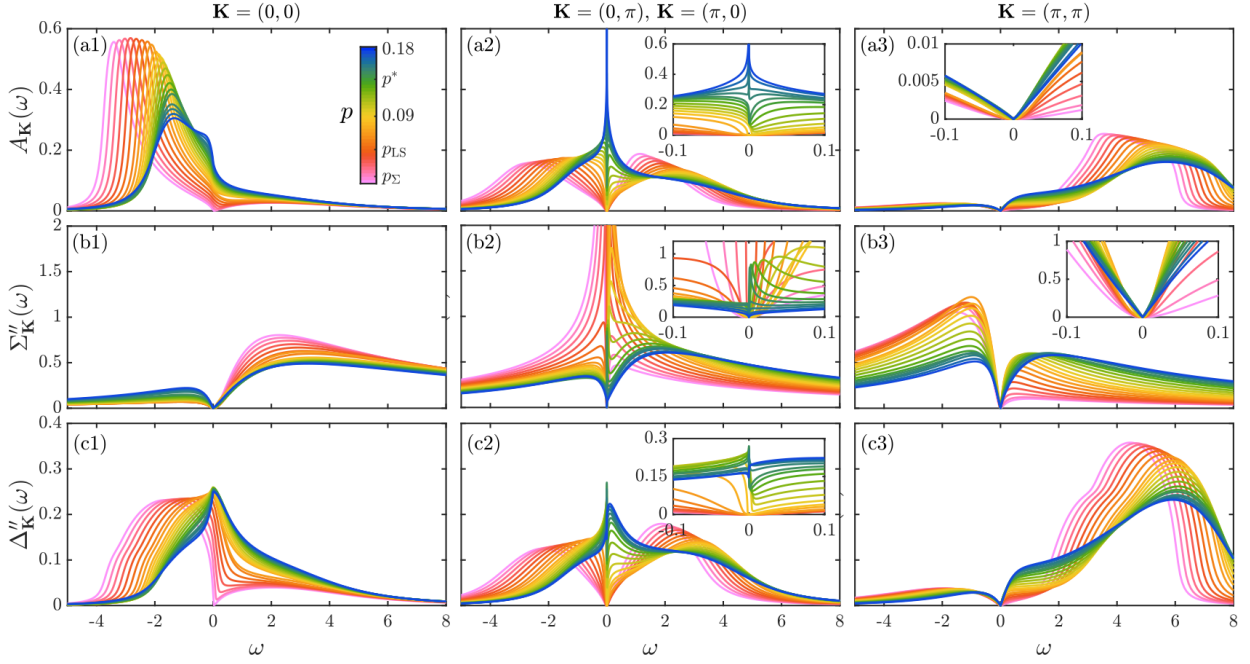


FIG. S5. Spectral parts of (a) the Green's function, (b) the self-energy and (c) the hybridization, plotted vs. frequency for various dopings (color scale). Columns (1-3) present, respectively, patch momenta $\mathbf{K} = (0,0)$, $\mathbf{K} = (0,\pi)$ or $\mathbf{K} = (\pi,0)$, and $\mathbf{K} = (\pi,\pi)$. Insets zoom in to small frequencies around $\omega = 0$.

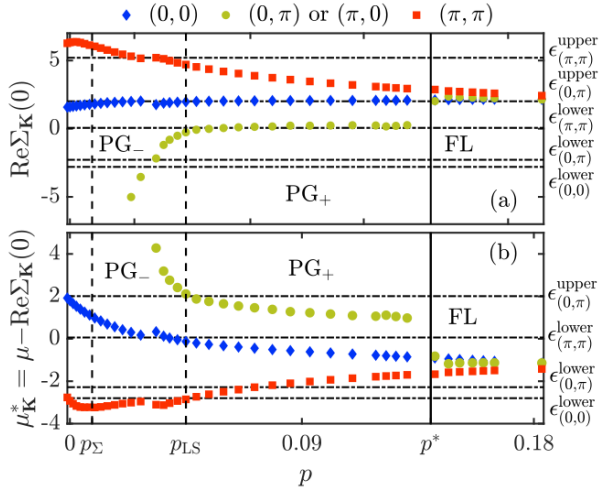


FIG. S6. (a) Real part of the self-energy at $\omega = 0$, $\text{Re}\Sigma_{\mathbf{K}}(0)$ as function of doping p . (b) $\text{Re}\Sigma_{\mathbf{K}}(0)$ shifted by the chemical potential μ . Vertical black lines indicate the characteristic dopings p_{Σ} , p_{LS} and p^* ; horizontal black lines mark $\epsilon_{\mathbf{K}}^{\text{lower}}$ and $\epsilon_{\mathbf{K}}^{\text{upper}}$, the lower and upper band edges of $\rho_{\mathbf{K}}(\epsilon)$ in Fig. S1, respectively. Here, $\epsilon_{(0,0)}^{\text{upper}} = \epsilon_{(0,\pi)}^{\text{upper}}$.

individual patches. They all exhibit significant features at p^* . Figure. S5 shows their spectral parts $X_{\mathbf{K}}''(\omega) =$

$-\frac{1}{\pi}\text{Im} X_{\mathbf{K}}(\omega)$, corresponding to $A_{\mathbf{K}}$, $\Sigma_{\mathbf{K}}''$ and $\Delta_{\mathbf{K}}''$, with color denoting doping p . As p is decreased towards p^* , the FL quasiparticle peak in $A_{(0,\pi)}$ (and $A_{(\pi,0)}$) weakens and then flips to a narrow gap-like feature [Fig. S5(a2)], while a self-energy peak in $\Sigma_{(0,\pi)}''$ emerges at $\omega = 0$ [Fig. S5(b2)]. Simultaneously, the hybridization spectrum $\Delta_{(0,\pi)}''$ becomes strongly particle-hole asymmetric around $\omega = 0$ [Fig. S5(c2)].

As p decreases, these features intensify and shift slightly to positive frequencies until reaching p_{LS} . There, the small self-energy peak in $\Sigma_{(0,\pi)}''$ merges with the upper Hubbard band, forming a broad peak that evolves into the Mott divergence as $p \rightarrow 0$. Correspondingly, $A_{(0,\pi)}(\omega)$ and $\Delta_{(0,\pi)}''(\omega)$ develop a broad gap-like feature, which evolves with the self-energy peak into the full Mott gap. Finally, when p drops below p_{Σ} , the location of the self-energy divergence changes sign from $\omega > 0$ to $\omega < 0$.

These features occur in the antinodal patches, which encompass the van Hove singularity of the non-interacting density of states [shown in Fig. S1(a)]. The nodal patch spectral functions $A_{(0,0)}$ and $A_{(\pi,\pi)}$ correspond to the lower and upper Hubbard bands, respectively. The upper edge of the lower Hubbard band lies above $\omega = 0$, yielding finite spectral weight for $A_{(\pi,\pi)}(0)$ and contributing to metallic behavior. By contrast, $A_{(\pi,\pi)}$ remains gapped at all dopings, while its self-energy spectrum $\Sigma_{(\pi,\pi)}''$ shows no weight at $\omega = 0$, but exhibits strong particle-hole asymmetry in high-

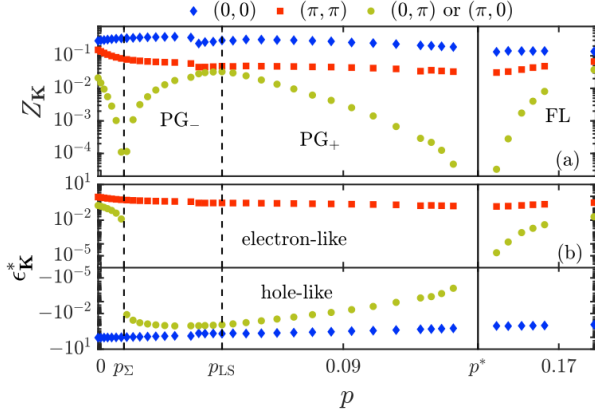


FIG. S7. (a) Quasiparticle weight $Z_{\mathbf{K}}$, and (b) energies $\epsilon_{\mathbf{K}}^*$, as function of p for momenta (blue) $\mathbf{K} = (0,0)$, (green) $\mathbf{K} = (0,\pi)$ or $\mathbf{K} = (\pi,0)$, and (red) $\mathbf{K} = (\pi,\pi)$.

energy features. The gap for $A_{(\pi,\pi)}$ occurs because $\mu_{(\pi,\pi)}^* = \mu - \text{Re}\Sigma_{(\pi,\pi)}(0)$, the effective chemical potential at $\omega = 0$, lies above the upper band edge $\epsilon_{(\pi,\pi)}^{\text{upper}}$ of the patch density of states $\rho_{(\pi,\pi)}(\epsilon)$ [c.f. Fig. S1(a)], so that $\rho_{(\pi,\pi)}(\mu_{(\pi,\pi)}^*) = 0$, see Fig. S6(a).

The Mott transition occurs at the critical doping p^* , where the self-energy pole in the antinodal patches emerges. The full gap opening in the antinodal patches at p_{LS} occurs because the effective chemical potential at $\omega = 0$, $\mu_{\mathbf{K}}^* = \mu - \text{Re}\Sigma_{\mathbf{K}}(0)$, continuously shifts outside of the patch bandwidth of the $\mathbf{K} = (0,\pi)$ and $\mathbf{K} = (\pi,0)$ patches, so that $A_{\mathbf{K}}(0) = \rho_{\mathbf{K}}(\mu_{\mathbf{K}}^*) = 0$, resulting in a full gap [see Figs. S6(a,b)]. The same occurs in the nodal patch as $p \rightarrow 0$, leading to a fully gapped Mott insulator. Neither p_{LS} nor $p = 0$ is associated with a critical point.

The antinodal self-energy exhibits a discontinuity at p^* , associated with the emergence of the pseudogap, while the nodal patches evolve smoothly with doping. The doping p_{LS} marks the point where $\mu_{(0,\pi)}^*$ crosses the band edge of $\rho_{(0,\pi)}(\epsilon)$, opening a full gap in the antinodal patch. This is consistent with the known patching dependence of the Hubbard model [63].

Notably, μ never shifts $\text{Re}\Sigma_{\mathbf{K}}(0)$ into the band edge regime of $\epsilon_{(\pi,\pi)}^{\text{lower}}$. This explains why the $\mathbf{K} = (\pi,\pi)$ patch remains gapped at all dopings, despite its relatively FL-like self energy. Interestingly, μ decreases with increasing doping p . While both the nodal $\mathbf{K} = (0,0)$ and antinodal patches follow this trend, the behavior of the $\mathbf{K} = (\pi,\pi)$ patch is opposite. This distinction is crucial: it prevents the Fermi surface from entering the $\mathbf{K} = (\pi,\pi)$ patch at low doping and thereby enables the Mott insulating state at half-filling.

B. Electronic quasiparticle

In this section we focus on the electronic quasiparticle behavior as function of doping. Figure S7 shows the p -dependence of patch quasiparticle (QP) weights and energy, defined as

$$Z_{\mathbf{K}} = (1 - \partial_{\omega}\Sigma'_{\mathbf{K}}(\omega)|_{\omega=0})^{-1}, \quad (\text{S16a})$$

$$\epsilon_{\mathbf{K}}^* = Z_{\mathbf{K}} [\epsilon_{\mathbf{K}} - \mu + \Sigma'_{\mathbf{K}}(0)], \quad (\text{S16b})$$

Colors blue, green, and red denote individual momenta.

The nodal quasiparticle weight $Z_{\mathbf{K}}$ in Fig. S7(a) exhibit an approximately linear dependence on doping, compared to the pronounced non-monotonic behavior of their antinodal counterparts. On a logarithmic scale, $Z_{(0,\pi)}$ (and equivalently $Z_{(\pi,0)}$) vanishes at p^* and p_{Σ} due to the emergence of a self-energy pole at $\omega = 0$. Between these dopings, $Z_{(0,\pi)}$ displays a maximum at p_{LS} .

Figure S7(b) shows the energies $\epsilon_{\mathbf{K}}^*$, which yield information about the electronic QP character. Across the entire doping range, the $\mathbf{K} = (0,0)$ and $\mathbf{K} = (\pi,\pi)$ patches retain hole- and electron-like character, respectively, consistent with conventional Fermi liquid behavior. In contrast, the antinodal energies change sign at the critical dopings p^* and p_{LS} . For $\Sigma_{\mathbf{K}}$, these sign changes are discontinuous, reflecting poles in the real part of the self-energy. By contrast, $\epsilon_{\mathbf{K}}^*$ evolves continuously, albeit with a very steep crossover near p_{Σ} . The shift from electron- to hole-like character is consistent with a transfer of coherence from the conventional electron-like Fermi liquid at $p > p^*$ to the emergent composite Fermi liquid at $p < p^*$.

C. Dependence on next nearest neighbor hopping t'

In this section, we discuss the dependence of the phase diagram on the next nearest neighbor hopping t' . In the main text, we focus on the representative case $t' = -0.3t$, which captures all qualitative features of the phase diagram. Here, we briefly comment on how these features evolve as a function of t' .

In Fig. S8, we show the critical dopings as a function of t' . The line labeled p^* marks the transition between the Fermi liquid (FL) regime and the pseudogap (PG) metal. This transition is characterized by a reconstruction of the Fermi surface and the simultaneous vanishing of the Fermi liquid coherence scale in multiple response functions. The doping p_{Σ} denotes the point at which the self-energy pole shifts from $\omega > 0$ for $p > p_{\Sigma}$ to $\omega < 0$ for $p < p_{\Sigma}$. The dopings p_{FS} and p_{LS} indicate changes in the topology of the Fermi surface (FS) and the Luttinger surface (LS), respectively.

The critical dopings shown in Fig. S8 are determined by characteristic changes in spectral behavior, which are equal to the $t' = -0.3t$ case presented in Fig. S5.

For $t' \geq 0.25t$, the critical dopings p^* and p_{FS} merge into a single transition. Apart from this merging, the

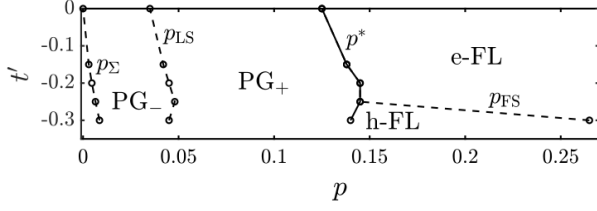


FIG. S8. Dependence of various critical doping values on next-nearest-neighbor hopping t' and doping p . The critical doping p^* marks the transition from the Fermi liquid (FL) to the pseudogap metal (PG). Dashed lines p_{FS} and p_{LS} denote topology changes of the Fermi surface (FS) and Luttinger surface (LS), respectively. The line p_{Σ} indicates the doping below which the self-energy pole shifts from $\omega > 0$ to $\omega < 0$.

qualitative behavior of the system remains unchanged across different values of $t' < 0$. Therefore, the choice $t' = -0.3t$ provides a representative description, and the conclusions drawn in the main text apply generally to other negative values of t' .

S-IV. MOMENTUM DEPENDENCE OF THE GREEN'S FUNCTION

In this section, we examine the doping evolution of the real part of the cluster Green's function at $\omega = 0$ across momentum and present the momentum dependence of the Green's function and self-energy near the critical transition complementary to the main text.

A. Fermi and Luttinger surface versus doping

This section provides insight into the evolution of the Fermi and Luttinger surfaces as a function of p . To this end, we use the cluster results for the real part of the Green's function at $\omega = 0$, $\text{Re } G_{\mathbf{k}}(0)$.

The DCA result for the Green's function gives

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)}, \quad (\text{S17})$$

with the self-energy given by $\Sigma_{\mathbf{k}}(\omega) = \theta_{\mathbf{k},\mathbf{K}} \Sigma_{\mathbf{K}}(\omega)$, where $\theta_{\mathbf{k},\mathbf{K}}$ is a patch-selective box function. Liouvillian interpolation replaces the latter piecewise constant form by a smoothly momentum-dependent version, obtained via a continued-fraction expansion [77].

Figure S9 shows the non-interpolated version of $\text{Re } G_{\mathbf{k}}(0)$. A sign change via a divergence within a patch (strong blue to strong red) define the Fermi surface, while small, step-like sign changes across patch boundaries (light-blue to light-red) indicate a Luttinger surface.

A Fermi surface topology change occurs at $p_{FS} \simeq 0.25$, where the Fermi surface changes smoothly from electron-like to hole-like. As p drops below p^* and decreases towards p_{LS} , we observe an increasing mismatch between

the Fermi surface of the nodal $\mathbf{K} = (0,0)$ patch and the antinodal patches. This is accompanied by the emergence of a Luttinger surface at the antinodal patch edges toward $\mathbf{K} = (\pi, \pi)$, driven by the PG_+ self-energy peak. In this regime, the Luttinger surface expands while the Fermi surface shrinks with decreasing doping.

When p drops below p_{LS} , the Fermi surface in the antinodal patches disappears and a closed Luttinger surface forms as the PG_+ self-energy peak merges with high-energy features, producing a Mott divergence in the antinodal patch. This constitutes a reconstruction of the Luttinger surface topology from open to closed. However, this is a crossover, not a thermodynamic transition, since previous studies showed that its details depend on the patching scheme chosen [63]. For example, improving the $\mathbf{k}$ -resolution by using a larger cluster, may well lead to different behavior for the Luttinger surface.

When p drops below p_{Σ} , the real part of the Green's function changes sign (positive to negative) in the antinodal patches, reflecting a sign change (positive to negative) in the location of the antinodal self-energy pole. However, Fermi surface and metallic behavior survive in the $\mathbf{K} = (0,0)$ patch throughout as p drops below p_{LS} and then p_{Σ} , vanishing only as $p \rightarrow 0$.

In the main text, Figs. 4(c1,c2) showed the zero-frequency spectral function $A_{\mathbf{k}}(0)$ for two doping values just above and below p^* , computed using a momentum-smooth self-energy $\Sigma_{\mathbf{k}}''$ obtained via Liouvillian interpolation [77]. To complement that discussion, Figs. S10(a,b) shows $A_{\mathbf{k}}(0)$ for the same two dopings, now computed without Liouvillian interpolation, i.e. using momentum-discontinuous patch self-energies $\Sigma_{\mathbf{K}}$. Whereas the nodal patches in for $p > p^*$ and $p < p^*$ hardly differ, implying a smooth evolution across p^* , the antinodal patches differ strongly, signaling a Fermi surface reconstruction across p^* . Note that for $p < p^*$, the region of non-zero spectral weight in the antinodal patches no longer crosses the antiferromagnetic zone boundary (for $p > p^*$, it did). The resulting Fermi surface represents a Fermi arc (albeit a discontinuous one, reflecting DCA patching) in that the antinodal surface does not extend to the boundary of the Brillouin zone. Figure 4(c1) shows the $\mathcal{L}$ -interpolated (continuous) version of this Fermi arc.

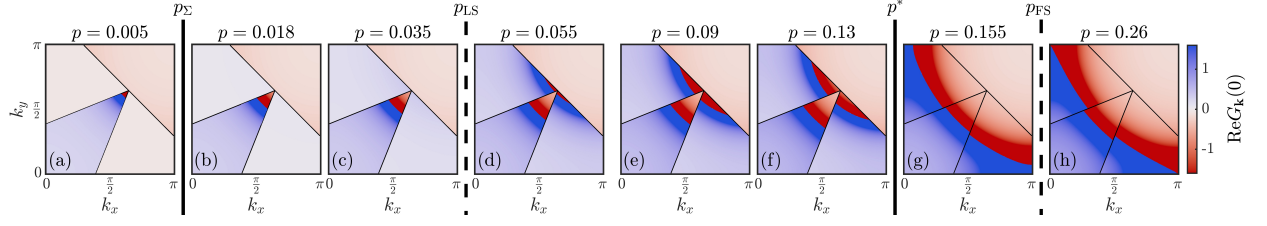


FIG. S9. Real part of the Green's function at $\omega = 0$, $\text{Re} G_{\mathbf{k}}(0)$, computed without $\mathcal{L}$ -interpolation, shown in a quadrant of the Brillouin zone for several values of doping p , increasing from (a) to (h). Black separators between panels mark characteristic dopings. Thin, straight black lines in each panel show patch boundaries. The Fermi surface is associated with a sign change via a divergence (strong-blue to strong-red), a Luttinger surface with a sign change via a small discontinuity (light-blue to light-red) at the patch boundaries.

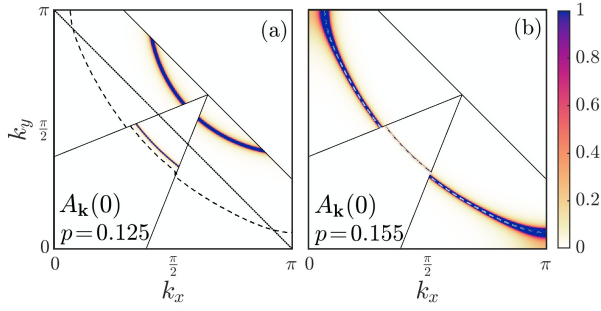


FIG. S10. Momentum-resolved spectral functions at $\omega = 0$, $A_{\mathbf{k}}(0)$, computed without $\mathcal{L}$ -interpolation for (a) $p = 0.125$ and (b) $p = 0.155$. Thin solid black lines indicate patch boundaries. In (a), the dotted line marks the antiferromagnetic zone boundary. In (b), the curved dashed line marks the locus of maximal $A_{\mathbf{k}}(0)$; it is shown in (a), too, as a reference for the unreconstructed Fermi surface. Figures 4(c2,c1) show the $\mathcal{L}$ -interpolated versions of (a,b).

Dynamical scaling near the pseudogap quantum critical point of the two-dimensional Hubbard model

by

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Dynamical scaling near the pseudogap quantum critical point of the two-dimensional Hubbard model

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We study dynamical scaling in the quantum-critical fan of the pseudogap-metal to Fermi-liquid transition of the two-dimensional Hubbard model. Using a four-patch dynamical cluster approximation with the numerical renormalization group as a cluster impurity solver, we access real-frequency dynamics over several decades at arbitrary temperatures. Close to the critical doping, the local spin and cluster-current susceptibility spectra exhibit $x = \omega/T$ scaling of the form $\chi''(\omega, T) \sim \tanh(x/2)$, and the cluster contribution to the optical conductivity obeys $T\sigma'_{cl}(\omega, T) \sim \tanh(x/2)/x$, implying a $1/T$ cluster dc conductivity. In the scaling regime, the vertex contribution to the cluster optical response is much larger than the bubble contribution. We further find evidence for a marginal-Fermi-liquid nodal self-energy. This, together with the $1/T$ vertex contribution to the conductivity, implies strange-metal optical transport in the quantum critical region. Our results describe several qualitative aspects of several experimental observations.

Introduction.— Hole-doped cuprates remain the superconductors with the highest transition temperatures at ambient pressure. Yet, almost four decades after their discovery, central aspects of their phase diagram, such as the underdoped pseudogap (PG) metal and the strange-metal regime near optimal doping, still lack a universally agreed-upon microscopic explanation [1].

It was suggested early on that the superconducting dome conceals a quantum critical point (QCP) at a critical doping p^* , separating the underdoped PG metal from the overdoped Fermi liquid (FL) [2–6]. This conjecture is supported experimentally by a singular specific heat coefficient [7] and a sharp transformation of the Fermi surface, indicated by Hall-effect [8, 9], angle-dependent magnetoresistance [10], quantum oscillation [11, 12], and ARPES measurements [13]. The latter reveals that low-energy electronic spectral weight is lost over a large part of the antinodal Fermi surface when decreasing doping from the overdoped FL into the underdoped PG metal, while the nodal region remains comparatively coherent [13–18]. Further, from this perspective, the strange metal observed near optimal doping is interpreted as the quantum-critical fan emanating from this QCP [19]. Experimental signatures of the strange metal include linear-in- T resistivity at low temperatures [20–22], a logarithmic temperature dependence of the specific-heat coefficient [7], and dynamical ω/T scaling of magnetic [23–26], charge [27], and optical responses [28–30]. The extended quantum critical region [13, 31] found in some experiments has been interpreted to be the result of disorder [32].

However, the aforementioned phenomena are difficult to reconcile with a Hertz–Millis–Moriya theory [33–35] without additional ingredients, and the nature of the putative QCP remains unclear. It is still debated whether

the transition is driven by a conventional (fluctuating) order parameter [36–43], by fractionalization or topological order [44–53], or whether disorder plays an important role [54–58]. An early phenomenological approach to strange metal dynamics was provided by the marginal Fermi liquid (MFL) proposal of Varma *et al.* [59]. There, bosonic fluctuations across many momenta exhibiting spectra proportional to $\tanh(\omega/2T)$ produce a single-particle scattering rate proportional to $\max(|\omega|, T)$ and give rise to a logarithmic temperature dependence of the specific-heat coefficient. Further, if vertex contributions to the conductivity are irrelevant, this gives rise to a linear-in- T resistivity. Recently, the Yukawa–Sachdev–Ye–Kitaev (YSYK) construction [56–58] has been put forward as a universal mechanism towards MFL physics, though spatially disordered interactions are required to relax momentum and ensure irrelevant vertex contributions. In clean lattices, current relaxation requires a separate mechanism, for instance, through Umklapp scattering [60–62].

In this Letter, we study the quantum-critical region of the PG-metal to Fermi-liquid QCP in the one-band Hubbard model, using a four-patch dynamical cluster approximation (DCA), a cluster extension of dynamical mean-field theory (DMFT) [63–66]. It has been established in a large body of previous work that cluster DMFT approximations capture central aspects of the hole-doped cuprates, in particular the existence of a PG metal [47, 48, 66–88]. Further, it seems that a four-site approach is enough to capture the qualitative aspects [65, 68, 71, 79, 82–87]. However, the existence of a QCP separating PG metal from FL has been controversial, with some work providing evidence for a QCP [76–78, 80, 81]. By contrast, Sordi *et al.* [82–87] have established in a certain parameter region ($t' = 0$, $U/t \leq 6$) that

the transition is first-order, and criticality is associated with a finite (but low) temperature critical endpoint.

In Ref. [89], we have made significant progress on this matter, by using four-patch DCA in conjunction with the numerical renormalization group (NRG) [90–95]. NRG is well-suited for this purpose, since it offers unprecedented real-frequency spectral resolution at arbitrarily low energies and temperatures. In a parameter regime relevant for cuprates, this has allowed us to establish the existence of a QCP that occurs between two distinct FLs (one is a PG metal) with different Fermi surfaces and quasiparticle content. At this transition, the Fermi-liquid scale is continuously suppressed to zero, suggesting that the QCP is governed by a non-Fermi-liquid (NFL) fixed point. Here, we study dynamical scaling in the quantum-critical fan emanating from this NFL fixed point.

Model and methods.— In this work, we aim to study universal dynamical phenomena in the quantum critical region of the pseudogap QCP in the cuprates. For that, we consider the two-dimensional square-lattice t - t' - U Hubbard model, which is believed to contain the necessary ingredients to describe cuprate physics [96],

$$H = - \sum_{\mathbf{r}\mathbf{r}'} t_{\mathbf{r}\mathbf{r}'} c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} - \mu \sum_{\mathbf{r}\sigma} n_{\mathbf{r}\sigma}. \quad (1)$$

The hopping matrix $t_{\mathbf{r}\mathbf{r}'}$ contains nearest and next-nearest neighbor matrix elements, denoted t and t' , respectively. We use $t' = -0.3t$ and $U = 7t$, appropriate for describing cuprates [97, 98]. In the following, we set $t = 1$ as our unit of energy. By tuning the chemical potential μ , we change the hole doping p (filling $n = 1 - p$) to drive this model through a quantum phase transition.

Physical quantities are computed within a four-patch DCA approximation, using the star patching scheme of Refs. [79, 89]. DCA approximates the self-energy as momentum-independent within each patch, which leads to discontinuities at the patch boundaries. The four patches are centered around momenta $\mathbf{K} \in \{(0, 0), (\pi, 0), (0, \pi), (\pi, \pi)\}$, which are also used as patch labels. The self-energy is computed from an effective four-impurity model, which we solve using NRG. Using the QSpace-based [99–101] MuNRG package [93, 102, 103], we exploit the $SU(2) \times U(1)$ spin and charge symmetries, use an interleaved Wilson chain with logarithmic discretization parameter $\Lambda = 8$, and keep up to $N_{\text{keep}} = 3 \cdot 10^4$ low-energy states during iterative diagonalization, resulting in a rescaled truncation energy of $E_{\text{trunc}} \geq 5$. An interleaved Wilson chain geometry [104, 105] is used to fully interleave the bath modes associated with the different patches (labeled by their patch momenta) in the order: $\mathbf{K}_1 = (0, 0)$, $\mathbf{K}_2 = (0, \pi)$, $\mathbf{K}_3 = (\pi, 0)$, $\mathbf{K}_4 = (\pi, \pi)$. We consider only non-symmetry-broken, normal-state solutions.

DCA+NRG yields access to real-frequency electronic spectral functions and self-energies with coarse-grained

momentum resolution. For our analysis, we further compute dynamical susceptibilities of the self-consistent cluster impurity model, which correspond to local or short-ranged dynamical susceptibilities of the lattice model.

Consider the retarded dynamical susceptibility of a bosonic cluster operator O (with $\langle \rangle$ a thermal average):

$$\chi[O](\omega, T) = -i \int_0^\infty dt e^{i(\omega + i0^+)t} \langle [O(t), O^\dagger] \rangle. \quad (2)$$

We compose it as $\chi = \chi' - i\pi\chi''$ into real and spectral parts. Within NRG, χ'' is computed via the Lehmann representation; the discrete raw spectrum is broadened with a log-Gaussian kernel [93], and χ' is subsequently obtained through a Kramers-Kronig relation. We further study the corresponding imaginary-time correlator,

$$\langle O(\tau)O^\dagger \rangle = \int_{-\infty}^\infty d\omega \frac{e^{-\tau\omega}}{1 - e^{-\omega/T}} \chi''[O](\omega, T). \quad (3)$$

We evaluate it using the discrete raw real-frequency spectrum as input, thus avoiding broadening artifacts.

We focus on the local spin $S_{\mathbf{r}}^z$ and the current density in x -direction on the cluster, j_{cl}^x , defined as

$$S_{\mathbf{r}}^z = \frac{1}{2}(c_{\mathbf{r}\uparrow}^\dagger c_{\mathbf{r}\uparrow} - c_{\mathbf{r}\downarrow}^\dagger c_{\mathbf{r}\downarrow}), \quad (4a)$$

$$j_{\text{cl}}^x = -\frac{1}{2}ie \sum_{\mathbf{r} \in R} \sum_{\mathbf{r}' \in L} \sum_{\sigma} t_{\mathbf{r}\mathbf{r}'} (c_{\mathbf{r},\sigma}^\dagger c_{\mathbf{r}',\sigma} - \text{h.c.}), \quad (4b)$$

where the sums on $\mathbf{r}$ or $\mathbf{r}'$ run over the two right (R) or the two left (L) sites of the square cluster, respectively.

Phase diagram.— The zero-temperature phase diagram and energy scales obtained through DCA+NRG are shown in Fig. 1(a). It displays the $T = 0$ imaginary-time exponent α of the local spin correlations, $\langle S_{\mathbf{r}}^z(\tau) S_{\mathbf{r}}^z \rangle \sim \tau^{-\gamma}$, for different doping levels p and imaginary time scales τ . At long times, $\tau^{-1} < T_{\text{FL}}$, where T_{FL} is the FL scale (white circles), we find $\gamma = 2$ (blue), characteristic of FL behavior. The scale T_{FL} continuously vanishes at a critical doping $p^* \simeq 0.14$, where a quantum phase transition between a PG metal with a reconstructed Fermi surface and a pseudogapped electronic spectral function and a normal FL occurs [89].

The vanishing FL scale in the vicinity of p^* gives rise to an intermediate NFL region, $T_{\text{FL}} < \tau^{-1} < T_{\text{NFL}}$, where T_{NFL} is the NFL scale (black circles). There, we find an SYK-like exponent, $\gamma = 1$, i.e. $\langle S_{\mathbf{r}}^z(\tau) S_{\mathbf{r}}^z \rangle \sim \tau^{-1}$ [yellow in Fig. 1(a)]. Our data suggest that this quantum critical region extends to $\tau^{-1} \rightarrow 0$ at p^* . This indicates that this region is controlled by an unstable NFL fixed point separating the PG metal from the normal FL. At short times, $\tau^{-1} > T_{\text{NFL}}$, the spin dynamics becomes very slow, with $\gamma < 0.5$, consistent with local-moment behavior.

We henceforth focus on $\mu = 1.24$. There, the system at $T = 0$ is a PG metal with filling $p \simeq 0.135$. The intermediate NFL window extends over ~ 4 decades, $[T_{\text{FL}}, T_{\text{NFL}}] = [10^{-5}, 10^{-1}]$. To elucidate the NFL behavior, we study the effects of non-zero temperature on

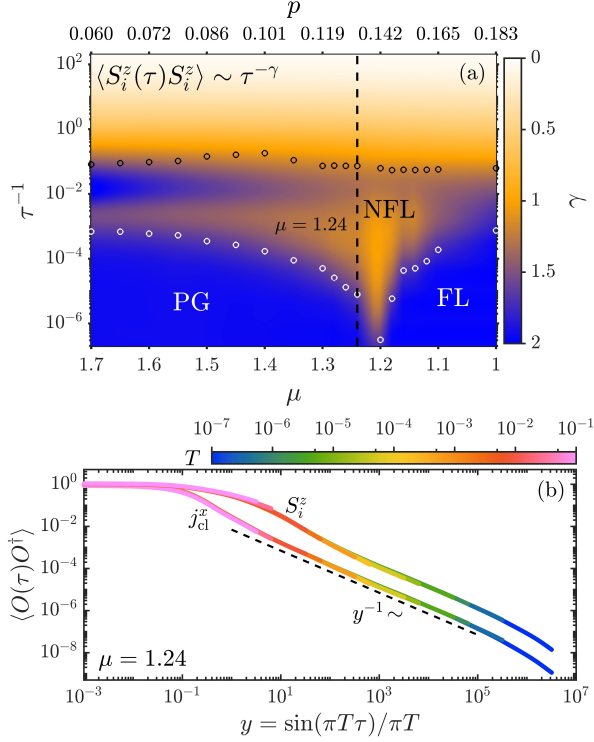


FIG. 1. (a) Zero-temperature phase diagram extracted from the power-law decay of the imaginary-time local spin correlator, $\langle S_{\mathbf{r}}^z(\tau) S_{\mathbf{r}}^z \rangle_{T=0} \sim \tau^{-\gamma}$. The color scale shows the exponent γ versus chemical potential μ and inverse imaginary time τ^{-1} . (Top abscissa: the corresponding hole doping p at $T = 0$.) Blue regions with $\gamma = 2$ indicate Fermi-liquid behavior at long times. The yellow region with $\gamma \simeq 1$ identifies the intermediate non-Fermi-liquid region emerging near the critical doping $p^* \simeq 0.14$. Black and white circles denote the crossover energies T_{NFL} and T_{FL} , respectively [106]. The vertical dashed line marks $\mu = 1.24$, where we study scaling. (b) Local spin and cluster-current correlators at $\mu = 1.24$, plotted vs. $y = \sin(\pi T \tau)/\pi T$ for $\tau \in [0, 1/2T]$ and 12 temperatures, indicated by ticks on the color bar. At intermediate temperatures and times, both correlators decay as y^{-1} (dashed line).

$\langle S_{\mathbf{r}}^z(\tau) S_{\mathbf{r}}^z \rangle$ and $\langle j_{\text{cl}}^x(\tau) j_{\text{cl}}^x \rangle$. When $\langle S_{\mathbf{r}}^z(\tau) S_{\mathbf{r}}^z \rangle$ is plotted vs. $y = \sin(\pi T \tau)/\pi T$ [107] [Fig. 1(b)], curves for different temperatures collapse onto a single curve, and likewise for $\langle j_{\text{cl}}^x(\tau) j_{\text{cl}}^x \rangle$; and for intermediate temperatures and times, $T, \tau^{-1} \in [T_{\text{FL}}, T_{\text{NFL}}]$, both correlators show power-law decay, $\sim y^{-\gamma}$, with $\gamma = 1$. Thus, both have the scaling form $\sim T^\gamma \mathcal{F}(\tau T)$, and in the NFL window, T is the only relevant energy scale, implying Planckian scaling.

Dynamical scaling.— Such τT scaling for imaginary-time correlators implies ω/T scaling for their real-frequency spectral functions, $\chi''(\omega, T) = T^\alpha \mathcal{X}''(\omega/T)$, with $\alpha = \gamma - 1 = 0$. For $\mathcal{F}(\tau T) = \pi/\sin(\pi \tau T)$, the scaling function is $\mathcal{X}''(x) = \mathcal{X}_0'' \tanh(x/2)$, where $\mathcal{X}_0''$ is a non-universal prefactor. Indeed, when the temperature-dependent spin spectrum, $\chi''[S_{\mathbf{r}}^z](\omega, T)$ [Fig. 2(a)] is

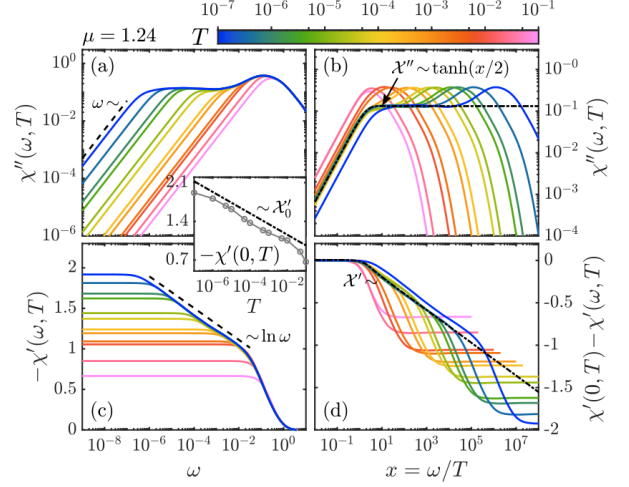


FIG. 2. Real-frequency scaling of the local spin susceptibility $\chi[S_{\mathbf{r}}^z](\omega, T)$ at $\mu = 1.24$. (a) Spectral part χ'' and (c) real part $-\chi'$, plotted vs. ω for 12 temperatures, indicated by ticks on the color bar. Upon lowering the temperature through the NFL window, χ'' develops an extended plateau for $T \lesssim |\omega| \lesssim T_{\text{NFL}}$, while the static response, $\chi'(0, T)$, grows approximately logarithmically (inset). (b) The spectral part, plotted as $\chi''(\omega, T)$ vs. $x = \omega/T$, shows a scaling collapse onto $\chi''(x) = \mathcal{X}_0'' \tanh(x/2)$. (d) After subtracting the static part, $\chi'(0, T) - \chi'(\omega, T)$, χ' shows a scaling collapse, too. Black dash-dotted curves depict the scaling functions; dashed lines are guides-to-the-eye.

plotted vs. $x = \omega/T$ [Fig. 2(b)], it exhibits a scaling collapse onto $\mathcal{X}_0'' \tanh(x/2)$ (black dash-dotted line). This Planckian dynamical scaling sets in around $T \simeq 10^{-2}$ – 10^{-3} and extends down to $T \simeq 10^{-6}$, implying scaling over 3 to 4 decades. The corresponding static susceptibility, $\chi'[S_{\mathbf{r}}^z](0, T)$ [Fig. 2, inset] depends on the high-frequency cutoff T_{NFL} and diverges logarithmically with T/T_{NFL} , $\chi'[S_{\mathbf{r}}^z](0, T) \sim \ln T/T_{\text{NFL}}$. When this static part is subtracted, $\chi'[S_{\mathbf{r}}^z](\omega, T) - \chi'[S_{\mathbf{r}}^z](0, T)$ [Fig. 2(c)] exhibits Planckian ω/T scaling, too [Fig. 2(d)], with a similar scaling range as χ'' and a scaling function $\mathcal{X}'(x)$ discussed in Ref. [108]. Our spin susceptibility thus follows the scaling form conjectured by Varma *et al.* [59] via phenomenological considerations.

Experimentally, ω/T scaling of spin fluctuations in the strange metal region has been measured in doped La_2CuO_4 [23–26]. A scaling analysis of the local susceptibility in Ref. [23] revealed an exponent of $\alpha = 0$, consistent with our calculations. To compare the temperature and frequency scales in the experiments to our data, we assume $t = 0.5 \text{ eV}$, suitable for most cuprates [97, 98]. Experimentally, the onset for scaling seems to be around $T \simeq 300 \text{ K}$ or $\hbar\omega \simeq 15 \text{ meV}$, which corresponds to around $10^{-2} t$, matching our scaling onset in order-of-magnitude.

Optical conductivity.— One of the most intriguing features of the strange metal observed in cuprates is its remarkably robust linear-in- T resistivity and dynamical scaling of the optical conductivity. The latter is deter-

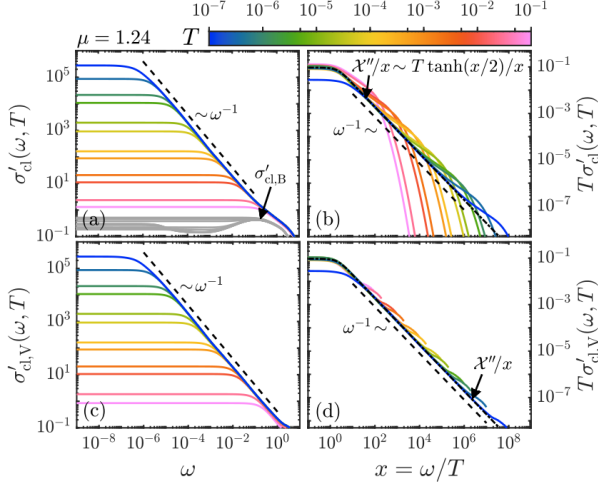


FIG. 3. Cluster contribution to the real part of the optical conductivity, $\sigma'_{\text{cl}}(\omega, T) = \chi''[j_{\text{cl}}^x](\omega, T)/\omega$, at $\mu = 1.24$. (a) $\sigma'_{\text{cl}}(\omega, T)$ vs. ω for 12 temperatures, indicated by ticks on the color bar; in the NFL regime, σ'_{cl} scales as ω^{-1} (dashed line). Grey curves show the cluster bubble contribution $\sigma'_{\text{cl},\text{B}}$, computed from dressed propagators without vertex contributions. (b) $T\sigma'_{\text{cl}}(\omega, T)$ vs. $x = \omega/T$, showing a scaling collapse onto $\tanh(x/2)/x$ (dash-dotted curve). (c) Vertex contribution $\sigma'_{\text{cl},\text{V}} = \sigma'_{\text{cl}} - \sigma'_{\text{cl},\text{B}}$, plotted vs. ω . In the NFL regime it is orders of magnitude larger than $\sigma'_{\text{cl},\text{B}}$, and (d) obeys the same ω/T scaling as the full cluster response σ'_{cl} .

mined by current fluctuations. Since the short-ranged cluster-current correlator shows τT scaling similar to the spin correlator [Fig. 1(b)], the cluster-current spectrum exhibits ω/T scaling in the NFL window, too, again of the form $\chi''[j_{\text{cl}}^x](\omega, T) \propto \tanh(\omega/2T)$. The corresponding cluster contribution to the real part of the optical conductivity, given by $\sigma'_{\text{cl}}(\omega, T) = \chi''[j_{\text{cl}}^x](\omega, T)/\omega$, is shown in Fig. 3(a) for different temperatures. In the NFL window, $T\sigma'_{\text{cl}}$ plotted vs. $x = \omega/T$ indeed exhibits a scaling collapse [Fig. 3(b)] onto $\tanh(x/2)/x$ (black dash-dotted line). Remarkably, this scaling implies that the cluster contribution to the static conductivity, $\sigma'_{\text{cl}}(0, T)$, exhibits $1/T$ behavior, reminiscent of the *uniform* conductivity in a strange metal. The ω/T scaling of $T\sigma'_{\text{cl}}$ sets in at higher temperatures than that of $\chi''[j_{\text{r}}^x]$ and extends over 5 decades, from at least $T = 10^{-1}t$ (highest T considered) down to $T = 10^{-6}t$. Using $t = 0.5$ eV, this roughly corresponds to temperatures from 600 K down to 6 mK. Experimentally, such a remarkably wide range is observed for the resistivity of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$: it is linear-in- T from around 1000 K [109, 110] down to at least 1.5 K [20] if superconductivity is suppressed by a magnetic field.

To further analyze $\sigma'_{\text{cl}}(\omega, T)$, we decompose it as $\sigma'_{\text{cl}} = \sigma'_{\text{cl},\text{B}} + \sigma'_{\text{cl},\text{V}}$ into bubble and vertex contributions, shown in grey or in color in Figs. 3(a) or 3(c), respectively. Deep in the NFL regime we find $\sigma'_{\text{cl},\text{V}} \gg \sigma'_{\text{cl},\text{B}}$ by orders of magnitude, hence the bubble contribution is irrelevant and σ'_{cl} is entirely dominated by the vertex contribu-

tion. Moreover, both $T\sigma'_{\text{cl}}$ and $T\sigma'_{\text{cl},\text{V}}$ exhibit ω/T scaling [Figs. 3(b,d)], the latter even cleaner than the former. By contrast, $T\sigma'_{\text{cl},\text{B}}$ does not exhibit scaling (not shown).

Large vertex contributions with the same scaling form as above have previously been reported [111] in a strange metal regime in the vicinity of a heavy-fermion QCP, found [112] in a cellular DMFT treatment of the 3-dimensional periodic Anderson model. There, the uniform lattice conductivity $\sigma'_{\text{latt}}(\omega, T)$ was approximated [111] by $\sigma'_{\text{latt}} \simeq \sigma'_{\text{latt},\text{B}} + \sigma'_{\text{cl},\text{V}}$, involving its bubble contribution and a vertex contribution restricted to the cluster, neglecting longer-ranged terms. In the strange metal regime this yielded $\sigma'_{\text{cl},\text{V}} \gg \sigma'_{\text{latt},\text{B}}$, i.e. the lattice bubble contribution is irrelevant, $\sigma'_{\text{latt}} \simeq \sigma'_{\text{cl},\text{V}}$, and $\sigma'_{\text{latt}}(0, T) \sim 1/T$. This is in strong contrast to MFL phenomenology, which assumes $\sigma'_{\text{latt}} \simeq \sigma'_{\text{B},\text{latt}}$. The periodic Anderson model was thus found to yield an intrinsic, short-ranged current decay mechanism without invoking disorder.

In the present case, very deep in the NFL region, for $\omega, T \lesssim 10^{-2}/T_{\text{NFL}}$, we likewise find $\sigma'_{\text{cl},\text{V}} \gg \sigma'_{\text{latt},\text{B}}$. That suggests a similar conclusion, in particular a strange-metal conductivity $\sigma'_{\text{latt}}(0, T) \propto 1/T$. However, we are unable to establish this with certainty, since our results for the scaling behavior of the self-energy $\Sigma(\omega, T)$, which determines that of $\sigma'_{\text{latt},\text{B}}(\omega, T)$, are not sufficiently accurate for very small ω and T [113].

For somewhat higher temperatures and frequencies, $\omega, T \in [10^{-2}T_{\text{NFL}}, T_{\text{NFL}}]$, we find evidence for a MFL self-energy at the node, discussed in detail below, leading to $\sigma'_{\text{latt},\text{B}}(0, T) \propto 1/T$ behavior, as discussed with Fig. 6 of the End Matter below. We expect that a more accurate determination of $\Sigma(\omega, T)$ [113] will confirm MFL behavior at least to leading order in the scattering of electrons off the spin fluctuations discussed in Fig. 2; then, $\sigma'_{\text{latt},\text{B}}(0, T)$ will not be more singular than $1/T$. All in all, our computations thus strongly suggest a strange-metal conductivity with $\sigma'_{\text{latt}}(0, T) \propto 1/T$.

Electronic spectra and self-energy.— Experimentally, it is established that the cuprates exhibit a Fermi surface with at least somewhat coherent electronic excitations in the strange metal region. Around optimal doping and in the underdoped region, these are mostly present in the nodal region, while the antinodal region appears to be much more incoherent, leading to Fermi arcs [19, 114–119]. Our DCA+NRG computations reproduce this behavior, see Figs. 4(a–c), which display momentum-dependent, zero-frequency spectral functions $A_{\mathbf{k}}(0)$ at different temperatures. (We obtained their smooth momentum dependence using Liouvillian interpolation [120] of the raw, momentum-discontinuous DCA self-energy (cf. Fig. S2 of the supplement [108]). The Fermi arcs of Figs. 4(a–c) show the typical behavior observed experimentally [115], becoming longer and more coherent as the temperature is lowered. Our choice of $\mu = 1.24$ yields a PG metal at the lowest temperatures.

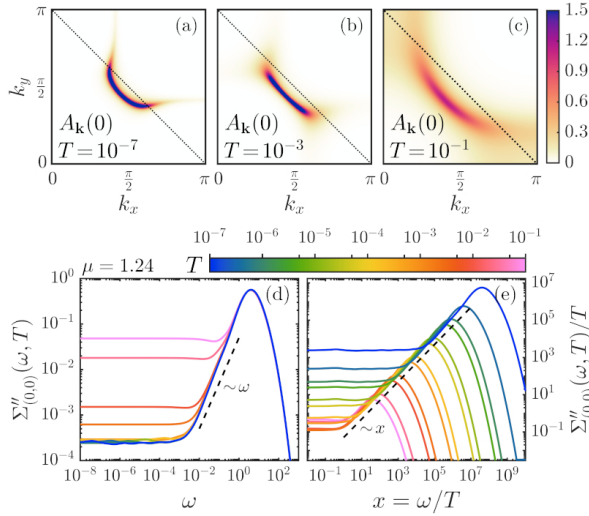


FIG. 4. The spectral function $A_{\mathbf{k}}(\omega = 0)$, computed at $\mu = 1.24$ for (a) the PG phase at $T = 10^{-7}t$, (b) the NFL at $T = 10^{-3}t$ and (c) the NFL at $T = 10^{-1}t$. The black dotted line indicates the antiferromagnetic zone boundary. (d) The spectral part of the self-energy at the nodal patch $\mathbf{K} = (0, 0)$, $\Sigma''_{(0,0)}(\omega, T)$ vs. ω , and (e) $\Sigma''_{(0,0)}(\omega, T)/T$ vs. $x = \omega/T$.

As established in Ref. [89], this PG metal exhibits FL quasiparticles with a reconstructed Fermi surface and a quasiparticle composition and weight with a strong nodal-antinodal dichotomy.

The degree of coherence in the nodal region is determined by the frequency and temperature dependence of the imaginary part of the self-energy, $\text{Im}\Sigma_{\mathbf{k}}(\omega, T)$. In our DCA approach, the self-energy at the node is determined by the self-energy of the $\mathbf{K} = (0, 0)$ patch, $\Sigma_{(0,0)}(\omega, T)$. For $T \gtrsim 10^{-3}$, its spectral part scales as $\Sigma'' \sim \omega$ for $\omega \gg T$, see Fig. 4(d), and roughly as $\Sigma'' \sim T$ for $\omega < T$, see Fig. 4(e), where Σ''/T vs. $x = \omega/T$ depends only weakly on T for $x < 1$ and $T > 10^{-3}$. (For $x < 1$ and $T < 10^{-3}$, however, the dependence of Σ'' on T saturates [Fig. 4(d)] and Σ''/T vs. x scaling breaks down [Fig. 4(e)]; this likely reflects numerical inaccuracies in the nodal self-energy at very low frequencies [113].) These results suggest that the nodal self-energy shows MFL behavior, $\Sigma''_{(0,0)}(\omega, T) \sim \max(\omega, T)$, but more accurate future computations are needed to solidify this claim.

Our results are consistent with Ref. [121], where a linear-in- T electronic scattering rate was found using DCA with 8 patches together with a Quantum Monte Carlo (QMC) impurity solver, in a similar parameter regime for $T > 0.02$. These 8-patch results were found to be consistent with 4-patch and 16-patch calculations, i.e. independent of cluster size. Experimentally, $\text{Im}\Sigma_{\mathbf{k}}(\omega, T)$ has been determined from momentum or energy distribution curves, and was found to be linear in frequency and temperature at the node and at optimal doping [13, 19, 114, 122], consistent with MFL phenomenol-

ogy and with DCA predictions for the Hubbard model.

Conclusion and outlook.— Using four-patch DCA+NRG, we studied scaling in the quantum critical region of the pseudogap quantum critical point of the Hubbard model. We find dynamical ω/T scaling for local spin and cluster-current susceptibilities, strong vertex contributions to the cluster conductivity, and evidence for a MFL self-energy in the nodal region. Our results strongly support a strange metal optical response in the quantum critical region. Important future goals are a more accurate computation of the DCA+NRG self-energy; a more in-depth analysis of the scaling of the optical response akin to Ref. [7]; and computing the NFL behavior of other observables such as the specific heat, the Hall response, or thermoelectric transport coefficients.

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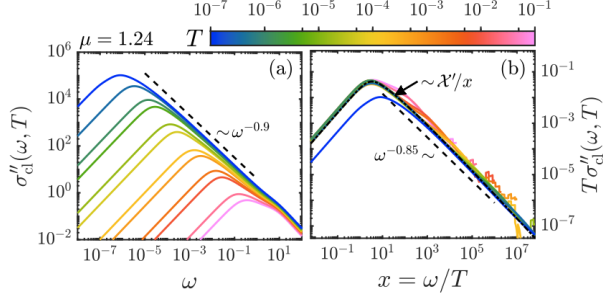


FIG. 5. Spectral part of the cluster optical conductivity, $\sigma''_{cl}(\omega, T)$, at $\mu = 1.24$. (a) σ''_{cl} vs. ω for 12 different temperatures, and (b) $T\sigma''_{cl}$ vs. $x = \omega/T$, showing a scaling collapse onto $\mathcal{X}''(x)/x$ (black dash-dotted curve). Black dashed lines indicate power law behavior.

I. IMAGINARY PART OF THE OPTICAL CONDUCTIVITY

In the main text, we discussed $\sigma'_{cl}(\omega, T)$, the real part of the cluster optical conductivity. Here, we discuss the corresponding spectral part, $\sigma''_{cl}(\omega, T)$, obtained via Kramers-Kronig. Figure 5(a) shows σ''_{cl} vs. ω ; for $\omega > T$, it decays slightly more slowly than $\omega^{-0.9}$ (dashed line). Figure 5(b) shows the corresponding scaling behavior of $T\sigma''_{cl}$ vs. $x = \omega/T$ (with some numerical artifacts at very high frequencies stemming from the Kramer-Kronig computation). Interestingly, the scaling collapse curve shows rather pure power-law decay, $\sim x^{-0.85}$ (dashed line). Similar exponents have been observed experimentally in Bi2212 and YBCO [123, 124]. Such a decay exponent slight smaller than 1 can be indicative of a logarithmic renormalization of the effective mass due to strong local vertex contributions, leading to logarithmic temperature scaling of the optical mass [30].

II. BUBBLE CONTRIBUTION

The bubble contribution to the optical conductivity is obtained from the $\mathbf{q} \rightarrow \mathbf{0}$ limit of the current-current correlator without vertex contributions. In this approximation, the conductivity is given by a sum over velocity-squared weights times products of Green's functions (or spectral functions), describing independent particle-hole excitations driven by a uniform electric field, with interactions entering only through the dressed propagators.

In this work, we considered two approaches for approximately computing the bubble contributions, using Green's functions computed on the cluster or the lattice, resulting in $\sigma'_{cl,B}(\omega, T)$ or $\sigma'_{latt,B}(\omega, T)$, respectively. The vertex contribution to the cluster conductivity, shown in

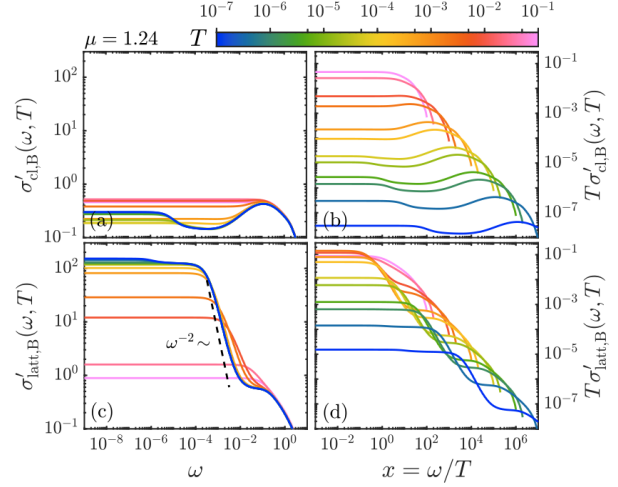


FIG. 6. Two approximations for the bubble contribution to the real part of the optical conductivity: (a,b) $\sigma'_{cl,B}(\omega, T)$, computed on the cluster, and (c,d) $\sigma'_{latt,B}(\omega, T)$, computed for the lattice. (a,c) show σ'_B vs. ω for several temperatures, (b,d) show $T\sigma'_B$ vs. $x = \omega/T$. For ease of comparison, panels (a,c) use the same range for the ordinate, likewise for (b,d).

the main text, is obtained as $\sigma'_{cl,V} = \sigma'_{cl} - \sigma'_{cl,B}$. For computational details, see the Supplemental Material [108].

Fig. 6 shows the two types of bubble contributions as functions of frequency, with colors indicating temperature. The cluster bubble contribution $\sigma'_{cl,B}$ [Fig. 6(a)] is negligible compared to the full cluster conductivity σ'_{cl} [cf. Fig. 3(a)], particularly at low temperatures, indicating that σ'_{cl} is dominated by vertex contributions [cf. Fig. 3(c)]. The lattice bubble $\sigma'_{latt,B}$ [Fig. 6(c)] is several orders of magnitude larger than the cluster bubble $\sigma'_{cl,B}$, but remains small relative to the full cluster conductivity σ'_{cl} [Fig. 6(a)]. At the lowest temperature, $\sigma'_{latt,B}$ exhibits the emergence of a precursor of a Drude peak, consistent with the onset of coherent transport in the pseudogap regime outside the quantum critical cone.

III. CURRENT-CURRENT CONTRIBUTIONS

In this section, we discuss the dependence of the cluster current-current correlation function $\chi''[j_{cl}^x](\omega, T)$ on its individual contributions. The definition (4) contains three types of terms, $j_{cl}^x = j_t + j_b + j_d$, describing hopping processes on the square cluster proceeding left-to-right along the top (t) rung, the bottom (b) rung, or along the two diagonals (d). Thus, the cluster-current susceptibility $\chi[j_{cl}^x]$ contains nine terms, which we group into four types: same-rung (t-t, b-b), opposite-rung (b-t,

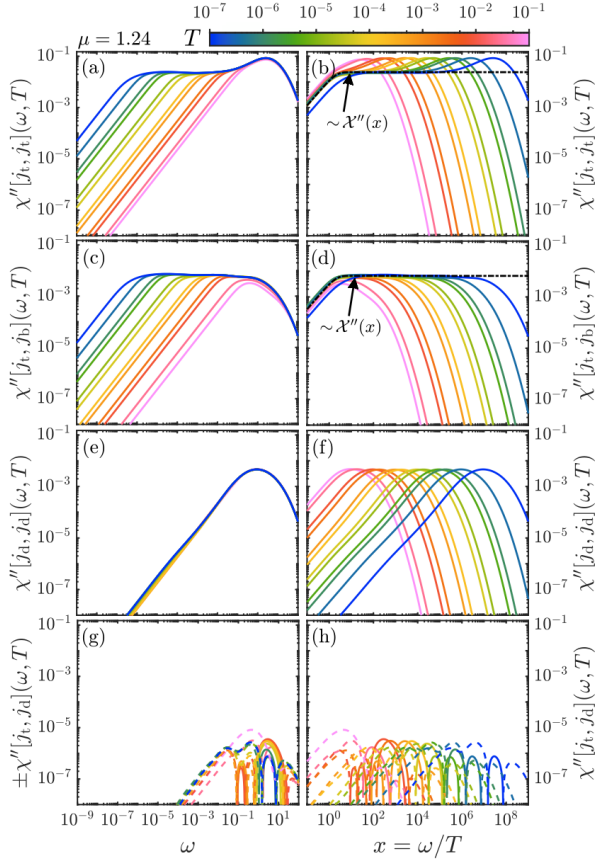


FIG. 7. Four types of contributions to the spectral part, $\chi''[j_t^x](\omega, T)$, of the cluster-current correlator, shown as functions of ω for 12 temperatures on the left, and as functions of $x = \omega/T$ on the right: (a,b) same-rung, (c,d) opposite-rung, (e,f) all-diagonal, and (g,h) rung-diagonal correlators. In (g,h) sign changes in $\chi''[j_t, j_d]$ are accounted for using solid or dashed lines to show $+\chi''$ or $-\chi''$, respectively. For ease of comparison, all panels use the same range for the ordinate. Black dashed lines indicate linear frequency behavior, while black dash-dotted lines correspond to the scaling function $\chi''(x) = \chi_0'' \tanh(x/2)$, with $\chi_0'' \simeq 0.024$ for $\chi''[j_t, j_t]$ and $\chi_0'' \simeq 0.0067$ for $\chi[j_t, j_b]$.

t-b), all-diagonal (d-d), and rung-diagonal (t-d, b-d, d-t, d-b) correlators, e.g.

$$\chi[j_t, j_b](\omega, T) = -i \int_0^\infty dt e^{i(\omega + i0^+)t} \langle [j_t(t), j_b] \rangle. \quad (5)$$

Figure 7 shows the (ω, T) dependence of one representative from each type (left panels), and its dependence on $x = \omega/T$ (right panels). The same-rung correlators [Figs. 7(a,b)], i.e. the most local ones, give the dominant contribution to the plateau in $\chi''[j_t^x]$ underlying Planckian scaling. The opposite-rung correlators also give plateau contributions, albeit smaller by roughly a factor of 2 [Figs. 7(c,d)]. The all-diagonal contributions

show no plateaus at all [Figs. 7(e,f)], while the rung-diagonal contributions, the only ones exhibiting sign changes, are several orders of magnitude smaller than all others [Figs. 7(g,h)].

We conclude that the plateau underlying Planckian scaling is dominated by the most short-ranged current-current correlations on the cluster, highlighting the strongly local character of the underlying quantum critical dynamics. It thus stands to reason that a marked plateau and Planckian scaling will also be found when studying larger clusters—although these will involve additional current correlators of longer range, their contributions will likely be even more sub-dominant than those considered here.

Supplemental Material for “Dynamical scaling near the pseudogap quantum critical point of the two-dimensional Hubbard model”

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S-I. SCALING FUNCTION

In the main text, we discussed Planckian ω/T scaling for two correlators whose spectral parts exhibit a plateau: $\chi[S_r^z]$ and $\chi[j_{cl}^x]$, the correlators for the local spin and the cluster-current in the x -direction, defined in Eqs. (4).

Our NRG impurity solver directly computes the corresponding real frequency spectra $\chi''[O](\omega, T)$. We use the discrete NRG data for the latter as input to evaluate the respective imaginary-time correlators $\langle O(\tau)O^\dagger \rangle$ via Eq. (3), thereby avoiding broadening artifacts.

In the imaginary-time domain, a correlator of the form

$$\langle O(\tau)O^\dagger \rangle \sim \frac{\pi T}{\sin(\pi T\tau)} \quad (S1)$$

represents scale-invariant finite-temperature behavior, where temperature sets the only energy scale and the dependence enters through the dimensionless combination $\pi T\tau$. The form (S1) has the imaginary-time periodicity properties required for finite-temperature correlators and can be viewed as the thermal generalization of a zero-temperature $1/\tau$ correlator.

The spectral function associated with the correlator (S1) has the form $\chi''[O](\omega, T) = \mathcal{X}''(x)$, where

$$\mathcal{X}''(x) = \mathcal{X}_0'' \tanh(x/2), \quad x = \omega/T. \quad (S2)$$

This has properties characteristic of Planckian scaling: linear in x for $x \ll 1$ and saturation to a plateau at $x \gg 1$. The parameter $\mathcal{X}_0''$ sets the overall scale.

We define the real part of the correlator, $\chi'[O](\omega, T)$, by the Kramer-Kronig relation

$$\mathcal{X}'(x, y) = \mathcal{P} \int_{-y}^y d\tilde{x} \frac{\mathcal{X}''(\tilde{x})}{x - \tilde{x}}, \quad (S3)$$

introducing y as an ultraviolet cutoff to regularize the integral, which diverges as $-\ln y$ for $y \rightarrow \infty$. To isolate the divergent part [111], we use $\frac{1}{x-\tilde{x}} = -\frac{1}{\tilde{x}} + \frac{x}{(x-\tilde{x})\tilde{x}}$ and write $\mathcal{X}'(x, y) \simeq \mathcal{X}'_0(y) + \mathcal{X}'(x)$, with

$$\mathcal{X}'_0(y) = -\mathcal{P} \int_{-y}^y d\tilde{x} \frac{\mathcal{X}''(\tilde{x})}{\tilde{x}}, \quad (S4a)$$

$$\mathcal{X}'(x) = \mathcal{P} \int_{-\infty}^{\infty} d\tilde{x} \frac{x\mathcal{X}''(\tilde{x})}{(x-\tilde{x})\tilde{x}}. \quad (S4b)$$

Here, $\mathcal{X}'_0(y) \simeq \mathcal{X}'(0, y)$ represents the singular, “static” contribution, and we took $y \rightarrow \infty$ in Eq. (S4b). All in all, we thus obtain a scaling function of the form

$$\mathcal{X}(x, y) \simeq \mathcal{X}'_0(y) + \mathcal{X}'(x) - i\pi\mathcal{X}''(x). \quad (S5)$$

In the main text, we employed this form to fit correlators $\chi(\omega, T)$ computed with DCA+NRG, using $y = T_{\text{NFL}}/T$ as ultraviolet cutoff [111]. Then, both $\chi''(\omega, T) = \mathcal{X}''(x)$ and $\chi'[O](\omega, T) - \chi'(0, T) = \mathcal{X}'(x)$ show scaling with $x = \omega/T$, and $\chi'[O](0, T) = \mathcal{X}'(T_{\text{NFL}}/T)$ describes the static part. When applied to the correlators $\mathcal{X}[S_r^z]$ and $\mathcal{X}[j_{cl}^x]$ discussed in the main text, fits of our numerical data for $\chi''(\omega, T)$ to Eq. (S2), with $\mathcal{X}_0''$ as fit parameter, yield $\mathcal{X}_0''[S_r^z] \simeq 0.132$ and $\mathcal{X}_0''[j_{cl}^x] \simeq 0.0189$.

S-II. SPECTRAL FUNCTIONS

In this section, we analyze the temperature evolution of the spectral parts of the patch Green’s functions $G_{\mathbf{K}}$, self-energies $\Sigma_{\mathbf{K}}$, and hybridization functions $\Delta_{\mathbf{K}}$ obtained from our DCA calculations at chemical potential $\mu = 1.24$. We denote their spectral parts, defined as $X_{\mathbf{K}}''(\omega) = -\frac{i}{2\pi}[X_{\mathbf{K}}(\omega) - X_{\mathbf{K}}^\dagger(\omega)]$, by $A_{\mathbf{K}}$, $\Sigma_{\mathbf{K}}''$ and $\Delta_{\mathbf{K}}''$, respectively. These are shown in the first, second and third rows of Fig. S1, with each column corresponding to a specified DCA patch momentum $\mathbf{K}$.

In the nodal patches $\mathbf{K} = (0, 0)$ and $\mathbf{K} = (\pi, \pi)$, which dominate the high- and low-frequency regimes and are associated with the upper and lower Hubbard bands, respectively, the spectral functions $A_{\mathbf{K}}$, $\Sigma_{\mathbf{K}}''$ and $\Delta_{\mathbf{K}}''$ all depend only very weakly on temperature. This implies that coherence is preserved as a function of temperature along the nodal direction.

By contrast, for the spectral functions for the degenerate antinodal patches, $\mathbf{K} = (0, \pi)$ and $\mathbf{K} = (\pi, 0)$, exhibit a pronounced temperature dependence. For $A_{(0,\pi)}$, we observe the well-known opening of a pseudogap as T decreases [Fig. S1(a2)]. Correspondingly, $\Sigma_{(0,\pi)}''$ develops a sharp peak, signaling the loss of coherence [Fig. S1(b2)]. For the hybridization function, a step-like feature emerges with decreasing temperature, leading to a strong particle-hole asymmetry at $\omega = 0$ [Fig. S1(c2)].

Figure S2 shows results for the spectral functions $A_{\mathbf{K}}(\omega = 0)$ computed using the raw (non-interpolated)

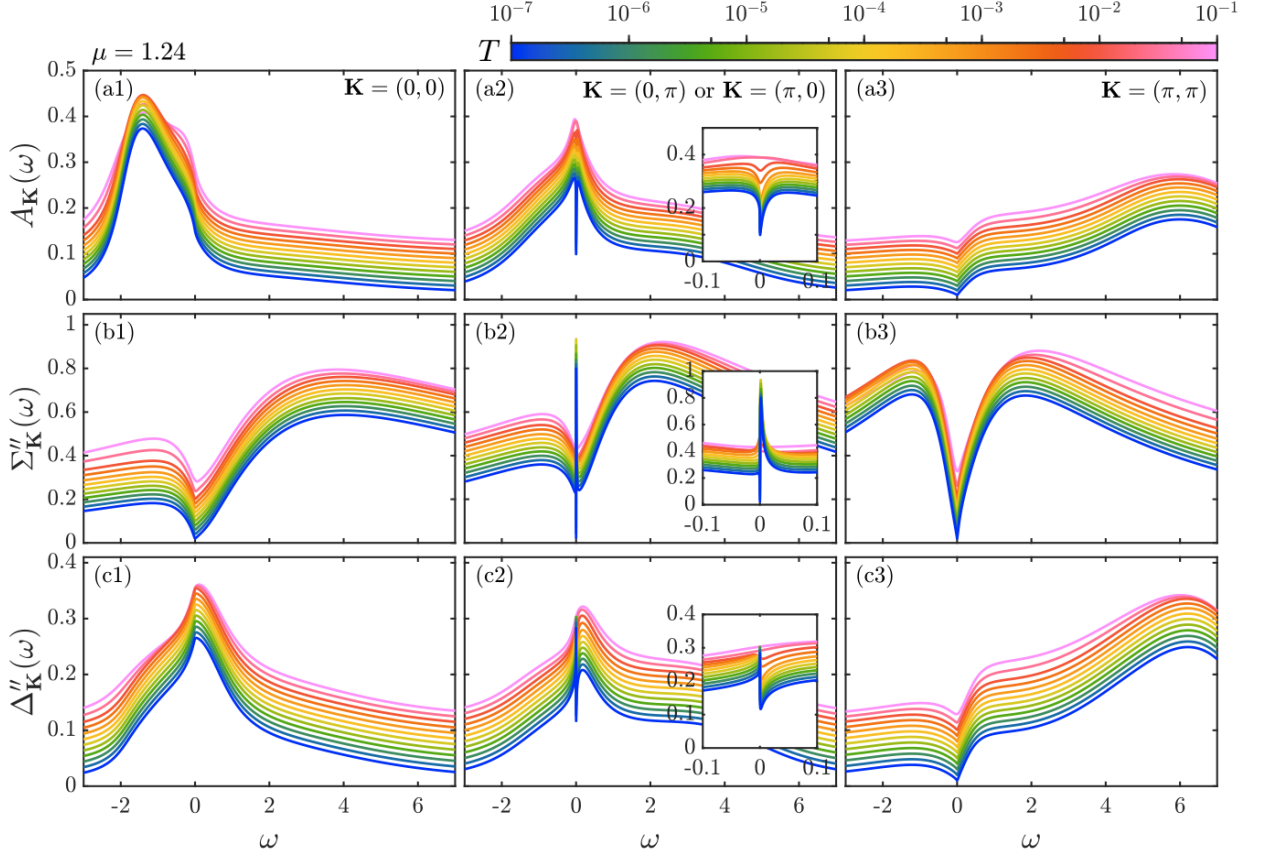


FIG. S1. Spectral functions of (a) the Green's function, (b) the self-energy, and (c) the hybridization at $\mu = 1.24$ as a function of ω for several temperatures T , denoted by different colors. Columns (1-3) depict DCA patch momenta $\mathbf{K} = (0,0)$, $\mathbf{K} = (0,\pi)$ or $\mathbf{K} = (\pi,0)$, and $\mathbf{K} = (\pi,\pi)$, respectively. For visual clarity, spectral functions for successive temperatures are vertically offset by 0.01 for $A_{\mathbf{K}}$ and $\Delta_{\mathbf{K}}''$, and by 0.02 for $\Sigma_{\mathbf{K}}''$. The insets for the anti nodal points show a zoom around $\omega = 0$.

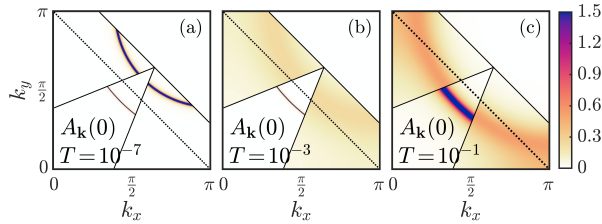


FIG. S2. Analogous to Fig. 4, but now showing spectral functions $A_{\mathbf{k}}(\omega = 0)$ computed using the non-interpolated DCA results for the patch self-energies $\Sigma_{\mathbf{K}}(\omega = 0)$. Black lines mark DCA patch boundaries.

DCA results for the patch self-energies $\Sigma_{\mathbf{K}}(\omega = 0)$ at three temperatures. (Figure 4 was computed analogously, but using a self-energy $\Sigma_{\mathbf{k}}$ obtained by Liouvillian interpolation [120].) Consistent with the spectral functions shown in Figs. S1 and 4, the nodal patches remain essentially unaffected by the change in temperature. In

contrast, the antinodal patches become strongly broadened as the temperature increases.

S-III. COMPUTATION OF THE BUBBLE CONTRIBUTIONS

In this section, we detail the formulas used to compute the bubble contributions to the optical conductivity, $\sigma'_{\text{cl,B}}(\omega, T)$ and $\sigma'_{\text{latt,B}}(\omega, T)$, computed for the cluster or the lattice, respectively. For numerical accuracy, we employ the integration method for the convolution of the bubble contribution introduced in Ref. [111].

A. Lattice Bubble

A conclusive determination of the resistivity scaling requires evaluating the lattice bubble rather than the local cluster bubble. In particular, the local vertex contribu-

tions computed on the cluster must dominate the low-frequency behavior over the lattice bubble term to yield the same linear-in- T scaling.

However, resolving this regime is numerically challenging. Solving a four-site cluster impurity within NRG is computationally demanding due to the exponential growth of the Hilbert space with cluster size. As a result, the very low-frequency regime ($\omega \lesssim T$) of the self energy, which is only visible on a logarithmic frequency grid, is not sufficiently reliable to accurately determine the lattice bubble contribution. Further numerical improvements are therefore required to establish scaling behavior beyond the local cluster level.

Nevertheless, we compute and show $\sigma_{\text{latt,B}}(\omega, T)$ compared to the cluster bubble for future reference. The lattice contribution to the optical conductivity is computed within the bubble approximation by explicitly retaining the dispersion dependence within each momentum patch. The total conductivity is obtained as an average over cluster momenta,

$$\sigma_{\text{latt,B}}(\omega) = \frac{1}{N_p} \sum_{\mathbf{K}} \sigma_{\mathbf{K}}^{\text{latt,B}}(\omega), \quad (\text{S6})$$

where each patch contribution $\sigma_{\mathbf{K}}^{\text{latt,B}}(\omega)$ is expressed as an integral over the band energy ϵ ,

$$\sigma_{\mathbf{K}}^{\text{latt,B}}(\omega) = 2\pi e^2 \int d\epsilon \Phi_{\mathbf{K}}^{xx}(\epsilon) \tilde{\sigma}_{\mathbf{K}}^{\text{latt,B}}(\epsilon, \omega), \quad (\text{S7})$$

Here, $\Phi_{\mathbf{K}}^{xx}(\epsilon)$ is the energy-resolved transport function, defined as the patch average of the squared band velocity weighted by the density of states,

$$\Phi_{\mathbf{K}}^{xx}(\epsilon) = \int_{V_{\mathbf{K}}} \frac{d\mathbf{k}}{V_{\mathbf{K}}} (v_{\mathbf{k}}^x)^2 \delta(\epsilon - \epsilon_{\mathbf{k}}), \quad (\text{S8})$$

where $v_{\mathbf{k}}^x = \partial\epsilon_{\mathbf{k}}/\partial k_x$ is the band velocity in the x -direction, and the integral is over momentum patch $\mathbf{K}$ with patch volume $V_{\mathbf{K}}$. The transport function $\Phi_{\mathbf{K}}^{xx}(\epsilon)$ captures the geometric contribution of the electronic dispersion to the optical response and weights the spectral functions involved in $\tilde{\sigma}_{\mathbf{K}}^{\text{latt,B}}$ [see Eq. (S9)] according to their current-carrying capability within each patch.

The dynamical part of the conductivity is encoded in the particle-hole bubble at band energy ϵ ,

$$\tilde{\sigma}_{\mathbf{K}}^{\text{latt,B}}(\epsilon, \omega) = \int d\tilde{\omega} \frac{f(\tilde{\omega}) - f(\tilde{\omega} + \omega)}{\omega} A_{\mathbf{K}}(\epsilon, \tilde{\omega}) A_{\mathbf{K}}(\epsilon, \tilde{\omega} + \omega). \quad (\text{S9})$$

Here, $f(\omega)$ is the Fermi-Dirac distribution, and the patch spectral function

$$A_{\mathbf{K}}(\epsilon, \omega) = -\frac{1}{\pi} \text{Im} \left[\frac{1}{\omega + \mu - \epsilon - \Sigma_{\mathbf{K}}(\omega)} \right] \quad (\text{S10})$$

depends on the patch self-energy $\Sigma_{\mathbf{K}}(\omega)$, which is momentum-independent within each patch. Finally, the

dc conductivity is obtained from the zero-frequency limit,

$$\sigma^{xx} = \lim_{\omega \rightarrow 0} \sigma(\omega). \quad (\text{S11})$$

The above formulation effectively separates the geometric (band-structure) contribution, captured by $\Phi_{\mathbf{K}}^{xx}(\epsilon)$, from the many-body dynamics encoded in the spectral functions. Compared to the cluster bubble discussed below, this approach replaces the patch-averaged velocity factor by an energy-resolved transport function, thereby improving numerical accuracy and capturing intra-patch dispersion effects.

B. Cluster Bubble

If the cluster contribution to the local optical conductivity is computed within the bubble approximation, one uses formulas analogous to but simpler than those above:

$$\sigma_{\text{cl,B}}(\omega) = \frac{1}{N_p} \sum_{\mathbf{K}} \sigma_{\mathbf{K}}^{\text{cl,B}}(\omega), \quad (\text{S12})$$

$$\sigma_{\mathbf{K}}^{\text{cl,B}}(\omega) = 2\pi e^2 \langle \Phi_{\mathbf{K}}^{xx} \rangle \tilde{\sigma}_{\mathbf{K}}^{\text{cl,B}}(\omega), \quad (\text{S13})$$

$$\tilde{\sigma}_{\mathbf{K}}^{\text{cl,B}}(\omega) = \int d\tilde{\omega} \frac{f(\tilde{\omega}) - f(\tilde{\omega} + \omega)}{\omega} A_{\mathbf{K}}(\tilde{\omega}) A_{\mathbf{K}}(\tilde{\omega} + \omega), \quad (\text{S14})$$

$$A_{\mathbf{K}}(\omega) = -\frac{1}{\pi} \text{Im} \left[\frac{1}{\omega + \mu - \epsilon_{\mathbf{K}} - \Delta_{\mathbf{K}}(\omega) - \Sigma_{\mathbf{K}}(\omega)} \right], \quad (\text{S15})$$

$$\langle \Phi_{\mathbf{K}}^{xx} \rangle = \int_{V_{\mathbf{K}}} \frac{d\mathbf{k}}{V_{\mathbf{K}}} (v_{\mathbf{k}}^x)^2, \quad \epsilon_{\mathbf{K}} = \int_{V_{\mathbf{K}}} \frac{d\mathbf{k}}{V_{\mathbf{K}}} \epsilon_{\mathbf{k}}. \quad (\text{S16})$$

$\tilde{\sigma}_{\mathbf{K}}^{\text{cl,B}}(\omega)$ is the particle-hole bubble, describing current-current correlations without vertex corrections; its frequency convolution encodes the creation of particle-hole excitations at energy ω , and the spectral functions occurring therein contain $\epsilon_{\mathbf{K}} + \Delta_{\mathbf{K}}(\omega)$ in the denominator rather than $\epsilon_{\mathbf{k}}$.

4 Conclusion and Outlook

In this section, we conclude from our findings that there is evidence for a quantum critical point and that our results provide a consistent picture with experimental studies [Che+19; RZP+19; MBR+23]. Our investigation also led to the development of a novel interpolation scheme for cluster dynamical mean-field theories.

Even though we made an extensive study of quantum criticality in the two-dimensional Hubbard model with conclusive results, there are still many interesting topics to investigate in the this regard on which we touch in an outlook.

4.1 Conclusion

In this thesis, we solve the Hubbard model embedded into a self-consistent bath. It serves as a minimal description of the CuO_2 plane in cuprate materials.

Despite the often argued necessity of additional orbital degrees of freedom to accurately describe the physical phenomena found in cuprates, we manage to simulate experimental findings of angle resolved photoemission spectroscopy (ARPES) and transport measurements with astonishing consistency. But not only do we find consistency with experiments, we are also able to answer the long-standing question of quantum criticality in the finite hole doping regime between the Fermi liquid and pseudogap phases.

Our major finding is a vanishing Fermi liquid scale at a critical doping $p^* \simeq 0.14$ providing proof of a quantum critical point (QCP). The Fermi liquid scale vanishes in various correlation function. This vanishing Fermi liquid scale manifests as a plateau extension towards p^* , i.e. strong increase of respective fluctuations. We find a momentum selective enhancement of charge $C_{\mathbf{K}}$ and spin $S_{\mathbf{K}}^z$ fluctuations. For the charge sector increasing fluctuations at momentum $\mathbf{Q} = (0, 0)$ and $\mathbf{Q} = (\pi, \pi)$ are indicative of charge order, often referenced in literature [Cho+20; WAC15; TL19; P  p+14; Mia+21]. The spin sector shows enhancement only at $\mathbf{Q} = (\pi, \pi)$ providing evidence for short-ranged antiferromagnetic correlations, driving the transition as found in Ref. [Wu+18].

We are able to observe the QCP due to suppressing superconductivity within our computations, nevertheless we observe a similar enhancement of fluctuations for $d_{x^2-y^2}$ -wave pairing, while s -wave and extended s -wave ($x^2 + y^2$) remain unaffected. This is indicative for the type of superconductivity found in the Hubbard model and cuprates being $d_{x^2-y^2}$ superconductivity.

Moreover, at p^* we observe a Fermi surface reconstruction from a full Fermi surface to Fermi arcs. The transition takes place at the antinodal point, where an emergent self-energy peak at $\omega = 0$ suppresses the spectral weight of the electronic Green's function. However, the nodal point $(\pi/2, \pi/2)$ seem to be unaffected. This is consistent with recent ARPES experiments [Che+19; RZP+19], which are reproduced to astonishing similarity by our Hubbard model computations.

We further investigate the temperature dependence of the local optical conductivity in the vicinity of the QCP. The plateau extension occurs not only as function of doping but also as function of temperature towards p^* . Within the quantum critical cone this extension equates to a ω/T -scaling, which fits Planckian scaling behavior as proposed in literature [MBR+23; Coo+09; Leg+19; Gri+21], indicative of linear-in- T resistivity. Due

to comparing our computations to the cluster and lattice bubble contribution we are able to conclude that vertex contributions play the major part in the emergence of the observed properties. The scaling in the susceptibility is accompanied by an suggestive marginal Fermi-liquid behavior in the nodal self-energy $\Sigma''_{(0,0)}(\omega, T) \sim \max(\omega, T)$, which is also found experimentally [Ols+90; Val+99; Cha+08; RZP+19].

Along our investigation of the Hubbard model we also explored various interpolation methods as post-processing methods to restore smooth momentum dependence within our cluster approximation. These interpolations are often plagued by causality issues and might not be able to resolve intrinsic structures [Ver+22b]. Inspired by Ref. [Ver+22b] we developed a novel method for interpolation of cluster dynamical mean field theories. We construct a continuous fraction expansion (CFE) of the self-energy whose coefficients are matrix elements of the one-particle irreducible Liouvillian. An interpolation of these matrix elements preserves causality, since the CFE coefficients are frequency independent.

4.2 Outlook

In future work, it would be interesting to establish a more detailed connection with previous cluster DMFT studies of the doped Hubbard model [Civ+05; SK06a; HK07; Sor+12a; Fer+09; Gul+10], in particular the work of *Sordi et al.* [Sor+12a].

Another interesting direction is the emergence of composite quasiparticles, similar to those discussed in Ref. [GK26]. Indeed, we observe the emergence of a coherent peak in the composite-quasiparticle propagator within the pseudogap phase, which warrants further investigation.

Since the employed NRG impurity solver enables the computation of a wide range of dynamical susceptibilities, the investigation of additional physical properties, as the ones discussed in Ref. [P4], is also possible.

Spin dynamics, such as the spin-lattice relaxation rate T_1^{-1} and the spin-echo decay rate T_{2G}^{-1} , can be obtained from dynamical spin susceptibilities (see Refs. [MM92; BP95; CLG17]). This enables further comparison with experiments on cuprate materials. Both T_1^{-1} and T_{2G}^{-1} are experimentally accessible via nuclear magnetic resonance (NMR). These quantities are directly linked to the dynamical spin susceptibility $\chi(\mathbf{q}, \omega)$ and are therefore sensitive to antiferromagnetic correlations, particularly in the $\mathbf{q} = (\pi, \pi)$ channel [Sli90]. They provide insight into the strength and dynamics of short-range antiferromagnetic fluctuations in the vicinity of the quantum critical point.

Other accessible observables include thermodynamic quantities. The impurity entropy is defined as $S_{\text{imp}}(T) = S_{\text{total}}(T) - S_{\text{bath}}(T)$, and is obtained from the computation of the total system and bath entropy. Within NRG, the entropy is evaluated from the expectation value of the Hamiltonian and the partition function via $S = \beta \langle H \rangle + \ln Z$ [BCP08]. An accurate lattice entropy $S_{\text{latt}}(T)$ can be obtained by including an additional correction term $S_{\text{corr}}(T)$, which accounts for the difference between the impurity and lattice descriptions. A general formulation of this correction term is currently the subject of ongoing work within our group.

Knowledge of the entropy further allows for the computation of the specific heat, providing an additional benchmark for the Hubbard model as a minimal description of cuprates. In particular, the experimentally observed behavior $C_V/T \propto \ln T$ [Gir+21; TS23] can be directly compared to theoretical results.

Further thermodynamic transport properties that exhibit anomalous behavior in the strange-metal and pseudogap regimes of cuprates include the thermopower, i.e., the

Seebeck effect. Their computation is possible using the Kelvin formula of Ref. [PS10], combined with the real-frequency information accessible from NRG.

Another important direction is the investigation of the superconducting phase. By relaxing enforced symmetries and allowing for spontaneous symmetry breaking, one can study dynamical quantities, such as pairing susceptibilities, within the superconducting dome in greater detail.

In addition to further investigating the parameter regime of the Hubbard model discussed in this thesis, similar studies can be carried out on the electron-doped side of the Hubbard model or using a minimal cluster of the Emery model.

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