

# Analytic Continuation of Multipoint Correlation Functions

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Conceptually, the Matsubara formalism (MF), using imaginary frequencies, and the Keldysh formalism (KF), formulated in real frequencies, give equivalent results for systems in thermal equilibrium. The MF has less complexity and is thus more convenient than the KF. However, computing dynamical observables in the MF requires the analytic continuation from imaginary to real frequencies. The analytic continuation is well-known for two-point correlation functions (having one frequency argument), but, for multipoint correlators, a straightforward recipe for deducing all Keldysh components from the MF correlator had not been formulated yet. Recently, a representation of MF and KF correlators in terms of formalism-independent partial spectral functions and formalism-specific kernels was introduced by Kugler, Lee, and von Delft [Phys. Rev. X 11, 041006 (2021)]. This representation is used to formally elucidate the connection between both formalisms. How a multipoint MF correlator can be analytically continued to recover all partial spectral functions and yield all Keldysh components of its KF counterpart is shown. The procedure is illustrated for various correlators of the Hubbard atom.

## 1. Introduction

Multipoint correlation functions, or correlators for short, are central objects of investigation in many-body physics. The fermionic one-particle or two-point (2p) correlator describes the propagation of a single particle, containing information on the spectrum of single-particle excitations. The two-particle or four-point (4p) correlator is associated with the effective interaction between two particles. Interesting observables, like optical and magnetic response functions, can be deduced from it. Additionally, the closely related 4p vertex, obtained by amputating all four external legs, is an essential ingredient in numerous many-body methods such as the functional renormalization group,<sup>[1]</sup> the parquet formalism,<sup>[2]</sup> and diagrammatic extensions of dynamical mean field theory.<sup>[3]</sup>

The most common framework for studying systems in thermal equilibrium at temperature  $T = 1/\beta$  is the imaginary-time Matsubara formalism (MF).<sup>[4]</sup> It exploits the cyclicity of the trace and the fact that the statistical weight of a thermal state for a Hamiltonian  $H$ ,  $e^{-\beta H}$ , corresponds to a time-evolution  $e^{-iHt}$  along the imaginary axis of the time argument. After a so-called Wick rotation,  $t \rightarrow -i\tau$ , the correlators are well-defined on the interval  $\tau \in [-\beta, \beta]$  and there satisfy (anti)periodicity relations with period  $\beta$ . Correspondingly, they can be expressed through a Fourier series using a discrete set of imaginary frequencies, the so-called Matsubara frequencies, ensuring this (anti)periodicity. Due to this periodicity, the Fourier transform of a MF correlator is a function defined on a discrete set of imaginary frequencies, so-called Matsubara frequencies. To obtain a correlator of real times or real frequencies, one has to “unwind” the Wick rotation by performing a suitable analytic continuation. Numerically, however, the analytic continuation to real frequencies is a highly challenging problem.<sup>[5,6]</sup>

The Keldysh formalism (KF) is another established framework.<sup>[7]</sup> Unlike the MF, it is not restricted to thermal equilibrium. It directly works with real times and frequencies, obviating the need for an analytic continuation. However, this comes at the cost of an increased complexity: the KF is formulated on a doubled time contour, and an  $\ell$ -point ( $\ell$ p) function has  $2^\ell$  components.<sup>[8,9]</sup> By contrast, every MF correlator is just a single function.

In thermal equilibrium, both MF and KF must in principle yield identical results for exact computations of any physical observable—the two formalisms only differ in the computational route to arrive at the result. In practice, though, it may be useful

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to transition from one formalism to the other, in order to exploit advantages from one or the other. The connection between the MF and KF by means of analytic continuation is well known for 2p functions, which effectively depend on a single time or frequency argument, see e.g., refs. [10–12]. For higher-point functions, progress has been made by various authors: Eliashberg discussed the analytic continuation of a specific 4p correlator from the MF to real frequencies.<sup>[13]</sup> Evans<sup>[14]</sup> and Kobes<sup>[15,16]</sup> studied the correspondence between both formalisms for 3p correlators in refs. [14–16]. Evans then considered  $\ell \geq 4$  multipoint correlators and showed that fully retarded and fully advanced Keldysh components can be obtained from analytic continuations of MF correlators.<sup>[17]</sup> Weldon conducted a thorough analysis of real-frequency  $\ell$ p functions and proved that these KF components are in fact the only ones that can be identified with an analytically continued MF function.<sup>[18,19]</sup> Taylor extended Evans' results to arbitrary Keldysh components of the fermionic 4p correlator, assuming the absence of so-called anomalous terms in the MF correlator.<sup>[20]</sup> (Anomalous terms can arise if the Lehmann representation of a correlator involves vanishing eigenenergy differences and zero bosonic Matsubara frequencies.) Guerin derived analogous results from diagrammatic arguments.<sup>[21,22]</sup>

In this paper, we solve the problem of analytic continuation of multipoint functions from the MF to the KF in full generality: We develop a strategy for analytically continuing an arbitrary MF  $\ell$ p correlator  $G$  (including anomalous terms) to all  $2^\ell$  components of the corresponding KF correlator  $G^k$  as functionals of  $G$ , i.e.,  $G^k = G^k[G]$ . We exemplify the procedure for the most relevant cases  $\ell \in \{2, 3, 4\}$ .

Our strategy builds upon the spectral representation of general  $\ell$ p correlators introduced in ref. [23]. There, the computation of MF and KF correlators is split into two parts: the calculation of formalism-independent but system-dependent partial spectral functions (PSFs), and their subsequent convolution with formalism-dependent but system-independent kernels. The main message of the present paper is that individual PSFs can be retrieved from the MF correlator, demonstrating the direct link between both formalisms.

In a nutshell, both MF and KF correlators have spectral representations involving sums over permutations of their constituent operators of the form

$$G(i\omega) = \sum_p G_p(i\omega_p), \quad G_p(i\omega_p) = (K * S_p)(i\omega_p) \quad (1a)$$

$$G^k(\omega) = \sum_p G_p^{k_p}(\omega_p), \quad G_p^{k_p}(\omega_p) = (K^{k_p} * S_p)(\omega_p) \quad (1b)$$

Here, the summands  $G_p$  and  $G_p^{k_p}$  are real-frequency convolutions (denoted by  $*$ ) of MF or KF kernels,  $K$  or  $K^{k_p}$ , with PSFs  $S_p$ . Importantly, the MF and KF correlators depend on the *same* PSFs,  $G = G[S_p]$  and  $G^k = G^k[S_p]$ . The key insight of this work is that the so-called regular part of the *partial* MF correlator  $G_p$ , denoted  $\tilde{G}_p$ , can be expressed as an imaginary-frequency convolution (denoted by  $\star$ ) of a kernel and the *full* MF correlator:

$$\tilde{G}_p(i\omega_p) = (\tilde{K} * S_p)(i\omega_p) = (K \star G)(i\omega_p) + \mathcal{O}(\frac{1}{\beta}) \quad (1c)$$

(The  $\mathcal{O}(\frac{1}{\beta})$  terms can be identified analytically and discarded.) From this, we can extract  $S_p$  as a functional of  $G$ , thus inverting the relation  $G[S_p] \rightarrow S_p[G]$ . That enables us to express KF through MF correlators,  $G^k = G^k[G]$ .

Our analysis not only provides relations between functions in the MF and the KF, but also between different Keldysh components of the KF correlator. As an application of our general results, we derive a complete set of generalized fluctuation-dissipation relations (gFDRs) for 3p and 4p functions. These reproduce the results of Wang and Heinzl<sup>[24]</sup> for real fields and the generalization to fermionic ones.<sup>[25]</sup> Moreover, we give a comprehensive discussion of the role of anomalous terms during analytic continuation and in gFDRs. Prior discussions of these topics have often neglected anomalous terms; indeed, their presence is acknowledged only in few works, such as refs. [26–28]. As an example of their physical importance, we mention that ref. [28] analyzed anomalous terms for the Mott–Hubbard metal–insulator transition in the Hubbard model using the dynamical mean-field theory and detected a degeneracy in the insulating regime by means of a finite anomalous term.

Conceptually, the Matsubara formalism (MF), using imaginary frequencies, and the Keldysh formalism (KF), formulated in real frequencies, give equivalent results for systems in thermal equilibrium. The MF has less complexity and is thus more convenient than the KF. However, computing dynamical observables in the MF requires the analytic continuation from imaginary to real frequencies. The analytic continuation is well-known for two-point correlation functions (having one frequency argument), but, for multipoint correlators, a straightforward recipe for deducing all Keldysh components from the MF correlator had not been formulated yet. Recently, a representation of MF and KF correlators in terms of formalism-independent partial spectral functions and formalism-specific kernels was introduced by Kugler, Lee, and von Delft. Regarding the number of independent components in the KF, one observes a general trend, obeyed by the known results for  $\ell \in \{2, 3, 4\}$ : Due to the doubled time contour, there are  $2^\ell$  Keldysh components. In the Keldysh basis,  $2^\ell - 1$  of them are nonzero, and  $\ell$  are fully retarded components. Now, there are  $2^{\ell-1}$  gFDRs (2, 4, 8 for  $\ell = 2, 3, 4$ ). Thus, the number of independent Keldysh components is  $2^{\ell-1} - 1$  (1, 3, 7 for  $\ell = 2, 3, 4$ ). It follows that, for  $\ell \geq 4$ , the fully retarded components do not suffice to encode the entire information of the Keldysh correlator.

The rest of the paper is organized as follows: In Section 2, we summarize the most important points of the spectral representation of  $\ell$ p MF and KF correlators introduced in ref. [23] (Sections 2.1–2.3) and then introduce our general recipe for the analytic continuation of arbitrary  $\ell$ p correlators (Sections 2.4 and 2.5). This recipe is applied to the 2p case in Section 3 and, after the investigation of analytic properties of regular  $\ell$ p MF correlators in Section 4, also to the 3p and 4p cases in Sections 5 and 6. The results also lead to gFDRs between different Keldysh components of the KF correlator. In Section 7, we perform explicit analytic continuations from MF to KF correlators for the Hubbard atom. The Hubbard atom is a good example for a system with anomalous contributions and, here, serves as a simple, exactly solvable model with just the right degree of complexity for illustrating our approach. Section 8 presents another application

**Table 1.** Overview of notation for correlators and their contributions. In the top, we list symbols for the MF correlator and its contributions, then, notation for analytic continuations and discontinuities, and, lastly, notation for Keldysh correlators.

Symbol	Description
$G$	full MF correlator, Equations (9)
$G_p$	partial MF correlator, Equation (11b)
$\tilde{G}, \hat{G}$	regular and anomalous part of the MF correlator, Equations (14a) and (A5)
$\tilde{G}_p$	regular part of the partial MF correlator, Equation (14c)
$\hat{G}_i, \hat{G}_i^\Delta, \hat{G}_i^\Delta$	further decomposition of the anomalous MF correlator, Equations (A5b) and (73)
$\tilde{G}_{z^+}, \hat{G}_{z^+}$	shorthand for analytic continuations of the regular/anomalous MF correlator, see Section 4.1
$\tilde{G}_{z^+}^\omega, \hat{G}_{z^+}^\omega$	discontinuities of the regular/anomalous MF correlator, Equation (67)
$G^k, G^{[n_1 \dots n_\alpha]}$	Keldysh correlator, Equations (19)
$G'^k, G'^{[n_1 \dots n_\alpha]}$	primed Keldysh correlator, Equations (25)

of our continuation formulas, namely for the computation of vertex corrections to susceptibilities. We conclude in Section 9.

In Appendix A and B, we give details on the MF kernels and PSFs used in calculations throughout the paper. Appendix C is devoted to detailed calculations concerning the analytic continuation of 3p correlators. In Appendix D, we extend insights from 2p and 3p results to deduce the relation between 4p PSFs and analytically continued MF correlators. The spectral representations of various useful combinations of analytically continued MF correlators and anomalous parts are presented in Appendix E. Appendix F expresses the spectral representation of KF correlators in a form especially suited for deriving their connection to MF functions. In Appendix G, we check the consistency of our results for PSFs by using equilibrium properties. Finally, Appendix H gives details about simplifications used for the analytic continuation of Hubbard atom correlators and includes full lists of the especially important fermionic 4p KF correlators.

## 2. Spectral Representations of Matsubara and Keldysh Correlators

To make our presentation self-contained, we summarize the key elements of the conventions and results of ref. [23] for common notions (Section 2.1), the MF (Section 2.2), and the KF (Section 2.3). Table 1 provides an overview of our symbols for correlators and their contributions. Our general strategy for the analytic continuation from MF to KF correlators is described in Sections 2.4 and 2.5.

### 2.1. Formalism-Independent Expectations Values

Consider a tuple of  $\ell$  operators  $\mathbf{O} = (O^1, \dots, O^\ell)$  at real times  $\mathbf{t} = (t_1, \dots, t_\ell)$ , obeying the Heisenberg time evolution  $O^j(t_i) = e^{iHt_i} O^j e^{-iHt_i}$  for a given Hamiltonian  $H$ .  $\mathbf{O}$  may include an even number of fermionic operators and any number of bosonic operators. Time-ordered products of such tuples, defined below,

involve permuted tuples  $\mathbf{O}_p = (O^{\bar{1}}, \dots, O^{\bar{\ell}})$  and  $\mathbf{t}_p = (t_{\bar{1}}, \dots, t_{\bar{\ell}})$ , where  $p = (\bar{1} \dots \bar{\ell})$  denotes the permutation of indices that replaces  $i$  by  $p(i) = \bar{i}$ . If  $\ell = 3$  and  $p = (\bar{123})$  is chosen as (312), e.g., then  $\mathbf{t}_p = (t_{\bar{1}}, t_{\bar{2}}, t_{\bar{3}}) = (t_3, t_1, t_2)$ . Thermal expectation values of permuted tuples are denoted by

$$S_p[\mathbf{O}_p](\mathbf{t}_p) = \zeta_p \left\langle \prod_{i=1}^{\ell} O^{\bar{i}}(t_{\bar{i}}) \right\rangle \quad (2)$$

For later convenience, the definition includes a sign factor  $\zeta_p$  which equals  $-1$  if the permutation from  $\mathbf{O}$  to  $\mathbf{O}_p$  involves an odd number of transpositions of fermionic operators; otherwise  $\zeta_p = 1$ . We will often suppress the operator arguments  $[\mathbf{O}_p]$  for brevity, since the subscript on  $S_p$  specifies their order. The real-frequency Fourier transform of  $S_p(\mathbf{t}_p)$  defines the so-called *partial spectral function* (PSF)

$$S_p(\boldsymbol{\varepsilon}_p) = \int_{-\infty}^{\infty} \frac{d^\ell \mathbf{t}_p}{(2\pi)^\ell} e^{i\boldsymbol{\varepsilon}_p \cdot \mathbf{t}_p} S_p(\mathbf{t}_p) \quad (3a)$$

Here,  $\boldsymbol{\varepsilon}_p = (\varepsilon_{\bar{1}}, \dots, \varepsilon_{\bar{\ell}})$  is a permuted version of  $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_\ell)$ , a tuple of continuous, real-frequency variables. We strictly associate each (integration) variable, such as  $t_i, \varepsilon_i$ , with the operator  $O^i$  carrying the same index. Time-translational invariance of  $S_p(\mathbf{t}_p)$  implies energy conservation for  $S_p(\boldsymbol{\varepsilon}_p)$ , which is expressed as

$$S_p(\boldsymbol{\varepsilon}_p) = \delta(\varepsilon_{\bar{1} \dots \bar{\ell}}) S_p(\boldsymbol{\varepsilon}_p) \quad (3b)$$

Here,  $\varepsilon_{\bar{1} \dots \bar{i}} = \varepsilon_{\bar{1}} + \dots + \varepsilon_{\bar{i}}$  is a shorthand for a frequency sum. We call it bosonic/fermionic if the frequencies  $(\varepsilon_{\bar{1}}, \dots, \varepsilon_{\bar{i}})$  are associated with an even/odd number of fermionic operators, i.e., if the sign  $\zeta^{\bar{1} \dots \bar{i}} = \zeta^{\bar{1}} \dots \zeta^{\bar{i}}$  equals  $\pm 1$  (with  $\zeta^j = \pm 1$  for bosonic/fermionic operators  $O^j$ ). The function  $S_p$  (calligraphic type) on the left of Equation (3b) is non-zero only if its arguments satisfy “energy conservation”,  $\varepsilon_{\bar{1} \dots \bar{\ell}} = 0$ ; for  $S_p$  (italic type) on the right, this condition on  $\boldsymbol{\varepsilon}_p$  is understood to hold by definition, e.g., by setting  $\varepsilon_{\bar{\ell}} = -\varepsilon_{\bar{1} \dots \bar{\ell}-1}$ . This convention for frequency arguments of functions typeset in calligraphics or italics also holds for the correlators,  $\mathcal{C}$  vs.  $G$ , and kernels,  $\mathcal{K}$  vs.  $K$ , defined below.

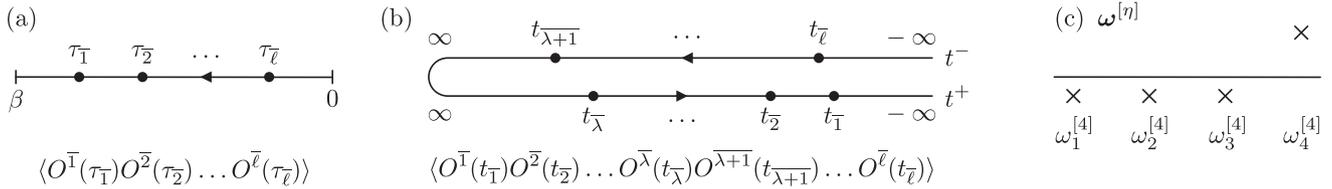
PSFs whose arguments are cyclically related are proportional to each other. For two cyclically related permutations, say  $p = (\bar{1} \dots \bar{\lambda} - 1 \bar{\lambda} \dots \bar{\ell})$  and  $p_\lambda = (\bar{\lambda} \dots \bar{\ell} \bar{1} \dots \bar{\lambda} - 1)$ , the cyclicity of the trace of operator products ensures the equilibrium condition (called cyclicity relation in ref. [23])

$$S_p(\boldsymbol{\varepsilon}_p) = \zeta_p \zeta_{p_\lambda} e^{\beta \varepsilon_{\bar{1} \dots \bar{\lambda}-1}} S_{p_\lambda}(\boldsymbol{\varepsilon}_{p_\lambda}), \quad \zeta_p \zeta_{p_\lambda} = \zeta^{\bar{1} \dots \bar{\lambda}-1} \quad (4)$$

Explicit Lehmann-type representations for PSFs in terms of a complete set of eigenenergies and eigenstates of  $H$  are given in refs. [23, 29] and exploited for numerical computations; however, they are not needed in this work. Here, it suffices to assume that  $S_p(\boldsymbol{\varepsilon}_p)$  may contain sums over Dirac delta functions and a part that is (piece-wise) continuous in its arguments. For future reference, we split it into *regular* and *anomalous* parts,

$$S_p(\boldsymbol{\varepsilon}_p) = \tilde{S}_p(\boldsymbol{\varepsilon}_p) + \hat{S}_p(\boldsymbol{\varepsilon}_p) \quad (5)$$

where the anomalous part,  $\hat{S}_p$ , comprises all terms containing bosonic Dirac  $\delta(\varepsilon_{\bar{1} \dots \bar{i}})$  factors (i.e. ones having bosonic arguments)



**Figure 1.** a) MF imaginary-time ordering: operators are arranged such that they are time-ordered (larger times to the left). b) KF real-time Keldysh ordering: operators are arranged such that all (forward-branch) times  $t^-$  appear to the right of all (backward-branch) times  $t^+$ , with  $t^-$  times time-ordered (larger ones to the left) and  $t^+$  times anti-time-ordered (smaller ones to the left). c) Depiction of imaginary shifts of frequencies  $\omega_i^{[\eta]} = \omega_i + i\gamma_i^{[\eta]}$  with  $i \in \{1, 2, 3, 4\}$  and  $\eta = 4$  according to Equation (21).

setting  $\varepsilon_{\bar{1}, \dots, \bar{i}} = 0$ , while  $\tilde{S}_p$  contains everything else (including fermionic Dirac deltas). We will see later that  $\hat{S}_p$  gives rise to anomalous contributions to MF correlators, whereas  $\tilde{S}_p$  does not.

In the ensuing analysis, we make *no* assumptions on the behavior of the PSFs (apart from cyclicity). Thus, our analysis is equally applicable to finite systems or infinite systems in the thermodynamic limit, and whether or not an ordered phase is present. Any such information is fully encoded in the PSFs.

## 2.2. Matsubara Formalism

A  $\ell$ p MF correlator  $\mathcal{G}$  is defined as a thermal expectation value of time-ordered operator products of the form

$$\mathcal{G}(\boldsymbol{\tau}) = (-1)^{\ell-1} \left\langle \mathcal{T} \prod_{i=1}^{\ell} O^i(-i\tau_i) \right\rangle \quad (6)$$

where  $\mathcal{T}$  denotes time-ordering along the imaginary time axis (see Figure 1a). This time-ordering ensures that  $\mathcal{G}(\boldsymbol{\tau})$  is periodic under  $\tau_i \rightarrow \tau_i + \beta$  if  $O^i$  is bosonic, and anti-periodic if  $O^i$  is fermionic. Therefore, it suffices to confine all times to the interval  $\tau_i \in [0, \beta)$ , and the Fourier transform of a MF correlator is defined as

$$\mathcal{G}(\boldsymbol{\omega}) = \int_0^{\beta} d^{\ell} \tau e^{i\boldsymbol{\omega} \cdot \boldsymbol{\tau}} \mathcal{G}(\boldsymbol{\tau}) = \beta \delta_{i\omega_{1, \dots, \ell}} G(\boldsymbol{\omega}) \quad (7)$$

where  $\boldsymbol{\omega} = (\omega_1, \dots, \omega_{\ell})$  is a tuple of discrete Matsubara frequencies (as indicated by the  $i$  in the argument of  $\mathcal{G}(\boldsymbol{\omega})$ ), with  $\omega_i$  bosonic/fermionic if  $O^i$  is bosonic/fermionic. On the right,  $\delta$  is the Kronecker delta for Matsubara frequencies,  $\delta_{i\omega=0} = 1$  and  $\delta_{i\omega \neq 0} = 0$ . In Equation (7), it enforces “energy conservation”,  $i\omega_{1, \dots, \ell} = 0$ . This condition originates from time translation invariance of  $\mathcal{G}(\boldsymbol{\tau})$ ; it is understood to hold for the argument of  $G(\boldsymbol{\omega})$  by definition.

As shown in ref. [23], it is possible to cleanly separate the analytical properties of correlators from the dynamical properties of the physical system of interest by expressing time-ordered products as sums over  $\ell!$  parts, reflecting the  $\ell!$  possible ways of ordering the time arguments:

$$\mathcal{G}(\boldsymbol{\tau}) = \sum_p \mathcal{G}_p(\boldsymbol{\tau}_p) \quad (8a)$$

$$\mathcal{G}_p(\boldsymbol{\tau}_p) = \mathcal{K}(\boldsymbol{\tau}_p) S_p(-i\boldsymbol{\tau}_p) \quad (8b)$$

$$\mathcal{K}(\boldsymbol{\tau}_p) = \prod_{i=1}^{\ell-1} [-\theta(\tau_i - \tau_{i+1})] \quad (8c)$$

Each *partial correlator*  $\mathcal{G}_p(\boldsymbol{\tau}_p)$  is a product of two factors:  $S_p(-i\boldsymbol{\tau}_p)$ , a thermal expectation value of imaginary-time operators obtained by Wick rotation of Equation (2); and a kernel  $\mathcal{K}(\boldsymbol{\tau}_p)$ , a product of Heaviside step functions enforcing time ordering: for given  $\boldsymbol{\tau}$ , only that partial correlator  $\mathcal{G}_p(\boldsymbol{\tau}_p)$  in Equation (8a) is nonzero for which the permuted tuple  $\boldsymbol{\tau}_p$  is time-ordered.  $\mathcal{K}$  is independent of the system and operators under consideration; all system-specific dynamical information is encoded in the PSFs  $S_p$ . Note that the (anti)periodic properties of  $\mathcal{G}(\boldsymbol{\tau})$  under  $\tau_i \rightarrow \tau_i + \beta$  do not hold for the individual partial correlators  $\mathcal{G}_p(\boldsymbol{\tau}_p)$ ; they emerge only once these are summed over all permutations, Equation (8a).

The product form of Equation (8b) for  $\mathcal{G}_p(\boldsymbol{\tau}_p)$  in the time domain implies that, in the Fourier domain,  $\mathcal{G}(\boldsymbol{\omega})$  can be expressed as a sum over convolutions:

$$\mathcal{G}(\boldsymbol{\omega}) = \sum_p \mathcal{G}_p(\boldsymbol{\omega}_p) \quad (9a)$$

$$\mathcal{G}_p(\boldsymbol{\omega}_p) = \int_0^{\beta} d^{\ell} \tau_p e^{i\boldsymbol{\omega}_p \cdot \boldsymbol{\tau}_p} \mathcal{G}_p(\boldsymbol{\tau}_p) \quad (9b)$$

$$= [\mathcal{K} * S_p](\boldsymbol{\omega}_p) \quad (9c)$$

Here, the convolution  $*$  is defined as

$$[\mathcal{K} * S_p](\boldsymbol{\omega}_p) = \int_{-\infty}^{\infty} d^{\ell} \varepsilon_p \delta(\varepsilon_{\bar{1}, \dots, \bar{\ell}}) \mathcal{K}(\boldsymbol{\omega}_p - \boldsymbol{\varepsilon}_p) S_p(\boldsymbol{\varepsilon}_p) \quad (9d)$$

where  $\varepsilon_p$  satisfies  $\varepsilon_{\bar{1}, \dots, \bar{\ell}} = 0$  (due to Equation (3b)), and the transformed kernel is defined as follows, with  $\boldsymbol{\Omega}_p = \boldsymbol{\omega}_p - \boldsymbol{\varepsilon}_p$ :

$$\mathcal{K}(\boldsymbol{\Omega}_p) = \int_0^{\beta} d^{\ell} \tau_p e^{\boldsymbol{\Omega}_p \cdot \boldsymbol{\tau}_p} \mathcal{K}(\boldsymbol{\tau}_p) \quad (10a)$$

$$= \beta \delta_{\Omega_{1, \dots, \ell}} K(\boldsymbol{\Omega}_p) + \mathcal{R}(\boldsymbol{\Omega}_p) \quad (10b)$$

In the second line,  $\mathcal{K}$  has been split into two contributions:  $\beta \delta_{\Omega_{1, \dots, \ell}}$  times a *primary part*  $K$ , with  $\Omega_{1, \dots, \ell} = 0$  understood for its argument, and a *residual part*,  $\mathcal{R}$  not containing  $\beta \delta_{\Omega_{1, \dots, \ell}}$ . Using  $\delta_{\Omega_{1, \dots, \ell}} = \delta_{i\omega_{1, \dots, \ell}}$  (since  $\varepsilon_{1, \dots, \ell} = 0$ ), each partial correlator  $\mathcal{G}_p(\boldsymbol{\omega}_p)$  can correspondingly be split into primary and residual parts,

$$\mathcal{G}_p(\boldsymbol{\omega}_p) = \beta \delta_{\omega_{1, \dots, \ell}} G_p(\boldsymbol{\omega}_p) + \mathcal{G}_p^{\mathcal{R}}(\boldsymbol{\omega}_p) \quad (11a)$$

$$G_p(\boldsymbol{\omega}_p) = [K * S_p](\boldsymbol{\omega}_p) \quad (11b)$$

with  $i\omega_{1, \dots, \ell} = 0$  understood for the argument of  $G(\boldsymbol{\omega}_p)$ , and  $\mathcal{G}_p^{\mathcal{R}} = [\mathcal{R} * S_p]$ . Since  $\mathcal{K}(\boldsymbol{\tau}_p)$  and  $\mathcal{G}_p(\boldsymbol{\tau}_p)$  lack the (anti)periodicity proper-

ties of  $\mathcal{G}(\tau)$ , the residual parts  $\mathcal{R}(\Omega_p)$  and  $\mathcal{G}_p^{\mathcal{R}}(i\omega_p)$  are nonzero *per se*. However, inserting Equation (11a) into Equation (9a) and noting from Equation (7) that  $\mathcal{G}(i\omega)$  is proportional to  $\beta\delta_{i\omega_{1\dots\ell}}$ , one concludes that

$$G(i\omega) = \sum_p G_p(i\omega_p) \quad (12)$$

and  $\sum_p \mathcal{G}_p^{\mathcal{R}}(i\omega_p) = 0$ . Thus, the *full* (summed over  $p$ ) MF correlator  $G$  involves only primary parts  $G_p$ ; the residual parts  $\mathcal{G}_p^{\mathcal{R}}$  cancel out in the sum over all permutations. In the discussions below, we will therefore focus only on the primary parts  $K$  and  $G_p$  (as done in ref. [23]), ignoring the residual parts  $\mathcal{R}$  and  $\mathcal{G}_p^{\mathcal{R}}$  for now. They will make a brief reappearance in Section 2.4, where we establish the connection between MF and KF correlators.

Explicit expressions for the primary kernel  $K$  were derived in refs. [23, 30] and are collected in Appendix A. Here, we just remark that  $K$  can be split into a *regular* kernel  $\tilde{K}$  and an *anomalous* kernel  $\hat{K}$ :

$$K(\Omega_p) = \begin{cases} \tilde{K}(\Omega_p) & \text{if } \prod_{i=1}^{\ell-1} \Omega_{\bar{1}\dots\bar{i}} \neq 0 \\ \hat{K}(\Omega_p) & \text{else} \end{cases} \quad (13a)$$

$$\tilde{K}(\Omega_p) = \prod_{i=1}^{\ell-1} \frac{1}{\Omega_{\bar{1}\dots\bar{i}}} \quad (13b)$$

The regular kernel  $\tilde{K}$  will play a crucial role for the analytic continuation of MF to KF correlators, since the latter can be expressed through kernels having the same structure as  $\tilde{K}$  (see Equation (19(d)) below). The anomalous kernel  $\hat{K}$  is nonzero only if we have  $\Omega_{\bar{1}\dots\bar{i}} = 0$  for one or more values of  $i < \ell$ , requiring both  $i\omega_{\bar{1}\dots\bar{i}} = 0$  and  $\varepsilon_{\bar{1}\dots\bar{i}} = 0$ . The first condition requires  $i\omega_{\bar{1}\dots\bar{i}}$  to be bosonic (with  $\zeta_{\bar{1}\dots\bar{i}} = +1$ ). The second condition requires the PSF  $S_p(\varepsilon_p)$  to have an anomalous contribution  $\hat{S}_p(\varepsilon_p)$  containing terms proportional to a bosonic Dirac  $\delta(\varepsilon_{\bar{1}\dots\bar{i}})$ ; then (and only then), the  $\varepsilon_p$  integrals in the convolution  $K * S_p$  receive a finite contribution from the point  $\varepsilon_{\bar{1}\dots\bar{i}} = 0$ . (See Appendix B.1 for a further discussion of this point.)

The regular/anomalous distinction made for the kernel implies, via Equations (11b) and (12), a corresponding decomposition of the full MF correlator  $G$  into regular ( $\tilde{G}$ ) and anomalous ( $\hat{G}$ ) parts:

$$G(i\omega) = \tilde{G}(i\omega) + \hat{G}(i\omega) \quad (14a)$$

$$\tilde{G}(i\omega) = \sum_p \tilde{G}_p(i\omega_p) \quad (14b)$$

$$\tilde{G}_p(i\omega_p) = [\tilde{K} * S_p](i\omega_p) \quad (14c)$$

$$= \int_{-\infty}^{\infty} d^\ell \varepsilon_p \delta(\varepsilon_{\bar{1}\dots\bar{\ell}}) \prod_{i=1}^{\ell-1} \frac{S_p(\varepsilon_p)}{i\omega_{\bar{1}\dots\bar{i}} - \varepsilon_{\bar{1}\dots\bar{i}}} \quad (14d)$$

The *regular partial correlators*  $\tilde{G}_p$ , constructed via the regular kernel  $\tilde{K}$ , will be the central objects for the analytic continuation from MF to KF correlators, as discussed in Section 2.4 below. Their sum over all permutations defines the *regular full correlator*  $\tilde{G}$ . The *anomalous full correlator*  $\hat{G}$  collects all other contributions

to  $G$ ; these contain one (or multiple) factors  $\beta\delta_{i\omega_{\bar{1}\dots\bar{i}}}$  with  $i < \ell$ , i.e. they involve vanishing partial frequency sums (see Appendix A.2 for details). The contribution of  $\hat{G}$  to MF-to-KF analytical continuation has been rather poorly understood to date. In this work, we fully clarify how it enters: not directly, but indirectly, in that the central objects  $\tilde{G}_p(i\omega_p)$  can be expressed explicitly through the full  $G = \tilde{G} + \hat{G}$  via imaginary-frequency convolutions of the form  $[K \star G](i\omega_p)$  (see Equation (31) below). There,  $\hat{G}$  must not be neglected.

### 2.3. Keldysh Formalism

A KF  $\ell$ -p correlator in the *contour basis* is defined as

$$\mathcal{G}^c(\mathbf{t}) = (-i)^{\ell-1} \left\langle \mathcal{T}_c \prod_{i=1}^{\ell} O^i(t_i^{c_i}) \right\rangle \quad (15a)$$

$$= \sum_p \mathcal{K}^{c_p}(\mathbf{t}_p) \mathcal{S}(\mathbf{t}_p) \quad (15b)$$

Here,  $\mathcal{T}_c$  denotes contour ordering on the Keldysh contour (see Figure 1b), and  $t_i^{c_i}$  are real times. They carry a tuple of contour indices  $\mathbf{c} = (c_1, \dots, c_\ell)$  with  $c_i = -$  or  $+$  if operator  $O^i$  resides on the forward (upper) or backward (lower) branch of the Keldysh contour, respectively. Equation (15b) is a permutation decomposition of the KF correlator  $\mathcal{G}^c(\mathbf{t})$ , analogous to Equation (8b) for  $\mathcal{G}(\tau)$  in the MF. Importantly, it employs the *same* PSFs  $\mathcal{S}(\mathbf{t}_p)$  as there (which is why the KF and MF formalisms have the same physical information content). The Keldysh kernel  $\mathcal{K}^{c_p}(\mathbf{t}_p)$  by definition (see ref. [23] for details) singles out that  $p$  for which the operators in  $S_p(\mathbf{t})$  are contour ordered.

The Fourier transform of the KF correlator is

$$\mathcal{G}^c(\omega) = \int d^\ell t e^{i\omega \cdot \mathbf{t}} \mathcal{G}^c(\mathbf{t}) = 2\pi \delta(\omega_{1\dots\ell}) \mathcal{G}^c(\omega) \quad (16)$$

Here, the Dirac  $\delta(\omega_{1\dots\ell})$ , following from time translation invariance, enforces  $\omega_{1\dots\ell} = 0$ ; this condition is understood for the argument of  $\mathcal{G}^c(\omega)$  by definition.

We now switch to the Keldysh basis. There, correlators  $\mathcal{G}^k(\omega)$  carry a tuple of Keldysh indices,  $\mathbf{k} = k_1 \dots k_\ell$ , with  $k_i \in \{1, 2\}$ . They are obtained by applying a linear transformation  $D$  to each contour index,

$$\mathcal{G}^k(\omega) = \frac{1}{2} \sum_{c_1, \dots, c_\ell} \prod_{i=1}^{\ell} [D^{k_i c_i}] \mathcal{G}^c(\omega), \quad D^{k_i c_i} = (-1)^{k_i \delta_{c_i, +}} \quad (17)$$

(This convention differs by a prefactor from ref. [23], with  $\mathcal{G}^k_{\text{here}} = 2^{\ell/2-1} \mathcal{G}^k_{\text{there}}$ , to avoid a proliferation of factors of  $2^{\ell/2-1}$  in later sections.) One thus obtains

$$\mathcal{G}^k(\omega) = \sum_p \mathcal{G}_p^{k_p}(\omega_p) \quad (18a)$$

$$\mathcal{G}_p^{k_p}(\omega_p) = (K^{k_p} * S_p)(\omega_p) \quad (18b)$$

$$= \int d^\ell \varepsilon_p \delta(\varepsilon_{\bar{1}\dots\bar{\ell}}) K^{k_p}(\omega_p - \varepsilon_p) S_p(\varepsilon_p) \quad (18c)$$

Remarkably, the same convolution structure emerges as for the MF correlator  $G(i\omega)$  (Equation (11b)), for the same reason (Fourier transforms of products yield convolutions). But now the frequency arguments are real, and the kernel  $K^{k_p}(\omega_p)$  carries Keldysh indices, with  $k_p = k_{\bar{1}} \dots k_{\bar{\ell}}$  a permuted version of the *external* Keldysh index  $k$  on  $G^k$ .

An explicit expression for this kernel, derived in ref. [23], is given in Equations (19) below. There, an alternative notation for Keldysh indices is employed. Each Keldysh index  $k$ , being a list with entries 1 or 2, is represented as a list  $k = [\eta_1 \dots \eta_\alpha]$ , where  $\alpha$  is the total number of 2's in  $k$  and  $\eta_i \in \{1, \dots, \ell\}$  denotes the position of the  $i$ th 2 in  $k$  in increasing order; e.g.,  $k = 1212 = [24]$ . Similarly, permuted Keldysh indices are represented as  $k_p = [\hat{\eta}_1 \dots \hat{\eta}_\alpha]$ , where  $\hat{\eta}_i$  denotes the position of the  $i$ th 2 in  $k_p$ . Its values can be deduced from the old  $\eta_j$ 's as follows: a 2 in slot  $\eta_j$  of  $k$  is moved by the permutation  $p$  to the new slot  $\mu_j = p^{-1}(\eta_j)$ ; denoting the list of new 2-slots by  $[\mu_1 \dots \mu_\alpha]$  and arranging it in increasing order yields the desired  $[\hat{\eta}_1 \dots \hat{\eta}_\alpha]$ . Note also that since  $\hat{\eta}_j \in \{p^{-1}(\eta_1), \dots, p^{-1}(\eta_\alpha)\}$ , we have  $\bar{\hat{\eta}}_1 \in \{\eta_1, \dots, \eta_\alpha\}$ ; hence,  $\bar{\hat{\eta}}_j$  is an element of the list specifying the *external* Keldysh index  $k = [\eta_1 \dots \eta_\alpha]$ . This will be crucial below. We illustrate these conventions for the permutation  $p = (4123)$  and  $k = 1212 = [24]$ . Then,  $k_p = 2121$ ,  $[\mu_1 \mu_2] = [31]$  and  $k_p = [\hat{\eta}_1 \hat{\eta}_2] = [13]$ ; moreover,  $\bar{\hat{\eta}}_1 = \bar{1} = 4$  and  $\bar{\hat{\eta}}_2 = \bar{3} = 2$  are both elements of  $k = [24]$ .

Expressed in this notation, Equations (18) read

$$G^{[\eta_1 \dots \eta_\alpha]}(\omega) = \sum_p G_p^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}(\omega_p) \quad (19a)$$

$$G_p^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}(\omega_p) = [K^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]} * S_p](\omega_p) \quad (19b)$$

with the permuted Keldysh kernel  $K^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}$  given by [23]

$$K^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}(\omega_p) = \sum_{j=1}^{\alpha} (-1)^{j-1} K^{[\hat{\eta}_j]}(\omega_p) \quad (19c)$$

$$K^{[\eta]}(\omega_p) = \prod_{i=1}^{\ell-1} \frac{1}{\omega_{1\dots i}^{[\eta]}} \quad (19d)$$

Equations (19) compactly express all partial correlators  $G_p^{k_p} = G_p^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}$ , and hence also the full KF correlator  $G^k = G^{[\eta_1 \dots \eta_\alpha]}$ , through a set of  $\ell$  so-called *fully retarded kernels*  $K^{[\eta]}$ . These are defined by Equation (19d) and depend on just a single index  $\eta$ , which takes the value  $\hat{\eta}_j$  in Equation (19c). The superscript on the frequencies occurring therein denotes imaginary shifts  $\omega_i \rightarrow \omega_i^{[\eta]} = \omega_i + i\gamma_i^{[\eta]}$ , with  $\gamma_i^{[\eta]} \in \mathbb{R}$  chosen such that  $\gamma_{i \neq \eta}^{[\eta]} < 0$ ,  $\gamma_\eta^{[\eta]} > 0$ , and  $\omega_{1\dots \ell} = \omega_{1\dots \ell}^{[\eta]} = 0$ . Shifts of precisely this form are needed to regularize the Fourier integrals expressing  $\mathcal{K}^{k_p}(\omega_p)$  through  $\mathcal{K}^{k_p}(\mathbf{t}_p)$ . Indeed, for infinitesimal  $\gamma_i^{[\eta]}$  each factor in Equation (19d) is the Fourier transform of a step function,

$$\pm i \int_{\mathbb{R}} dt \theta(\pm t) e^{i\omega t} = \frac{1}{\omega \pm i0^+} = P\left(\frac{1}{\omega}\right) \mp i\pi\delta(\omega) \quad (20)$$

giving the kernels both principal-value P and Dirac- $\delta$  contributions. We choose the same convention as in ref. [23],

$$\gamma_{i \neq \eta}^{[\eta]} = -\gamma_0, \quad \gamma_\eta^{[\eta]} = (\ell - 1)\gamma_0 \quad (21)$$

see Figure 1c, with  $\gamma_0$  taken to be infinitesimal,  $\gamma_0 = 0^+$ , for analytical considerations. Below, we also use the shorthand  $\omega_{i\dots j}^\pm = \omega_{i\dots j} \pm i0^+$  to indicate infinitesimal imaginary shifts for sums of frequencies.

Comparing the fully retarded kernel  $K^{[\eta]}$  of Equation (19d) with the regular Matsubara kernel  $\tilde{K}$  of Equation (13b), we find that the former is the analytic continuation of the latter:

$$K^{[\eta]}(\omega_p) = \tilde{K}(i\omega_p \rightarrow \omega_p^{[\eta]}) \quad (22)$$

This remarkable relation between MF and KF kernels constitutes the nucleus from which we will develop our strategy for obtaining KF correlators via analytic continuation of MF correlators. Here, we just note that, by Equations (13b) and (20), the analytical continuation of the *regular* MF kernel on the right of Equation (22) generally yields both principal-value and Dirac- $\delta$  contributions. By contrast, we will find below that the analytic continuation of *anomalous* MF kernels yields solely Dirac- $\delta$  contributions in KF correlators [cf. Equations (84) and (101)].

Two well-known statements on general  $\ell$ p correlators follow immediately from Equations (19). First, for  $\alpha = 0$ , they imply  $G^{[]} = G^{1\dots 1} = 0$ . Second, for  $\alpha = 1$ , we have  $\bar{\hat{\eta}}_1 = \eta_1$ . Thus,  $K^{[\hat{\eta}_1]}(\omega_p) = \tilde{K}(\omega_p^{[\eta_1]})$  by Equation (22), and Equation (19b) yields

$$G_p^{[\hat{\eta}_1]}(\omega) = [\tilde{K} * S_p](\omega_p^{[\eta_1]}) = \tilde{G}_p(i\omega_p \rightarrow \omega_p^{[\eta_1]}) \quad (23)$$

For the second step, we evoked Equation (14c). Importantly, the superscript on  $\omega_p^{[\eta]}$  on the right, which specifies its imaginary frequency shifts, is fully determined by the external Keldysh index  $\eta$  and *not* dependent on  $p$ . It thus remains unchanged throughout the sum on  $p$  in Equation (18a) for the full correlator  $G^{[\eta]}(\omega)$ , which hence can be expressed as

$$G^{[\eta]}(\omega) = \tilde{G}(i\omega \rightarrow \omega^{[\eta]}) \quad (24)$$

The fully retarded ( $\alpha = 1$ ) components of KF correlators are therefore fully determined, via analytic continuation, by the *regular* parts of MF correlators. Conversely, anomalous parts of MF correlators can only influence Keldysh components with  $\alpha \geq 2$ .

For later use, we also define primed partial correlators

$$G'^{[\eta_1 \dots \eta_\alpha]}(\omega) = \sum_p G_p'^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}(\omega_p) \quad (25a)$$

$$G_p'^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]}(\omega_p) = [(K^{[\hat{\eta}_1 \dots \hat{\eta}_\alpha]})^* * S_p](\omega_p) \quad (25b)$$

They differ from the unprimed correlators of Equation (19b) by the complex conjugation of the kernel, replacing  $\omega_i + i\gamma_i^{[\eta]}$  by  $\omega_i - i\gamma_i^{[\eta]}$ , with  $\gamma_i^{[\eta]}$  still determined by the rule Equation (21). For  $\alpha = 1$ , the corresponding  $G'^{[\eta]}$  will be called *fully advanced* correlators. For fully retarded or advanced correlators,  $G^{[\eta]}$  or  $G'^{[\eta]}$ , all frequencies  $\omega_{i \neq \eta}$  acquire negative or positive imaginary shifts, respectively. Note that primed correlators  $G'^k$  may differ from

complex conjugated correlators  $G^{*k}$  as the complex conjugation generally affects the PSFs, too.

This concludes our summary of the results of ref. [23] needed for present purposes. In the next section, we introduce a general strategy for expressing KF correlators through analytically-continued MF correlators. It is well-known how to do this for all components of  $2p$  correlators, and, as discussed above, for the fully retarded and advanced components of  $\ell p$  correlators. Our goal is a strategy applicable for all components of  $\ell p$  correlators.

## 2.4. The Bridge between the MF and KF Formalisms

Equation (23), expressing KF partial correlators through MF partial correlators for  $\alpha = 1$ , has a counterpart for arbitrary  $\alpha$ , obtained via Equations (19), (22), and (14c):

$$G_p^{[\hat{n}_1 \dots \hat{n}_\alpha]}(\omega_p) = \sum_{j=1}^{\alpha} (-1)^{j-1} [\tilde{K} * S_p](\omega_p^{[\hat{n}_j]}) \quad (26a)$$

$$= \sum_{j=1}^{\alpha} (-1)^{j-1} \tilde{G}_p \left( i\omega_p \rightarrow \omega_p^{[\hat{n}_j]} \right) \quad (26b)$$

with  $\bar{\eta}_j \in \{\eta_1, \dots, \eta_\alpha\}$ . This is already one of our main results: The partial correlators serve as a bridge between the MF and KF. All components of the partial KF correlator  $G_p^{k_p} = G_p^{[\hat{n}_1 \dots \hat{n}_\alpha]}$  can be obtained by taking linear combinations of analytic continuations of partial regular MF correlators,  $\tilde{G}_p(i\omega_p \rightarrow \omega_p^{[\hat{n}_j]})$ . The external Keldysh indices  $\mathbf{k} = [\eta_1 \dots \eta_\alpha]$  and the permutation  $p$  together specify the imaginary frequency shifts, encoded in  $\omega_p^{[\hat{n}_j]}$ , to be used.

Equation (23), expressing the full ( $p$ -summed) KF correlators through MF ones for  $\alpha = 1$ , does not have a counterpart for  $\alpha > 1$ . Then, the full correlators, given by

$$G^{[n_1 \dots n_\alpha]}(\omega) = \sum_p [K^{[\hat{n}_1 \dots \hat{n}_\alpha]} * S_p](\omega_p) \quad (27a)$$

$$= \sum_p \sum_{j=1}^{\alpha} (-1)^{j-1} \tilde{G}_p \left( i\omega_p \rightarrow \omega_p^{[\hat{n}_j]} \right) \quad (27b)$$

involve a sum  $\sum_j$ . The  $\bar{\eta}_j$  indices on the right now depend on  $p$ , so that the imaginary frequency shifts vary from one permutation to the next. As a result, the full  $G^{[n_1 \dots n_\alpha]}$ , unlike  $G^{[n]}$ , does not depend on a single set of frequency shifts and cannot be directly expressed through a mere analytic continuation of  $\tilde{G}(i\omega)$ . Instead, Equation (27b) requires separate knowledge of each individual  $\tilde{G}_p(i\omega_p)$ . Most computational methods capable of computing the full MF correlator  $G(i\omega)$  do not have access to the separate partial MF correlators  $\tilde{G}_p(i\omega_p)$ . In the following, we therefore develop a strategy for extracting the partial MF correlators  $\tilde{G}_p(i\omega_p)$  from a full MF correlator  $G(i\omega)$  given as input, assuming the latter to be known analytically. By writing the resulting functions  $\tilde{G}_p(i\omega)$  in the form  $[\tilde{K} * S_p](i\omega)$ , one can deduce explicit expressions for the PSFs  $S_p[G]$  as functionals of the input  $G$ . By inserting these  $S_p$  into Equation (27a), one obtains  $G^{[n_1 \dots n_\alpha]}[G]$  as a functional of  $G$ , thereby achieving the desired MF-to-KF analytic continuation.

We start in the MF time domain. There, a specific partial MF correlator  $\mathcal{G}_p(\tau_p)$  can be obtained from the full  $\mathcal{G}(\tau) = \sum_p \mathcal{G}_p(\tau_p)$  (Equations (8)) using the projector property of MF kernels in the time domain,  $\mathcal{K}(\tau_p)\mathcal{K}(\tau_{p'}) = (-1)^{\ell-1}\mathcal{K}(\tau_p)$  if  $p = p'$  and 0 otherwise. Hence, we can express the partial correlator as

$$\mathcal{G}_p(\tau_p) = (-1)^{\ell-1}\mathcal{K}(\tau_p)\mathcal{G}(\tau) \quad (28)$$

Computing the discrete Fourier transform of Equation (28) according to Equation (9b), we obtain

$$\mathcal{G}_p(i\omega_p) = [\mathcal{K} \star G](i\omega_p) \quad (29a)$$

with the imaginary-frequency convolution  $\star$  defined as

$$[\mathcal{K} \star G](i\omega_p) = \frac{1}{(-\beta)^{\ell-1}} \sum_{i\omega'_p} \delta_{i\omega'_p, \bar{i}} \mathcal{K}(i\omega_p - i\omega'_p)G(i\omega') \quad (29b)$$

We will typically sum over the  $\ell - 1$  independent Matsubara frequency variables  $i\omega'_{\bar{1} \dots \bar{i}}$ , with  $i \in \{1, \dots, \ell - 1\}$ . Note that the arguments of  $G(i\omega')$  appear in *unpermuted* order, but are to be viewed as functions of the summation variables, i.e.,  $i\omega' = i\omega'(\omega'_p)$ . We will often make this explicit using the notation  $G_{i\omega'_p} = G(i\omega'(\omega'_p))$ , where the subscript is a label indicating the  $\ell - 1$  independent frequencies chosen to parametrize  $i\omega'$ . Consider, e.g.,  $\ell = 3$  and choose  $i\omega_{\bar{1}}, i\omega_{\bar{2}}$  as summation variables. For the permutation  $p = (132)$ , the correlator is then represented as  $G_{i\omega_{\bar{1}}, i\omega_{\bar{2}}} = G_{i\omega_1, i\omega_{13}} = G(i\omega(i\omega_1, i\omega_{13})) = G(i\omega_1, -i\omega_{13}, i\omega_{13} - i\omega_1)$ .

Using Equation (11a) for  $\mathcal{G}_p(i\omega_p)$  and Equation (10b) for  $\mathcal{K}(i\omega_p)$  in Equation (29a), we obtain

$$\beta \delta_{i\omega_{1 \dots \ell}} G_p(i\omega_p) + G_p^R(i\omega_p) = \beta \delta_{i\omega_{1 \dots \ell}} [K \star G](i\omega_p) + [\mathcal{R} \star G](i\omega_p) \quad (30)$$

By construction, neither  $G_p^R$  nor  $\mathcal{R}$  contain an overall factor of  $\beta$ ; in this sense, they are  $\mathcal{O}(\beta^0)$ . Likewise,  $\mathcal{R} \star G$  is  $\mathcal{O}(\beta^0)$ , for reasons explained below. Moreover, recall that MF-to-KF continuation via Equation (27b) requires only the regular part  $\tilde{G}_p(i\omega_p)$ . We avoid anomalous contributions to  $G_p(i\omega_p)$  in Equation (30) by imposing the condition  $i\omega_{\bar{1} \dots \bar{i}} \neq 0$  on the external frequencies. Setting  $i\omega_{1 \dots \ell} = 0$ , we conclude that

$$\begin{aligned} \tilde{G}_p(i\omega_p) + \mathcal{O}\left(\frac{1}{\beta}\right) &= [K \star G](i\omega_p), \quad (i\omega_{\bar{1} \dots \bar{i}} \neq 0, \forall i < \ell) \\ &= \frac{1}{(-\beta)^{\ell-1}} \sum_{i\omega'_p} \delta_{i\omega'_p, \bar{i}} K(i\omega_p - i\omega'_p)G_{i\omega'_p} \end{aligned} \quad (31)$$

To find  $\tilde{G}_p(i\omega_p)$ , we should thus compute  $K \star G$  with  $i\omega_{\bar{1} \dots \bar{i}} \neq 0$  and retain only the  $\mathcal{O}(\beta^0)$  terms, ignoring all  $\mathcal{O}(1/\beta^{i \geq 1})$  contributions. Note, however, that the full information on  $K$  and  $G$ , including both regular and anomalous terms, is needed on the right-hand side to obtain  $\tilde{G}_p$  on the left.

Equation (31) is an important intermediate result. It provides a recipe for extracting partial regular MF correlators from the full MF correlator by performing Matsubara sums  $\sum_{i\omega'_p}$ . After performing the sums, the final results will be analytically continued to yield  $\tilde{G}_p(i\omega_p \rightarrow \omega_p^{[n]})$  through which all Keldysh correlators can

be expressed (Equation (27b)). However, we choose to fully evaluate the Matsubara sums *before* performing this analytic continuation. The reason is that we will evaluate the sums using contour integration and contour deformation. For the latter step, it is convenient if the arguments of  $\tilde{G}_p(i\omega_p)$  all lie safely on the imaginary axis, where they do not impede contour deformation.

## 2.5. Converting Matsubara Sums to Contour Integrals

Next, we discuss three technical points relevant for performing Matsubara sums explicitly. To be concrete, we illustrate our general statements for the case  $\ell = 2$ . Other cases are discussed in subsequent sections.

### 2.5.1. Singularity-Free Kernels

The argument of the kernel  $K(\Omega_p)$  in Equation (31) has the form  $\Omega_p = i\omega_p - i\omega'_p$ . This is always bosonic, being the difference of two same-type Matsubara frequencies. The Matsubara sums  $\sum_{i\omega'_p}$  will thus contain terms with  $\Omega_{1\dots i} = 0$ . To facilitate dealing with these, we assume that the kernel has been expressed in “singularity-free” form, where case distinctions ensure that factors of  $1/\Omega_{1\dots i}$  occur only if  $\Omega_{1\dots i} \neq 0$ . This is possible for the presented correlators, as shown in ref. [30] and discussed in Appendix A.1. These case distinctions are expressed via the symbol

$$\Delta_{\Omega_{1\dots i}} = \begin{cases} \frac{1}{\Omega_{1\dots i}} & \text{if } \Omega_{1\dots i} \neq 0 \\ 0 & \text{if } \Omega_{1\dots i} = 0 \end{cases} \quad (32)$$

Thus,  $K(\Omega_p)$  is assumed to contain  $1/\Omega_{1\dots i}$  only via  $\Delta_{\Omega_{1\dots i}}$ . A sum over a  $\Delta$  symbol becomes a restricted sum, lacking the summand for which  $\Delta = 0$ . For  $\ell = 2$ , e.g., we have  $K(\Omega_p) = \Delta_{\Omega_{\bar{1}}} - \frac{1}{2}\beta\delta_{\Omega_{\bar{1}}}$  (see Equation (A2a)), so that Equation (31) yields

$$\tilde{G}_p(i\omega_p) + \mathcal{O}\left(\frac{1}{\beta}\right) \stackrel{\ell=2}{=} \frac{1}{(-\beta)} \sum_{i\omega'_{\bar{1}}}^{\neq i\omega_{\bar{1}}} \frac{G_{i\omega'_{\bar{1}}}}{i\omega_{\bar{1}} - i\omega'_{\bar{1}}} + \frac{G_{i\omega_{\bar{1}}}}{2} \quad (33)$$

This involves a restricted sum and an  $\mathcal{O}(\beta^0)$  term resulting from  $\beta\delta_{\Omega_{\bar{1}}}$  collapsing the sum  $\frac{1}{(-\beta)} \sum_{i\omega'_{\bar{1}}}$  in Equation (31).

### 2.5.2. $\beta\delta$ Expansion of $G$

To facilitate the identification of the leading-in- $\beta$  contributions to Equation (31), we assume that the anomalous  $\tilde{G}$  contribution to  $G_{i\omega'_p} = (\tilde{G} + \hat{G})_{i\omega'_p}$  has been expressed as an expansion in powers of  $\beta\delta_{\Omega_{1\dots i}}$ . Such a  $\beta\delta$  expansion is always possible for the correlators under consideration in this work, as discussed in Appendix A.2. Whenever  $\beta\delta_{i\omega'}$  appears in a Matsubara sum  $\frac{1}{(-\beta)} \sum_{i\omega'}$ , the sum collapses and their  $\beta$  factors cancel. (This cancellation is why  $\mathcal{R} \star G$  in Equation (30) is  $\mathcal{O}(\beta^0)$ , as stated above, even if  $G$  contains anomalous terms.) For  $\ell = 2$ , e.g., we have  $G_{i\omega'_{\bar{1}}} = \tilde{G}_{i\omega'_{\bar{1}}} + \beta\delta_{i\omega'_{\bar{1}}} \hat{G}_{\bar{1}}$ , with  $\tilde{G}_{i\omega'_{\bar{1}}}$  singularity-free at all Matsubara frequencies  $i\omega'_{\bar{1}}$  and  $\hat{G}_{\bar{1}}$  a constant (see Equation (40)). Thus,

Equation (33) becomes

$$\tilde{G}_p(i\omega_p) + \mathcal{O}\left(\frac{1}{\beta}\right) \stackrel{\ell=2}{=} \frac{1}{(-\beta)} \sum_{i\omega'_{\bar{1}}}^{\neq i\omega_{\bar{1}}} \frac{\tilde{G}_{i\omega'_{\bar{1}}}}{i\omega_{\bar{1}} - i\omega'_{\bar{1}}} + \frac{\tilde{G}_{i\omega_{\bar{1}}}}{2} - \frac{\hat{G}_{\bar{1}}}{i\omega_{\bar{1}}} \quad (34)$$

Here, the condition  $i\omega_{\bar{1}} \neq 0$  on the left was evoked to replace  $\frac{1}{2}G_{i\omega_{\bar{1}}}$  by  $\frac{1}{2}\tilde{G}_{i\omega_{\bar{1}}}$  on the right.

### 2.5.3. Converting Sums to Integrals

By restricting or collapsing Matsubara sums containing  $\Delta$  or  $\delta$  factors, one can ensure that the remaining sums are all of the form  $\frac{1}{(-\beta)} \sum_{i\omega'} f(i\omega')$  or  $\frac{1}{(-\beta)} \sum_{i\omega'}^{\neq i\omega} f(i\omega')$ , where  $f(z)$ , viewed as a function of  $z \in \mathbb{C}$ , is *analytic* at each  $i\omega'$  visited by the sum. (More precisely, for each  $i\omega'$  in the sum,  $f(z)$  is analytic in an open domain containing that  $i\omega'$ .) We express such sums in standard fashion as contour integrals:

$$\frac{1}{(-\beta)} \sum_{i\omega'} f(i\omega') = \oint_z n_z f(z) \quad (35a)$$

$$\frac{1}{(-\beta)} \sum_{i\omega'}^{\neq i\omega} f(i\omega') = \oint_z n_z f(z) - \text{Res}_{z=i\omega} (n_z f(z)) \quad (35b)$$

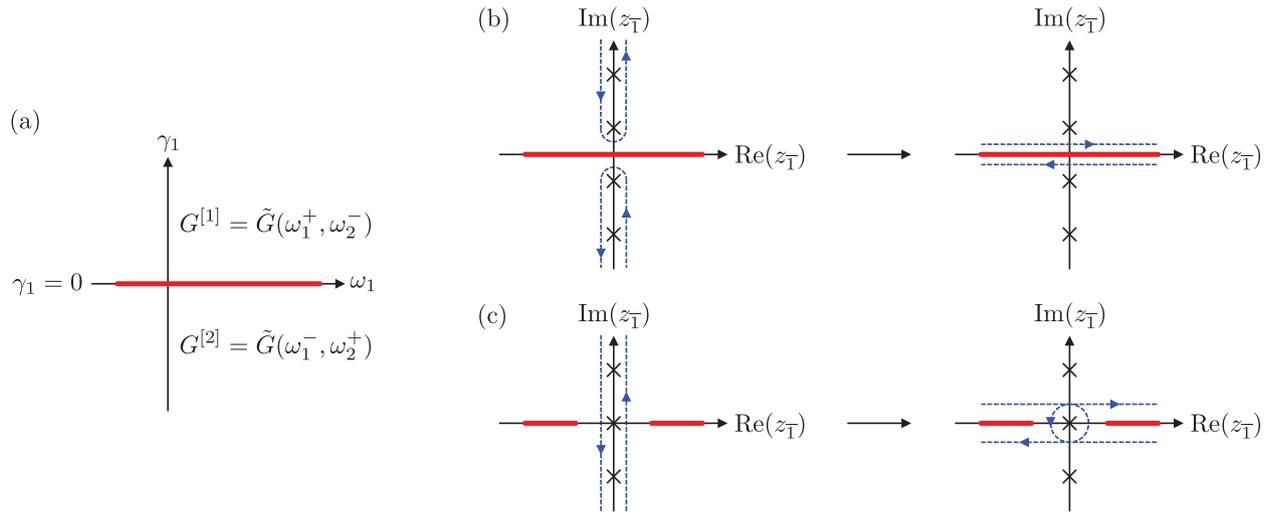
Here,  $\oint_z = \oint_{2\pi i}$  denotes counterclockwise integration around all points  $i\omega'$  visited by the sum, and  $n_z$  is a Matsubara weighting function (MWF). We choose it as

$$n_z = \frac{\zeta}{e^{-\beta z} - \zeta} = \frac{1}{(-\beta)} \frac{1}{z - i\omega} - \frac{1}{2} + \mathcal{O}(z - i\omega) \quad (36)$$

with  $\zeta = \pm$  for bosonic/fermionic  $i\omega'$ . ( $n_z$  is related to standard Fermi and Bose distribution functions by  $-\zeta(1 + n_z) = 1/(e^{\beta z} - \zeta)$ .) The Laurent expansion on the right of Equation (36) shows that  $n_z$  has first-order poles with residues  $1/(-\beta)$  at all Matsubara frequencies  $i\omega'$ . Therefore, the integral  $\oint_z$  along a contour including all  $i\omega'$  frequencies recovers the unrestricted Matsubara sum of Equation (35a) (see left parts of Figure 2b,c). For the restricted sum of Equation (35b), the first term on the right represents an unrestricted sum, i.e. the restricted sum plus a contribution from  $i\omega' = i\omega$ , and the residue correction subtracts the latter. For example, consider the case, needed below, that  $f(i\omega') = \tilde{f}(i\omega')/(i\omega - i\omega')$ , with  $\tilde{f}(z)$  analytic at  $z = i\omega$ . Then,  $n_z f(z)$  has a pole of second order at  $i\omega$ , with

$$\begin{aligned} \text{Res}_{z=i\omega} \left( \frac{n_z \tilde{f}(z)}{i\omega - z} \right) &= \left( \partial_z [(i\omega - z)n_z \tilde{f}(z)] \right)_{z=i\omega} \\ &= \frac{1}{2} \tilde{f}(i\omega) + \frac{1}{\beta} \left( \partial_z \tilde{f}(z) \right)_{z=i\omega} \end{aligned} \quad (37)$$

Note that Equations (35) remain valid under shifts of the MWF by a constant,  $n_z \rightarrow n_z + c$ . We purposefully exploited this freedom to choose  $n_z$  to have  $-\frac{1}{2}$  as the second term in the Laurent expansion. The reason is that this leads to a convenient cancellation between terms arising from a  $\delta$  in  $K$  and residue corrections arising from  $\Delta$  restrictions. For example, when evaluating



**Figure 2.** a) Analytic regions of a regular 2p MF correlator as a function of a complex frequency  $\omega_1 + i\gamma_1$  with  $\omega_1, \gamma_1 \in \mathbb{R}$ . The thick red line on the real axis depicts a possible branch cut of the correlator. b,c) Contours to evaluate the Matsubara summation in the (b) fermionic and (c) bosonic case, see Equations (43) and (44), respectively. Crosses indicate the poles of the MWF  $n_{z_T}$  at the Matsubara frequencies on the imaginary axis. The dashed blue contours, initially enclosing all Matsubara frequencies, are deformed away from the imaginary axis to run infinitesimally above and below the real axis. In the bosonic 2p case (c), the branch cut does not extend to  $z_T = 0$  as the correlator, by definition, is free of any singularities at vanishing Matsubara frequencies.

the Matsubara sum in Equation (34) using Equations (35b) with  $f(i\omega') = \tilde{G}_{i\omega'} / (i\omega - i\omega')$ , we obtain:

$$\tilde{G}_p(i\omega_p) + \mathcal{O}\left(\frac{1}{\beta}\right)_{i\omega_T \neq 0} = \oint_{z_T} \frac{n_{z_T} \tilde{G}_{z_T}}{i\omega_1 - z_T} - \text{Res}_{z_T=i\omega_T} \left( \frac{n_{z_T} \tilde{G}_{z_T}}{i\omega_1 - z_T} \right) + \frac{\tilde{G}_{i\omega_T}}{2} - \frac{\hat{G}_T}{i\omega_T} \quad (38a)$$

$$= \oint_{z_T} \frac{n_{z_T} \tilde{G}_{z_T}}{i\omega_1 - z_T} - \frac{1}{\beta} \left( \partial_{z_T} \tilde{G}_{z_T} \right)_{z_T \rightarrow i\omega_T} - \frac{\hat{G}_T}{i\omega_T} \quad (38b)$$

The  $\frac{1}{2} \tilde{G}_{i\omega_T}$  term in Equation (38a) conveniently cancels a contribution from the residue correction, evaluated using Equation (37). This cancellation results from our choice of  $n_z$  having  $-\frac{1}{2}$  in its Laurent expansion. (Similar cancellations occur for  $\ell > 2$ ; see, e.g., Appendix C.2.1.) The  $-\frac{1}{\beta} (\partial_z \tilde{G}_z)_{z \rightarrow i\omega}$  term in Equation (38b) is an example of an  $\mathcal{O}\left(\frac{1}{\beta}\right)$  contribution that arises from  $K \star G$  but is not part of  $\tilde{G}_p$ .

Having worked through the example of  $\ell = 2$ , we conclude this section with some general remarks about Equation (31) for  $\tilde{G}_p$ . Once the Matsubara sums from the imaginary-frequency convolution  $K \star G$  have been expressed through contour integrals, one obtains the general form<sup>[31]</sup>

$$\tilde{G}_p(i\omega_p) + \mathcal{O}\left(\frac{1}{\beta}\right)_{i\omega_{1..l} \neq 0} = \oint_{z_T} \dots \oint_{z_{1..l-1}} \tilde{K}(i\omega_p - z_p) n_{z_T} \dots n_{z_{1..l-1}} \tilde{G}_{z_T, \dots, z_{1..l-1}} + \text{contributions from } \hat{G} \quad (39)$$

Here, the  $(\ell - 1)$ -fold contour integrals involve only the *regular* part,  $\tilde{G}$ , of the full MF correlator. Its anomalous part,  $\hat{G}$ , comes with factors  $\beta\delta$  that collapse one or multiple sums in Equation (31). Therefore, contributions from  $\hat{G}$  to  $\tilde{G}_p$  contain at most  $\ell - 2$  contour integrals.

The next step, discussed in detail in Section 3.2, is to deform the integration contour in such a way that it runs infinitesimally above and below the real axis. The anomalous contributions from  $\hat{G}$  can then be reincorporated into the real integrals using bosonic Dirac delta functions. As a result, one recovers precisely the form  $\tilde{G}_p = \tilde{K} \star S_p$  of the spectral representation (14d): regular kernels  $\tilde{K}$  convolved with other functions, built from MWFs and analytic continuations of the various components of  $\tilde{G}$  and  $\hat{G}$ , the latter multiplied by bosonic Dirac  $\delta$  functions. These other functions can thus be identified with the PSFs  $S_p = \tilde{S}_p + \hat{S}_p$ , now expressed through analytic continuations of  $G$ . This clarifies, on a conceptual level, how the information contained in the full MF correlator  $G$  needs to be repackaged to obtain PSFs, and the explicit formulas for  $\ell = 2, 3, 4$  in Equations (47), (74), and (88) constitute the main results of this paper. These, in turn, can then be used to obtain KF correlators via Equation (27a).

To summarize, the MF-to-KF analytic continuation of arbitrary  $\ell$ p correlation functions can be achieved via the following three-step strategy:

**Step 1. Matsubara summation through contour integration:** Insert the MF kernel  $K$  (expressed in singularity-free form) and the MF correlator  $G$  (expressed as a  $\beta\delta$  expansion), including all regular and anomalous contributions, into Equation (31) for  $\tilde{G}_p$ . Restrict or collapse Matsubara sums containing  $\Delta$  or  $\beta\delta$  factors and express the remaining sums through contour integrals using Equations (35), to arrive at Equation (39).

- Step 2. *Extraction of PSFs:* Deform the contours away from the imaginary axis to run along the real axis, while carefully tracking possible singularities of the MF correlators. Reincorporate anomalous contributions via bosonic Dirac delta functions. This results in a spectral representation of the form  $\tilde{G}_p = \tilde{K} * S_p$ . From this, read off the PSFs  $S_p[G]$ , expressed through products of MWFs and MF correlators, analytically continued to real frequencies (see, e.g., Equation (47)).
- Step 3. *Construction of KF correlators:* Construct the full KF correlator  $G^{[\hat{n}_1 \dots \hat{n}_a]}$ , involving a sum  $\sum_p$  over terms of the form  $[K^{[\hat{n}_1 \dots \hat{n}_a]} * S_p](i\omega_p)$  (Equation (27a)). Simplify the kernels  $K^{[\hat{n}_1 \dots \hat{n}_a]}$  via a set of kernel identities (see, e.g., Equations (57)) and combine terms with similar structure from the sum  $\sum_p$ . Insert into the resulting expressions the PSFs from Step 2, and then compute the integrals involved in the  $*$  convolution. This leads to equations expressing KF correlators through analytically continued MF correlators,  $G^{[\hat{n}_1 \dots \hat{n}_a]}[G]$ .

The result of Step 2 already constitutes an analytic continuation since the PSFs  $S_p$  suffice to construct the KF correlators via the spectral representation. Step 3 serves to give direct relations between both formalisms.

In Appendix G.2, we follow an independent approach and use the equilibrium condition to explicitly perform the following consistency check: given an arbitrary set of PSFs  $S_p$  as input, compute the MF correlator  $G = \sum_p K * S_p$  and verify that the formulas  $S_p[G]$  correctly recover the input PSFs from  $G$ , giving  $S_p[G] = S_p$ . This consistency check is presented for general 2p and 3p and for fermionic 4p correlators.

The next sections are devoted to explicitly working out the details of this strategy. To demonstrate its basic ideas, we first revisit the well-known 2p case in the following section. Though that is textbook material, we present it in a manner that readily generalizes to the higher-point correlators discussed in subsequent sections: 3p correlators in Section 5 and 4p correlators in Section 6.

### 3. Analytic Continuation of 2p Functions

In this section, we carry through the strategy outlined in Section 2.5 to obtain the MF-to-KF analytic continuation in the well-known 2p case. While our strategy may seem more cumbersome than traditional textbook discussions (see, e.g., ref. [32]), it has the merit of readily generalizing to  $\ell > 2$ . We first recapitulate the spectral representation and analytic properties of general 2p MF correlators (Section 3.1). Then, we express the PSFs in terms of analytically continued MF correlators (Section 3.2). Finally, we use these to recover familiar expressions for the retarded, advanced, and Keldysh components of the KF 2p correlator (Section 3.3).

#### 3.1. Analytic Properties of the 2p MF Correlator

We begin by reviewing well-known analytical properties of the 2p MF correlator. This also serves to give concrete examples for our notational conventions.

$G(i\omega) = G(i\omega_1, i\omega_2)$  explicitly depends on one Matsubara frequency,  $i\omega_1$  or  $i\omega_2$ , while the other frequency is fixed by energy conservation,  $i\omega_2 = 0$ . Since we want to compute Equation (31) for arbitrary permutations  $p = \overline{(12)}$ , it proves useful to develop an unbiased notation for the frequency dependence. The chosen explicit frequency dependence is indicated by a subscript in  $G_{i\omega_{\bar{p}}}$ , such that  $G_{i\omega_1} = G(i\omega(\omega_1)) = G(i\omega_1, -i\omega_1)$  and  $G_{i\omega_2} = G(i\omega(\omega_2)) = G(-i\omega_2, i\omega_2)$ . The most general form of  $G_{i\omega_{\bar{p}}}$ , covering both fermionic and bosonic cases, reads

$$G(i\omega(\omega_{\bar{p}})) = G_{i\omega_{\bar{p}}} = \tilde{G}_{i\omega_{\bar{p}}} + \beta \delta_{i\omega_{\bar{p}}} \hat{G}_{\bar{p}} \quad (40)$$

in agreement with the general form Equation (A5). The regular part,  $\tilde{G}_{i\omega_{\bar{p}}}$ , is singularity-free for all  $i\omega_{\bar{p}}$ , including 0.  $\hat{G}_{\bar{p}}$  denotes the anomalous part, a constant, contributing only for  $i\omega_{\bar{p}} = 0$ . The relation  $G_{i\omega_1} = G_{i\omega_2}$  enforces  $\hat{G}_1 = \hat{G}_2$ .

One of the next steps involves the deformation of the integration contour  $\oint_{z_{\bar{p}}}$  from the imaginary axis toward the real axis. This requires knowledge of the analytic structure of the MF correlator. It can be made explicit via the spectral representation of  $G_{z_1}$  (Equations (14)), with the PSFs  $S_p$  viewed as input. For the regular part, we obtain

$$\tilde{G}_{z_1} = \int d^2 \epsilon \delta(\epsilon_{12}) \left[ \frac{S_{(12)}(\epsilon_1)}{z_1 - \epsilon_1} + \frac{S_{(21)}(\epsilon_2)}{-z_1 - \epsilon_2} \right] = \int d\epsilon_1 \frac{S_{\text{std}}(\epsilon_1)}{z_1 - \epsilon_1} \quad (41)$$

Here, we introduced the “standard” spectral function  $S_{\text{std}}$ , given by a commutator of PSFs resulting from the sum over the two permutations  $p = (12)$  and  $(21)$ :

$$S_{\text{std}}(\epsilon_1) = S_{[1,2]_{\pm}}(\epsilon_1, -\epsilon_1) = S_{(12)}(\epsilon_1) - S_{(21)}(-\epsilon_1) \quad (42a)$$

$$S_{[1,2]_{\pm}}(\epsilon) = S_{(12)}(\epsilon_1) \pm S_{(21)}(\epsilon_2) \quad (42b)$$

Here,  $\epsilon_{12} = 0$  is understood for the argument of  $S_{[1,2]_{\pm}}(\epsilon)$ . For PSF (anti)commutators, we always display the unpermuted  $\epsilon$  and insert the permuted  $\epsilon_p$  only for individual PSFs, as done on the right of Equation (42b). Evidently,  $\tilde{G}_{z_1}$  has poles (or branch cuts for continuous spectra) whenever the denominator  $z_1 - \epsilon_1$  vanishes. This can happen only if  $\text{Im}(z_1) = 0$  (or, more generally,  $\text{Im}(z_{\bar{p}}) = 0$ ), indicated in Figure 2 by thick, red lines on the real axis. Hence, the upper and the lower complex half plane are analytic regions of  $\tilde{G}_{z_1}$ , separated by a branch cut at  $\text{Im}(z_1) = 0$ .

#### 3.2. Extraction of PSFs from Partial MF Correlators

In Section 2.5, we expressed the regular partial MF correlators  $\tilde{G}_p(i\omega_p)$  for  $\ell = 2$  in terms of a contour integral  $\oint_{z_{\bar{p}}}$  involving the regular MF correlator  $\tilde{G}_{z_{\bar{p}}}$ , see Equation (38b). That amounted to Step 1 of the three-step strategy. Turning to Step 2, we write  $\tilde{G}_p(i\omega_p)$  in the form of a convolution  $[\tilde{K} * S_p](i\omega_p)$ , from which we then read out expressions for the PSFs  $S_p[G]$ .

To this end, we exploit the analyticity of  $\tilde{G}_{z_{\bar{p}}}$  in the upper and lower half-plane to deform the contours in  $\oint_{z_{\bar{p}}}$  from enclosing the imaginary axis to running infinitesimally above and below the branch cut. We denote the corresponding integration variables

along the branch cut by  $\varepsilon_{\mp}^{\pm} = \varepsilon_{\mp} \pm i0^{+}$ , with  $\varepsilon_{\mp} = \text{Re}(z_{\mp})$  now being a real variable and  $\pm i0^{+}$  infinitesimal shifts.

We discuss the cases of fermionic or bosonic frequencies separately. For fermions, the contour deformation of  $\oint_{z_{\mp}} \tilde{G}_{z_{\mp}}$  in Equation (38b) is straightforward and yields (see Figure 2b)

$$\oint \frac{dz_{\mp}}{2\pi i} \frac{n_{z_{\mp}} \tilde{G}_{z_{\mp}}}{i\omega_{\mp} - z_{\mp}} = \int_{-\infty}^{\infty} \frac{d\varepsilon_{\mp}}{2\pi i} \frac{n_{\varepsilon_{\mp}} \tilde{G}_{\varepsilon_{\mp}}}{i\omega_{\mp} - \varepsilon_{\mp}} \quad (43)$$

Here, we defined  $\tilde{G}_{\varepsilon_{\mp}}^{\varepsilon_{\mp}} = \tilde{G}_{\varepsilon_{\mp}^{+}} - \tilde{G}_{\varepsilon_{\mp}^{-}}$  as the discontinuity of  $\tilde{G}_{z_{\mp}}$  across the branch cut at  $\text{Im}(z_{\mp}) = 0$ . Moreover, we extended the subscript notation introduced after Equation (29b) to real frequencies with infinitesimal imaginary shifts. (This notation is further discussed after Equation (47).)

In the bosonic case, the pole at  $z_{\mp} = 0$  has to be treated separately (see Figure 2c):

$$\begin{aligned} \oint \frac{dz_{\mp}}{2\pi i} \frac{n_{z_{\mp}} \tilde{G}_{z_{\mp}}}{i\omega_{\mp} - z_{\mp}} &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\varepsilon_{\mp}}{2\pi i} \frac{n_{\varepsilon_{\mp}} \tilde{G}_{\varepsilon_{\mp}}}{i\omega_{\mp} - \varepsilon_{\mp}} + \text{Res}_{z_{\mp}=0} \left( \frac{n_{z_{\mp}} \tilde{G}_{z_{\mp}}}{i\omega_{\mp} - z_{\mp}} \right) \\ &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\varepsilon_{\mp}}{2\pi i} \frac{n_{\varepsilon_{\mp}} \tilde{G}_{\varepsilon_{\mp}}}{i\omega_{\mp} - \varepsilon_{\mp}} + \mathcal{O}\left(\frac{1}{\beta}\right) \end{aligned} \quad (44)$$

Here,  $\mathcal{P}$  indicates a principal-value integral. The residue evaluates to a contribution of order  $\mathcal{O}\left(\frac{1}{\beta}\right)$  as the bosonic MWF  $n_{z_{\mp}}$  is the only factor having a pole at  $z_{\mp} = 0$ , with residue  $1/(-\beta)$  there (remember that  $i\omega_{\mp} \neq 0$ ). Combining Equations (43), (44), and (38b), and omitting  $\mathcal{O}\left(\frac{1}{\beta}\right)$  terms, we finally find

$$\tilde{G}_p(i\omega_p) = \int_{\varepsilon_{\mp}} \frac{n_{\varepsilon_{\mp}} \tilde{G}_{\varepsilon_{\mp}}}{i\omega_{\mp} - \varepsilon_{\mp}} - \frac{\hat{G}_{\mp}}{i\omega_{\mp}} = \int_{\varepsilon_{\mp}} \frac{n_{\varepsilon_{\mp}} \tilde{G}_{\varepsilon_{\mp}} + \hat{\delta}(\varepsilon_{\mp}) \hat{G}_{\mp}}{i\omega_{\mp} - \varepsilon_{\mp}} \quad (45)$$

On the right, we absorbed the anomalous  $\hat{G}$  contribution into the integral, defining  $\hat{\delta}(\varepsilon_{\mp}) = -2\pi i \delta(\varepsilon_{\mp})$ . Moreover, we introduced the symbol  $\int_{\varepsilon_i}$  as

$$\int_{\varepsilon_i} \dots = \begin{cases} \int_{-\infty}^{\infty} \frac{d\varepsilon_i}{2\pi i} \dots & \text{for fermionic } \varepsilon_i \text{ or anomalous frequency,} \\ \mathcal{P} \int_{-\infty}^{\infty} \frac{d\varepsilon_i}{2\pi i} \dots & \text{for bosonic } \varepsilon_i \text{ and regular frequency.} \end{cases} \quad (46)$$

We call a frequency  $\varepsilon_i$  *anomalous* if it is directly set to zero by a Dirac  $\hat{\delta}(\varepsilon_i)$  in the integrand, and *regular* otherwise. Since the anomalous contribution arose from a Kronecker  $\delta_{i\omega_{\mp}}$ , we arrive at a rule of thumb: when performing Matsubara sums via contour integration and contour deformation to the real axis, Kronecker deltas with Matsubara arguments lead to Dirac deltas with real arguments.

Importantly, Equation (45) has precisely the same form as Equation (14d) for  $\ell = 2$ , with the correspondence

$$(2\pi i) S_p(\varepsilon_{\mp}) = n_{\varepsilon_{\mp}} \tilde{G}_{\varepsilon_{\mp}}^{\varepsilon_{\mp}} + \hat{\delta}(\varepsilon_{\mp}) \hat{G}_{\mp} \quad (47)$$

This remarkable formula is the first central result of this section: it shows that a suitable analytic continuation of the MF correlator

$G(i\omega)$ , combined with a MWF, fully determines the PSF and thus, via the spectral representation Equations (27a), the KF correlator  $G^k$ . It also clarifies the role of anomalous contributions. In subsequent sections, we will find analogous results for  $\ell = 3, 4$ .

To conclude this section, we elaborate on the meaning of the super- and subscript notation used above. The discontinuity in Equation (47),  $\tilde{G}^{\varepsilon_{\mp}} = \tilde{G}_{\varepsilon_{\mp}^{+}} - \tilde{G}_{\varepsilon_{\mp}^{-}}$ , consists of analytically continued MF correlators,  $\tilde{G}(i\omega) \rightarrow \tilde{G}(z)$ . Here, the entries of  $z = (\varepsilon_{\mp}^{\pm}, \varepsilon_{\mp}^{\mp})$  are infinitesimally shifted by  $+i0^{+}$  or  $-i0^{+}$ , but constrained by energy conservation,  $\varepsilon_{12} = 0$ . The subscript on  $\tilde{G}_{\varepsilon_{\mp}^{\pm}}$  has the same meaning as for imaginary frequencies (see paragraph after Equation (29b)): it indicates the chosen explicit (real-)frequency dependence of  $\tilde{G}(z)$ , i.e.,  $\tilde{G}_{\varepsilon_{\mp}^{\pm}} = \tilde{G}(z(\varepsilon_{\mp}^{\pm}))$ , uniquely determining the imaginary shifts in each entry of  $z$ . To be explicit, we have

$$\tilde{G}^{\varepsilon_1} = \tilde{G}(\varepsilon_1^{+}, -\varepsilon_1^{+}) - \tilde{G}(\varepsilon_1^{-}, -\varepsilon_1^{-}) \quad (48a)$$

$$\tilde{G}^{\varepsilon_2} = \tilde{G}(-\varepsilon_2^{+}, \varepsilon_2^{+}) - \tilde{G}(-\varepsilon_2^{-}, \varepsilon_2^{-}) \quad (48b)$$

Since  $\varepsilon_2 = -\varepsilon_1$  (energy conservation) and hence  $\varepsilon_2^{+} = -\varepsilon_1^{-}$ , we have  $\tilde{G}^{\varepsilon_1} = -\tilde{G}^{\varepsilon_2} = \tilde{G}^{-\varepsilon_2}$ . (Check for negative superscripts:  $\tilde{G}^{-\varepsilon_2} = \tilde{G}_{(-\varepsilon_2)^{+}} - \tilde{G}_{(-\varepsilon_2)^{-}} = \tilde{G}_{-\varepsilon_2^{-}} - \tilde{G}_{-\varepsilon_2^{+}} = -\tilde{G}^{\varepsilon_2}$ .)

For illustration, we give explicit formulas for  $S_p$  for the permutations  $p = (12)$  and  $p = (21)$ ,

$$\begin{aligned} (2\pi i) S_{(12)}(\varepsilon_1) &= n_{\varepsilon_1} [\tilde{G}(\varepsilon_1^{+}, -\varepsilon_1^{+}) - \tilde{G}(\varepsilon_1^{-}, -\varepsilon_1^{-})] + \hat{\delta}(\varepsilon_1) \hat{G}_1 \\ (2\pi i) S_{(21)}(\varepsilon_2) &= n_{\varepsilon_2} [\tilde{G}(-\varepsilon_2^{+}, \varepsilon_2^{+}) - \tilde{G}(-\varepsilon_2^{-}, \varepsilon_2^{-})] + \hat{\delta}(\varepsilon_2) \hat{G}_2 \end{aligned} \quad (49)$$

where we inserted Equation (48) for the discontinuities. The anomalous contributions satisfy  $\hat{G}_1 = \hat{G}_2$  (as explained after Equation (40)) and exist only for bosonic correlators ( $\zeta = 1$ ). Energy conservation  $\varepsilon_2 = -\varepsilon_1$  then gives

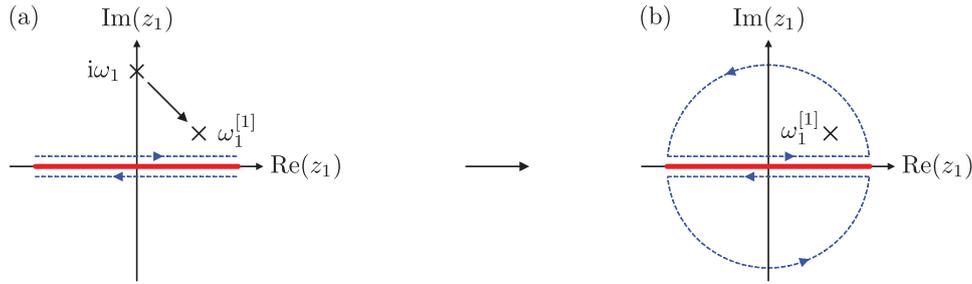
$$\begin{aligned} (2\pi i) S_{(21)}(-\varepsilon_1) &= n_{-\varepsilon_1} [\tilde{G}(\varepsilon_1^{-}, -\varepsilon_1^{-}) - \tilde{G}(\varepsilon_1^{+}, -\varepsilon_1^{+})] + \hat{\delta}(\varepsilon_1) \hat{G}_2 \\ &= \zeta e^{-\beta\varepsilon_1} (2\pi i) S_{(12)}(\varepsilon_1) \end{aligned} \quad (50)$$

For the last step, we used the identity  $-n_{-\varepsilon_1} = \zeta e^{-\beta\varepsilon_1} n_{\varepsilon_1}$ . As a useful consistency check, we note that Equation (50) corresponds to the equilibrium condition Equation (4) for PSFs (with  $p = (21)$ ,  $p_{\lambda} = (12)$  there, implying  $\zeta_p = \zeta$ ,  $\zeta_{p_{\lambda}} = +1$  and  $\varepsilon_{\mp} = \varepsilon_2 = -\varepsilon_1$ ,  $\varepsilon_{p_{\lambda}(1)} = \varepsilon_1$ ).

Expressing the standard spectral function  $S_{\text{std}}(\varepsilon_1)$  from Equation (42a) in terms of Equation (47), we find

$$\begin{aligned} (2\pi i) S_{\text{std}}(\varepsilon_1) &= n_{\varepsilon_1} \tilde{G}_{\varepsilon_1}^{\varepsilon_1} + \hat{\delta}(\varepsilon_1) \hat{G}_1 - n_{-\varepsilon_1} \tilde{G}_{-\varepsilon_1}^{-\varepsilon_1} - \hat{\delta}(-\varepsilon_1) \hat{G}_2 \\ &= n_{\varepsilon_1} \tilde{G}_{\varepsilon_1}^{\varepsilon_1} - n_{-\varepsilon_1} \tilde{G}_{-\varepsilon_1}^{-\varepsilon_1} = (n_{\varepsilon_1} + n_{-\varepsilon_1}) \tilde{G}_{\varepsilon_1}^{\varepsilon_1} \\ &= -\tilde{G}_{\varepsilon_1}^{\varepsilon_1} \end{aligned} \quad (51)$$

where we used  $\tilde{G}_{-\varepsilon_1}^{-\varepsilon_1} = -\tilde{G}_{\varepsilon_1}^{\varepsilon_1}$ . Thus, the discontinuity  $\tilde{G}_{\varepsilon_1}^{\varepsilon_1}$  in the PSFs (47) encodes  $S_{\text{std}}(\varepsilon_1)$ . Conversely, however,  $S_{\text{std}}(\varepsilon_1)$  retains only the discontinuity  $\tilde{G}_{\varepsilon_1}^{\varepsilon_1}$  in the PSFs (47), while the information on the MWF and the anomalous part, both contained in the  $S_p$  (49), is lost. In Appendix G.2, we use Equation (51) and the equilibrium condition to explicitly perform the following consistency



**Figure 3.** a) Analytic continuation of the Matsubara frequency  $i\omega_1 \rightarrow \omega_1^{[1]} = \omega_1 + i\gamma_0$  in Equations (52) for fermionic frequencies. The imaginary part of the external frequency  $\omega_1^{[1]}$  has to be larger than the imaginary parts of  $\varepsilon_1^\pm$  used to integrate infinitesimally above and below the real axis. The transition from (a) to (b) illustrates the closing of the contour in the upper/lower half-planes to evaluate the integral in Equation (53). As the integrand is independent of the fermionic MWF  $n_{\varepsilon_1}$ , the only contribution to the integral originates from the simple pole at  $z_1 = \omega_1^{[1]}$ .

tency check: given an arbitrary set of PSFs as input, compute the MF correlator  $G = \sum_p K * S_p$  and verify that Equation (47) for  $S_p$  correctly recovers the input PSFs.

### 3.3. Keldysh Correlator

Next, we turn to Step 3 of our three-step strategy: we use the PSFs obtained above to explicitly construct the Keldysh components  $G^{[1]}$ ,  $G^{[2]}$ , and  $G^{[12]}$ , expressed through analytically continued MF correlators. As the structure of KF correlators becomes more intricate with an increasing number of 2's in the Keldysh component, denoted by  $\alpha$  in Equations (19), we discuss the different values of  $\alpha$  separately in the following and throughout the rest of the paper.

#### 3.3.1. Keldysh Components $G^{[n]}$

For  $\alpha = 1$ , the fully retarded or fully advanced Keldysh components  $G^{[n]}$  can be deduced from the regular part of MF correlators alone (Equation (23)). Here, we follow the alternative and equivalent strategy of Step 3: we insert the PSFs from Equation (47) into the spectral representation (27a):

$$G^{[n]}(\omega) = \sum_p [K^{[n]} * S_p](\omega_p) = \sum_p [\tilde{K} * S_p](\omega_p^{[n]}) \quad (52a)$$

$$= \int d^2\varepsilon \delta(\varepsilon_{12}) \left( \frac{S_{(12)}(\varepsilon_1)}{\omega_1^{[n]} - \varepsilon_1} + \frac{S_{(21)}(\varepsilon_2)}{\omega_2^{[n]} - \varepsilon_2} \right) \quad (52b)$$

$$= \int d\varepsilon_1 \frac{S_{[1,2]_-(\varepsilon_1, -\varepsilon_1)}}{\omega_1^{[n]} - \varepsilon_1} \quad (52c)$$

Here, we used  $\omega_2^{[n]} = -\omega_1^{[n]}$  (Equation (21)) and that the sum over both permutations,  $p = (12)$  and  $(21)$ , leads to the appearance of the PSF commutator  $S_{[1,2]_-}$  (equalling  $S_{\text{std}}$ , cf. Equation (42)).

Before proceeding, a general remark is in order: When the external variables  $\omega_p^{[n]}$  appear in  $*$  convolution integrals such as  $\int_{\varepsilon_1}$  in Equations (52), it is essential to maintain the hierarchy  $\gamma_0 \gg 0^+$  for the infinitesimal imaginary shifts  $\pm i\gamma_0$  and  $\pm i0^\pm$  contained in the external frequencies  $\omega_p^{[n]}$  and the integration variables  $\varepsilon_1^\pm$ , respectively. The reason is that the contour deformation

from  $\int_{z_1}$  to  $\int_{\varepsilon_1}$  has been performed *before* the analytic continuation  $i\omega_p \rightarrow \omega_p^{[n]}$  underlying Equations (27) and leading to Equation (52) (see Figure 3a). This hierarchy is particularly relevant for principle-value integrals  $\mathcal{P}$  (needed below); these exclude an interval  $[-0^+, 0^+]$  around the origin, and  $\gamma_0$  must lie outside this interval.

Inserting  $S_{[1,2]_-(\varepsilon_1, -\varepsilon_1)} = S_{\text{std}}(\varepsilon_1) = \tilde{G}^{\varepsilon_1}/(-2\pi i)$  (from Equations (42a) and (51)), we find

$$G^{[n]}(\omega) = - \int_{\varepsilon_1} \frac{\tilde{G}^{\varepsilon_1}}{\omega_1^{[n]} - \varepsilon_1} = - \int_{\varepsilon_1} \frac{\tilde{G}_{\varepsilon_1^+} - \tilde{G}_{\varepsilon_1^-}}{\omega_1^{[n]} - \varepsilon_1} = \tilde{G}_{\omega_1^{[n]}} \quad (53)$$

Importantly, no MWFs  $n_{\varepsilon_1}$  occur in Equation (53). For the last step, we were thus able to close the forward (backward) integration contour involving  $\tilde{G}_{\varepsilon_1^+}$  ( $\tilde{G}_{\varepsilon_1^-}$ ) in the upper (lower) half-plane. We then used Cauchy's integral formula for the simple pole at  $\omega_1^{[n]}$  (see Figure 3b). Equation (53) expresses the fully retarded Keldysh correlators through analytic continuations of MF correlators,  $G^{[n]}[G]$ , as desired. To make contact with standard notation, we recall that the retarded and advanced  $2p$  components are given by  $G^R = G^{21} = G^{[1]}$  and  $G^A = G^{12} = G^{[2]}$ . Reinstating frequency dependencies, with  $\omega_1^{[1]} = \omega_1 + i\gamma_0 \equiv \omega_1^+$  and  $\omega_1^{[2]} = \omega_1 - i\gamma_0 \equiv \omega_1^-$ , we get

$$G^R(\omega) = \tilde{G}(\omega_1^+, \omega_2^-), \quad G^A(\omega) = \tilde{G}(\omega_1^-, \omega_2^+) \quad (54)$$

This implies the well-known relation

$$G^{rR}(\omega) = G^A(\omega), \quad G^{rA}(\omega) = G^R(\omega) \quad (55)$$

#### 3.3.2. Keldysh Component $G^{[12]}$

For  $\alpha = 2$ , both Keldysh indices equal 2,  $G^{22} = G^{[12]}$ . Then, the spectral representation in Equation (27a) requires the kernel (Equation (19c))

$$K^{[\hat{n}_1 \hat{n}_2]}(\omega_p) = (K^{[\hat{n}_1]} - K^{[\hat{n}_2]})(\omega_p) = \tilde{K}(\omega_p^{[\hat{n}_1]}) - \tilde{K}(\omega_p^{[\hat{n}_2]}) \quad (56)$$

for the case  $[\eta_1, \eta_1] = [12] = [\hat{\eta}_1, \hat{\eta}_2]$ . Evaluating this for  $p = (12)$  and  $(21)$ , we find

$$\begin{aligned} K^{[12]}(\omega_{(12)}) &= \tilde{K}(\omega_{(12)}^{[1]}) - \tilde{K}(\omega_{(12)}^{[2]}) \\ &= \frac{1}{\omega_1^{[1]}} - \frac{1}{\omega_1^{[2]}} = \frac{-2i\gamma_0}{\omega_1^2 + \gamma_0^2} = \hat{\delta}_{\gamma_0}(\omega_1) \end{aligned} \quad (57a)$$

$$\begin{aligned} K^{[12]}(\omega_{(21)}) &= \tilde{K}(\omega_{(21)}^{[2]}) - \tilde{K}(\omega_{(21)}^{[1]}) \\ &= \frac{1}{\omega_2^{[2]}} - \frac{1}{\omega_2^{[1]}} = \frac{-2i\gamma_0}{\omega_2^2 + \gamma_0^2} = \hat{\delta}_{\gamma_0}(\omega_1) \end{aligned} \quad (57b)$$

On the right, we introduced a Lorentzian representation of a broadened Dirac delta function:

$$\hat{\delta}_{\gamma_0}(x) = \frac{-2i\gamma_0}{x^2 + \gamma_0^2}, \quad \lim_{\gamma_0 \rightarrow 0^+} \hat{\delta}_{\gamma_0}(x) = -2\pi i \delta(x) = \hat{\delta}(x) \quad (58)$$

Finally, we obtain  $G^{[12]}$  by convolving the kernels (57) with the PSFs (47) according to Equation (27a):

$$\begin{aligned} G^{[12]} &= \sum_p [K^{[\hat{1}2]} * S_p](\omega_p) \\ &= \int_{\varepsilon_1} (2\pi i) S_{[1,2]_x}(\varepsilon_1, -\varepsilon_1) \hat{\delta}_{\gamma_0}(\omega_1 - \varepsilon_1) \\ &= \int_{\varepsilon_1} [(1 + 2n_{\varepsilon_1}) \tilde{G}^{\varepsilon_1} + 2\hat{\delta}(\varepsilon_1) \hat{G}_1] \hat{\delta}_{\gamma_0}(\omega_1 - \varepsilon_1) \\ &= N_{\omega_1} \tilde{G}^{\omega_1} + 4\pi i \delta(\omega_1) \hat{G}_1 \end{aligned} \quad (59)$$

For the last step we defined

$$N_{\omega_i} = -1 - 2n_{\omega_i} = \coth[\beta\omega_i/2]^{s_i} \quad (60)$$

For bosonic correlators,  $N_{\omega_1}$  is singular at  $\omega_1 = 0$ , so that a principle-value integral is implied in Equation (59). Then, the product  $N_{\omega_1} \tilde{G}^{\omega_1}$  should be evaluated via the limit  $(N_{\omega_1} \tilde{G}^{\omega_1})_{\omega_1 \rightarrow 0}$ . More precisely, three limits are involved:  $0^+$ ,  $\gamma_0$ , and  $\omega_1$  should all be sent to zero, while respecting  $0^+ \ll \gamma_0 \ll |\omega_1|$  (see discussion after Equation (52)). In the following, we suppress the subscript  $\gamma_0$  in Equation (58) and always take  $\gamma_0 \rightarrow 0^+$  after evaluating a principal-value integral (if present).

Summarizing, all Keldysh components can be expressed through analytically continued MF functions. Comparing Equations (59) and (40), we find that the anomalous part,  $\hat{G}_1$ , enters  $G^{[12]}$  with a prefactor of  $4\pi i \delta(\omega_1)$ . Using our previous results from Equation (54), yielding  $\tilde{G}^{\omega_1} = G^R(\omega_1) - G^A(\omega_1)$ , and defining  $G^{[12]} = G^K$ , the above relation (59) can be identified as the FDR

$$G^K(\omega_1) = N_{\omega_1} [G^R(\omega_1) - G^A(\omega_1)] + 4\pi i \delta(\omega_1) \hat{G}_1 \quad (61)$$

Hence, the way in which anomalous MF terms appear in KF correlators is via Keldysh correlator  $G^K$ . The anomalous term contributes only if  $\omega_1$  is bosonic and vanishes.

We will refer to general relations between components of KF correlators in thermal equilibrium as *generalized fluctuation-*

*dissipation relations* (gFDRs). Equations (55) and (61) constitute the two gFDRs available for  $\ell = 2$ . In the absence of anomalous contributions, they reduce the three nonzero KF components to a single independent one (typically chosen as  $G^R$ ).

## 4. Analytic Regions and Discontinuities of the MF Correlator

Step 2 of our three-step strategy, the extraction of PSFs, requires knowledge of possible singularities of the MF correlators. In the 2p case, for  $\tilde{G}_{z_1}$ , a branch cut divides the complex  $z_1$  plain into two analytic regions (see Figure 2a), and the discontinuity across the branch cut is given by the difference of the analytic continuations  $\tilde{G}_{\omega_1^\pm}$ . In this section, we generalize the concepts of and notations for branch cuts, analytic regions, and discontinuities to general  $\ell$ , enabling a concise discussion of the analytic continuation of 3p and 4p MF correlators in Sections 5 and 6, respectively. We focus on the regular parts  $\tilde{G}$  of the MF correlators; the anomalous parts will be discussed separately in the sections for  $\ell = 3$  and 4.

### 4.1. Analytic Regions of $\tilde{G}(z)$

Possible singularities of the regular part can be inferred from the spectral representation in Equation (14d)

$$\tilde{G}(z) = \int d^\ell \varepsilon_p \delta(\varepsilon_{\bar{1}\dots\bar{\ell}}) \sum_p \frac{S_p(\varepsilon_p)}{\prod_{i=1}^{\ell-1} (z_{\bar{1}\dots\bar{i}} - \varepsilon_{\bar{1}\dots\bar{i}})} \quad (62)$$

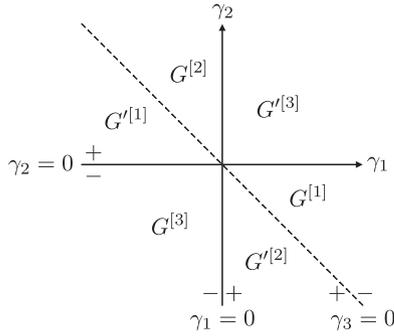
with  $z_i = \omega_i + i\gamma_i$  and  $z_{1\dots\ell} = 0$ . Singularities can be located at the points where the imaginary part of the denominator vanishes, defining branch cuts by the condition

$$\text{Im}(z_I) = \gamma_I = 0 \quad (63)$$

where  $z_I = \sum_{i \in I} z_i$  denotes a frequency sum over the elements of a non-empty subset  $I \subseteq \{1, \dots, \ell\}$ . In total, condition (63) defines  $2^{\ell-1} - 1$  distinct branch cuts since frequency conservation implies  $\text{Im}(z_I) = -\text{Im}(z_{I^c})$  where  $I^c = \{1, \dots, \ell\} \setminus I$  is the complement of  $I$ , so that  $\text{Im}(z_I) = 0$  and  $\text{Im}(z_{I^c}) = 0$  describe the same branch cut. The branch cuts divide  $\mathbb{C}^\ell$  into regions of analyticity (regions without singularities), each corresponding to one particular analytic continuation of  $\tilde{G}$ .

We henceforth focus on the case, needed for Equation (27b), that all arguments of  $\tilde{G}(z)$  are real, up to infinitesimal shifts. To be specific, we take the imaginary shifts of the frequency sums  $z_I$  to be infinitesimal,  $|\gamma_I| = 0^+$  (with signs determined via conventions described below). Then,  $\tilde{G}(z)$  is a function of  $\ell - 1$  independent real frequencies  $\omega_i$ , and the analytic region is indicated by including the  $2^{\ell-1} - 1$  shift directions  $\gamma_I = \pm 0^+$  in the argument of  $\tilde{G}(z)$ . Thus, for 2p, 3p, and 4p correlators, we need 1, 3, and 7 imaginary parts, respectively (see examples below for  $\ell = 3, 4$  in Equations (65) and (66)).

For a compact presentation of our results, it is convenient to introduce notation that specifies all imaginary shifts via a  $(\ell - 1)$ -tuple  $\check{z}$  whose components  $\check{z}_i = \check{\omega}_i + i\check{\gamma}_i$  are frequency sums of the form  $\check{z}_i = z_I$ . Then, the argument of  $\tilde{G}(z)$  is expressed as  $z(\check{z})$ , and the imaginary shifts of  $z$  are determined by those chosen for



**Figure 4.** Regions of analyticity of regular 3p MF correlators. Lines with  $\gamma_i = 0$  denote possible branch cuts of the correlators. (Figure adapted from ref. [17].) We label each region by that specific Keldysh correlator,  $G^{[n]}$  or  $G'^{[n]}$ , whose imaginary shifts  $\gamma_i$  lie within that region: For  $G^{[1]}$ , only  $\omega_1$  has a positive imaginary shift, i.e.,  $\gamma_1 > 0$ ,  $\gamma_2 < 0$ , and  $\gamma_3 < 0$ , implying  $G^{[1]}(\omega) = \tilde{G}(\omega_1^+, \omega_2^-, \omega_3^-)$ . Primed correlators (Equations (25)) have inverted imaginary shifts, such that  $G'^{[1]}(\omega) = \tilde{G}(\omega_1^-, \omega_2^+, \omega_3^+)$ .

$\check{z}$ . We will specify the  $\ell - 1$  independent frequencies  $\check{z}$  chosen to parametrize  $z(\check{z})$  using subscripts,  $\tilde{G}_z = \tilde{G}(z(\check{z}))$ , extending the subscript notation developed in Section 3.1 for  $\ell = 2$  to the regular parts of  $\ell$ p correlators. To uniquely determine the imaginary shifts in  $z_i(\check{z})$ , and hence the analytic region for  $\tilde{G}_z$ , we implicitly assign imaginary shifts to all  $\check{z}_i$  via the rule

$$2|\check{\gamma}_{i-1}| \leq |\check{\gamma}_i|, \quad \text{for } 1 < i < \ell \quad (64)$$

It ensures that the imaginary part of any  $\text{Im}z_i$  is always nonzero, and that its sign is specified uniquely through the sign choices made for the shifts  $\pm|\check{\gamma}_i|$ . We specify these sign choices using superscripts on the corresponding real frequencies  $\check{\omega}_i$ , writing  $\check{z}_i = \check{\omega}_i^\pm = \check{\omega}_i \pm i|\check{\gamma}_i|$ .

**Examples for  $\ell = 3$ :** For  $\ell = 3$ , the branch cuts are given by  $\gamma_1 = 0$ ,  $\gamma_2 = 0$ , and  $\gamma_3 = 0$ , see **Figure 4**. Therefore, three imaginary parts are required to uniquely identify one analytic region for a regular MF correlator  $\tilde{G}(z)$ , with  $z = (z_1, z_2, z_3)$  and  $z_i = \omega_i^\pm$ . Consider, e.g., the set of independent frequencies  $\check{z} = (\omega_1^+, \omega_2^-)$  with infinitesimal imaginary shifts fulfilling Equation (64). It yields the analytic continuation (see **Figure 4** for the labels of analytic regions):

$$\tilde{G}_{\omega_1^+, \omega_2^-} = \tilde{G}(\omega_1^+, \omega_2^-, -\omega_{12}^-) = \tilde{G}(\omega_1^+, \omega_2^-, \omega_3^+) = G'^{[2]}(\omega) \quad (65a)$$

The third argument,  $z_3 = -z_{12} = -\check{z}_1 - \check{z}_2 = -\omega_1^+ - \omega_2^-$ , has a positive imaginary shift since  $\text{Im}(z_3) = -\text{Im}(|\check{\gamma}_1| - |\check{\gamma}_2|) > 0$ , by Equation (64). By contrast, for  $\check{z} = (\omega_2^-, \omega_1^+)$ , we obtain

$$\tilde{G}_{\omega_2^-, \omega_1^+} = \tilde{G}(\omega_1^+, \omega_2^-, -\omega_{12}^+) = \tilde{G}(\omega_1^+, \omega_2^-, \omega_3^-) = G^{[1]}(\omega) \quad (65b)$$

Evidently,  $\tilde{G}_{\omega_2^-, \omega_1^+} \neq \tilde{G}_{\omega_1^+, \omega_2^-}$ , because switching  $\omega_1^+ \rightarrow \omega_2^-$  in the argument list of  $\check{z}$  also switches the relative magnitudes of their imaginary parts, due to Equation (64).

Note that the representation via subscripts is not unique. For instance,  $G^{[1]}(\omega)$  can also be written as  $\tilde{G}_{\omega_{12}^+, \omega_1^+}$ , since the subscript  $\check{z} = (\omega_{12}^+, \omega_1^+)$  yields  $z(\check{z}) = (\omega_1^+, \omega_{12}^+ - \omega_1^+, -\omega_{12}^+) = (\omega_1^+, \omega_2^-, \omega_3^-)$ , matching the arguments found in Equation (65b).

For the last step, the sign of the imaginary shift of the second argument follows from  $\text{Im}(z_2) = \text{Im}(\omega_{12}^+ - \omega_1^+) = |\check{\gamma}_1| - |\check{\gamma}_2| < 0$ .

**Example for  $\ell = 4$ :** For  $\ell = 4$ , the branch cuts are located at vanishing  $\gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_{12}, \gamma_{13}$ , and  $\gamma_{14}$ , see **Figure 5**. Thus, seven imaginary parts are needed to uniquely identify one analytic region for a regular MF correlator  $\tilde{G}(z)$ . We therefore write its argument as  $z = (z_1, z_2, z_3, z_4; z_{12}, z_{13}, z_{14})$ , with  $z_i = \omega_i^\pm$ , also listing the arguments after the semicolon since the signs of their imaginary parts are needed to fully specify the analytic region. Consider, e.g.,  $\check{z} = (\omega_{13}^+, \omega_2^-, \omega_3^+)$ . Then,  $z_4 = -z_{123} = -\check{z}_1 - \check{z}_2 = -\omega_{13}^+ - \omega_2^- = -\omega_{123}^- = \omega_4^+$ ,  $z_{12} = \check{z}_1 + \check{z}_2 - \check{z}_3 = \omega_{13}^+ + \omega_2^- - \omega_3^+ = \omega_{12}^-$ , and  $z_{14} = -z_{23} = -z_2 - z_3 = -\omega_2^- - \omega_3^+ = -\omega_{23}^+$ ; the signs of the imaginary shifts on the right sides follow via Equation (64). We thus obtain

$$\begin{aligned} \tilde{G}_{\omega_{13}^+, \omega_2^-, \omega_3^+} &= \tilde{G}(\omega_1^-, \omega_2^-, \omega_3^+, -\omega_{123}^-; \omega_{12}^-, \omega_{13}^+, -\omega_{23}^+) \\ &= \tilde{G}(\omega_1^-, \omega_2^-, \omega_3^+, \omega_4^+; \omega_{12}^-, \omega_{13}^+, \omega_{14}^-) = C_{IV}^{(34)} \end{aligned} \quad (66)$$

In the last line, the frequency arguments were expressed through those used to label the analytic regions in **Figure 5**.

## 4.2. Discontinuities of $\tilde{G}(z)$

The discontinuity of  $\tilde{G}(z)$  across a given branch cut, defined by  $\text{Im}z_I = \gamma_I = 0$ , quantifies the difference between two neighboring analytic regions,  $R_+$  and  $R_-$ , separated by  $\gamma_I = 0$ . We denote this discontinuity by  $\tilde{G}(z^{R_+}) - \tilde{G}(z^{R_-})$ . Explicitly, we have opposite imaginary shifts  $\gamma_I$  in the analytic regions,  $\gamma_I^{R_+} = 0^+ = -\gamma_I^{R_-}$ , and equivalent shifts for all other  $\gamma_J^{R_+} = \gamma_J^{R_-}$  with  $J \not\subseteq \{1, \dots, \ell\}$  and  $J \neq I$ . To describe this discontinuity using  $\check{z}$  notation, we write  $\check{z}^{R_\pm} = (\check{z}_1^{R_\pm}, \check{z}^*)$ , where the first variable is chosen as the one whose imaginary part changes sign across the branch cut,  $\check{z}_1^{R_\pm} = \omega_I^\pm$ , and  $\check{z}^*$  denotes a tuple of  $\ell - 2$  other, independent frequencies, with imaginary shifts given by the prescription (64). Then, extending the superscript notation from Section 3.1, we can express the discontinuity of  $\tilde{G}(z)$  across  $\text{Im}z_I = 0$  as

$$\tilde{G}_{\check{z}^*}^{\omega_I} = \tilde{G}_{\omega_I^+, \check{z}^*} - \tilde{G}_{\omega_I^-, \check{z}^*} = \tilde{G}_{\check{z}^{R_+}} - \tilde{G}_{\check{z}^{R_-}} \quad (67)$$

Similarly, we define consecutive discontinuities across two branch cuts,  $\gamma_I = 0$  and  $\gamma_J = 0$ , to be evaluated as

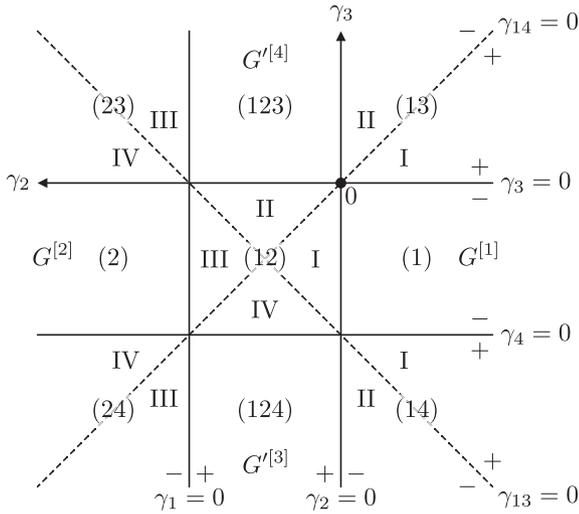
$$\tilde{G}_{\check{z}_3, \dots, \check{z}_{\ell-1}}^{\omega_1, \omega_J} = \tilde{G}_{\omega_1^+, \check{z}_3, \dots, \check{z}_{\ell-1}} - \tilde{G}_{\omega_J^+, \check{z}_3, \dots, \check{z}_{\ell-1}} \quad (68)$$

where we have  $\check{z}_1 = \omega_I^\pm$  and  $\check{z}_2 = \omega_J^\pm$ .

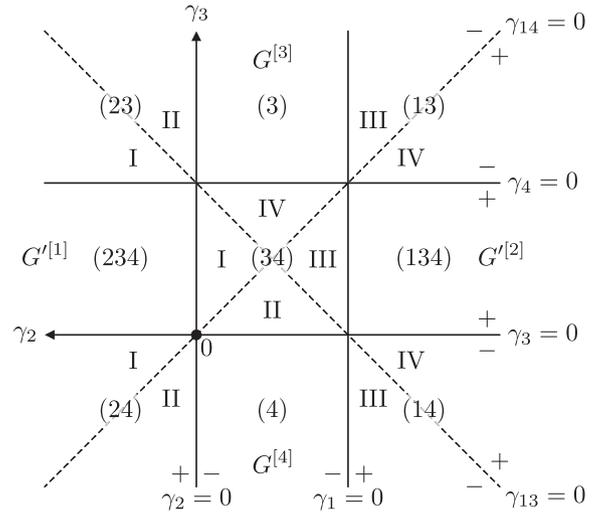
**Examples for  $\ell = 3$ :** For a discontinuity across  $\gamma_2 = 0$  and  $\check{z}^* = \omega_1^+$ , we find

$$\begin{aligned} \tilde{G}_{\omega_1^+}^{\omega_2} &= \tilde{G}_{\omega_2^+, \omega_1^+} - \tilde{G}_{\omega_2^-, \omega_1^+} \\ &= \tilde{G}(\omega_1^+, \omega_2^+, -\omega_{12}^+) - \tilde{G}(\omega_1^+, \omega_2^-, -\omega_{12}^+) \\ &= \tilde{G}(\omega_1^+, \omega_2^+, \omega_3^-) - \tilde{G}(\omega_1^+, \omega_2^-, \omega_3^-) \\ &= G'^{[3]}(\omega) - G^{[1]}(\omega) \end{aligned} \quad (69)$$

$\gamma_{12} > 0$ :



$\gamma_{12} < 0$ :



**Figure 5.** Regions of analyticity of regular 4p MF correlators (analogous to ref. [13]). Lines with  $\text{Im } z_i = \gamma_i = 0$  and  $\text{Im } z_{ij} = \gamma_{ij} = 0$  denote possible branch cuts. The rectangular regions are labeled by arabic numbers indicating which  $\gamma_i$  are positive; e.g., for region (124), we have  $\gamma_1, \gamma_2, \gamma_4 > 0$  but  $\gamma_3 < 0$ . Consequently, regions composed of one or three arabic numbers correspond to fully retarded or advanced Keldysh components. Regions with two of the  $\gamma_i$  positive, like region (12), are further divided into four subregions by the branch cuts in  $\gamma_{ij}$  and are distinguished by roman numbers I – IV.

Two consecutive discontinuities across, e.g.,  $\gamma_1 = 0$  and  $\gamma_2 = 0$  yield

$$\begin{aligned} \tilde{G}^{\omega_1, \omega_2} &= \tilde{G}_{\omega_2^+}^{\omega_1} - \tilde{G}_{\omega_2^-}^{\omega_1} = \tilde{G}_{\omega_1^+, \omega_2^+} - \tilde{G}_{\omega_1^-, \omega_2^+} - \tilde{G}_{\omega_1^+, \omega_2^-} + \tilde{G}_{\omega_1^-, \omega_2^-} \\ &= \tilde{G}(\omega_1^+, \omega_2^+, -\omega_{12}^+) - \tilde{G}(\omega_1^-, \omega_2^+, -\omega_{12}^+) \\ &\quad - \tilde{G}(\omega_1^+, \omega_2^-, -\omega_{12}^-) + \tilde{G}(\omega_1^-, \omega_2^-, -\omega_{12}^-) \\ &= G^{[3]} - G^{[2]} - G'^{[2]} + G^{[3]} \end{aligned} \quad (70)$$

*Example for  $\ell = 4$ :* The discontinuity for, e.g.,  $\gamma_{123} = 0$  and  $\tilde{z}^r = (\omega_3^+, \omega_1^-)$  evaluates to

$$\begin{aligned} \tilde{G}_{\omega_3^+, \omega_1^-}^{\omega_{123}} &= \tilde{G}_{\omega_{123}^+, \omega_3^+, \omega_1^-} - \tilde{G}_{\omega_{123}^-, \omega_3^+, \omega_1^-} \\ &= \tilde{G}(\omega_1^-, \omega_2^+, \omega_3^+, -\omega_{123}^+; \omega_{12}^-, \omega_{13}^-, -\omega_{23}^-) \\ &\quad - \tilde{G}(\omega_1^-, \omega_2^+, \omega_3^+, -\omega_{123}^-; \omega_{12}^-, \omega_{13}^-, -\omega_{23}^-) \\ &= C_1^{(23)} - C^{(234)} \end{aligned} \quad (71)$$

## 5. Analytic Continuation of 3p Correlators

The notation introduced in the previous section enables a concise discussion of the analytic continuation of 3p MF correlators in the following. Section 5.1 is devoted to the general structure of these correlators and the connection of their analytical continuations to 3p PSFs. In contrast to the 2p case, the derivation of these PSFs, constituting Steps 1 and 2 of our three-step strategy, is discussed in Appendix C.2; in the main text, we merely state the final result. In Section 5.2, we show that the PSFs yield all components of the KF correlator as linear combinations of analytically continued MF correlators.

### 5.1. Extraction of PSFs

A general 3p correlator can be decomposed into a regular and various anomalous parts (see Equation (A5) and Appendix C.1):

$$\begin{aligned} G(i\omega(\omega_1^-, \omega_2^-)) &= G_{i\omega_1^-, i\omega_2^-} \\ &= \tilde{G}_{i\omega_1^-, i\omega_2^-} + \beta \delta_{i\omega_1^-} \hat{G}_{1; i\omega_2^-} + \beta \delta_{i\omega_2^-} \hat{G}_{2; i\omega_1^-} \\ &\quad + \beta \delta_{i\omega_{12}^-} \hat{G}_{12; i\omega_1^-} + \beta^2 \delta_{i\omega_1^-} \delta_{i\omega_2^-} \hat{G}_{1, \bar{2}} \end{aligned} \quad (72)$$

Here,  $\tilde{G}$  denotes the regular part, whereas  $\hat{G}_i$  represents the anomalous part w.r.t. frequency  $i\omega_i$ , i.e.,  $\hat{G}_i$  comes with a factor of  $\beta \delta_{i\omega_i}$  and is independent of  $i\omega_i$ .  $\hat{G}_{1,2}$  is anomalous w.r.t. all frequencies and is a frequency-independent constant. (Note that, e.g.,  $\beta \delta_{i\omega_3} \hat{G}_3$  can be written as  $\beta \delta_{i\omega_{12}} \hat{G}_{12}$  in the  $\beta \delta$  expansion in Equation (72), implying relations like  $\hat{G}_{12} = \hat{G}_3$ . This unbiased notation allows us to write formulas that hold for any permutation  $p$ .)

The full correlator  $G$  as well as the components  $\tilde{G}$  and  $\hat{G}_i$  are, by definition, singularity-free for all Matsubara frequencies. For the anomalous contributions, we further have the decomposition

$$\hat{G}_{3; i\omega_1} = \hat{G}_{3; i\omega_1}^{\Delta} + \Delta_{i\omega_1} \hat{G}_{3; 1}^{\Delta} \quad (73)$$

where  $\Delta_{i\omega_i}$  is defined in Equation (32) for a purely imaginary  $\Omega_i = i\omega_i$ . Here,  $\hat{G}_{3; 1}^{\Delta}$  comprises all terms proportional to a  $\Delta_{i\omega_1}$  symbol, and  $\hat{G}_{3; i\omega_1}^{\Delta}$  contains the rest. Analogous definitions hold for all anomalous terms  $\hat{G}_i$ , see Appendix C.1 for a detailed discussion. The distinction between  $\hat{G}_i^{\Delta}$  and  $\hat{G}_i^{\Delta}$  is only needed if all three operators are bosonic, in which case all anomalous terms in Equation (72) can occur. For two fermionic and one bosonic

operator, all following results equally hold by replacing  $\hat{G}_i^{\Delta} \rightarrow \hat{G}_i$  and  $\hat{G}_i^{\Delta} \rightarrow 0$ .

In Appendix C.2, we show that the PSFs can be expressed via analytic continuations of the general constituents of the 3p correlator [Equation (72)]:

$$(2\pi i)^2 S_p(\varepsilon_{\bar{1}}, \varepsilon_{\bar{2}}) = n_{\varepsilon_{\bar{1}}} n_{\varepsilon_{\bar{2}}} \tilde{G}^{\varepsilon_{\bar{2}}, \varepsilon_{\bar{1}}} + n_{\varepsilon_{\bar{1}}} n_{\varepsilon_{\bar{1}\bar{2}}} \tilde{G}^{\varepsilon_{\bar{1}\bar{2}}, \varepsilon_{\bar{1}}} + \delta(\varepsilon_{\bar{1}}) n_{\varepsilon_{\bar{2}}} \hat{G}_{\bar{1}}^{\Delta, \varepsilon_{\bar{2}}} + \delta(\varepsilon_{\bar{2}}) n_{\varepsilon_{\bar{1}}} \hat{G}_{\bar{2}}^{\Delta, \varepsilon_{\bar{1}}} + \delta(\varepsilon_{\bar{3}}) n_{\varepsilon_{\bar{1}}} \hat{G}_{\bar{3}}^{\Delta, \varepsilon_{\bar{1}}} + \delta(\varepsilon_{\bar{1}}) \delta(\varepsilon_{\bar{2}}) \left( \hat{G}_{\bar{1}\bar{2}}^{\Delta} - \frac{1}{2} \hat{G}_{\bar{3}\bar{1}}^{\Delta} \right) \quad (74)$$

This is our main result for  $\ell = 3$ . Explicit expressions of the PSFs for individual permutations are obtained by inserting the permuted indices into the above equation. In Equations (C26), we provide an overview of all possibly occurring discontinuities expressed through the analytic regions in Figure 4. As for 2p PSFs, we provide a consistency check of Equation (74) in Appendix G.

## 5.2. 3p Keldysh Correlators

In the following two sections, we demonstrate how to construct KF correlators as linear combinations of analytically continued MF correlators using the PSFs in Equation (74), corresponding to Step 3 of our strategy. For  $\alpha = 1$ , Equation (23) gives the analytic continuation of  $G$  to fully retarded components  $G^{[n]}$  for general  $\ell$ . Therefore, we directly consider the more challenging cases of  $\alpha = 2, 3$  in Sections 5.2.1 and 5.2.2, respectively. Lastly, in Section 5.2.3 we provide an overview of all Keldysh components and present gFDRs.

### 5.2.1. Keldysh Components $G^{[n_1, n_2]}$

To recapitulate, in Section 3.3.2 we performed manipulations on the level of the Keldysh kernels for  $\ell = 2$  and  $\alpha = 2$  by using the identity (58), which directly allowed us to evaluate the convolution with the PSFs. Even though the kernels for  $\ell = 3$  are more complicated due to an additional factor in the denominator (see Equation (19d)), similar manipulations are presented in Appendix C.3.1 for the Keldysh component  $G^{212} = G^{[13]}$ . There, it is shown that simplifications of the 3p KF kernel  $K^{[n_1, n_2]}$  (Equation (19c)) yield

$$G^{[13]}(\omega) = \int_{\varepsilon_1, \varepsilon_2} \delta(\omega_1 - \varepsilon_1) \frac{(2\pi i)^2}{\omega_2^- - \varepsilon_2} S_{[1,2,3]_{-}}(\varepsilon_1, \varepsilon_2, -\varepsilon_{12}) - \int_{\varepsilon_1, \varepsilon_2} \delta(\omega_{12} - \varepsilon_{12}) \frac{(2\pi i)^2}{\omega_2^- - \varepsilon_2} S_{[[1,2]_{-}, 3]_{+}}(\varepsilon_1, \varepsilon_2, -\varepsilon_{12}) \quad (75)$$

Similarly to the 2p case, we always display the unpermuted  $\varepsilon$  for PSF (anti)commutators and insert permuted  $\varepsilon_p$  only for individual PSFs, implying, e.g.,  $S_{2[3,1]_{+}}(\varepsilon) = S_{(231)}(\varepsilon_2, \varepsilon_3) \pm S_{(213)}(\varepsilon_2, \varepsilon_1)$ . For the integrations in Equation (75), we fixed the two independent frequencies  $\varepsilon_1$  and  $\varepsilon_2$  as integration variables. We thus ob-

tain, e.g.,

$$S_{[1,2,3]_{-}}(\varepsilon) = S_{1[2,3]_{-}}(\varepsilon) + S_{[2,3]_{-}1}(\varepsilon) = S_{(123)}(\varepsilon_1, \varepsilon_2) - S_{(132)}(\varepsilon_1, \varepsilon_3) + S_{(231)}(\varepsilon_2, \varepsilon_3) - S_{(321)}(\varepsilon_3, \varepsilon_2) \quad (76)$$

with  $\varepsilon_3 = -\varepsilon_{12}$  being understood.

To relate the KF to the MF correlator, we insert Equation (74) into the PSF (anti)commutators of Equation (76) and simplify the results using relations for the discontinuities such as  $\tilde{G}^{\varepsilon_2, \varepsilon_3} = -\tilde{G}^{\varepsilon_2, \varepsilon_1}$ . Such identities follow by explicitly expressing the discontinuities in terms of  $G^{[n]}$  and  $G'^{[n]}$  correlators (see Equations (C26)). Then, the PSF (anti)commutator in Equation (76), e.g., reads

$$(2\pi i)^2 S_{[1,2,3]_{-}}(\varepsilon_1, \varepsilon_2, -\varepsilon_{12}) = N_{\varepsilon_1} \tilde{G}^{\varepsilon_1, \varepsilon_2} - 2\delta(\varepsilon_1) \hat{G}_1^{\Delta, \varepsilon_2} - 2\delta(\varepsilon_1) \delta(\varepsilon_2) \hat{G}_{1,2}^{\Delta} \quad (77)$$

Inserting Equation (77) (and a similar expression for  $S_{[[1,2]_{-}, 3]_{+}}$ , see Equation (C31b)) into Equation (75) and evaluating one of the integrals via the  $\delta$ -function, we find

$$G^{[13]}(\omega) = -N_{\omega_1} \int_{\varepsilon_2} \frac{\tilde{G}^{\omega_1, \varepsilon_2}}{\omega_2^- - \varepsilon_2} + 2\delta(\omega_1) \left( \int_{\varepsilon_2} \frac{\hat{G}_1^{\Delta, \varepsilon_2}}{\omega_2^- - \varepsilon_2} - \frac{\hat{G}_{1,2}^{\Delta}}{\omega_2^-} \right) - N_{\omega_{12}} \int_{\varepsilon_2} \frac{\tilde{G}^{\omega_{12}, \varepsilon_2}}{\omega_2^- - \varepsilon_2} + 2\delta(\omega_{12}) \left( \int_{\varepsilon_2} \frac{\hat{G}_3^{\Delta, \varepsilon_2}}{\omega_2^- - \varepsilon_2} - \frac{\hat{G}_{3,2}^{\Delta}}{\omega_2^-} \right) \quad (78)$$

Here, it becomes apparent why collecting PSFs in terms of (anti)commutators is beneficial. The integrands in Equation (78) do not contain any MWFs depending on the integration variable  $\varepsilon_2$ , so that the only pole away from  $\text{Im}(z_2) = 0$  comes from the denominators. Consequently, the integrals over  $\varepsilon_2$  can be evaluated by closing the forward/backward integration contours in the upper/lower half-planes. Then, only the pole at  $z_2 = \omega_2^-$  contributes (as illustrated in Figure 3 for the integral in Equation (53)), and the final result for the Keldysh correlator  $G^{[13]}$  reads

$$G^{[13]} = N_{\omega_1} \tilde{G}_{\omega_2^-}^{\omega_1} + N_{\omega_{12}} \tilde{G}_{\omega_2^-}^{\omega_{12}} + 4\pi i \delta(\omega_1) \hat{G}_{1, \omega_2^-}^{\Delta} + 4\pi i \delta(\omega_{12}) \hat{G}_{3, \omega_2^-}^{\Delta} = N_{\omega_1} (G'^{[2]} - G^{[3]}) + N_{\omega_3} (G'^{[2]} - G^{[1]}) + 4\pi i \delta(\omega_1) \hat{G}_1^{\Delta} + 4\pi i \delta(\omega_3) \hat{G}_3^{\Delta} \quad (79)$$

Here, we used  $N_{\omega_{12}} = -N_{\omega_3}$ , expressed  $\tilde{G}_{\omega_2^-}^{\omega_1}$  and  $\tilde{G}_{\omega_2^-}^{\omega_{12}}$  in terms of the analytic regions in Figure 4, and defined the shorthand

$$\hat{G}_{i, \omega_j^{\pm}}^{\Delta} = \hat{G}_{i, \omega_j^{\pm}}^{\Delta} + \frac{\hat{G}_{ij}^{\Delta}}{\omega_j^{\pm}} \quad (80)$$

We emphasize that Equation (80) should not be interpreted as a direct analytic continuation of Equation (73). Rather, it can

be obtained from Equation (73) by replacing  $\Delta_{i\omega_j} \rightarrow 1/(i\omega_j)$  and only afterwards analytically continuing the resulting expression  $i\omega_j \rightarrow \omega_j^\pm$ . Additionally, we defined the shorthand  $\hat{G}_i^{[n]} = \hat{G}_i(\omega^{[n]})$ , such that, e.g.,  $\hat{G}_{1,\omega_2^-} = \hat{G}_{1,\omega_2^+} = \hat{G}_1^{[3]}$ . The other two Keldysh components with  $\alpha = 2$ ,  $G^{[12]}$  and  $G^{[23]}$ , can be derived similarly, and their results are shown in Equations (84a) and (84c), respectively.

### 5.2.2. Keldysh Component $G^{[123]}$

In this section, we relate the Keldysh component  $G^{[123]}$  to the analytic continued MF correlator. In the derivation of Equation (78), using the identity (58) for the  $\alpha = 2$  kernel  $K^{[\tilde{n}_1, \tilde{n}_2]}$  was essential. However, the Keldysh kernel for  $G^{[123]}$ ,  $K^{[\tilde{n}_1, \tilde{n}_2, \tilde{n}_3]}$ , involves three retarded kernels according to Equation (19c), impeding the direct application of Equation (58).

In Appendix C.3.2, we show that this problem can be circumvented by subtracting a fully retarded component, say,  $G^{[3]}$ . An analysis of the spectral representation of  $G^{[123]} - G^{[3]}$  then leads to

$$\begin{aligned} & \frac{1}{(2\pi i)^2} (G^{[123]} - G^{[3]})(\omega) \\ &= \int_{\varepsilon_1, \varepsilon_2} \hat{\delta}(\omega_1 - \varepsilon_1) \hat{\delta}(\omega_2 - \varepsilon_2) S_{[[1,2]_+, 3]_+}(\varepsilon_1, \varepsilon_2, -\varepsilon_{12}) \\ &+ \int_{\varepsilon_1, \varepsilon_2} \hat{\delta}(\omega_1 - \varepsilon_1) \frac{1}{\omega_2^- - \varepsilon_2} S_{[1, [2, 3]_-]}(\varepsilon_1, \varepsilon_2, -\varepsilon_{12}) \\ &+ \int_{\varepsilon_1, \varepsilon_2} \hat{\delta}(\omega_2 - \varepsilon_2) \frac{1}{\omega_1^- - \varepsilon_1} S_{[2, [1, 3]_-]}(\varepsilon_1, \varepsilon_2, -\varepsilon_{12}) \end{aligned} \quad (81)$$

Similar to Equations (76) and (78), we evaluate the PSF (anti)commutators by inserting Equation (74) (see Equation (C36)), and subsequently evaluate the integrals either via the  $\delta$ -functions or via Cauchy's integral formula, yielding

$$\begin{aligned} & (G^{[123]} - G^{[3]})(\omega) \\ &= (1 + N_{\omega_1} N_{\omega_2}) \tilde{G}^{\omega_2, \omega_1} + N_{\omega_{12}} N_{\omega_1} \tilde{G}^{\omega_{12}, \omega_1} + \tilde{G}_{\omega_2^-}^{\omega_1} + \tilde{G}_{\omega_1^-}^{\omega_2} \\ &+ 4\pi i \delta(\omega_1) N_{\omega_2} \hat{G}_1^{\hat{\omega}_2} + 4\pi i \delta(\omega_2) N_{\omega_1} \hat{G}_2^{\hat{\omega}_1} \\ &+ 4\pi i \hat{\delta}(\omega_{12}) N_{\omega_1} \hat{G}_3^{\hat{\omega}_1} + (4\pi i)^2 \delta(\omega_1) \delta(\omega_2) \hat{G}_{1,2} \end{aligned} \quad (82)$$

A more symmetric form of this result (see Equation (84d)) can be obtained by expressing all discontinuities in terms of the analytic regions in Figure 4 and applying the identity

$$1 + N_{\omega_1} N_{\omega_2} + N_{\omega_1} N_{\omega_3} + N_{\omega_2} N_{\omega_3} = 0 \quad (83)$$

which holds for  $\ell = 3$  due to frequency conservation.

### 5.2.3. 3p Generalized Fluctuation-Dissipation Relations

Expressing all Keldysh components with  $\alpha \geq 2$  through analytic continuations of MF correlators is equivalent to relating them to

fully retarded and advanced components. Indeed, as in the 2p case, knowledge of the fully retarded and advanced components *and* the anomalous terms suffices to obtain all Keldysh components, as brought to bear by the 3p gFDRs (where  $N_i = N_{\omega_i}$ )

$$\begin{aligned} G^{[12]} &= N_1 (\tilde{G}^{[3]} - \tilde{G}^{[2]}) + N_2 (\tilde{G}^{[3]} - \tilde{G}^{[1]}) \\ &+ 4\pi i \delta(\omega_1) \hat{G}_1^{[2]} + 4\pi i \delta(\omega_2) \hat{G}_2^{[1]} \end{aligned} \quad (84a)$$

$$\begin{aligned} G^{[13]} &= N_1 (\tilde{G}^{[2]} - \tilde{G}^{[3]}) + N_3 (\tilde{G}^{[2]} - \tilde{G}^{[1]}) \\ &+ 4\pi i \delta(\omega_1) \hat{G}_1^{[3]} + 4\pi i \delta(\omega_3) \hat{G}_3^{[1]} \end{aligned} \quad (84b)$$

$$\begin{aligned} G^{[23]} &= N_2 (\tilde{G}^{[1]} - \tilde{G}^{[3]}) + N_3 (\tilde{G}^{[1]} - \tilde{G}^{[2]}) \\ &+ 4\pi i \delta(\omega_2) \hat{G}_2^{[3]} + 4\pi i \delta(\omega_3) \hat{G}_3^{[2]} \end{aligned} \quad (84c)$$

$$\begin{aligned} G^{[123]} &= N_2 N_3 G^{[1]} + N_1 N_3 G^{[2]} + N_1 N_2 G^{[3]} \\ &+ (1 + N_2 N_3) G^{[1]} + (1 + N_1 N_3) G^{[2]} + (1 + N_1 N_2) G^{[3]} \\ &+ 4\pi i \left[ \delta(\omega_1) N_2 (\hat{G}_1^{\hat{\omega}_2} - \hat{G}_1^{\hat{\omega}_3}) + \delta(\omega_2) N_3 (\hat{G}_2^{\hat{\omega}_3} - \hat{G}_2^{\hat{\omega}_1}) \right. \\ &\left. + \delta(\omega_3) N_1 (\hat{G}_3^{\hat{\omega}_1} - \hat{G}_3^{\hat{\omega}_2}) \right] + (4\pi i)^2 \delta(\omega_1) \delta(\omega_2) \hat{G}_{1,2} \end{aligned} \quad (84d)$$

These gFDRs agree with the results in ref. [24], and generalize those by also including anomalous contributions. Applications of these formulas to the Hubbard atom are presented in Section 7.

## 6. Analytic Continuation of 4p Correlators

In this section, we demonstrate the MF-to-KF analytic continuation of fermionic 4p correlators. In Section 6.1, we first discuss our convention for labelling analytic regions and provide the expression of PSFs in terms of analytically continued MF correlators. In Section 6.2, we then generalize the key concept for the construction of 3p KF correlators, namely rewriting the KF spectral representation using kernel identities and PSF (anti)commutators, to arbitrary  $\ell$ , and apply it to the relevant case  $\ell = 4$ .

### 6.1. Analytic Regions and Extraction of PSFs

As discussed in Section 4.1, the possible singularities of a regular 4p MF correlator are located at seven branch cuts, splitting the complex plane into a total of 32 regions (see Figure 5). Importantly, for  $\ell \geq 4$ , only few of these regions correspond to fully retarded or advanced Keldysh components, in contrast to  $\ell = 2, 3$ . We label analytic continuations of MF correlators by  $C$ , e.g.,

$$\tilde{G}(\omega_1^+, \omega_2^-, \omega_3^+, \omega_4^-; \omega_{12}^-, \omega_{13}^+, \omega_{14}^-) = C_{\text{III}}^{(13)} \quad (85)$$

The superscript of  $C_{\text{III}}^{(13)}$  indicates which  $\omega_i$  (with  $1 \leq i \leq 4$ ) have a positive imaginary shift. Analytic regions with two  $\omega_i$ 's having positive shifts are further divided into four subregions, denoted by roman numbers I – IV in the subscripts of  $C$ . This is necessary because for  $C_{\text{III}}^{(13)}$ , e.g., the superscripts do not uniquely determine

the imaginary parts of  $\omega_1^+ + \omega_2^- = \omega_{12}^\pm$  and  $\omega_1^+ + \omega_4^- = \omega_{14}^\pm$ . Fully retarded or advanced Keldysh components, on the other hand, are directly related to analytic regions,  $G^{[\eta]} = C^{(i)}$  with  $i = \eta$  and  $G^{[\eta]} = C^{(ijk)}$  with  $i, j, k \neq \eta$ , as depicted in Figure 5.

Priming correlators, i.e., complex conjugation of the imaginary parts of frequencies (Equation (25)), is directly applicable to the analytic regions. Consider, e.g.,  $C^{(1)}$ , where only  $\omega_1$  has a positive imaginary part; then, priming  $C^{(1)}$  yields  $(C^{(1)})' = (G^{[1]})' = G^{[1]} = C^{(234)}$ , where only  $\omega_1$  has a negative imaginary part. The roman subscripts are chosen such that they are unaffected by complex conjugation of imaginary parts, so that, e.g.,  $(C_{II}^{(14)})' = C_{II}^{(23)}$ .

Finally, we note that double bosonic discontinuities, e.g.,  $\tilde{G}_{\omega_1^+}^{\omega_{13}, \omega_{14}}$ , vanish since the fermionic 4p kernel contains only one bosonic frequency, see Appendix E.1.2. This implies that not all analytic regions displayed in Figure 5 are independent, since the following relations hold:

$$C_I^{(ij)} - C_{II}^{(ij)} + C_{III}^{(ij)} - C_{IV}^{(ij)} = 0, \quad \text{with } 1 \leq i < j \leq 4 \quad (86)$$

The identity for  $(ij) = (12)$ , e.g., follows from  $\tilde{G}_{\omega_1^+}^{\omega_{13}, \omega_{14}} = 0$ .

After establishing our convention for labeling analytic regions, we now apply our strategy for the analytic continuation to fermionic 4p MF correlators. Anomalous terms, requiring bosonic Matsubara frequencies, only occur for sums of two fermionic Matsubara frequencies, implying the general form (Equation (A5))

$$\begin{aligned} G(i\omega(\omega_1, \omega_2, \omega_3)) &= G_{i\omega_1, i\omega_2, i\omega_3} \\ &= \tilde{G}_{i\omega_1, i\omega_2, i\omega_3} + \beta \delta_{i\omega_{12}} \hat{G}_{12; i\omega_1, i\omega_3} \\ &\quad + \beta \delta_{i\omega_{13}} \hat{G}_{13; i\omega_1, i\omega_2} + \beta \delta_{i\omega_{14}} \hat{G}_{14; i\omega_1, i\omega_2} \end{aligned} \quad (87)$$

The anomalous terms need not be further distinguished by factors of  $\Delta_{i\omega}$  as in Equation (73), since the remaining frequency arguments are fermionic ( $i\omega_i \neq 0$ ).

Using Equation (87), Steps 1 and 2 of our three-step strategy are discussed in Appendix D; they yield the PSFs

$$\begin{aligned} (2\pi i)^3 S_p(\varepsilon_1, \varepsilon_2, \varepsilon_3) &= n_{\varepsilon_1} n_{\varepsilon_2} n_{\varepsilon_3} \tilde{G}^{\varepsilon_1, \varepsilon_2, \varepsilon_3} + n_{\varepsilon_1} n_{\varepsilon_2} n_{\varepsilon_{123}} \tilde{G}^{\varepsilon_{123}, \varepsilon_2, \varepsilon_1} \\ &\quad + n_{\varepsilon_1} n_{\varepsilon_2} n_{\varepsilon_{13}} \tilde{G}^{\varepsilon_{13}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_1} n_{\varepsilon_2} n_{\varepsilon_{23}} \tilde{G}^{\varepsilon_{23}, \varepsilon_2, \varepsilon_1} \\ &\quad + n_{\varepsilon_1} n_{\varepsilon_{12}} n_{\varepsilon_3} \tilde{G}^{\varepsilon_3, \varepsilon_{12}, \varepsilon_1} + n_{\varepsilon_1} n_{\varepsilon_{12}} n_{\varepsilon_{123}} \tilde{G}^{\varepsilon_{123}, \varepsilon_{12}, \varepsilon_1} \\ &\quad + n_{\varepsilon_1} n_{\varepsilon_3} \delta(\varepsilon_{12}) \hat{G}_{12}^{\varepsilon_3, \varepsilon_1} + n_{\varepsilon_1} n_{\varepsilon_2} \delta(\varepsilon_{13}) \hat{G}_{13}^{\varepsilon_2, \varepsilon_1} \\ &\quad + n_{\varepsilon_1} n_{\varepsilon_2} \delta(\varepsilon_{14}) \hat{G}_{14}^{\varepsilon_2, \varepsilon_1} \end{aligned} \quad (88)$$

This is our main result for  $\ell = 4$ . Equations (D11) give an overview over all possibly occurring discontinuities expressed through the analytic regions in Figure 5. As for the 2p and 3p cases, we provide a consistency check of Equation (88) in Appendix G.

To conclude this section, we further comment on properties of the anomalous parts. As discussed in Appendix D.2, the anomalous contribution  $\hat{G}_{13; i\omega_1, i\omega_2}$ , e.g., can only depend on the frequencies  $\omega_1$  and  $\omega_2$  separately, but not on  $i\omega_{12}$ . For anomalous parts, the complex frequency plane is thus divided into only four analytic regions corresponding to the imaginary parts of  $\varepsilon_1^\pm$  and  $\varepsilon_3^\pm$ , in contrast to the six analytic regions for 3p correlators. This directly implies symmetries for discontinuities, such as  $\hat{G}_{13}^{\varepsilon_2, \varepsilon_1} = \hat{G}_{13}^{\varepsilon_1, \varepsilon_2}$ . Similarly as for the regular parts, we label analytic continuations of anomalous parts with  $\hat{C}$ , e.g.,

ous contribution  $\hat{G}_{13; i\omega_1, i\omega_2}$ , e.g., can only depend on the frequencies  $\omega_1$  and  $\omega_2$  separately, but not on  $i\omega_{12}$ . For anomalous parts, the complex frequency plane is thus divided into only four analytic regions corresponding to the imaginary parts of  $\varepsilon_1^\pm$  and  $\varepsilon_3^\pm$ , in contrast to the six analytic regions for 3p correlators. This directly implies symmetries for discontinuities, such as  $\hat{G}_{13}^{\varepsilon_2, \varepsilon_1} = \hat{G}_{13}^{\varepsilon_1, \varepsilon_2}$ . Similarly as for the regular parts, we label analytic continuations of anomalous parts with  $\hat{C}$ , e.g.,

$$\hat{G}_{12; \omega_1^+, \omega_3^-} = \hat{C}_{12}^{(14)} \quad (89)$$

with the difference that subscripts indicate the anomalous contributions. Since  $\hat{G}_{12; \omega_1^+, \omega_3^-}$  is always multiplied by  $\delta(\omega_{12})$ , the remaining frequencies must have imaginary parts  $\omega_2^-$  and  $\omega_4^+$ . Accordingly, the superscript of  $\hat{C}_{12}^{(14)}$  indicates the positive imaginary shifts of  $\omega_1$  and  $\omega_4$ .

## 6.2. 4p Keldysh Correlators

In this section, we discuss the construction of KF correlators as linear combinations of analytically continued MF correlators. In Equations (59), (75), and (81), we expressed various Keldysh components via a convolution of PSF (anti)commutators with modified KF kernels, which originated from kernel identities presented in Equations (57) and Appendix C.3. To generalize these insights to arbitrary  $\ell$ p correlators and to present our results in a concise way, we now introduce further notation. The goal of this notation is to collect terms which are related to discontinuities, each expressible via a sum over restricted permutations, such as the  $\sum_{\vec{I}^1 | \vec{I}^2}$  terms in Equation (93).

The set of all indices  $L = \{1, \dots, \ell\}$  can be partitioned into  $\alpha$  subsets  $\vec{I}$  of length  $|\vec{I}|$ , such that  $L = \bigcup_{j=1}^{\alpha} \vec{I}^j$  with  $\vec{I}^j \cap \vec{I}^{j'} = \emptyset$  for  $j \neq j'$  and  $\ell = \sum_{j=1}^{\alpha} |\vec{I}^j|$ . For a general Keldysh component  $[\eta_1 \dots \eta_\alpha]$ , we define the subsets  $\vec{I}$  to contain at least the element  $\eta_j \in \vec{I}$  for all  $j \in \{1, \dots, \alpha\}$ , implying  $|\vec{I}| \geq 1$ . For example, a possible choice of the subsets for  $\ell = 4$  and  $[\eta_1 \eta_2] = [12]$  is given by  $\vec{I}^1 = \{1, 3\}$  and  $\vec{I}^2 = \{2, 4\}$ . With  $\sum_{\vec{I}^1 | \vec{I}^2}$ , we denote sums over restricted permutations  $p = \vec{I}^1 | \vec{I}^2$  for which all indices in subset  $\vec{I}^1$  appear to the left of those in subset  $\vec{I}^2$ . Then, in the previous example,  $\sum_{\vec{I}^1 | \vec{I}^2}$  sums over  $\vec{I}^1 | \vec{I}^2 \in \{(1324), (3124), (1342), (3142)\}$ .

Consequently, we always find  $|\vec{I}^j| = |\vec{I}^j|$  and  $\eta_j \in \vec{I}^j$  for all  $j \in \{1, \dots, \alpha\}$ . In the following, we denote the elements of  $\vec{I}^j$  by  $\vec{I}_i^j$  with  $i \in \{1, \dots, |\vec{I}^j|\}$ .

We further define the *retarded product kernel*

$$\tilde{K}_{\vec{I}^1 | \dots | \vec{I}^{\alpha}} \left( \omega_{\vec{I}^1 | \dots | \vec{I}^{\alpha}}^{[\eta_1 \dots \eta_\alpha]} \right) = \prod_{j=1}^{\alpha-1} \left[ \hat{\delta}(\omega_{\vec{I}^j}) \right] \prod_{j=1}^{\alpha} \left[ \tilde{K} \left( \omega_{\vec{I}^j}^{[\eta_j]} \right) \right] \quad (90a)$$

$$\tilde{K} \left( \omega_{\vec{I}^j} \right) = \prod_{i=1}^{|\vec{I}^j|-1} \frac{1}{\omega_{\vec{I}_i^j \dots \vec{I}_i^j}} \quad (90b)$$

The regular kernel in the last line is defined according to Equation (19d) but restricted to the subtuple of frequencies  $\omega_{\vec{I}^j} = (\omega_{\vec{I}_1^j}, \dots, \omega_{\vec{I}_{|\vec{I}^j}^j})$ . Additionally, we defined the shorthand

$\hat{\delta}(\omega_{\vec{j}}) = -2\pi i \delta(\omega_{\vec{j}})$  and  $\omega_{\vec{j}} = \omega_{\vec{j}} = \sum_{i \in \vec{j}} \omega_i$ . The superscript on  $\omega_{\vec{I}^1 \dots \vec{I}^\alpha}$  indicates that the frequencies carry imaginary parts  $\omega_i + i\gamma_i^{[\eta_j]}$  for  $i \in \vec{I}^j$  and  $j \in \{1, \dots, \alpha\}$ , such that  $\gamma_{\eta_j}^{[\eta_j]} > 0$  and  $\gamma_{i \neq \eta_j}^{[\eta_j]} < 0$ . The Dirac delta function also ensures conservation of imaginary parts,  $\gamma_{\vec{j}} = 0$ .

As an example, consider again  $\ell = 4$  and  $[\eta_1 \eta_2] = [12]$  with  $\vec{I}^1 = \{3, 1\}$  and  $\vec{I}^2 = \{2, 4\}$ . Then, we find

$$\begin{aligned} \tilde{K}_{\vec{I}^1 \vec{I}^2} \left( \omega_{\vec{I}^1 \vec{I}^2}^{[\eta_1][\eta_2]} \right) &= \hat{\delta}(\omega_{\vec{I}^1}) \tilde{K} \left( \omega_{\vec{I}^1}^{[\eta_1]} \right) \tilde{K} \left( \omega_{\vec{I}^2}^{[\eta_2]} \right) \\ &= \hat{\delta}(\omega_{13}) \frac{1}{\omega_3} \frac{1}{\omega_2} \end{aligned} \quad (91)$$

The retarded product kernels, together with PSF (anti)commutators, constitute the central objects for expressing Equations (19) in a form particularly suitable for relating KF components to analytically continued MF correlators.

### 6.2.1. Keldysh Components $G^{[\eta_1 \eta_2]}$

In Equations (42b) and (76), we introduced PSF (anti)commutators for  $\ell = 2$  and  $\ell = 3$ , respectively. We generalize this notation to arbitrary subsets by defining

$$S_{\vec{I}^1 \vec{I}^2}(\epsilon) = S_{\vec{I}^1 \vec{I}^2}(\epsilon_{\vec{I}^1 \vec{I}^2}) \pm S_{\vec{I}^2 \vec{I}^1}(\epsilon_{\vec{I}^2 \vec{I}^1}) \quad (92)$$

where the PSF (anti)commutator takes unpermuted variables  $\epsilon$  as its argument. In Appendix F.2, we then show that Keldysh components with  $\alpha = 2$  can be rewritten as

$$G^{[\eta_1 \eta_2]}(\omega) = \sum_{(I^1, I^2) \in \mathcal{I}^{12}} \sum_{\vec{I}^1 \vec{I}^2} \left( \tilde{K}_{\vec{I}^1 \vec{I}^2} \diamond S_{\vec{I}^1 \vec{I}^2} \right) \left( \omega_{\vec{I}^1 \vec{I}^2}^{[\eta_1][\eta_2]} \right) \quad (93)$$

Here,  $\mathcal{I}^{12} = \{(I^1, I^2) \mid \eta_1 \in I^1, \eta_2 \in I^2, I^1 \cup I^2 = L, I^1 \cap I^2 = \emptyset\}$  is the set of all possibilities to partition  $L = \{1, \dots, \ell\}$  into two non-empty subsets,  $I^1$  and  $I^2$ , such that  $\eta_1 \in I^1$  and  $\eta_2 \in I^2$ . The convolution of a kernel with a PSF (anti)commutator is defined as

$$\begin{aligned} &\left( \tilde{K}_{\vec{I}^1 \vec{I}^2} \diamond S_{\vec{I}^1 \vec{I}^2} \right) \left( \omega_{\vec{I}^1 \vec{I}^2}^{[\eta_1][\eta_2]} \right) \\ &= \int d^\ell \epsilon \delta(\epsilon_{1 \dots \ell}) \tilde{K}_{\vec{I}^1 \vec{I}^2} \left( \omega_{\vec{I}^1 \vec{I}^2}^{[\eta_1][\eta_2]} - \epsilon_{\vec{I}^1 \vec{I}^2} \right) S_{\vec{I}^1 \vec{I}^2}(\epsilon) \end{aligned} \quad (94)$$

Further, as shown in Equation (F10), Equation (93) can be expressed in terms of analytically continued Matsubara correlators,

$$G^{[\eta_1 \eta_2]}(\omega) = \sum_{I^1 \in \mathcal{I}^1} \left[ N_{\omega_{I^1}} \tilde{G}_{\omega^*}^{\omega_{I^1}} + 4\pi i \delta(\omega_{I^1}) \hat{G}_{I^1, \omega^*} \right] \quad (95)$$

with  $\mathcal{I}^1 = \{I^1 \subsetneq L \mid \eta_1 \in I^1, \eta_2 \notin I^1\}$  the set of all subtuples of  $L$  containing  $\eta_1$  but not  $\eta_2$ . The  $\ell - 2$  frequencies in  $\omega^* = \{\omega_i \mid i \neq \eta_1, i \neq \eta_2\}$  all carry negative imaginary shifts, in accordance with the definition of  $\omega^{[\eta_1 \eta_2]}$ . The anomalous part  $\hat{G}_{I^1, \omega^*} = \hat{G}_{I^1}(z(\omega^*))$  for complex  $z$ , which is independent of the anomalous frequency

$\omega_i$  and parametrized via  $\omega^*$ , is defined as

$$\hat{G}_{I^1, \omega^*} = \left[ \hat{G}_{I^1}(i\omega) \right]_{\Delta_{i\omega} \rightarrow \frac{1}{i\omega}, i\omega \rightarrow z(\omega^*)} \quad (96)$$

We first replaced the symbol  $\Delta_{i\omega}$  by  $1/(i\omega)$  to obtain a functional form that we can analytically continue, and then continue it as  $i\omega \rightarrow z(\omega^*)$ . Remarkably, Equation (95) holds for arbitrary  $\ell$ ,  $\eta_1$ , and  $\eta_2$ , and elucidates how anomalous terms enter the Keldysh components with  $\alpha = 2$ . Examples are found in Equation (59) for  $\ell = 2$ , where  $[\eta_1 \eta_2] = [12]$ ,  $\mathcal{I}^1 = \{1\}$ , and  $\omega^*$  is an empty set, or in Equation (79) for  $\ell = 3$ , where  $[\eta_1 \eta_2] = [13]$ ,  $\mathcal{I}^1 = \{1, 12\}$ , and  $\omega^* = \omega_2^-$ .

For  $\ell = 4$ , consider  $[\eta_1 \eta_2] = [12]$ , implying the set  $\mathcal{I}^1 = \{1, 13, 14, 134\}$  and  $\omega^* = \omega_3^-, \omega_4^-$ . Then, Equation (95) directly yields

$$\begin{aligned} G^{[12]}(\omega) &= N_1 \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_1} + N_{13} \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_{13}} + N_{14} \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_{14}} + N_{134} \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_{134}} \\ &\quad + 4\pi i \delta(\omega_{13}) \hat{G}_{13; \omega_3^-, \omega_4^-} + 4\pi i \delta(\omega_{14}) \hat{G}_{14; \omega_3^-, \omega_4^-} \end{aligned} \quad (97)$$

An expression for  $G^{[12]}$  expressed in terms of analytic regions is given in Equation (102). Additionally, a full list of all  $G^{[\eta_1 \eta_2]}$  is provided in Equations (101a)–(101f) (with relations such as  $N_{134} \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_{134}} = -N_2 \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_2} = N_2 \tilde{G}_{\omega_3^-, \omega_4^-}^{\omega_2}$  used).

### 6.2.2. Other Keldysh Components

The derivation of  $G^{[123]} - G^{[3]}$  in Section 5.2.2 can be extended to arbitrary  $\ell$  and  $[\eta_1 \eta_2 \eta_3]$  by keeping track of permutations that are cyclically related, generalizing Equation (81) to (see Appendix F.3 for details)

$$\begin{aligned} &(G^{[\eta_1 \eta_2 \eta_3]} - G^{[\eta_3]})(\omega) \\ &= \sum_{(I^1, I^{23}) \in \mathcal{I}^{123}} \sum_{\vec{I}^1 \vec{I}^{23}} \left[ \tilde{K}_{\vec{I}^1 \vec{I}^{23}} \diamond S_{\vec{I}^1 \vec{I}^{23}} \right] \left( \omega_{\vec{I}^1 \vec{I}^{23}}^{[\eta_1][\eta_2][\eta_3]} \right) \\ &\quad + \sum_{(I^2, I^{13}) \in \mathcal{I}^{213}} \sum_{\vec{I}^2 \vec{I}^{13}} \left[ \tilde{K}_{\vec{I}^2 \vec{I}^{13}} \diamond S_{\vec{I}^2 \vec{I}^{13}} \right] \left( \omega_{\vec{I}^2 \vec{I}^{13}}^{[\eta_2][\eta_1][\eta_3]} \right) \\ &\quad + \sum_{(I^1, I^2, I^3) \in \mathcal{I}^{123}} \sum_{\vec{I}^1 \vec{I}^2 \vec{I}^3} \left[ \tilde{K}_{\vec{I}^1 \vec{I}^2 \vec{I}^3} \diamond S_{\vec{I}^1 \vec{I}^2 \vec{I}^3} \right] \left( \omega_{\vec{I}^1 \vec{I}^2 \vec{I}^3}^{[\eta_1][\eta_2][\eta_3]} \right) \end{aligned} \quad (98)$$

Here,  $\mathcal{I}^{123} = \{(I^1, I^2, I^3) \mid \eta_1 \in I^1, \eta_2 \in I^2, \eta_3 \in I^3, I^j \cap I^{j'} = \emptyset \text{ for } j \neq j'\}$  is the set of all possibilities to partition  $L = \{1, \dots, \ell\}$  into three subsets, each of which contains one of the indices  $\eta_j \in I^j$ . The remaining sets are defined as

$$\mathcal{I}^{123} = \{(I^1, I^{23}) \mid \eta_1 \in I^1, \eta_2, \eta_3 \in I^{23}, I^1 \cap I^{23} = \emptyset\} \quad (99a)$$

$$\mathcal{I}^{213} = \{(I^2, I^{13}) \mid \eta_2 \in I^2, \eta_1, \eta_3 \in I^{13}, I^2 \cap I^{13} = \emptyset\} \quad (99b)$$

Then, Equation (81) provides an example for  $\ell = 3$  and  $[\eta_1 \eta_2 \eta_3] = [123]$ , where  $\mathcal{I}^{123} = \{(1, 23)\}$ ,  $\mathcal{I}^{213} = \{(2, 13)\}$  and  $\mathcal{I}^{123} = \{(1, 2, 3)\}$ .

For  $\ell = 4$ , consider  $[\eta_1 \eta_2 \eta_3] = [123]$ . Compared to the 3p case, the additional index allows for larger sets  $I^{1|23} = \{(1, 234), (14, 23)\}$ ,  $I^{2|13} = \{(2, 134), (24, 13)\}$ , and  $I^{3|12} = \{(1, 2, 34), (1, 24, 3), (14, 2, 3)\}$ , resulting in (suppressing the frequency arguments of PSF (anti)commutators)

$$\begin{aligned} (G^{[123]} - G^{[3]}) (\boldsymbol{\omega}) &= \tilde{G}_{\omega_2^- \omega_4^-}^{\omega_1} + \tilde{G}_{\omega_2^- \omega_4^-}^{\omega_2} + \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_2} + \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_{24}} \\ &+ \int_{\varepsilon_1 \varepsilon_2 \varepsilon_3} \left[ \hat{\delta}(\omega_1 - \varepsilon_1) \hat{\delta}(\omega_2 - \varepsilon_2) \frac{(2\pi i)^3}{\omega_3^+ - \varepsilon_3} S_{[[1,2]_+, [3,4]_-]_+} \right. \\ &+ \hat{\delta}(\omega_1 - \varepsilon_1) \hat{\delta}(\omega_3 - \varepsilon_3) \frac{(2\pi i)^3}{\omega_2^+ - \varepsilon_2} S_{[[1, [2,4]_-]_+, 3]_+} \\ &\left. + \hat{\delta}(\omega_2 - \varepsilon_2) \hat{\delta}(\omega_3 - \varepsilon_3) \frac{(2\pi i)^3}{\omega_1^+ - \varepsilon_1} S_{[[1, [4]_-]_+, 2]_+, 3]_+} \right] \quad (100) \end{aligned}$$

Here, we identified the terms in the first line of Equation (98) with discontinuities (see Appendix E.1). After inserting the PSFs (see Equations (F15)) and performing the remaining integrations using Cauchy's integral formula, we obtain Equation (101g).

For  $\alpha \geq 4$ , expressing the spectral representation of  $G^{[\eta_1 \dots \eta_\alpha]}$  in terms of retarded product kernels and PSF (anti)commutators becomes increasingly challenging. Nevertheless, we provide a formula for  $G^{[1234]}$  and  $\ell = 4$  in Equation (F16), with a list of all relevant PSF (anti)commutators given in Equation (F17). Equation (101k) then displays the result after evaluating all convolution integrals.

### 6.2.3. Overview of Keldysh Components

To summarize the results of the previous sections, we give an overview of all Keldysh components with  $\alpha > 1$ :

$$G^{[12]} (\boldsymbol{\omega}) = N_1 \tilde{G}_{\omega_3^- \omega_4^-}^{\omega_1} + N_2 \tilde{G}_{\omega_3^- \omega_4^-}^{\omega_2} + N_{13} \tilde{G}_{\omega_3^- \omega_4^-}^{\omega_{13}} + N_{14} \tilde{G}_{\omega_3^- \omega_4^-}^{\omega_{14}} + 4\pi i \delta(\omega_{13}) \hat{G}_{13; \omega_3^- \omega_4^-} + 4\pi i \delta(\omega_{14}) \hat{G}_{14; \omega_3^- \omega_4^-} \quad (101a)$$

$$G^{[34]} (\boldsymbol{\omega}) = N_3 \tilde{G}_{\omega_1^- \omega_2^-}^{\omega_3} + N_{13} \tilde{G}_{\omega_1^- \omega_2^-}^{\omega_{13}} + N_{14} \tilde{G}_{\omega_1^- \omega_2^-}^{\omega_{14}} + N_4 \tilde{G}_{\omega_1^- \omega_2^-}^{\omega_4} + 4\pi i \delta(\omega_{13}) \hat{G}_{13; \omega_1^- \omega_2^-} + 4\pi i \delta(\omega_{14}) \hat{G}_{14; \omega_1^- \omega_2^-} \quad (101b)$$

$$G^{[13]} (\boldsymbol{\omega}) = N_1 \tilde{G}_{\omega_2^- \omega_4^-}^{\omega_1} + N_{12} \tilde{G}_{\omega_2^- \omega_4^-}^{\omega_{12}} + N_{14} \tilde{G}_{\omega_2^- \omega_4^-}^{\omega_{14}} + N_3 \tilde{G}_{\omega_2^- \omega_4^-}^{\omega_3} + 4\pi i \delta(\omega_{12}) \hat{G}_{12; \omega_2^- \omega_4^-} + 4\pi i \delta(\omega_{14}) \hat{G}_{14; \omega_2^- \omega_4^-} \quad (101c)$$

$$G^{[24]} (\boldsymbol{\omega}) = N_2 \tilde{G}_{\omega_1^- \omega_3^-}^{\omega_2} + N_{12} \tilde{G}_{\omega_1^- \omega_3^-}^{\omega_{12}} + N_{14} \tilde{G}_{\omega_1^- \omega_3^-}^{\omega_{14}} + N_4 \tilde{G}_{\omega_1^- \omega_3^-}^{\omega_4} + 4\pi i \delta(\omega_{12}) \hat{G}_{12; \omega_1^- \omega_3^-} + 4\pi i \delta(\omega_{14}) \hat{G}_{14; \omega_1^- \omega_3^-} \quad (101d)$$

$$G^{[14]} (\boldsymbol{\omega}) = N_1 \tilde{G}_{\omega_2^- \omega_3^-}^{\omega_1} + N_{12} \tilde{G}_{\omega_2^- \omega_3^-}^{\omega_{12}} + N_{13} \tilde{G}_{\omega_2^- \omega_3^-}^{\omega_{13}} + N_4 \tilde{G}_{\omega_2^- \omega_3^-}^{\omega_4} + 4\pi i \delta(\omega_{12}) \hat{G}_{12; \omega_2^- \omega_3^-} + 4\pi i \delta(\omega_{13}) \hat{G}_{13; \omega_2^- \omega_3^-} \quad (101e)$$

$$G^{[23]} (\boldsymbol{\omega}) = N_2 \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_2} + N_{12} \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_{12}} + N_{13} \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_{13}} + N_3 \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_3} + 4\pi i \delta(\omega_{12}) \hat{G}_{12; \omega_1^- \omega_4^-} + 4\pi i \delta(\omega_{13}) \hat{G}_{13; \omega_1^- \omega_4^-} \quad (101f)$$

$$\begin{aligned} (G^{[123]} - G^{[3]}) (\boldsymbol{\omega}) &= (N_1 N_2 + 1) \tilde{G}_{\omega_3^+}^{\omega_2, \omega_1} + N_1 N_{12} \tilde{G}_{\omega_3^+}^{\omega_{12}, \omega_1} + N_1 N_3 \tilde{G}_{\omega_3^+}^{\omega_3, \omega_1} + (N_1 N_{13} - 1) \tilde{G}_{\omega_2^+}^{\omega_{13}, \omega_1} + N_2 N_3 \tilde{G}_{\omega_1^+}^{\omega_3, \omega_2} + (N_2 N_{23} - 1) \tilde{G}_{\omega_1^+}^{\omega_{23}, \omega_2} \\ &+ \tilde{G}_{\omega_2^- \omega_3^+}^{\omega_1} - \tilde{G}_{\omega_1^+ \omega_2^-}^{\omega_{23}} + \tilde{G}_{\omega_1^- \omega_3^+}^{\omega_2} - \tilde{G}_{\omega_2^+ \omega_1^-}^{\omega_{13}} + 4\pi i \delta(\omega_{12}) N_1 \hat{G}_{12; \omega_3^+}^{\omega_1} + 4\pi i \delta(\omega_{13}) N_1 \hat{G}_{13; \omega_2^+}^{\omega_1} + 4\pi i \delta(\omega_{14}) N_2 \hat{G}_{14; \omega_1^+}^{\omega_2} \quad (101g) \end{aligned}$$

$$\begin{aligned} (G^{[124]} - G^{[4]}) (\boldsymbol{\omega}) &= (N_1 N_2 + 1) \tilde{G}_{\omega_4^+}^{\omega_2, \omega_1} + N_1 N_{12} \tilde{G}_{\omega_4^+}^{\omega_{12}, \omega_1} + N_1 N_4 \tilde{G}_{\omega_4^+}^{\omega_4, \omega_1} + (N_1 N_{14} - 1) \tilde{G}_{\omega_2^+}^{\omega_{14}, \omega_1} + N_2 N_4 \tilde{G}_{\omega_1^+}^{\omega_4, \omega_2} + (N_2 N_{24} - 1) \tilde{G}_{\omega_1^+}^{\omega_{24}, \omega_2} \\ &+ \tilde{G}_{\omega_2^- \omega_4^+}^{\omega_1} - \tilde{G}_{\omega_1^+ \omega_2^-}^{\omega_{24}} + \tilde{G}_{\omega_1^- \omega_4^+}^{\omega_2} - \tilde{G}_{\omega_2^+ \omega_1^-}^{\omega_{14}} + 4\pi i \delta(\omega_{12}) N_1 \hat{G}_{12; \omega_4^+}^{\omega_1} + 4\pi i \delta(\omega_{13}) N_2 \hat{G}_{13; \omega_1^+}^{\omega_2} + 4\pi i \delta(\omega_{14}) N_1 \hat{G}_{14; \omega_2^+}^{\omega_1} \quad (101h) \end{aligned}$$

$$\begin{aligned} (G^{[134]} - G^{[4]}) (\boldsymbol{\omega}) &= (N_1 N_3 + 1) \tilde{G}_{\omega_4^+}^{\omega_3, \omega_1} + N_1 N_{13} \tilde{G}_{\omega_4^+}^{\omega_{13}, \omega_1} + N_1 N_4 \tilde{G}_{\omega_4^+}^{\omega_4, \omega_1} + (N_1 N_{14} - 1) \tilde{G}_{\omega_3^+}^{\omega_{14}, \omega_1} + N_3 N_4 \tilde{G}_{\omega_1^+}^{\omega_4, \omega_3} + (N_3 N_{34} - 1) \tilde{G}_{\omega_1^+}^{\omega_{34}, \omega_3} \\ &+ \tilde{G}_{\omega_3^- \omega_4^+}^{\omega_1} - \tilde{G}_{\omega_1^+ \omega_3^-}^{\omega_{34}} + \tilde{G}_{\omega_1^- \omega_4^+}^{\omega_3} - \tilde{G}_{\omega_3^+ \omega_1^-}^{\omega_{14}} + 4\pi i \delta(\omega_{12}) N_3 \hat{G}_{12; \omega_4^+}^{\omega_1} + 4\pi i \delta(\omega_{13}) N_1 \hat{G}_{13; \omega_4^+}^{\omega_1} + 4\pi i \delta(\omega_{14}) N_1 \hat{G}_{14; \omega_3^+}^{\omega_1} \quad (101i) \end{aligned}$$

$$\begin{aligned} (G^{[234]} - G^{[4]}) (\boldsymbol{\omega}) &= (N_2 N_3 + 1) \tilde{G}_{\omega_4^+}^{\omega_3, \omega_2} + N_2 N_{23} \tilde{G}_{\omega_4^+}^{\omega_{23}, \omega_2} + N_2 N_4 \tilde{G}_{\omega_4^+}^{\omega_4, \omega_2} + (N_2 N_{24} - 1) \tilde{G}_{\omega_3^+}^{\omega_{24}, \omega_2} + N_3 N_4 \tilde{G}_{\omega_2^+}^{\omega_4, \omega_3} + (N_3 N_{34} - 1) \tilde{G}_{\omega_2^+}^{\omega_{34}, \omega_3} \\ &+ \tilde{G}_{\omega_3^- \omega_4^+}^{\omega_2} - \tilde{G}_{\omega_2^+ \omega_3^-}^{\omega_{34}} + \tilde{G}_{\omega_2^- \omega_4^+}^{\omega_3} - \tilde{G}_{\omega_3^+ \omega_2^-}^{\omega_{24}} + 4\pi i \delta(\omega_{12}) N_3 \hat{G}_{12; \omega_4^+}^{\omega_3} + 4\pi i \delta(\omega_{13}) N_2 \hat{G}_{13; \omega_3^+}^{\omega_2} + 4\pi i \delta(\omega_{14}) N_2 \hat{G}_{14; \omega_4^+}^{\omega_2} \quad (101j) \end{aligned}$$

$$\begin{aligned} G^{[1234]} (\boldsymbol{\omega}) &= N_1 \tilde{G}_{\omega_2^- \omega_3^-}^{\omega_1} + N_2 \tilde{G}_{\omega_3^- \omega_4^-}^{\omega_2} + N_3 \tilde{G}_{\omega_1^- \omega_4^-}^{\omega_3} + N_4 \tilde{G}_{\omega_1^- \omega_2^-}^{\omega_4} + N_3 \tilde{G}_{\omega_2^+}^{\omega_3, \omega_4} + N_2 \tilde{G}_{\omega_1^+}^{\omega_2, \omega_3} + N_4 \tilde{G}_{\omega_3^+}^{\omega_4, \omega_1} + N_1 \tilde{G}_{\omega_4^+}^{\omega_1, \omega_2} + N_2 \tilde{G}_{\omega_3^+}^{\omega_2, \omega_4} \\ &+ N_4 \tilde{G}_{\omega_3^+}^{\omega_4, \omega_2} + N_1 \tilde{G}_{\omega_4^+}^{\omega_1, \omega_3} + N_3 \tilde{G}_{\omega_4^+}^{\omega_3, \omega_1} + (N_1 N_2 N_3 + N_1 + N_3) \tilde{G}_{\omega_4^+}^{\omega_3, \omega_2, \omega_1} + (N_1 N_2 N_4 + N_4 + N_2) \tilde{G}_{\omega_4^+}^{\omega_4, \omega_2, \omega_1} \\ &+ (N_1 N_2 N_{13} + N_1 - N_2) \tilde{G}_{\omega_3^+}^{\omega_{13}, \omega_2, \omega_1} + (N_1 N_2 N_{23}) \tilde{G}_{\omega_3^+}^{\omega_{23}, \omega_2, \omega_1} + N_1 (1 + N_{12} N_3) \tilde{G}_{\omega_3^+}^{\omega_3, \omega_{12}, \omega_1} + N_1 N_{12} N_4 \tilde{G}_{\omega_3^+}^{\omega_4, \omega_2, \omega_1} \\ &+ 4\pi i N_1 N_3 \delta(\omega_{12}) \hat{G}_{12}^{\omega_1, \omega_3} + 4\pi i N_1 N_2 \left[ \delta(\omega_{13}) \hat{G}_{13}^{\omega_1, \omega_2} + \delta(\omega_{13}) \hat{G}_{14}^{\omega_1, \omega_2} \right] \quad (101k) \end{aligned}$$

These equations constitute the main results of the MF-to-KF analytic continuation: They relate all components of a fermionic KF 4p correlator to linear combinations of analytically continued regular and anomalous parts of the corresponding MF correlator, expressed in terms of discontinuities and statistical factors  $N_i$ .

#### 6.2.4. 4p gFDRs

For 4p correlators, there are several regions of analyticity that cannot be identified with a KF correlator. Therefore, in contrast to  $\ell \leq 3$ , fully retarded and advanced Keldysh components do not suffice to determine all other Keldysh components. Nevertheless, different Keldysh components can be related to each other. We now present the strategy for deriving these gFDRs for the Keldysh component  $G^{[12]}$ .

Since every Keldysh component can be represented as a linear combination of analytically continued MF correlators, the analytic regions can serve as a basis to find relations among different Keldysh components. Expressing the discontinuities in Equation (101a) via analytic regions, the KF correlator  $G^{[12]}$  reads

$$G^{[12]} = N_1 \left( C_{\text{III}}^{(12)} - G^{[2]} \right) + N_{13} \left( C_{\text{II}}^{(12)} - C_{\text{III}}^{(12)} \right) + N_{14} \left( C_{\text{IV}}^{(12)} - C_{\text{III}}^{(12)} \right) + N_2 \left( C_1^{(12)} - G^{[1]} \right) + 4\pi i \delta(\omega_{13}) \hat{C}_{13}^{(12)} + 4\pi i \delta(\omega_{14}) \hat{C}_{14}^{(12)} \quad (102)$$

where we inserted  $G^{[1]} = C^{(1)}$  and  $G^{[2]} = C^{(2)}$ . Evidently,  $G^{[12]}$  cannot be expressed in terms of fully retarded and advanced components only (modulo anomalous terms) due to the occurrence of  $C_{\text{I/III/IV}}^{(12)}$ . However, these analytic regions and the same anomalous contributions appear in the primed KF correlator  $G'^{[34]}$  as well:

$$G'^{[34]} = N_3 \left( C_{\text{II}}^{(12)} - G'^{[4]} \right) + N_{13} \left( C_{\text{III}}^{(12)} - C_{\text{II}}^{(12)} \right) + N_{14} \left( C_{\text{IV}}^{(12)} - C_{\text{III}}^{(12)} \right) + N_4 \left( C_{\text{IV}}^{(12)} - G'^{[3]} \right) - 4\pi i \delta(\omega_{13}) \hat{C}_{13}^{(12)} - 4\pi i \delta(\omega_{14}) \hat{C}_{14}^{(12)} \quad (103)$$

Note that priming the  $i\delta(\dots)$  factors amounts to complex conjugation, as these arise from the identity (58), i.e.,  $[i\delta(\dots)]' = -i\delta(\dots)$ . Therefore, we make the ansatz of expressing  $G^{[12]}$  as a linear combination of  $G'^{[34]}$ ,  $G^{[1]}$ ,  $G^{[2]}$ ,  $G'^{[3]}$ , and  $G'^{[4]}$ , where the coefficients are determined by comparing terms proportional to the same analytic regions. Even though the resulting set of equations is overdetermined (including anomalous contributions, we have ten equations for five coefficients), we find the gFDR

$$G^{[12]} = -N_1 G^{[2]} - N_2 G^{[1]} + \frac{N_1 + N_2}{N_3 + N_4} \left[ G'^{[34]} + N_3 G'^{[4]} + N_4 G'^{[3]} \right] \quad (104a)$$

The anomalous terms enter the right-hand side only implicitly via  $G'^{[34]}$ . However, using  $\frac{N_1 + N_2}{N_3 + N_4} \delta(\omega_{13}) = -\delta(\omega_{13})$  and  $\frac{N_1 + N_2}{N_3 + N_4} \delta(\omega_{14}) =$

$-\delta(\omega_{14})$ , it is straightforward to show that the  $\hat{C}_{13}^{(12)}$  and  $\hat{C}_{14}^{(12)}$  contributions in the last line of Equation (102) are recovered by the corresponding terms in Equation (103) via Equation (104a). Conversely, the gFDR for  $G^{[34]}$  can be derived from Equation (104a) by solving for  $G'^{[34]}$  and priming all correlators.

The gFDRs for all other Keldysh components with  $\alpha \geq 2$  follow from the same strategy: Express Keldysh components in terms of linearly independent analytic regions and find relations between different components by solving a set of equations to determine coefficients. In addition to Equation (104a), we then obtain for  $\alpha = 2$

$$G^{[13]} = -N_1 G^{[3]} - N_3 G^{[1]} + \frac{N_1 + N_3}{N_2 + N_4} \left[ G'^{[24]} + N_2 G'^{[4]} + N_4 G'^{[2]} \right] \quad (104b)$$

$$G^{[14]} = -N_1 G^{[4]} - N_4 G^{[1]} + \frac{N_1 + N_4}{N_2 + N_3} \left[ G'^{[23]} + N_2 G'^{[3]} + N_3 G'^{[2]} \right] \quad (104c)$$

for  $\alpha = 3$

$$G^{[234]} = (1 + N_2 N_4 + N_2 N_3 + N_3 N_4) G'^{[1]} - N_3 N_4 G^{[2]} - N_2 N_4 G^{[3]} - N_2 N_3 G^{[4]} - N_4 G^{[23]} - N_3 G^{[24]} - N_2 G^{[34]} \quad (104d)$$

$$G^{[134]} = (1 + N_1 N_4 + N_1 N_3 + N_3 N_4) G'^{[2]} - N_3 N_4 G^{[1]} - N_1 N_4 G^{[3]} - N_1 N_3 G^{[4]} - N_4 G^{[13]} - N_3 G^{[14]} - N_1 G^{[34]} \quad (104e)$$

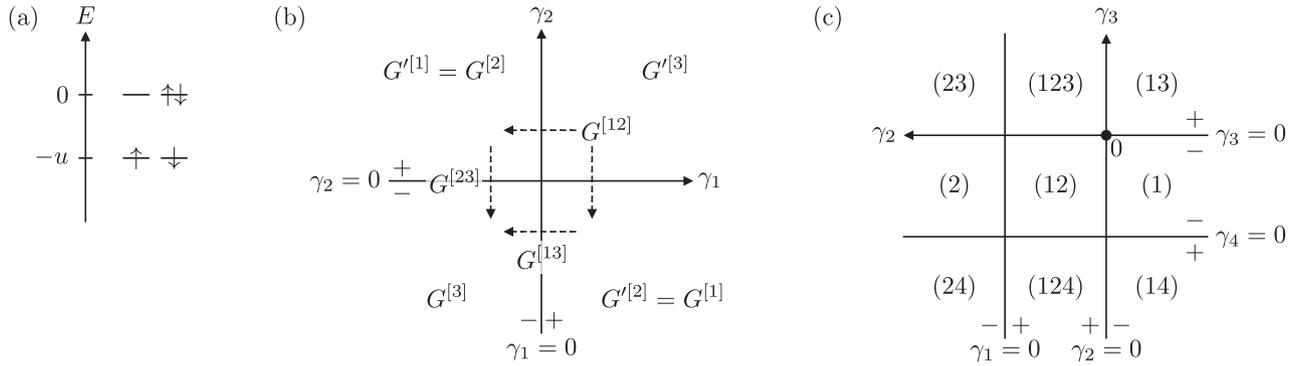
$$G^{[124]} = (1 + N_1 N_2 + N_1 N_3 + N_2 N_4) G'^{[3]} - N_2 N_4 G^{[1]} - N_1 N_4 G^{[2]} - N_1 N_2 G^{[4]} - N_4 G^{[12]} - N_2 G^{[14]} - N_1 G^{[24]} \quad (104f)$$

$$G^{[123]} = (1 + N_1 N_2 + N_1 N_3 + N_2 N_3) G'^{[4]} - N_2 N_3 G^{[1]} - N_1 N_3 G^{[2]} - N_1 N_2 G^{[3]} - N_1 G^{[23]} - N_2 G^{[13]} - N_3 G^{[12]} \quad (104g)$$

and for  $\alpha = 4$

$$G^{[1234]} = 2N_2 N_3 N_4 G^{[1]} + (N_2 N_3 N_4 + N_2 + N_3 + N_4) G'^{[1]} + 2N_1 N_3 N_4 G^{[2]} + (N_1 N_3 N_4 + N_1 + N_3 + N_4) G'^{[2]} + 2N_1 N_2 N_4 G^{[3]} + (N_1 N_2 N_4 + N_1 + N_2 + N_4) G'^{[3]} + 2N_2 N_3 N_4 G^{[4]} + (N_1 N_2 N_3 + N_1 + N_2 + N_3) G'^{[4]} + N_3 N_4 G^{[12]} + N_2 N_4 G^{[13]} + N_2 N_3 G^{[14]} + N_1 N_4 G^{[23]} + N_1 N_3 G^{[24]} + N_1 N_2 G^{[34]} \quad (104h)$$

These results agree with the FDRs found in ref. [24], and therefore provide a consistency check for our approach. Moreover, we checked that the anomalous parts fulfill the same gFDRs. They enter Equations (104) only implicitly through  $G^{[n_1 n_2]}$  and  $G'^{[n_1 n_2]}$  on the right-hand sides, which contain anomalous parts via Equations (101a)–(101f). This is in contrast to the 2p and 3p cases in Equations (61) and (84), respectively. There, only fully retarded and advanced Keldysh correlators, which solely depend on the



**Figure 6.** a) Degenerate energy levels of the half-filled Hubbard atom for  $u > 0$ . b) Relevant analytic regions of the regular part of the 3p electron-density correlator in Equation (113). As the correlator is independent of  $i\omega_3 = -i\omega_2$ , there are no poles on the line  $\gamma_3 = 0$  in Figure 4, resulting in  $G^{[1]} = G^{[2]}$  and  $G'^{[2]} = G^{[1]}$ . The dashed arrows indicate the relevant discontinuities for the different Keldysh components with  $\alpha = 2$ , see Equation (84). c) Reduced analytic regions of the regular part of the fermionic 4p correlator in Equation (119). The regions labeled by (3), (4), (34), (134), and (234) in Figure 5 are missing.

regular part  $\tilde{G}$  of the corresponding MF correlator (see Equation (23)), occur on the right-hand side, and thus the anomalous parts have to enter the gFDRs explicitly.

## 7. Hubbard Atom

To illustrate the use of our analytic continuation formulas, we consider the Hubbard atom (HA) with the Hamiltonian

$$H = Un_{\uparrow}n_{\downarrow} - \mu(n_{\uparrow} + n_{\downarrow}) \quad (105)$$

It describes an interacting system of spin- $\frac{1}{2}$  electrons on a single site, created by  $d_{\sigma}^{\dagger}$ , with  $n_{\sigma} = d_{\sigma}^{\dagger}d_{\sigma}$  the number operator for spin  $\sigma \in \{\uparrow, \downarrow\}$ . The chemical potential  $\mu$  is set to the half-filling value  $\mu = u = U/2$  for compact results, where  $U$  is the interaction parameter. The Hilbert space of the HA is only four-dimensional, with the site being either unoccupied,  $|0\rangle$ , singly occupied,  $|\uparrow\rangle$  or  $|\downarrow\rangle$ , or doubly occupied,  $|\uparrow\downarrow\rangle$ . The eigenenergies are (see Figure 6a)

$$E_0 = E_{\uparrow\downarrow} = 0, \quad E_{\uparrow} = E_{\downarrow} = -u \quad (106)$$

The partition sum evaluates to  $Z = \text{tr}(e^{-\beta H}) = 2 + 2e^{\beta u}$ .

This very simple model is interesting as it is accessible via analytically exact computations. It describes the Hubbard model and the single-impurity Anderson model in the atomic limit (where the interaction  $U$  dominates over all other energy scales) and can thus serve as a benchmark for numerical methods.<sup>[23,33–35]</sup> Several correlators of the Hubbard atom were computed in the MF and studied extensively, like fermionic 2p (one-particle) and 4p (two-particle) correlators.<sup>[36–40]</sup> Also its 3p MF functions have been computed and applied in previous works.<sup>[41–43]</sup> The vertex of the Hubbard atom, obtained from the fermionic 4p correlator by dividing out external legs, was used as a starting point for an expansion around strong coupling.<sup>[37,38,44,45]</sup> Additionally, it was found that (despite the simplicity of the model) the two-particle irreducible (2PI) vertices display a complicated frequency dependence, and their divergencies are subject to ongoing research.<sup>[46–49]</sup> Such divergencies have been related

to the breakdown of the perturbative expansion due to the multivaluedness of the Luttinger–Ward functional<sup>[46,50–52]</sup> and to the local moment formation in generalized susceptibilities.<sup>[53,54]</sup>

2p and 3p bosonic correlators have gained interest in recent years as well. They describe not only the asymptotic behaviour of the 4p vertex for large frequencies<sup>[40]</sup> or the interaction of electrons via the exchange of effective bosons,<sup>[55,56]</sup> but they are also the central objects of linear and non-linear response theory.<sup>[57,58]</sup>

KF correlators for the HA (beyond  $\ell = 2$ ) were of smaller interest due to the lack of numerical real-frequency studies. However, substantial progress has been made in this direction.<sup>[23,29,59–61]</sup> Hence, we exemplify the analytic continuation from MF to KF correlators on the example of the HA for various correlators of interest.

One further comment is in order: The following MF correlators are derived by first computing the PSFs, followed by a convolution with the MF kernels. From our experience, a direct insertion of these PSFs into the spectral representation of KF correlators yields cluttered expressions, cumbersome to simplify due to the infinitesimal imaginary shifts  $\gamma_0$ . With the analytic continuation formulas, on the other hand, terms are conveniently preorganized, collecting those contributions with the same imaginary shifts. Additionally, the discontinuities conveniently yield Dirac delta contributions, as we will show below. In order to derive, e.g., our first results for the 4p correlator, Equations (H18), it is much more convenient to start from the analytic continuation formulas, Equations (101), than from the original KF Equation (19).

For a compact presentation of our results, we distinguish different correlators with operators in subscripts, e.g.,  $G[O^1, O^2](i\omega) = G_{O^1 O^2}(i\omega)$ . Furthermore, we will make use of the identities (proven in Appendix H.1)

$$\frac{\omega^+}{(\omega^+)^2 - u^2} - \frac{\omega^-}{(\omega^-)^2 - u^2} = \frac{\pi}{i} [\delta(\omega + u) + \delta(\omega - u)] \quad (107a)$$

$$\frac{1}{(\omega^+)^2 - u^2} - \frac{1}{(\omega^-)^2 - u^2} = \frac{\pi i}{u} [\delta(\omega + u) - \delta(\omega - u)] \quad (107b)$$

All following correlators refer to the connected part.

## 7.1. Examples for $\ell = 2$

### 7.1.1. Fermionic 2p Correlator

To begin with, we consider the fermionic 2p correlator (propagator), with  $\mathbf{O} = (d_1, d_1^\dagger)$ . By  $SU(2)$  spin symmetry, reversing all spins leaves the correlator invariant. As the nonzero matrix elements are  $\langle \uparrow | d_1^\dagger | 0 \rangle = \langle \uparrow \downarrow | d_1^\dagger | \downarrow \rangle = 1$  and  $\langle 0 | d_1 | \uparrow \rangle = \langle \downarrow | d_1 | \uparrow \downarrow \rangle = 1$ , we can readily compute the PSFs,  $S_p$ , via Equation (22b) in ref. [23]. Evaluating the spectral representation yields

$$G_{d_1, d_1^\dagger}(i\omega) = \frac{i\omega}{(i\omega)^2 - u^2} = \tilde{G}(i\omega) \quad (108)$$

By construction, there is no anomalous part  $\hat{G}_1 = 0$ . The retarded and advanced component are directly obtained from Equation (54):

$$G_{d_1, d_1^\dagger}^{[1/2]}(\omega) = \frac{\omega^\pm}{(\omega^\pm)^2 - u^2} \quad (109)$$

The Keldysh component involves the difference of the retarded and advanced component. Via Equation (107a), one gets

$$G_{d_1, d_1^\dagger}^{[12]}(\omega) = \pi i t [\delta(\omega + u) - \delta(\omega - u)] \quad (110)$$

where we used  $N_{-\omega} = -N_\omega$  and defined  $t = \tanh(\beta u/2)$ .

### 7.1.2. Density–Density Correlator

Our second example is the density–density correlator  $\mathbf{O} = (n_-, n_+)$ . The spectral representation in the MF yields a purely anomalous result

$$G_{n_-, n_+}(i\omega) = \beta \delta_{i\omega, \frac{1}{4}} t = \beta \delta_{i\omega} \hat{G}_1 \quad (111)$$

The correlator  $G_{n_-, n_+}$  discussed above describes the linear response of the spin-up occupation to a shift of the spin-down energy level, which lifts the degeneracy of the singly-occupied energy levels in Figure 6a. For decreasing temperatures, the system becomes increasingly susceptible to such perturbations. This is reflected by the  $\beta = 1/T$  divergence for  $T \rightarrow 0$  in the MF correlator of Equation (111), and the  $\delta(\omega)$  behavior in Equation (112) for its Keldysh counterpart.

Using Equations (54) and (61), the Keldysh components read

$$\begin{aligned} G_{n_-, n_+}^{[1]}(\omega) &= G_{n_+, n_-}^{[2]}(\omega) = 0, \\ G_{n_-, n_+}^{[12]}(\omega) &= 4\pi i \delta(\omega) \frac{1}{4} t \end{aligned} \quad (112)$$

We again emphasize the importance of the anomalous term in the gFDR. If it were discarded, the Keldysh component  $G_{n_-, n_+}^{[12]}$  would falsely vanish entirely.

## 7.2. Examples for $\ell = 3$

### 7.2.1. 3p Electron-Density Correlator

Our first example for  $\ell = 3$  involves the operators  $\mathbf{O} = (d_1, d_1^\dagger, n_1)$ . As only the third operator is bosonic, there is at most one anomalous term if  $i\omega_3 = -i\omega_{12} = 0$ . Indeed, the spectral representation evaluates to

ous term if  $i\omega_3 = -i\omega_{12} = 0$ . Indeed, the spectral representation evaluates to

$$\begin{aligned} G_{d_1, d_1^\dagger, n_1}(i\omega) &= \frac{u^2 - i\omega_1 i\omega_2}{[(i\omega_1)^2 - u^2][(i\omega_2)^2 - u^2]} + \beta \delta_{i\omega_{12}, 0} \frac{u t}{2} \frac{1}{(i\omega_1)^2 - u^2} \\ &= \tilde{G}(i\omega) + \beta \delta_{i\omega_{12}} \hat{G}_3(i\omega_1). \end{aligned} \quad (113)$$

Since the fully retarded and fully advanced components of the correlator trivially follow from the regular part, we focus on the  $\alpha \geq 2$  components in the following. We begin with the Keldysh component  $G^{[13]}$  in Equation (84b): The regular part is independent of  $i\omega_3 = -i\omega_{12}$ , such that the discontinuity across  $\gamma_3 = -\gamma_{12} = 0$  vanishes, implying  $G^{[2]} - G^{[1]} = 0$  (see Figure 6b). The discontinuity  $G^{[2]} - G^{[3]}$ , on the other hand, is nonzero and can be easily evaluated using Equations (107), leading to (see Appendix H.2)

$$\begin{aligned} G_{d_1, d_1^\dagger, n_1}^{[13]}(\omega) &= N_1 (\tilde{G}(\omega_1^+, \omega_2^-) - \tilde{G}(\omega_1^-, \omega_2^-)) + 4\pi i \delta(\omega_{12}) \hat{G}_3(\omega_1^+) \\ &= \pi i t \left[ \frac{\delta(\omega_1 - u)}{\omega_2^- + u} - \frac{\delta(\omega_1 + u)}{\omega_2^- - u} \right] \\ &\quad + 4\pi i \delta(\omega_{12}) \frac{u t}{2} \frac{1}{(\omega_1^+)^2 - u^2} \end{aligned} \quad (114)$$

Similarly, the remaining components with  $\alpha = 2$ , as well as the Keldysh component with  $\alpha = 3$ , read

$$\begin{aligned} G_{d_1, d_1^\dagger, n_1}^{[23]}(\omega) &= \pi i t \left[ \frac{\delta(\omega_2 - u)}{\omega_1^- + u} - \frac{\delta(\omega_2 + u)}{\omega_1^- - u} \right] \\ &\quad + 4\pi i \delta(\omega_{12}) \frac{u t}{2} \frac{1}{(\omega_1^-)^2 - u^2}, \\ G_{d_1, d_1^\dagger, n_1}^{[12]}(\omega) &= \pi i t \left[ \frac{\delta(\omega_1 - u)}{\omega_2^+ + u} - \frac{\delta(\omega_1 + u)}{\omega_2^+ - u} \right] \\ &\quad + \pi i t \left[ \frac{\delta(\omega_2 - u)}{\omega_1^+ + u} - \frac{\delta(\omega_2 + u)}{\omega_1^+ - u} \right], \\ G_{d_1, d_1^\dagger, n_1}^{[123]}(\omega) &= \frac{u^2 - \omega_1^+ \omega_2^+}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]} \end{aligned} \quad (115)$$

Here,  $G_{d_1, d_1^\dagger, n_1}^{[12]}$  includes two discontinuities across  $\gamma_1 = 0$  and  $\gamma_2 = 0$ , but no contribution from  $\hat{G}_3$ , leading to the different structure compared to the other two Keldysh components with  $\alpha = 2$ . Surprisingly,  $G_{d_1, d_1^\dagger, n_1}^{[123]}$  is directly determined by  $G^{[3]}$ . All other contributions from regular and anomalous parts mutually cancel, see Appendix H.2.

### 7.2.2. Three-Spin Correlator

3p bosonic correlators are the central objects in non-linear response theory. Here, we consider the correlator for the spin operators  $\mathbf{O} = (S_x, S_y, S_z)$ , describing second-order changes in the magnetization by applying an external magnetic field. The spin

operators are given by

$$S_x = \frac{1}{2} (d_1^\dagger d_1 + d_1^\dagger d_1), \quad S_y = -\frac{i}{2} (d_1^\dagger d_1 - d_1^\dagger d_1),$$

$$S_z = \frac{1}{2} (n_1 - n_1) \quad (116)$$

The spectral representation, using the MF kernel in Equation (A4b), then yields

$$G_{S_x S_y S_z}(\mathbf{i}\omega) = -\beta \delta_{i\omega_1} \tilde{Z} \Delta_{i\omega_2} + \beta \delta_{i\omega_2} \tilde{Z} \Delta_{i\omega_1} - \beta \delta_{i\omega_2} \tilde{Z} \Delta_{i\omega_1}$$

$$= \beta \delta_{i\omega_1} \hat{G}_1^\Delta(i\omega_2) + \beta \delta_{i\omega_2} \hat{G}_2^\Delta(i\omega_1) + \beta \delta_{i\omega_3} \hat{G}_3^\Delta(i\omega_1) \quad (117)$$

where  $\tilde{Z} = ie^{\beta u} / (2Z)$ .

From Equations (84a)–(84d), we deduce the only nonzero Keldysh components as

$$G_{S_x S_y S_z}^{[12]}(\omega) = -4\pi i \delta(\omega_1) \frac{\tilde{Z}}{\omega_2^+} + 4\pi i \delta(\omega_2) \frac{\tilde{Z}}{\omega_1^+},$$

$$G_{S_x S_y S_z}^{[13]}(\omega) = -4\pi i \delta(\omega_1) \frac{\tilde{Z}}{\omega_2^-} - 4\pi i \delta(\omega_2) \frac{\tilde{Z}}{\omega_1^-}, \quad (118)$$

$$G_{S_x S_y S_z}^{[23]}(\omega) = 4\pi i \delta(\omega_1) \frac{\tilde{Z}}{\omega_1^-} - 4\pi i \delta(\omega_2) \frac{\tilde{Z}}{\omega_1^-}$$

Even though anomalous parts contribute to  $G^{[123]}$  as well, they solely originate from the  $\hat{G}_i^{\Delta}$  terms, such that  $G^{[123]}$  vanishes in this case.

### 7.3. Example for $\ell = 4$ : Fermionic 4p Correlator

Finally, we consider the 4p correlator  $G_{\sigma\sigma'}$  involving the operators  $\mathbf{O} = (d_\sigma, d_\sigma^\dagger, d_{\sigma'}, d_{\sigma'}^\dagger)$ . Let us showcase the analytic continuation for  $G_{\uparrow\downarrow}$ , which evaluates in the MF to

$$G_{\uparrow\downarrow}(\mathbf{i}\omega) = \frac{2u \prod_{i=1}^4 (i\omega_i) + u^3 \sum_{i=1}^4 (i\omega_i)^2 - 6u^5}{\prod_{i=1}^4 [(i\omega_i)^2 - u^2]}$$

$$+ \frac{u^2 [\beta \delta_{i\omega_{12}} t + \beta \delta_{i\omega_{13}} (t-1) + \beta \delta_{i\omega_{14}} (t+1)]}{\prod_{i=1}^4 (i\omega_i + u)}$$

$$= \tilde{G}(\mathbf{i}\omega) + \beta \delta_{i\omega_{12}} \hat{G}_{12}(\mathbf{i}\omega) + \beta \delta_{i\omega_{13}} \hat{G}_{13}(\mathbf{i}\omega)$$

$$+ \beta \delta_{i\omega_{14}} \hat{G}_{14}(\mathbf{i}\omega) \quad (119)$$

We study the analytic continuation to the Keldysh component  $G^{[12]}$ , expressed in terms of the analytic regions from Equation (102). Since the regular part only depends on the frequencies  $i\omega_i$  individually, the discontinuities across  $\gamma_{12} = 0$ ,  $\gamma_{13} = 0$ , and  $\gamma_{14} = 0$  vanish (Figure 6c), resulting in

$$G_{\uparrow\downarrow}^{[12]}(\omega) = N_1 (C_{111}^{(12)} - C^{(2)}) + N_2 (C_1^{(12)} - C^{(1)})$$

$$+ 4\pi i \delta(\omega_{13}) \hat{C}_{13}^{(12)} + 4\pi i \delta(\omega_{14}) \hat{C}_{14}^{(12)} \quad (120)$$

The remaining discontinuities can be computed without further complications. From Equation (119), we can already infer

some of their structures. Since the regular part has poles at  $i\omega_1 \rightarrow z_1 = \pm u$  (or  $i\omega_2 \rightarrow z_2 = \pm u$ ), we expect the discontinuity across  $\gamma_1 = 0$  (or  $\gamma_2 = 0$ ) to select these poles. Indeed, we find (see Appendix H.3)

$$G_{\uparrow\downarrow}^{[12]}(\omega) = 2\pi i u t \frac{\delta(\omega_1 - u) - \delta(\omega_1 + u)}{(\omega_2^+)^2 - u^2} \left( \frac{1}{\omega_{13}^-} + \frac{1}{\omega_{14}^-} \right)$$

$$+ (1 \leftrightarrow 2) + 4\pi i u^2 \frac{\delta(\omega_{13})(t-1) + \delta(\omega_{14})(t+1)}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]} \quad (121)$$

where  $1 \rightarrow 2$  indicates that indices 1 and 2 are exchanged compared to the first term. This expression can be simplified even further by collecting terms proportional to  $t$  and rewriting the  $\delta$ -functions in the resulting prefactor using Equations (58) and (107b). We eventually obtain

$$G_{\uparrow\downarrow}^{[12]}(\omega) = 4\pi i u^2 \frac{\delta(\omega_{14}) - \delta(\omega_{13})}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]}$$

$$+ 2u^2 t \left[ \frac{1}{(\omega_1^+)^2 - u^2} \frac{1}{(\omega_2^-)^2 - u^2} \left( \frac{1}{\omega_{23}^-} + \frac{1}{\omega_{24}^-} \right) - \text{c.c.} \right] \quad (122)$$

where c.c. is the complex conjugate. The other Keldysh components follow by similar calculations, see Appendix H.4.

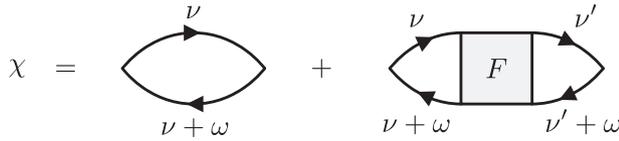
This concludes the section on HA examples for the analytic continuation of multipoint correlators. We again stress the simplicity of the analytic continuation procedure using our results for the Keldysh components expressed through analytic regions.

## 8. Vertex Corrections to Conductance

In this section, we consider a specific application of the analytic continuation of 4p functions regarding vertex corrections to the conductivity. One can deduce vertex corrections to real-frequency susceptibilities either by working directly in the KF or by using the MF and the analytic continuation method. The latter strategy was pursued by Eliashberg,<sup>[13]</sup> converting Matsubara sums into contour integrals and thereby obtaining various vertex contributions which consist of linear combinations of the MF vertex analytically continued to specific regions. For the special case of the linear conductance through an interacting region coupled to two noninteracting leads, Oguri<sup>[62]</sup> subsequently found that only one of these many vertex corrections contributes to the final result. A very similar formula for the linear conductance was later derived by Heyder et al.<sup>[63]</sup> with a different line of argument, working entirely in the KF. With our insights on 4p analytic continuation and gFDRs, we can demonstrate the equivalence between the results by Oguri and Heyder et al. and connect the MF and KF derivations.

A general susceptibility  $\chi$  can be expressed as in Figure 7. The first (“bubble”) term merely comprises two 2p correlators. We thus focus on the second term, the vertex correction, which in the MF reads

$$\chi_F(i\omega) = \frac{1}{\beta^2} \sum_{iv, iv'} G(iv) G(iv+i\omega) F(iv, iv', i\omega) G(iv') G(iv'+i\omega) \quad (123)$$



**Figure 7.** Diagrammatic representation of the susceptibility  $\chi$  consisting of a bubble and a vertex contribution. Lines represent propagators  $G$ , and the square is a vertex  $F$ .

Definitions of the propagator  $G$  and vertex  $F$  can be found in Section III A of ref. [23]. The summand in Equation (123) is the connected 4p correlator. Due to their close relation, the vertex  $F$  inherits its analytic properties from the correlator. In fact, by a transformation of Keldysh correlators to the  $R/A$  basis,<sup>[64,65]</sup> it can be easily shown that our formulas in Equation (101) identically hold for  $F$ , and we thus use the same symbols  $C$  to denote analytic continuations of  $F$  (see, e.g., Equation (124b)). Note that the Keldysh indices 1 and 2 exchange their meaning for  $F$ , such that, e.g., a fully retarded component reads  $F^{[1]} = F^{1222}$  (while  $G^{[1]} = G^{2111}$ ).

In ref. [13], Eliashberg converted the Matsubara sums in Equation (123) to contour integrals, thereby analytically continuing the MF functions and picking up contributions from all regions of analyticity (see Figure 5). In ref. [62], Oguri showed that the  $\omega$ -linear part, needed for the linear conductance (lc), stems from only one function,  $F^{(0)}$ , see Equation (2.34) in ref. [62]. The corresponding vertex correction to the retarded susceptibility reads

$$\chi_{F,lc}^R(\omega) = - \int \int \frac{d\nu d\nu'}{(4\pi i)^2} G^R(\nu + \omega) G^A(\nu) G^A(\nu') G^R(\nu' + \omega) \times \left[ \tanh\left(\frac{\nu + \omega}{2T}\right) - \tanh\left(\frac{\nu}{2T}\right) \right] F_O(\nu, \nu', \omega) \quad (124a)$$

$$F_O = -N_{\omega_3} C_{II}^{(12)} - N_{\omega_4} C_{IV}^{(12)} + N_{\omega_{13}} [C_{II}^{(12)} - C_{III}^{(12)}] + N_{\omega_{14}} [C_{IV}^{(12)} - C_{III}^{(12)}] \quad (124b)$$

where we used

$$(\omega_1, \omega_2, \omega_3, \omega_4) = (\nu + \omega, -\nu, \nu', -\nu' - \omega) \quad (125)$$

as frequency parametrization. Note that the results by Oguri and Eliashberg differ in their choice of the MWF; Equation (124b) corresponds to  $\mathcal{T}_{22}$  in Equation (12) of ref. [13].

An analogous result with an independent KF derivation was obtained in Equations (11) and (17) of ref. [63] by Heyder et al. There, the vertex correction to the linear conductance corresponds to

$$\chi_{F,lc}^R(\omega) = \int \int \frac{d\nu d\nu'}{(4\pi i)^2} G^R(\nu + \omega) G^A(\nu) G^A(\nu') G^R(\nu' + \omega) \times \left[ \tanh\left(\frac{\nu + \omega}{2T}\right) - \tanh\left(\frac{\nu}{2T}\right) \right] F_H(\nu, \nu', \omega) \quad (126a)$$

$$F_H = - (F^{[12]} + N_{\omega_1} F^{[2]} + N_{\omega_2} F^{[1]}) \quad (126b)$$

For an easier comparison with Equation (124a), we here used the tanh function instead of the Fermi distribution function. We also

absorbed a factor of 2 due to our choice of convention for the Keldysh rotation of multipoint functions (cf. Equation (17)).

To show that Equations (124a) and (126a) are equivalent, we translate the analytic continuations of the MF vertex in Equation (124b) to Keldysh components. First, we note that the linear combination of terms comprising  $F_O$  in Equation (124b) can also be expressed as follows, using (103):

$$F^{[34]} + N_{\omega_3} F^{[4]} + N_{\omega_4} F^{[3]} = N_{\omega_3} C_{II}^{(12)} + N_{\omega_4} C_{IV}^{(12)} + N_{\omega_{13}} [C_{III}^{(12)} - C_{II}^{(12)}] + N_{\omega_{14}} [C_{III}^{(12)} - C_{IV}^{(12)}] = -F_O \quad (127)$$

where we assumed vanishing anomalous parts. Next, we use the gFDR in Equation (104a) for vertices,

$$(N_{\omega_3} + N_{\omega_4})(F^{[12]} + N_{\omega_1} F^{[2]} + N_{\omega_2} F^{[1]}) = (N_{\omega_1} + N_{\omega_2})(F^{[34]} + N_{\omega_3} F^{[4]} + N_{\omega_4} F^{[3]}) \quad (128)$$

Together with Equation (125), this implies the equivalence of Equations (124a) and (126a) as

$$(N_{\omega_3} + N_{\omega_4})F_H = (N_{\omega_1} + N_{\omega_2})F_O \quad (129)$$

With the analytic continuation formulas and the gFDRs, we have thereby shown that both results agree and provided a direct transcription between two independent MF and KF derivations.

## 9. Conclusion

We showed how to perform the analytic continuation of multipoint correlators in thermal equilibrium from the imaginary-frequency MF to the real-frequency KF. To this end, we used the spectral representation derived in ref. [23], separating the correlator into formalism-independent partial spectral functions (PSFs) and formalism-specific kernels. From this analytical starting point, we showed that it is possible to fully recover all  $2^\ell$  components of the  $\ell$ p KF correlator from the one  $\ell$ p MF correlator. Our main result is that each of the ( $\ell!$ ) PSFs can be obtained by linear combinations of analytic continuations of the MF correlator multiplied with combinations of Matsubara weighting functions (MWFs). Explicit formulas are given in Equations (47) and (74) for arbitrary 2p and 3p correlators, respectively, and Equation (88) for fermionic 4p correlators. For these cases, we additionally derived direct MF-to-KF continuation formulas in Equation (61) ( $\ell = 2$ ), Equations (84) ( $\ell = 3$ ), and Equations (101) ( $\ell = 4$ ), complementing the general Equation (23) for any  $\ell$ .

We approached the problem of analytic continuation by comparing the spectral representations of general  $\ell$ p MF ( $G$ ) and KF ( $G^{[n_1 \dots n_\ell]}$ ) correlators and by identifying the regular partial MF correlators,  $\tilde{G}_p$ , as the central link between them. A key insight was that the partial MF correlators can be obtained by an imaginary-frequency convolution of MF kernels with the full MF correlator,  $\tilde{G}_p(i\omega_p) + \mathcal{O}(\frac{1}{\beta}) = (K \star G)(i\omega_p)$ . Building on this formula, we developed a three-step strategy for the MF-to-KF analytic continuation, applicable to arbitrary  $\ell$ p correlators and explicitly presented in the aforementioned cases  $\ell \leq 4$ . In the first step, we

used the kernel representation of ref. [30] to express the Matsubara sums, inherent in the imaginary-frequency convolution, through contour integrals enclosing the imaginary axis. In the second step, we deformed the contours toward the real axis, carefully tracking possible singularities of the MF correlator. This resulted in a spectral representation  $\tilde{G}_p(i\omega_p) = (\tilde{K} * S_p)(i\omega_p)$ , which allowed us to extract the PSFs,  $S_p[G]$ , as functionals of the regular and the various anomalous parts of  $G$  multiplied with MWFs. In the third and final step, we simplified the spectral representation for the KF components  $G^{[n_1 \dots n_\ell]}$ , inserted the PSFs from the second step, and evaluated all real-frequency integrals to express the KF correlators as linear combinations of analytically continued MF correlators.

In our analysis, we explicitly considered so-called anomalous parts of the MF correlator which can occur, e.g., for conserved quantities or in finite systems with degenerate energy eigenstates. The analytical continuations of these terms do not contribute to fully retarded correlators, but they do contribute to other components of the KF correlator. In the KF, the notion of “anomalous terms” is not needed; instead, the corresponding contributions are included via  $\delta$ -terms in the kernels, see Equation (20) and Equations (57)–(59) for  $\ell = 2$ .

Exploiting the relations between KF correlators and analytically continued MF functions, we derived generalized fluctuation-dissipation relations (gFDRs) for 3p and 4p correlators, Equations (84) and (104), establishing relations between the different KF components. We thereby reproduced the results of refs. [24, 25], while additionally including the anomalous terms.

We expect that similar results can be obtained for multipoint ( $\ell > 2$ ) out-of-time-ordering correlators (OTOCs)<sup>[66]</sup> which generalize the KF by additional copies of the Keldysh contour. Multipoint OTOCs, too, can be written as a sum over permutations of PSFs and kernels which encode the ordering on the desired number of branches. Importantly, the PSFs arising in this manner are precisely the same as those used in this work. Hence, the steps presented in Sections 3.3, 5.2 and 6.2 should be generalizable to multipoint OTOCs. Expressing the PSFs in terms of analytically continued MF correlators, analogous calculations would then reveal direct MF-to-OTOC continuation formulas. We leave this to future work.

As an application of our results, we considered various correlators of the Hubbard atom. Starting from their MF expressions, we calculated all components of the corresponding KF correlators using analytic continuation. For the fermionic 4p correlator, a full list of all Keldysh components for the two relevant spin configurations is given in Equations (H18) and (H20).

We further used our formulas to find KF expressions of the MF results derived in refs. [13, 62] for the linear conductance through an interacting system. There, the authors showed that only few analytic continuations of the vertex function are required for the vertex corrections to the linear conductance. Similar results were derived in ref. [63] working entirely in the KF. We reproduced their real-frequency results by analytic continuation and could thus provide a direct transcription between two independent derivations in the MF and the KF.

For future investigations, it would be interesting to apply our formulas in conjunction with the algorithmic Matsubara integration technique.<sup>[60]</sup> There, the evaluation of Feynman diagrams yields an exact symbolic expression for  $G(i\omega)$  that can

be readily continued to full Keldysh correlators or to PSFs. If, by contrast, the Matsubara results are only available as numerical data, the numerical analytic continuation is an ill-conditioned problem. Nevertheless, recent advances suggest that it can possibly be tamed to some extent by exploiting further information on mathematical properties of the function.<sup>[67–69]</sup>

Numerically representing multipoint MF correlators is another fruitful direction to explore. References<sup>[70,71]</sup> showed that 2p MF functions can be represented compactly by a suitable basis expansion. Yet, for multipoint functions, ref. [33] found that the overcompleteness of the basis hinders an extraction of the basis coefficients by projection. Here, a numerical counterpart of our method for recovering individual PSFs  $S_p$  (or partial correlators  $G_p$ ) from a full correlator  $G(i\omega)$  might be helpful. Finally, our formulas might also be useful for evaluating diagrammatic relations typically formulated for correlators while using the PSFs as the main information carriers. For recent developments regarding the numerical computation of MF or KF multipoint correlators using symmetric improved estimators, see ref. [61].

## Appendix A: MF Kernels

This appendix is devoted to a discussion of the full primary MF kernel  $K$ , including both regular and anomalous terms. It is defined via Equation (10a) for the MF kernel  $\mathcal{K}(\Omega_p)$ . In ref. [23], it was shown that it can be computed via

$$\begin{aligned} \mathcal{K}(\Omega_p) &= \int_0^\beta d\tau'_\ell e^{\Omega_{\tau'_\ell} \tau'_\ell} \prod_{i=\ell-1}^1 \left[ - \int_0^{\beta-\tau'_{i+1}} d\tau'_i e^{\Omega_{\tau'_i} \tau'_i} \right] \\ &= \beta \delta_{\Omega_{\tau'_\ell} \bar{\tau}} K(\Omega_p) + \mathcal{R}(\Omega_p) \end{aligned} \quad (\text{A1})$$

The residual part  $\mathcal{R}$  is not of interest, for reasons explained after Equation (12). The primary part  $K(\Omega_p)$  is obtained<sup>[72]</sup> by collecting all contributions multiplying  $\beta \delta_{\Omega_{\tau'_\ell} \bar{\tau}}$ , and its argument satisfies  $\Omega_{\tau'_\ell} \bar{\tau} = 0$  by definition. Before presenting explicit expressions for  $K$ , let us briefly recall where it is needed in the main text.

The analytical continuation of MF to KF correlators, based on  $\tilde{C}_p(i\omega_p \rightarrow \omega_p^{[n]})$  (Equation (26)), utilizes regular partial MF correlators,  $\tilde{C}_p(i\omega_p) = [\tilde{K} * S_p](i\omega_p)$  (Equation (14c)). These are expressed through regular MF kernels  $\tilde{K}(\Omega_p)$  having a simple product form,  $\prod_{i=1}^{\ell-1} \Omega_{\tau'_i, \bar{\tau}_i}^{-1}$ , with  $\Omega_{\tau'_i, \bar{\tau}_i} = 0$  understood. The more complicated primary kernel  $K(\Omega_p)$  is defined implicitly via Equation (10a). It includes both regular and anomalous parts, the latter involving vanishing partial frequency sums,  $\Omega_{\tau'_i, \bar{\tau}_i} = 0$  with  $i < \ell$ . The primary kernel arises in two distinct contexts, involving either (i) imaginary-frequency convolutions  $\star$  or (ii) real-frequency convolutions  $*$ , with different requirements for the bookkeeping of anomalous contributions. We discuss them in turn.

- (i) For a specified permutation  $p$ , the regular partial  $\tilde{C}_p(i\omega_p)$  can be extracted from the full MF correlator  $G(i\omega')$  via a imaginary-frequency convolution,  $[K \star G](i\omega_p)$  (Equation (31)). There, the argument of  $K(\Omega_p)$  has the form  $\Omega_p = i\omega_p - i\omega'_p$ . This is always bosonic, being the difference of two same-type Matsubara frequencies. The convolution  $\star$  involves Matsubara sums  $\sum_{i\omega'_p}$ , generating many anomalous contributions with  $\Omega_{\tau'_i, \bar{\tau}_i} = 0$ . For these sums to be well-defined, the kernel  $K(\Omega_p)$  must thus be represented in a form that (in contrast to  $\tilde{K}(\Omega_p)$ ) is manifestly singularity-free for all values of  $\Omega_{\tau'_i, \bar{\tau}_i}$ , including 0.
- (ii) In Equation (31),  $\tilde{C}_p$  is given by that part of  $[K \star G]$  that is  $\mathcal{O}(\beta^0)$ ; subleading powers of  $\beta$  are not needed. Therefore, we seek the MF  $G(i\omega')$  in the form of an  $\beta\delta$  expansion, i.e. an expansion in powers of  $\beta\delta_{\omega'_\ell, \bar{\tau}_\ell}$ .

Then each of them can collapse one Matsubara sum  $1/(-\beta) \sum_{\Omega'_{1\dots i}}$  while their  $\beta$  factors cancel. To obtain a  $\beta\delta$  expansion for  $G(i\omega')$ , it is convenient to express it via a permutation sum of real-frequency convolutions,  $\sum_p [K * S_p](i\omega')$  (Equation (11b)), and represent the kernel  $K(\Omega_p)$ , with argument  $\Omega_p = i\omega'_p - \epsilon_p$ , as a  $\beta\delta$  expansion in powers of  $\beta\delta_{\Omega'_{1\dots i}}$ .

Fortunately, suitable representations of  $K$  satisfying the respective requirements of either (i) or (ii) are available in the literature.<sup>[23,30,73,74]</sup> We discuss them for  $\ell \leq 4$  in Appendices A.1 and A.2, respectively.

### A.1. Singularity-Free Representation of $K$

Consider case (i), involving  $K \star G$ , where the argument of  $K(\Omega_p)$  is a bosonic Matsubara frequency. We seek a singularity-free (sf) representation for  $K$ , to be denoted  $K^{sf}$  for the purpose of this appendix. That such a representation exists is obvious from the form of integrals in Equation (A1): inserting  $\Omega_{\bar{1}\dots\bar{j}} = 0$  there reduces an exponential function to 1, so no contributions singular in  $\Omega_{\bar{1}\dots\bar{j}}$  can arise. To find  $K^{sf}$ , one simply has to perform the integrals explicitly, treating the cases  $\Omega_{\bar{1}\dots\bar{j}} \neq 0$  or  $= 0$  separately and distinguish them using Kronecker symbols.

Such a direct computation of Equation (A1) has been performed in ref. [30] for arbitrary  $\ell$  and an arbitrary number of vanishing partial frequency sums,  $\Omega_{\bar{1}\dots\bar{j}} = 0$ . The following equations summarize their results for  $\ell \leq 4$ :

$$K^{sf}(\Omega_p)^{\ell=2} = \Delta_{\Omega_{\bar{1}}} - \frac{\beta}{2} \delta_{\Omega_{\bar{1}}} \quad (\text{A2a})$$

$$K^{sf}(\Omega_p)^{\ell=3} = \Delta_{\Omega_{\bar{1}\bar{2}}} \left( \Delta_{\Omega_{\bar{1}}} - \frac{\beta}{2} \delta_{\Omega_{\bar{1}}} \right) - \delta_{\Omega_{\bar{1}\bar{2}}} \left( \Delta_{\Omega_{\bar{1}}}^2 + \frac{\beta}{2} \Delta_{\Omega_{\bar{1}}} - \frac{\beta^2}{6} \delta_{\Omega_{\bar{1}}} \right) \quad (\text{A2b})$$

$$K^{sf}(\Omega_p)^{\ell=4} = \Delta_{\Omega_{\bar{1}\bar{2}\bar{3}}} \left[ \Delta_{\Omega_{\bar{1}\bar{2}}} \left( \Delta_{\Omega_{\bar{1}}} - \frac{\beta}{2} \delta_{\Omega_{\bar{1}}} \right) - \delta_{\Omega_{\bar{1}\bar{2}}} \left( \Delta_{\Omega_{\bar{1}}}^2 + \frac{\beta}{2} \Delta_{\Omega_{\bar{1}}} - \frac{\beta^2}{6} \delta_{\Omega_{\bar{1}}} \right) \right] \\ - \delta_{\Omega_{\bar{1}\bar{2}\bar{3}}} \left[ \Delta_{\Omega_{\bar{1}\bar{2}}} \Delta_{\Omega_{\bar{1}}} \left( \Delta_{\Omega_{\bar{1}\bar{2}}} + \Delta_{\Omega_{\bar{1}}} + \frac{\beta}{2} \right) - \frac{\beta}{2} \Delta_{\Omega_{\bar{1}\bar{2}}} \delta_{\Omega_{\bar{1}}} \left( \Delta_{\Omega_{\bar{1}\bar{2}}} + \frac{\beta}{3} \right) \right] \\ - \delta_{\Omega_{\bar{1}\bar{2}\bar{3}}} \Delta_{\Omega_{\bar{1}}} \left( \Delta_{\Omega_{\bar{1}}}^2 + \frac{\beta}{2} \Delta_{\Omega_{\bar{1}}} + \frac{\beta^2}{6} \right) + \frac{\beta^3}{24} \delta_{\Omega_{\bar{1}\bar{2}}} \delta_{\Omega_{\bar{1}}} \right] \quad (\text{A2c})$$

Equations (A2) are manifestly singularity-free for all values of their frequency arguments—including those with  $\Omega_{\bar{1}\dots\bar{j}} = 0$ , for which  $\Delta_{\Omega_{\bar{1}\dots\bar{j}}}$  terms vanish by definition (Equation (32)).

### A.2. $\beta\delta$ Expansion for $K$

Next, consider case (ii), involving  $G = \sum_p K * S_p$  (Equations (11b) and (12)), where the argument of  $K(\Omega_p)$  has the form  $\Omega_p = i\omega_p - \epsilon_p$ , and we seek a  $\beta\delta$  expansion for  $G$ . For this purpose, the kernels  $K^{sf}$  of Equations (A2) are inconvenient, because they contain some  $\delta$  factors not accompanied by  $\beta$ . Instead,  $G$  can be expressed through an alternative kernel, to be denoted  $K^{alt}$ , which constitutes a  $\beta\delta$  expansion itself and hence differs from  $K^{sf}$ , but yields the same result for  $G$  when summed over all permutations, so that

$$G(i\omega) = \sum_p [K^{sf} * S_p](i\omega) = \sum_p [K^{alt} * S_p](i\omega) \quad (\text{A3})$$

Explicit expressions for  $K^{alt}$  were given in ref. [23] for up to one potentially vanishing frequency (general 2p correlators, 3p correlators with one bosonic operator, and fermionic 4p correlators). By also allowing general 3p correlators, these results are extended to

$$K^{alt}(\Omega_p)^{\ell=2} = \frac{1}{\Omega_{\bar{1}}} - \frac{\beta}{2} \delta_{\Omega_{\bar{1}}} \quad (\text{A4a})$$

$$K^{alt}(\Omega_p)^{\ell=3} = \frac{1}{\Omega_{\bar{1}}\Omega_{\bar{2}}} - \frac{\beta}{2} \left( \delta_{\Omega_{\bar{1}\bar{2}}} \Delta_{\Omega_{\bar{1}}} + \delta_{\Omega_{\bar{1}}}\Delta_{\Omega_{\bar{2}}} \right) + \frac{\beta^2}{6} \delta_{\Omega_{\bar{1}}}\delta_{\Omega_{\bar{2}}} \quad (\text{A4b})$$

$$K^{alt}(\Omega_p)^{\ell=4} = \frac{1}{\Omega_{\bar{1}}\Omega_{\bar{2}}\Omega_{\bar{3}}} - \frac{\beta}{2} \delta_{\Omega_{\bar{1}\bar{2}}} \frac{1}{\Omega_{\bar{1}}\Omega_{\bar{3}}} \quad (\text{A4c})$$

The kernels (A4) have the form  $K^{alt} = \tilde{K} + \hat{K}^{alt}$ , with regular part  $\tilde{K}$  as given in Equation (13b), while the anomalous part,  $\hat{K}^{alt}$ , comprises terms multiplied by one or multiple factors  $\beta\delta_{\Omega_{\bar{1}\dots\bar{j}}}$ . (We remark that the nomenclature *regular* and *anomalous* is used non-uniformly in the literature and our usage here may differ from refs. [23, 30, 73].) Whether or not  $\Omega_{\bar{1}\dots\bar{j}} = i\omega_{\bar{1}\dots\bar{j}} - \epsilon_{\bar{1}\dots\bar{j}}$  can vanish at all depends on the fermionic or bosonic nature of the Matsubara frequencies. Take, e.g.,  $\ell = 4$  and all operators fermionic. Then, in Equation (A2c), all terms multiplied by  $\delta_{\Omega_{\bar{1}\bar{2}\bar{3}}}$  evaluate to  $\delta_{\Omega_{\bar{1}\bar{2}\bar{3}}} = 0$ , since  $i\omega_{\bar{1}\bar{2}\bar{3}} \neq 0$  is a fermionic Matsubara frequency. For the computation of fermionic 4p correlators, all terms proportional to  $\delta_{\Omega_{\bar{1}}}$  and  $\delta_{\Omega_{\bar{1}\bar{2}}}$  can thus be dropped. Even if  $i\omega_{\bar{1}\dots\bar{j}}$  is bosonic and vanishes,  $\Omega_{\bar{1}\dots\bar{j}} = 0$  additionally requires  $\epsilon_{\bar{1}\dots\bar{j}} = 0$ , enforced by a Dirac  $\delta(\epsilon_{\bar{1}\dots\bar{j}})$  in the PSFs; see Appendix B.1 for further discussion of this point.

For a specified permutation  $p$ , the kernels  $K^{alt}$  are not singularity-free. In particular, the regular part  $\tilde{K}$  diverges if one (or multiple)  $\Omega_{\bar{1}\dots\bar{j}} \rightarrow 0$ . However, that singularity is canceled by  $1/\Omega_{\bar{1}\dots\bar{j}} = -1/\Omega_{\bar{1}\dots\bar{j}}$  from a cyclically related permutation in the sum over permutations in Equation (A3). This can be shown explicitly by treating nominally vanishing denominators as infinitesimal and tracking the cancellation of divergent terms while exploiting the equilibrium condition (4) (see Appendix B of ref. [23]).

The kernels  $K^{alt}$ , inserted into Equation (A4), result in the general form for MF correlators given in Equation (14):

$$G(i\omega) = \tilde{G}(i\omega) + \hat{G}(i\omega) \quad (\text{A5a})$$

$$\hat{G}(i\omega) = \sum_{j=1}^{\ell-1} \beta \delta_{i\omega_j} \hat{G}_j(i\omega) + \sum_{j=1}^{\ell-1} \sum_{k>j}^{\ell-1} \left( \beta \delta_{i\omega_j} \hat{G}_{jk}(i\omega) + \beta^2 \delta_{i\omega_j} \delta_{i\omega_k} \hat{G}_{j,k}(i\omega) \right) \quad (\text{A5b})$$

As for Equation (A4), this form of the anomalous part of the correlator applies to general 2p and 3p correlators as well as fermionic 4p correlators. The subscripts of  $\hat{G}$  indicate the frequency in which they are anomalous. Even though their arguments nominally include all frequencies  $i\omega$ , they are independent of their respective anomalous frequency; e.g.,  $\hat{G}_1(i\omega_1, i\omega_2) = \hat{G}_1(i\omega_2)$  for  $\ell = 3$ . Note that this decomposition of the correlator is convenient for the analytic continuation because the components, such as  $\tilde{G}$  and  $\hat{G}_j$ , have a functional form that allows their arguments to be analytically continued,  $i\omega_i \rightarrow z_i$ . In anomalous components this functional form is obtained by symbolically replacing all  $\Delta_{i\omega}$  by  $\frac{1}{i\omega}$  (see, e.g., Equation (80) and the discussion thereafter).

## Appendix B: Discussion of PSFs

In Appendix B.1, we clarify the functional structure of PSFs and motivate their decomposition into regular and anomalous contributions,  $S_p = \tilde{S}_p + \hat{S}_p$  (Equation (5)), analogous to that for MF correlators. This decomposition aids investigations in subsequent appendices. As an immediate application of the decomposition, we present an analysis of the effect of fully anomalous PSFs on 3p MF correlators in Appendix B.2.

### B.1. Decomposition of PSFs

Interacting thermal systems typically have a continuum of energy levels. Ref. [27] argues that, in general, PSFs may contain contributions which diverge as  $P(\frac{1}{\epsilon})$  for vanishing bosonic frequencies  $\epsilon$ , with  $P$  the principal value. As our derivations do not make assumptions on the shape

of continuous PSF contributions, such terms require no further consideration. However, Dirac delta contributions in  $S_p$  can arise for finite systems or in the presence of conserved quantities. When these are present, MF partial correlators  $G_p = K * S_p$  (Equation (11b)) can contain anomalous terms,  $\hat{G}_p$ , containing at least one factor  $\delta_{i\omega_{\tau\dots j}}$  with  $i < \ell$ . These arise from anomalous  $\delta_{\Omega_{\tau\dots j}}$  terms in the MF kernel  $K(\Omega_p)$ , with argument  $\Omega_p = i\omega_p - \epsilon_p$  (Equations (A3), (A4)). Such terms can contribute if  $\Omega_{\tau\dots j} = 0$ , requiring  $i\omega_{\tau\dots j} = 0$  and  $\epsilon_{\tau\dots j} = 0$ . The first condition requires that  $i\omega_{\tau\dots j}$  is bosonic. This is the case if the sign  $\zeta^{\tau\dots j} = \zeta^{\tau\dots 1} \dots \zeta^{\tau\dots j}$  equals +1 (with  $\zeta^j = \pm 1$  for bosonic/fermionic operators  $O^j$ ). Then, the associated  $\epsilon_{\tau\dots j}$  is bosonic, too, according to the nomenclature introduced after Equation (3b). The second condition is met if the PSF  $S_p(\epsilon_p)$  contains a term proportional to a bosonic Dirac delta, i.e. one having a bosonic  $\epsilon_{\tau\dots j}$  as argument, e.g.  $\delta(\epsilon_{\tau\dots j})\check{S}_{\tau\dots j}$ . Then, the  $\epsilon_p$  integrals in the convolution  $K * S_p$  receive a finite contribution from the point  $\epsilon_{\tau\dots j} = 0$ . We summarize these conditions via the symbolic notation

$$\delta_{\Omega_{\tau\dots j}} = \delta_{i\omega_{\tau\dots j}} \delta_{\epsilon_{\tau\dots j}} \quad (\text{B1})$$

needed only for bosonic  $\Omega_{\tau\dots j}$ . Here  $\delta_{\epsilon_{\tau\dots j}}$ , carrying a continuous variable as subscript, is defined only for bosonic  $\epsilon_{\tau\dots j}$  and by definition “acts on”  $S_p(\epsilon_p)$  by extracting only those parts (if present) containing bosonic Dirac  $\delta(\epsilon_{\tau\dots j})$  factors. For the example above,  $\delta_{\epsilon_{\tau\dots j}}$  acts on  $S_p(\epsilon_p)$  as

$$\delta_{\epsilon_{\tau\dots j}} S_p(\epsilon_p) = \delta_{\epsilon_{\tau\dots j}} \hat{S}_p(\epsilon_p) \sim \delta(\epsilon_{\tau\dots j}) \quad (\text{B2})$$

As we always assume an even number of fermionic operators,  $\zeta^{1\dots\ell} = +1$  follows.

The motivation for splitting PSFs as  $S_p = \check{S}_p + \hat{S}_p$  is now clear. The anomalous  $\hat{S}_p$  comprises all terms containing bosonic Dirac  $\delta(\epsilon_{\tau\dots j})$  factors, the regular  $\check{S}$  everything else. The regular part of the MF correlator,  $\hat{G}$ , receives contributions from both  $\check{S}_p$  and  $\hat{S}_p$ ; the anomalous part,  $\hat{G}$ , receives contributions only from  $\hat{S}_p$ , i.e. if  $\hat{S}_p = 0$  for all  $p$ , then  $\hat{G} = 0$ .

For  $\ell = 2$ , the anomalous contribution consists of one term,

$$\hat{S}_p(\epsilon_p) = \delta(\epsilon_{\bar{1}})\check{S}_{p;\bar{1}} \quad (\text{B3})$$

where  $\check{S}_{p;\bar{1}}$  is a constant. Due to the equilibrium condition (4), we can further conclude  $\check{S}_{(12);1} = \check{S}_{(21);2}$ .

For  $\ell = 3$ , the anomalous  $\hat{S}_p$  reads

$$\hat{S}_p(\epsilon_p) = \delta(\epsilon_{\bar{1}})\check{S}_{p;\bar{1}}(\circ, \epsilon_{\bar{2}}, \epsilon_{\bar{3}}) + \delta(\epsilon_{\bar{3}})\check{S}_{p;\bar{3}}(\epsilon_{\bar{1}}, \epsilon_{\bar{2}}, \circ) + \delta(\epsilon_{\bar{2}})\check{S}_{p;\bar{2}}(\epsilon_{\bar{1}}, \circ, \epsilon_{\bar{3}}) \quad (\text{B4})$$

Here, we inserted  $\circ$ 's to emphasize that functions do not depend on these arguments, and  $\check{S}_{p;\bar{1}}(\circ, \epsilon_{\bar{2}}, \epsilon_{\bar{3}})$  is a constant. For bosonic 3p functions,  $\check{S}_{p;\bar{1}}$  and  $\check{S}_{p;\bar{3}}$  do not contain further  $\delta$ -factors that lead to anomalous parts, e.g.,  $\delta_{\epsilon_{\bar{3}}}\check{S}_{p;\bar{1}}(\circ, \epsilon_{\bar{2}}, \epsilon_{\bar{3}}) = 0$ .

To further illustrate the symbolic  $\delta_{\epsilon_{\tau\dots j}}$  notation introduced in Equation (B1), it yields the following relations when applied to the above definitions, for bosonic  $\epsilon_{\bar{1}}$ :

$$\delta_{\epsilon_{\bar{1}}} S_p(\epsilon_p) = \delta(\epsilon_{\bar{1}})\check{S}_{p;\bar{1}}(\epsilon_p) + \delta(\epsilon_{\bar{1}})\delta(\epsilon_{\bar{2}})\check{S}_{p;\bar{1};\bar{2}} \quad (\text{B5a})$$

$$\delta_{\epsilon_{\bar{1}}}\delta_{\epsilon_{\bar{2}}} S_p(\epsilon_p) = \delta(\epsilon_{\bar{1}})\delta(\epsilon_{\bar{2}})\check{S}_{p;\bar{1};\bar{2}} \quad (\text{B5b})$$

For fermionic  $\ell = 4$ , we only need

$$\hat{S}_p(\epsilon_p) = \delta(\epsilon_{\bar{1}\bar{2}})\check{S}_{p;\bar{1}\bar{2}}(\epsilon_p) \quad (\text{B6})$$

since, e.g., terms in the kernel proportional to  $\delta_{i\omega_{\bar{1}}-\epsilon_{\bar{1}}}$  do not lead to anomalous contributions by the fermionic nature of  $i\omega_{\bar{1}}$ .

## B.2. Effect of Fully Anomalous PSFs on 3p MF Correlators

In the Appendix C.1 below, we discuss the general structure of 3p MF correlators inferred by the decomposition of the PSFs. The regular PSFs,  $\check{S}_p$ , can only contribute to the regular part of the correlator. However, the effect of anomalous PSFs,  $\hat{S}_p$ , is more involved and is studied in detail in the following.

To this end, we consider PSFs with finite weight at vanishing frequency arguments. In particular, we assume the maximally anomalous form  $S_p^{\text{ma}}(\epsilon_{\bar{1}}, \epsilon_{\bar{2}}) = \delta(\epsilon_{\bar{1}})\delta(\epsilon_{\bar{2}})\check{S}_{p;\bar{1}\bar{2}}$  (see Equation (B5b)). Then, the equilibrium condition Equation (4) implies  $\check{S}_{(123);1;2} = \check{S}_{(231);2;3} = \check{S}_{(312);3;1}$  and  $\check{S}_{(132);1;3} = \check{S}_{(321);3;2} = \check{S}_{(213);2;1}$ , since  $\zeta_p = \zeta_{p_i} = 1$  for purely bosonic correlators. For such PSFs, the 3p correlator evaluates to

$$\begin{aligned} G^{\text{ma}}(i\omega) &= \sum_p [K * S_p^{\text{ma}}](i\omega_p) \\ &= \left[ \frac{\beta}{2} (\delta_{i\omega_1} \Delta_{i\omega_{12}} + \Delta_{i\omega_1} \delta_{i\omega_{12}}) + \frac{\beta^2}{6} \delta_{i\omega_1} \delta_{i\omega_{12}} \right] \check{S}_{(123);1,2} \\ &\quad + \left[ \frac{\beta}{2} (\delta_{i\omega_2} \Delta_{i\omega_{23}} + \Delta_{i\omega_2} \delta_{i\omega_{23}}) + \frac{\beta^2}{6} \delta_{i\omega_2} \delta_{i\omega_{23}} \right] \check{S}_{(231);2,3} \\ &\quad + \left[ \frac{\beta}{2} (\delta_{i\omega_3} \Delta_{i\omega_{31}} + \Delta_{i\omega_3} \delta_{i\omega_{31}}) + \frac{\beta^2}{6} \delta_{i\omega_3} \delta_{i\omega_{31}} \right] \check{S}_{(312);3,1} \\ &\quad + (2 \leftrightarrow 3) \\ &= \beta (\delta_{i\omega_1} \Delta_{i\omega_2} + \delta_{i\omega_2} \Delta_{i\omega_3} + \delta_{i\omega_3} \Delta_{i\omega_1}) (\check{S}_{(123);1,2} - \check{S}_{(132);1,3}) \\ &\quad + \frac{\beta^2}{2} \delta_{i\omega_1} \delta_{i\omega_2} (\check{S}_{(123);1,2} + \check{S}_{(132);1,3}) \end{aligned} \quad (\text{B7})$$

where  $(2 \leftrightarrow 3)$  exchanges the indices of the frequencies and PSFs. The contribution of the regular kernel in Equation (A4b) vanishes due to  $\frac{1}{i\omega_1 i\omega_{12}} + \frac{1}{i\omega_2 i\omega_{23}} + \frac{1}{i\omega_3 i\omega_{31}} = 0$  with  $i\omega_3 = -i\omega_{12}$ .

For later reference (see Appendices C.1 and E.2), we define the constants

$$\hat{G}_{1,2} = \frac{1}{2} (\check{S}_{(123);1,2} + \check{S}_{(132);1,3}) \quad (\text{B8a})$$

$$\hat{G}_{1,2}^{\Delta} = \hat{G}_{2,3}^{\Delta} = \hat{G}_{3,1}^{\Delta} = \check{S}_{(132);1,3} - \check{S}_{(123);1,2} \quad (\text{B8b})$$

such that  $G^{\text{ma}}$  reads

$$\begin{aligned} \hat{G}^{\text{ma}}(i\omega) &= \beta (\delta_{i\omega_1} \Delta_{i\omega_2} \hat{G}_{1,2}^{\Delta} + \delta_{i\omega_2} \Delta_{i\omega_3} \hat{G}_{2,3}^{\Delta} + \delta_{i\omega_3} \Delta_{i\omega_1} \hat{G}_{3,1}^{\Delta}) \\ &\quad + \beta^2 \delta_{i\omega_1} \delta_{i\omega_2} \hat{G}_{1,2} \end{aligned} \quad (\text{B8c})$$

We emphasize that  $\hat{G}_{ij}^{\Delta}$  and  $\hat{G}_{1,2}$  are nonzero only if the full PSFs  $S_p$  contain fully anomalous contributions  $S_p^{\text{ma}}$ , which is only the case for all operators being bosonic. In the next section, the most general form of 3p correlators is discussed.

## Appendix C: Calculations for 3p Correlators

This appendix is devoted to computations for the analytic continuation of 3p correlators, complementing the discussions in Section 5. First, in Appendix C.1, we discuss the general structure of MF correlators, needed in Appendix C.2 for the derivation of an explicit formula for partial MF correlators and the subsequent extraction of PSFs. In Appendix C.3, we then present manipulations needed to construct KF correlators from analytically continued MF correlators.

### C.1. Structure of 3p Correlators

For 3p correlators, Equation (A5) implies the general form

$$\begin{aligned} G_{i\omega_1, i\omega_2} &= \tilde{G}_{i\omega_1, i\omega_2} + \hat{G}_{i\omega_1, i\omega_2} \\ \hat{G}_{i\omega_1, i\omega_2} &= \beta \delta_{i\omega_1} \hat{G}_{1; i\omega_2} + \beta \delta_{i\omega_2} \hat{G}_{2; i\omega_1} + \beta \delta_{i\omega_3} \hat{G}_{3; i\omega_1} + \beta^2 \delta_{i\omega_1} \delta_{i\omega_2} \hat{G}_{1,2} \end{aligned} \quad (C1)$$

Here, we used the subscript notation introduced in Section 4.

For the conversion of Matsubara sums to contour integrals we distinguish restricted from unrestricted sums (see e.g. Equation (35b)). Therefore we explicitly distinguish terms with  $\Delta_{i\omega}$  factors, writing (cf. Equation (73))

$$\hat{G}_{i; i\omega_j}^\Delta = \hat{G}_{i; i\omega_j}^\Delta + \Delta_{i\omega_j} \hat{G}_{i; i\omega_j}^\Delta \quad (C2)$$

In Equation (B8b), we have identified the constants  $\hat{G}^\Delta$  with (maximally anomalous) PSFs. For alternative frequency parametrizations in Equations (B8), the constants in Equation (C2) read

$$\hat{G}_{1,2}^\Delta = -\hat{G}_{1,3}^\Delta = -\hat{G}_{2,1}^\Delta = \hat{G}_{2,3}^\Delta = \hat{G}_{3,1}^\Delta = -\hat{G}_{3,2}^\Delta \quad (C3)$$

such that, e.g.,  $\delta_{i\omega_1} \Delta_{i\omega_2} \hat{G}_{1,2}^\Delta = -\delta_{i\omega_1} \Delta_{i\omega_3} \hat{G}_{1,2}^\Delta = \delta_{i\omega_1} \Delta_{i\omega_2} \hat{G}_{1,3}^\Delta$ , which follows from frequency conservation,  $i\omega_{1\dots\ell} = 0$ , and the  $\delta_{i\omega_i}$  factor multiplying  $\hat{G}_i$ .

### C.2. Partial MF 3p Correlators

In this appendix, we present explicit calculations concerning Steps 1 and 2 of our 3-step strategy. First, we introduce two identities used for simplifications in Step 1.

Consider the restricted Matsubara sum of Equation (35b) for  $f(i\omega')$  =  $\tilde{f}(i\omega')/(i\omega - i\omega')$ . Using Equation (37) for the residue term, one obtains

$$\frac{1}{(-\beta)^2} \sum_{i\omega'} \left( \Delta_{i\omega - i\omega'} - \frac{\beta}{2} \delta_{i\omega - i\omega'} \right) \tilde{f}(i\omega') = \oint_z \frac{n_z \tilde{f}(z)}{i\omega - z} + \mathcal{O}\left(\frac{1}{\beta}\right) \quad (C4)$$

Here, the restriction of the sum is implicit in the  $\Delta$  symbol (Equation (32)), and the first term of Equation (37) was incorporated into the sum using the Kronecker  $\delta$ . We can identify the summand on the left of Equation (C4) as the singularity-free 2p kernel of Equation (A2a), and therefore this identity constitutes the convenient cancellation in Equations (38) already on the level of kernels. Following the same line of arguments, one can show that

$$\frac{1}{(-\beta)^2} \sum_{i\omega'} \left( \Delta_{i\omega - i\omega'}^2 + \frac{\beta^2}{12} \delta_{i\omega - i\omega'} \right) \tilde{f}(i\omega') = \mathcal{O}\left(\frac{1}{\beta}\right) \quad (C5)$$

In the following, we focus on evaluating

$$\tilde{G}_{(123)}(i\omega_{(123)}) + \mathcal{O}\left(\frac{1}{\beta}\right) = [K \star G](i\omega_{(123)}) \quad (C6)$$

using the 3p kernel given in Equation (A2b) (with  $\Omega_{(123)} = i\omega_{(123)} - i\omega'_{(123)}$ ), and the general form of the 3p correlator displayed in Equation (C1). For convenience, we focus on the identity permutation  $p = (123)$ ; all other permutations can be obtained by replacing indices with their permuted ones,  $i \rightarrow \bar{i}$ . We split the calculation of Equation (C6) into regular (r) and anomalous (a) contributions from  $G$ :

$$\tilde{G}_{(123)}^r(i\omega_{(123)}) + \mathcal{O}\left(\frac{1}{\beta}\right) = [K \star \tilde{G}^r](i\omega_{(123)}) \quad (C7a)$$

$$\tilde{G}_{(123)}^a(i\omega_{(123)}) + \mathcal{O}\left(\frac{1}{\beta}\right) = [K \star \hat{G}^a](i\omega_{(123)}) \quad (C7b)$$

The computations are presented in Appendices C.2.1 and C.2.2, respectively, with the final result  $\tilde{G}_{(123)} = \tilde{G}_{(123)}^r + \tilde{G}_{(123)}^a$  discussed in Appendix C.2.3. Additionally, we will use the super- and subscript notation introduced in Section 4 and suppress the frequency argument of  $\tilde{G}_{(123)}^r$  and  $\tilde{G}_{(123)}^a$ .

#### C.2.1. Contributions from Regular Part

Step 1. *Matsubara summation through contour integration*: First, we concentrate on evaluating Equation (C7a):

$$\begin{aligned} \tilde{G}_{(123)}^r + \mathcal{O}\left(\frac{1}{\beta}\right) &= K \star \tilde{G} \\ &= \frac{1}{(-\beta)^2} \sum_{i\omega'_1, i\omega'_{12}} \left[ \Delta_{\Omega_{12}} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \right. \\ &\quad \left. + \delta_{\Omega_{12}} \left( -\Delta_{\Omega_1}^2 - \frac{\beta}{2} \Delta_{\Omega_1} + \frac{\beta^2}{6} \delta_{\Omega_1} \right) \right] \tilde{G}_{i\omega'_1, i\omega'_{12}} \\ &= \frac{1}{(-\beta)^2} \sum_{i\omega'_1} \sum_{i\omega'_{12}}^{\neq i\omega_{12}} \frac{1}{i\omega_{12} - i\omega'_{12}} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \tilde{G}_{i\omega'_1, i\omega'_{12}} \\ &\quad + \frac{1}{(-\beta)^2} \sum_{i\omega'_1} \sum_{i\omega'_{12}} \delta_{\Omega_{12}} \left( -\Delta_{\Omega_1}^2 - \frac{\beta}{2} \Delta_{\Omega_1} + \frac{\beta^2}{6} \delta_{\Omega_1} \right) \tilde{G}_{i\omega'_1, i\omega'_{12}} \end{aligned} \quad (C8)$$

The restricted sum over  $i\omega'_{12}$  can be rewritten using Equation (C4), and collecting all resulting terms  $\sim \delta_{\Omega_{12}}$  yields

$$\begin{aligned} \tilde{G}_{(123)}^r + \mathcal{O}\left(\frac{1}{\beta}\right) &= \frac{1}{(-\beta)^2} \sum_{i\omega'_1} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \oint_{z_{12}} \frac{n_{z_{12}} \tilde{G}_{i\omega'_1, z_{12}}}{i\omega_{12} - z_{12}} \\ &\quad + \frac{1}{(-\beta)^2} \sum_{i\omega'_1} \sum_{i\omega'_{12}} \delta_{\Omega_{12}} \left( -\Delta_{\Omega_1}^2 - \frac{\beta^2}{12} \delta_{\Omega_1} \right) \tilde{G}_{i\omega'_1, i\omega'_{12}} \end{aligned} \quad (C9)$$

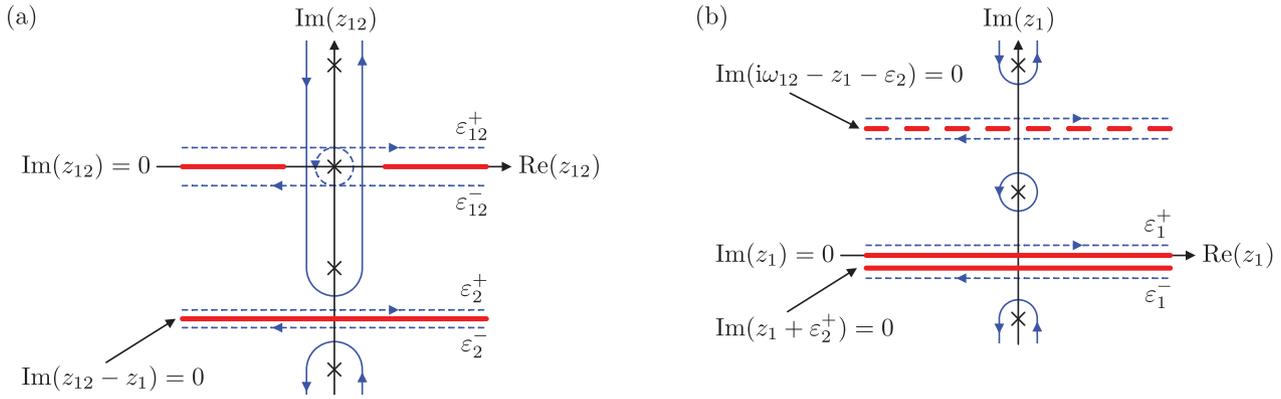
The  $i\omega'_1$  sums can be further simplified with the help of Equations (C4) and (C5) for the second and third line, respectively, reproducing Equation (39) for  $\ell = 3$ ,

$$\tilde{G}_{(123)}^r + \mathcal{O}\left(\frac{1}{\beta}\right) = \oint_{z_1, z_{12}} \frac{n_{z_1} n_{z_{12}} \tilde{G}_{z_1, z_{12}}}{(i\omega_1 - z_1)(i\omega_{12} - z_{12})} + \mathcal{O}\left(\frac{1}{\beta}\right) \quad (C10)$$

with  $\oint_{z_1, z_{12}} = \oint_{z_1} \oint_{z_{12}}$ .

Step 2. *Extraction of PSFs*: Next, we deform the contours away from the imaginary axis, beginning with the contour integral over  $z_{12}$ . During the contour deformation, we have to carefully track possible singularities of  $\tilde{G}_{z_1, z_{12}} = \tilde{G}(z_1, z_{12} - z_1, -z_{12})$ . As explained in Section 4, possible branch cuts in the complex  $z_{12}$  plane lie on the lines defined by  $\text{Im}(z_{12}) = 0$  or  $\text{Im}(z_{12} - z_1) = 0$ , see Figure C1a. The branch cut at  $\text{Im}(z_{12}) = 0$  is taken into account by integrating infinitesimally above and below the real  $z_{12}$  axis, denoted by  $\varepsilon_{12}^\pm$  with  $\text{Re}(z_{12}) = \varepsilon_{12}$ .

The second branch cut  $\text{Im}(z_{12} - z_1) = 0$  is included by substituting  $z_{12} \rightarrow z_2 = z_{12} - z_1$ , with  $z_2$  being the new integration variable. Therefore, the contour is shifted onto the line  $\text{Im}(z_{12} - z_1) = 0 \rightarrow \text{Im}(z_2) = 0$ , i.e., onto the real axis of the complex  $z_2$  plane, and integrating infinitesimally above and below the real axis of  $z_2$ , denoted by  $\varepsilon_2^\pm$  with  $\text{Re}(z_2) = \varepsilon_2$ . The substitution also affects the argument of the MWF in Equation (C10). However, since the  $z_1$  contour encloses only the poles of  $n_{z_1}$ ,  $z_1$  can be



**Figure C1.** a) Contour deformation used in Equation (C12) for fermionic  $z_1$  and  $z_2$ , therefore bosonic  $z_{12}$ . Black crosses denote the poles of  $n_{z_{12}}$  on the imaginary axis given by bosonic Matsubara frequencies. The blue, solid contour encloses all the poles on the imaginary axis. It is deformed into the blue, dashed contour to integrate along the possible branch cuts of  $\tilde{G}_{z_1, z_{12}}$  denoted by the red, thick lines, located at  $\text{Im}(z_{12}) = 0$  and  $\text{Im}(z_{12} - z_1) = 0$ . (b) Contour deformation used to obtain Equation (C15). The branch cut at  $\text{Im}(z_1 + \epsilon_2^+) = 0$  lies infinitesimally close to the branch cut  $\text{Im}(z_1) = 0$ . Therefore, we integrate along the deformed blue, dashed contour, infinitesimally above and below the real axis, where the infinitesimal imaginary part of  $\epsilon_1^+$ , with  $\text{Re}(z_1) = \epsilon_1$ , has to be larger than that of  $\epsilon_2^+$ , i.e.,  $|\text{Im}(\epsilon_1^+)| > |\text{Im}(\epsilon_2^+)|$ . The thick, red, dashed line denotes the pole at  $\text{Im}(i\omega_{12} - z_1 - \epsilon_2)$  coming from the kernel. However, these poles only contribute at  $\mathcal{O}(\frac{1}{\beta})$  and can be neglected, see the discussion after Equation (C17).

treated as a Matsubara frequency, implying  $e^{-\beta z_1} = \zeta^1$  and therefore

$$\begin{aligned} n_{z_{12}} &= \frac{\zeta^{12}}{e^{-\beta z_{12}} - \zeta^{12}} \stackrel{z_{12} \rightarrow z_1 + z_2}{=} \frac{\zeta^1 \zeta^2}{e^{-\beta z_1} e^{-\beta z_2} - \zeta^1 \zeta^2} \\ &= \frac{\zeta^2}{e^{-\beta z_2} - \zeta^2} = n_{z_2} \end{aligned} \quad (\text{C11})$$

Adding the contributions from both branch cuts, the  $z_{12}$  dependent terms in Equation (C10) evaluate to

$$\oint_{z_{12}} \frac{n_{z_{12}} \tilde{G}_{z_1, z_{12}}}{i\omega_{12} - z_{12}} = \int_{\epsilon_{12}} \frac{n_{\epsilon_{12}} \tilde{G}_{z_1}^{\epsilon_{12}}}{i\omega_{12} - \epsilon_{12}} + \int_{\epsilon_2} \frac{n_{\epsilon_2} \tilde{G}_{z_1}^{\epsilon_2}}{i\omega_{12} - z_1 - \epsilon_2} + \mathcal{O}(\frac{1}{\beta}) \quad (\text{C12})$$

see also Figure C1a. The term  $\mathcal{O}(\frac{1}{\beta})$  comes from the possible poles at  $z_{12} = 0$  or  $z_2 = 0$  (if  $z_{12}$  or  $z_2$  are bosonic) which do not contribute at  $\mathcal{O}(1)$ , see Equation (44).

Inserting Equation (C12) into Equation (C10) yields

$$\begin{aligned} \tilde{G}_{(123)}^r + \mathcal{O}(\frac{1}{\beta}) &= \oint_{z_1} \frac{n_{z_1}}{i\omega_1 - z_1} \int_{\epsilon_2} \frac{n_{\epsilon_2} \tilde{G}_{z_1}^{\epsilon_2}}{i\omega_{12} - z_1 - \epsilon_2} \\ &+ \oint_{z_1} \frac{n_{z_1}}{i\omega_1 - z_1} \int_{\epsilon_{12}} \frac{n_{\epsilon_{12}} \tilde{G}_{z_1}^{\epsilon_{12}}}{i\omega_{12} - \epsilon_{12}} \end{aligned} \quad (\text{C13})$$

Next we focus on the contour deformation of  $z_1$ . For the first term, we have illustrated possible branch cuts and the contours before and after the deformation in Figure C1b. As the  $z_1$  contour is deformed away from the Matsubara frequencies, we merely have to consider the singularities in the integrand of the  $\epsilon_2$  integral. After Equation (C17), we will show that the singularities at  $z_1 = i\omega_{12} - \epsilon_2$  contribute at order  $\mathcal{O}(\frac{1}{\beta})$ . We can thus focus on the branch cut in  $\tilde{G}_{z_1}^{\epsilon_2}$ . Previously we have taken the infinitesimal limit for the imaginary shifts of  $\epsilon_2^\pm$ . Thus, during the  $z_1$  contour deformation we have to ensure  $|\text{Im}(\epsilon_2^\pm)| < |\text{Im}(\epsilon_1^\pm)|$ , see Figure C1b. The  $z_1$  contours infinitesimally above and below  $\text{Re}(z_1)$  are summarized in a discontinuity

$$\tilde{G}^{\epsilon_2, \epsilon_1} = \tilde{G}_{\epsilon_1^+}^{\epsilon_2} - \tilde{G}_{\epsilon_1^-}^{\epsilon_2} \quad (\text{C14})$$

and we thus find for the first term in Equation (C13):

$$\oint_{z_1} \frac{n_{z_1}}{i\omega_1 - z_1} \int_{\epsilon_2} \frac{n_{\epsilon_2} \tilde{G}_{z_1}^{\epsilon_2}}{i\omega_{12} - z_1 - \epsilon_2} = \int_{\epsilon_1} \int_{\epsilon_2} \frac{n_{\epsilon_1} n_{\epsilon_2} \tilde{G}^{\epsilon_2, \epsilon_1}}{(i\omega_1 - \epsilon_1)(i\omega_{12} - \epsilon_{12})} + \mathcal{O}(\frac{1}{\beta}) \quad (\text{C15})$$

Repeating an analogous  $z_1$  contour deformation for the second term in Equation (C13), we finally obtain

$$\tilde{G}_{(123)}^r = \int_{\epsilon_1, \epsilon_2} \frac{n_{\epsilon_1} n_{\epsilon_2} \tilde{G}^{\epsilon_2, \epsilon_1} + n_{\epsilon_1} n_{\epsilon_{12}} \tilde{G}^{\epsilon_{12}, \epsilon_1}}{(i\omega_1 - \epsilon_1)(i\omega_{12} - \epsilon_{12})} \quad (\text{C16})$$

which resembles the spectral representation in Equation (14d) for  $\ell = 3$ .

The term  $\mathcal{O}(\frac{1}{\beta})$  on the right of Equation (C15) originates from the pole at  $z_1 = i\omega_{12} - \epsilon_2$  in the denominator on the left, yielding

$$\mathcal{O}(\frac{1}{\beta}) = - \int_{\epsilon_2} \frac{n_{\epsilon_2} n_{-\epsilon_2} \tilde{G}_{i\omega_{12}}^{\epsilon_2}}{i\omega_2 - \epsilon_2} \quad (\text{C17})$$

with  $\tilde{G}_{i\omega_{12}}^{\epsilon_2} = \tilde{G}(i\omega_{12} - \epsilon_2^+, \epsilon_2^+, -i\omega_{12}) - \tilde{G}(i\omega_{12} - \epsilon_2^-, \epsilon_2^-, -i\omega_{12})$ . That the integral on the right indeed is  $\mathcal{O}(\frac{1}{\beta})$ , although it lacks an explicit prefactor  $1/\beta$ , can be seen by the following argument: The product of two MWFs  $n_{\epsilon_2} n_{-\epsilon_2}$  has finite support on an interval  $\epsilon_2 \in [-1/\beta, 1/\beta]$ . Therefore, the integral scales as  $1/\beta$ .

To demonstrate this claim more explicitly, we proceed as follows. We note that we evaluated the imaginary-frequency convolution in Equation (C8) by evaluating first the  $\omega'_{12}$  and then the  $\omega'_1$  sum. Due to frequency conservation, we could have also evaluated the convolution by first summing over, e.g.,  $\omega'_2$  and then  $\omega'_{12}$ , or  $\omega'_1$  and then  $\omega'_2$ , yielding

$$\begin{aligned} \omega'_2, \text{ then } \omega'_{12}: \quad K \star \tilde{G} &= \tilde{G}_{(123)}^r - \int_{\epsilon_2} \frac{n_{\epsilon_2} n_{-\epsilon_2} \tilde{G}_{i\omega_1}^{\epsilon_2}}{i\omega_2 - \epsilon_2} + \mathcal{O}(\frac{1}{\beta}) \\ \omega'_1, \text{ then } \omega'_2: \quad K \star \tilde{G} &= \tilde{G}_{(123)}^r - \int_{\epsilon_2} \frac{n_{\epsilon_2} n_{-\epsilon_2} \tilde{G}_{i\omega_{12}}^{\epsilon_2}}{i\omega_2 - \epsilon_2} \\ &+ \int_{\epsilon_{12}} \frac{n_{\epsilon_{12}} n_{-\epsilon_{12}} \tilde{G}_{i\omega_1}^{\epsilon_{12}}}{i\omega_{12} - \epsilon_{12}} + \mathcal{O}(\frac{1}{\beta}) \end{aligned} \quad (\text{C18})$$

Equating the two expressions yields a proof for Equation (C17):

$$\begin{aligned}
 & \int_{\varepsilon_2} \frac{n_{\varepsilon_2} n_{-\varepsilon_2} \tilde{G}_{i\omega_{12}}^{\varepsilon_2}}{i\omega_2 - \varepsilon_2} \\
 &= \int_{\varepsilon_2} \frac{n_{\varepsilon_2} n_{-\varepsilon_2} \tilde{G}_{i\omega_1}^{\varepsilon_2}}{i\omega_2 - \varepsilon_2} + \int_{\varepsilon_{12}} \frac{n_{\varepsilon_{12}} n_{-\varepsilon_{12}} \tilde{G}_{i\omega_{12}}^{\varepsilon_{12}}}{i\omega_{12} - \varepsilon_{12}} + \mathcal{O}\left(\frac{1}{\beta}\right) \\
 &= \oint_{z_2} \frac{n_{z_2} n_{-z_2} \tilde{G}_{i\omega_1, z_2}}{i\omega_2 - z_2} + \mathcal{O}\left(\frac{1}{\beta}\right) \\
 &= -\frac{1}{(-\beta)^2} \sum_{i\omega'_2}^{\neq i\omega_2} \frac{\tilde{G}_{i\omega_1, i\omega'_2}}{(i\omega_2 - i\omega'_2)^2} - \frac{1}{12} \tilde{G}_{i\omega_1, i\omega_2} + \mathcal{O}\left(\frac{1}{\beta}\right) \\
 &= \mathcal{O}\left(\frac{1}{\beta}\right) \tag{C19}
 \end{aligned}$$

We obtained the third line by a contour deformation in analogy to the derivation of Equation (C12). Here, the second line can be expressed as a contour integral along the branch cuts at  $\text{Im}(z_2) = 0$  and  $\text{Im}(z_{12}) = 0$  (blue dashed lines in Figure C1a) and the contour in the third line encloses the Matsubara frequencies (blue solid lines in Figure C1a). For the last step, we used Equation (C5).

### C.2.2. Contributions from Anomalous Parts

**Step 1. Matsubara summation through contour integration:** To evaluate Equation (C7b), we first focus on  $\beta \delta_{i\omega'_3} \hat{G}_{3; i\omega'_1}$ , yielding  $\tilde{G}_{3; (123)}^a$  in a decomposition  $\tilde{G}_{(123)}^a = \sum_{i=1}^3 \tilde{G}_{i; (123)}^a$ ; the contributions from  $\tilde{G}_{1; (123)}^a$  and  $\tilde{G}_{2; (123)}^a$  follow from analogous calculations. Then, the imaginary-frequency convolution of the 3p kernel with  $\beta \delta_{i\omega'_3} \hat{G}_{3; i\omega'_1}$  can be rewritten as

$$\begin{aligned}
 \tilde{G}_{3; (123)}^a + \mathcal{O}\left(\frac{1}{\beta}\right) &= K \star \hat{G}_3 \\
 &= \frac{1}{(-\beta)^2} \sum_{i\omega'_1, i\omega'_{12}} \left[ \Delta_{\Omega_{12}} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \right. \\
 &\quad \left. + \delta_{\Omega_{12}} \left( -\Delta_{\Omega_1}^2 - \frac{\beta}{2} \Delta_{\Omega_1} + \frac{\beta^2}{6} \delta_{\Omega_1} \right) \right] \beta \delta_{i\omega'_{12}} \hat{G}_{3; i\omega'_1} \\
 &= -\frac{1}{i\omega_{12}} \frac{1}{(-\beta)} \sum_{i\omega'_1} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \hat{G}_{3; i\omega'_1} \\
 &= -\frac{1}{i\omega_{12}} \frac{1}{(-\beta)} \sum_{i\omega'_1} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \hat{G}_{3; i\omega'_1}^{\Delta} \\
 &\quad - \frac{1}{i\omega_{12}} \frac{1}{(-\beta)} \sum_{i\omega'_1}^{\neq 0} \left( \Delta_{\Omega_1} - \frac{\beta}{2} \delta_{\Omega_1} \right) \frac{\hat{G}_{3; 1}^{\Delta}}{i\omega'_1} \tag{C20}
 \end{aligned}$$

In the second step, we carried out the sum over  $i\omega'_{12}$  and used  $\delta_{\Omega_{12}} \delta_{i\omega'_{12}} = \delta_{i\omega_{12}} \delta_{i\omega'_{12}} = 0$ , since we enforce the external Matsubara frequencies to be nonzero. In the third step, we further split the anomalous part according to Equation (C2).

The sums can be evaluated using Equation (C4) and yield

$$\begin{aligned}
 \tilde{G}_{3; (123)}^a + \mathcal{O}\left(\frac{1}{\beta}\right) &= -\frac{1}{i\omega_{12}} \oint_{z_1} \frac{n_{z_1} \hat{G}_{3; z_1}^{\Delta}}{i\omega_1 - z_1} - \frac{1}{i\omega_{12}} \oint_{z_1} \frac{n_{z_1}}{(i\omega_1 - z_1)} \frac{\hat{G}_{3; 1}^{\Delta}}{z_1} \\
 &\quad + \frac{1}{i\omega_{12}} \text{Res}_{z_1=0} \left( \frac{n_{z_1} \hat{G}_{3; 1}^{\Delta}}{(i\omega_1 - z_1)} \frac{1}{z_1} \right) + \mathcal{O}\left(\frac{1}{\beta}\right) \tag{C21}
 \end{aligned}$$

where we excluded the contribution from  $i\omega'_1 \rightarrow z_1 = 0$  by subtracting the residue.

**Step 2. Extraction of PSFs:** The first contour integral in Equation (C21) can be deformed analogously to the 2p case in Section 3.2. The integrand of the second contour integral only has poles on the imaginary axis since  $\hat{G}_{3; 1}^{\Delta}$  is a constant. Thus, the integral vanishes by closing the contour in the left and right half of the complex  $z_1$  plane. Further evaluating the residue, we then obtain

$$\begin{aligned}
 \tilde{G}_{3; (123)}^a &= -\frac{1}{i\omega_{12}} \int_{\varepsilon_1} \frac{n_{\varepsilon_1} \hat{G}_3^{\Delta; \varepsilon_1}}{i\omega_1 - \varepsilon_1} - \frac{1}{2} \frac{\hat{G}_{3; 1}^{\Delta}}{i\omega_1 i\omega_{12}} \\
 &= \int_{\varepsilon_1, \varepsilon_2} \frac{\hat{\delta}(\varepsilon_{12}) n_{\varepsilon_1} \hat{G}_3^{\Delta; \varepsilon_1} - \frac{1}{2} \hat{\delta}(\varepsilon_1) \hat{\delta}(\varepsilon_{12}) \hat{G}_{3; 1}^{\Delta}}{(i\omega_1 - \varepsilon_1)(i\omega_{12} - \varepsilon_{12})} \tag{C22}
 \end{aligned}$$

where we recovered the form of the spectral representation in Equation (14d) by introducing Dirac delta functions.

Similarly, the contributions from  $\hat{G}_1$ ,  $\hat{G}_2$ , and also  $\hat{G}_{1,2}$  to Equation (C7b) can be derived, leading to the general result

$$\begin{aligned}
 \tilde{G}_{(123)}^a &= \int_{\varepsilon_1, \varepsilon_2} \frac{1}{(i\omega_1 - \varepsilon_1)(i\omega_{12} - \varepsilon_{12})} \\
 &\quad \times \left[ \hat{\delta}(\varepsilon_1) n_{\varepsilon_2} \hat{G}_1^{\Delta; \varepsilon_2} + \hat{\delta}(\varepsilon_2) n_{\varepsilon_1} \hat{G}_2^{\Delta; \varepsilon_1} + \hat{\delta}(\varepsilon_{12}) n_{\varepsilon_1} \hat{G}_3^{\Delta; \varepsilon_1} \right. \\
 &\quad \left. + \hat{\delta}(\varepsilon_1) \hat{\delta}(\varepsilon_2) \left( \hat{G}_{1,2} - \frac{1}{2} \hat{G}_{3; 1}^{\Delta} \right) \right] \tag{C23}
 \end{aligned}$$

Here, only  $\hat{G}_{3; 1}^{\Delta}$  enters, since contributions from  $\hat{G}_{1,2}$  and  $\hat{G}_{2; 1}$  cancel to due Equation (C3).

### C.2.3. Final Result

The main results of the previous sections are Equations (C16) and (C23), yielding the spectral representation for  $\tilde{G}_{(123)} = \tilde{G}_{(123)}^r + \tilde{G}_{(123)}^a$ . The partial MF correlator  $\tilde{G}_p = \tilde{G}_p^r + \tilde{G}_p^a$  for a general permutation  $p$  is then obtained by replacing any index by its permuted counterpart,  $i \rightarrow p(i) = \bar{i}$ . Thus, we obtain our final result

$$\tilde{G}_p(i\omega_p) = \int_{\varepsilon_{\bar{1}}, \varepsilon_{\bar{2}}} \frac{(2\pi i)^2 S_p(\varepsilon_{\bar{1}}, \varepsilon_{\bar{2}})}{(i\omega_{\bar{1}} - \varepsilon_{\bar{1}})(i\omega_{\bar{2}} - \varepsilon_{\bar{2}})} \tag{C24}$$

with the PSFs given by

$$\begin{aligned}
 (2\pi i)^2 S_p(\varepsilon_{\bar{1}}, \varepsilon_{\bar{2}}) &= n_{\varepsilon_{\bar{1}}} n_{\varepsilon_{\bar{2}}} \tilde{G}^{\varepsilon_{\bar{2}}, \varepsilon_{\bar{1}}} + n_{\varepsilon_{\bar{1}}} n_{\varepsilon_{\bar{2}}} \tilde{G}^{\varepsilon_{\bar{1}}, \varepsilon_{\bar{2}}} + \hat{\delta}(\varepsilon_{\bar{1}}) n_{\varepsilon_{\bar{2}}} \hat{G}_{\bar{1}}^{\Delta; \varepsilon_{\bar{2}}} \\
 &\quad + \hat{\delta}(\varepsilon_{\bar{2}}) n_{\varepsilon_{\bar{1}}} \hat{G}_{\bar{2}}^{\Delta; \varepsilon_{\bar{1}}} + \hat{\delta}(\varepsilon_{\bar{1}}) \hat{\delta}(\varepsilon_{\bar{2}}) \left( \hat{G}_{\bar{1}, \bar{2}} - \frac{1}{2} \hat{G}_{\bar{3}; \bar{1}}^{\Delta} \right) \tag{C25}
 \end{aligned}$$

PSFs for all six permutations are recovered by inserting the respective  $\bar{i}$  into above equation. They can be expressed in terms of analytic regions (cf. Figure 4) using

$$\tilde{G}^{\varepsilon_2, \varepsilon_1} = -\tilde{G}^{\varepsilon_1, \varepsilon_2} = -\tilde{G}^{\varepsilon_2, \varepsilon_3} = \tilde{G}^{\varepsilon_1, \varepsilon_3} = \tilde{G}^{[3]} - \tilde{G}^{[1]} - \tilde{G}^{[1]} + \tilde{G}^{[3]} \tag{C26a}$$

$$\tilde{G}^{\varepsilon_1, \varepsilon_2} = -\tilde{G}^{\varepsilon_2, \varepsilon_1} = -\tilde{G}^{\varepsilon_1, \varepsilon_3} = \tilde{G}^{\varepsilon_2, \varepsilon_3} = \tilde{G}^{[3]} - \tilde{G}^{[2]} - \tilde{G}^{[2]} + \tilde{G}^{[3]} \tag{C26b}$$

$$\tilde{G}^{\varepsilon_3, \varepsilon_1} = -\tilde{G}^{\varepsilon_1, \varepsilon_3} = -\tilde{G}^{\varepsilon_3, \varepsilon_2} = \tilde{G}^{\varepsilon_2, \varepsilon_1} = \tilde{G}^{[2]} - \tilde{G}^{[1]} - \tilde{G}^{[1]} + \tilde{G}^{[2]} \tag{C26c}$$

$$\hat{G}_1^{\Delta; \varepsilon_2} = -\hat{G}_1^{\Delta; \varepsilon_3} = \hat{G}_1^{\Delta; [2]} - \hat{G}_1^{\Delta; [3]} \quad (\text{C26d})$$

$$\hat{G}_2^{\Delta; \varepsilon_1} = -\hat{G}_2^{\Delta; \varepsilon_2} = \hat{G}_2^{\Delta; [1]} - \hat{G}_2^{\Delta; [3]} \quad (\text{C26e})$$

$$\hat{G}_3^{\Delta; \varepsilon_1} = -\hat{G}_3^{\Delta; \varepsilon_2} = \hat{G}_3^{\Delta; [1]} - \hat{G}_3^{\Delta; [2]} \quad (\text{C26f})$$

$$\hat{G}_{1;2}^{\Delta} = -\hat{G}_{1;3}^{\Delta} = -\hat{G}_{2;1}^{\Delta} = \hat{G}_{2;3}^{\Delta} = \hat{G}_{3;1}^{\Delta} = -\hat{G}_{3;2}^{\Delta} \quad (\text{C26g})$$

$$\hat{G}_{\bar{1};\bar{2}} = \hat{G}_{1,2} \quad (\text{C26h})$$

with the definitions introduced in Section 5

$$G^{[1]} = \tilde{G}(\varepsilon_1^+, \varepsilon_2^-, \varepsilon_3^-), \quad G^{[1]} = \tilde{G}(\varepsilon_1^-, \varepsilon_2^+, \varepsilon_3^+) \quad (\text{C27a})$$

$$G^{[2]} = \tilde{G}(\varepsilon_1^-, \varepsilon_2^+, \varepsilon_3^-), \quad G^{[2]} = \tilde{G}(\varepsilon_1^+, \varepsilon_2^-, \varepsilon_3^+) \quad (\text{C27b})$$

$$G^{[3]} = \tilde{G}(\varepsilon_1^-, \varepsilon_2^-, \varepsilon_3^+), \quad G^{[3]} = \tilde{G}(\varepsilon_1^+, \varepsilon_2^+, \varepsilon_3^-) \quad (\text{C27c})$$

$$\hat{G}_1^{\Delta; [2]} = \hat{G}_1^{\Delta}(\circ, \varepsilon_2^+, \varepsilon_3^-), \quad \hat{G}_1^{\Delta; [3]} = \hat{G}_1^{\Delta}(\circ, \varepsilon_2^-, \varepsilon_3^+) \quad (\text{C27d})$$

$$\hat{G}_2^{\Delta; [1]} = \hat{G}_1^{\Delta}(\varepsilon_1^+, \circ, \varepsilon_3^-), \quad \hat{G}_2^{\Delta; [3]} = \hat{G}_1^{\Delta}(\varepsilon_1^-, \circ, \varepsilon_3^+) \quad (\text{C27e})$$

$$\hat{G}_3^{\Delta; [1]} = \hat{G}_1^{\Delta}(\varepsilon_1^+, \varepsilon_2^-, \circ), \quad \hat{G}_3^{\Delta; [2]} = \hat{G}_1^{\Delta}(\varepsilon_1^-, \varepsilon_2^+, \circ) \quad (\text{C27f})$$

Here, we have inserted a  $\circ$  at the position of the frequency arguments on which the function does not depend. Note that Equations (C26a)–(C26c) also imply, e.g.,  $\tilde{G}^{\varepsilon_2, \varepsilon_1} = \tilde{G}^{\varepsilon_1, \varepsilon_2} + \tilde{G}^{\varepsilon_3, \varepsilon_1}$ . Relations of this form can be used to simplify PSF (anti)commutators, which appear in Section 5.2.

One additional comment is in order for the regular contributions in Equation (C25). Consider, e.g., permutation  $p = (123)$  and  $n_{\varepsilon_1}$  a bosonic MWF. Then, if the regular contributions  $\tilde{G}^{\varepsilon_2, \varepsilon_1}$  and  $\tilde{G}^{\varepsilon_1, \varepsilon_2}$  contain terms proportional to Dirac  $\delta(\varepsilon_1)$ , the combination  $n_{\varepsilon_1} \delta(\varepsilon_1)$  is ill-defined as the MWF diverges for vanishing frequencies. For their evaluation, however, we can use Equations (C26a)–(C26c) to rewrite

$$\begin{aligned} & (2\pi i)^2 \tilde{S}_{(123)}(\varepsilon_1, \varepsilon_2) \\ &= n_{\varepsilon_1} n_{\varepsilon_2} \tilde{G}^{\varepsilon_2, \varepsilon_1} + n_{\varepsilon_1} n_{\varepsilon_{12}} (\tilde{G}^{\varepsilon_1, \varepsilon_{12}} - \tilde{G}^{\varepsilon_2, \varepsilon_1}) \\ &= -n_{-\varepsilon_2} n_{\varepsilon_{12}} \tilde{G}^{\varepsilon_2, \varepsilon_1} + n_{\varepsilon_1} n_{\varepsilon_{12}} \tilde{G}^{\varepsilon_1, \varepsilon_{12}} \end{aligned} \quad (\text{C28})$$

Here, the first term does not include  $n_{\varepsilon_1}$ , and the discontinuity  $\tilde{G}^{\varepsilon_1, \varepsilon_{12}}$  in the second term does not contain  $\delta(\varepsilon_1)$  contributions (see, e.g., Equations (G10) and discussion thereafter), circumventing the occurrence of bosonic  $n_{\varepsilon_1} \delta(\varepsilon_1)$  contributions.

### C.3. Simplifications for KF Correlators for $\ell = 3$

In the following, we show that the spectral representation of Keldysh components can be recast into a form that is formally equivalent to Equations (19), but more convenient for the purpose of analytic continuation. The new representation enables us to insert the PSFs in Equation (C25) and obtain expressions for the Keldysh components in terms of analytic continuations of MF correlators. This constitutes Step 3 of our three-step strategy.

While the following calculations are demonstrated for explicit examples of 3p KF components, they can be generalized to arbitrary KF components and even to arbitrary  $\ell$ p functions (see Appendix F).

**Table C1.**  $\ell = 3$ : Simplification of the Keldysh kernel (19c) for the KF correlator  $G^{[13]}$  for all permutations by application of the identity (58). For permutations  $p = (123)$  and  $p = (321)$ , manipulations presented in Equation (C30) were performed. Additionally, energy conservation and the constraints enforced by the  $\delta$ -functions allow us to express all denominators through  $\omega_2^-$ .

$p$	$k_p$	$[\eta_1, \eta_2]$	$[\bar{\eta}_1, \bar{\eta}_2]$	$K^{[\eta_1, \eta_2]}(\omega_p) = \tilde{K}(\omega_p^{\eta_1}) - \tilde{K}(\omega_p^{\eta_2})$
(123)	212	[13]	[13]	$\tilde{K}(\omega_{(123)}^{[1]}) - \tilde{K}(\omega_{(123)}^{[3]}) = \hat{\delta}(\omega_1) \frac{1}{\omega_2^-} - \hat{\delta}(\omega_{12}) \frac{1}{\omega_2^-}$
(132)	221	[12]	[13]	$\tilde{K}(\omega_{(132)}^{[1]}) - \tilde{K}(\omega_{(132)}^{[3]}) = -\hat{\delta}(\omega_1) \frac{1}{\omega_2^-}$
(213)	122	[23]	[13]	$\tilde{K}(\omega_{(213)}^{[1]}) - \tilde{K}(\omega_{(213)}^{[3]}) = \hat{\delta}(\omega_{12}) \frac{1}{\omega_2^-}$
(231)	122	[23]	[31]	$\tilde{K}(\omega_{(231)}^{[3]}) - \tilde{K}(\omega_{(231)}^{[1]}) = \hat{\delta}(\omega_1) \frac{1}{\omega_2^-}$
(312)	221	[12]	[31]	$\tilde{K}(\omega_{(312)}^{[3]}) - \tilde{K}(\omega_{(312)}^{[1]}) = -\hat{\delta}(\omega_{12}) \frac{1}{\omega_2^-}$
(321)	212	[13]	[31]	$\tilde{K}(\omega_{(321)}^{[3]}) - \tilde{K}(\omega_{(321)}^{[1]}) = -\hat{\delta}(\omega_1) \frac{1}{\omega_2^-} + \hat{\delta}(\omega_{12}) \frac{1}{\omega_2^-}$

#### C.3.1. Simplifications for KF Correlator $G^{[\eta_1, \eta_2]}$

We begin with outlining the necessary steps to express the KF component  $G^{[\eta_1, \eta_2]}$  in terms of analytically continued MF correlators on the example  $G^{[13]}$ . The simplifications rely on repeated application of identity (58).

The spectral representation in Equations (19) serves as our starting point. As a first step, we bring the Keldysh kernel  $K^{[\eta_1, \eta_2]}$  in a more convenient form, starting with permutation  $p = (123)$ , where  $[\eta_1, \eta_2] = [13]$  and therefore

$$K^{[13]}(\omega_{(123)}) = \tilde{K}(\omega_{(123)}^{[1]}) - \tilde{K}(\omega_{(123)}^{[3]}) = \frac{1}{\omega_1^{[1]} \omega_{12}^{[1]}} - \frac{1}{\omega_1^{[3]} \omega_{12}^{[3]}} \quad (\text{C29})$$

In the first term, all frequency combinations in the denominator acquire a positive imaginary shift, whereas in the second term they obtain a negative imaginary shift. Adding and subtracting  $1/(\omega_1^{[1]} \omega_{12}^{[3]})$ , identity (58) leads to

$$\begin{aligned} K^{[13]}(\omega_{(123)}) &= \left( \frac{1}{\omega_1^{[1]}} - \frac{1}{\omega_1^{[3]}} \right) \frac{1}{\omega_{12}^{[3]}} + \left( \frac{1}{\omega_1^{[1]}} - \frac{1}{\omega_1^{[3]}} \right) \frac{1}{\omega_1^{[1]}} \\ &= \hat{\delta}(\omega_1) \frac{1}{\omega_2^-} + \hat{\delta}(\omega_{12}) \frac{1}{\omega_1^+} \end{aligned} \quad (\text{C30})$$

The kernels for all other permutations can be simplified in a similar manner, and the results are summarized in Table C1. Collecting all contributions proportional to either  $\hat{\delta}(\omega_1)/\omega_2^-$  or  $\hat{\delta}(\omega_{12})/\omega_2^-$  yields Equation (75). The PSF (anti)commutators therein are evaluated using the relations in Equations (C26) and result in

$$S_{[1, [2, 3]_+]} = S_{(123)} - S_{(132)} + S_{(231)} - S_{(321)} \quad (\text{C31a})$$

$$= N_{\varepsilon_1} \tilde{G}^{\varepsilon_1, \varepsilon_2} - 2\hat{\delta}(\varepsilon_1) \hat{G}_1^{\Delta; \varepsilon_2} - 2\hat{\delta}(\varepsilon_1) \hat{\delta}(\varepsilon_2) \hat{G}_{1;2}^{\Delta}$$

$$S_{[[1, 2]_+, 3]} = S_{(123)} - S_{(213)} + S_{(312)} - S_{(321)} \quad (\text{C31b})$$

$$= -N_{\varepsilon_{12}} \tilde{G}^{\varepsilon_{12}, \varepsilon_2} + 2\hat{\delta}(\varepsilon_{12}) \hat{G}_3^{\Delta; \varepsilon_2} + 2\hat{\delta}(\varepsilon_1) \hat{\delta}(\varepsilon_2) \hat{G}_{3;2}^{\Delta}$$

where we suppressed the frequency arguments of the PSFs.

#### C.3.2. Simplifications for KF Correlator $G^{[\eta_1, \eta_2, \eta_3]}$

In Section 5.2.2 it was pointed out that the Keldysh component  $G^{[123]}$  can be computed by subtracting a fully retarded correlator, e.g.  $G^{[3]}$ , in order to reuse identity (58).

**Table C2.**  $\ell = 3$ : Keldysh kernel for  $G^{[123]} - G^{[3]}$  in Equation (C32), evaluated for all permutations.

$p$	Kernel of $G^{[123]} - G^{[3]}$
(123)	$K^{[123]}(\omega_{(123)}) - \tilde{K}(\omega_{(123)}^{[3]}) = \hat{\delta}(\omega_1)\hat{\delta}(\omega_2) + \hat{\delta}(\omega_1)\frac{1}{\omega_2^-}$
(132)	$K^{[123]}(\omega_{(132)}) - \tilde{K}(\omega_{(132)}^{[3]}) = -\hat{\delta}(\omega_1)\frac{1}{\omega_2^-} - \hat{\delta}(\omega_2)\frac{1}{\omega_1^-}$
(213)	$K^{[123]}(\omega_{(213)}) - \tilde{K}(\omega_{(213)}^{[3]}) = \hat{\delta}(\omega_1)\hat{\delta}(\omega_2) + \hat{\delta}(\omega_2)\frac{1}{\omega_1^-}$
(231)	$K^{[123]}(\omega_{(231)}) - \tilde{K}(\omega_{(231)}^{[3]}) = -\hat{\delta}(\omega_2)\frac{1}{\omega_1^-} - \hat{\delta}(\omega_1)\frac{1}{\omega_2^-}$
(312)	$K^{[123]}(\omega_{(312)}) - \tilde{K}(\omega_{(312)}^{[3]}) = \hat{\delta}(\omega_1)\hat{\delta}(\omega_2) + \hat{\delta}(\omega_2)\frac{1}{\omega_1^-}$
(321)	$K^{[123]}(\omega_{(321)}) - \tilde{K}(\omega_{(321)}^{[3]}) = \hat{\delta}(\omega_1)\hat{\delta}(\omega_2) + \hat{\delta}(\omega_1)\frac{1}{\omega_2^-}$

The kernel of  $G^{[3]}$  is simply given by  $K^{[3]}(\omega_p) = \tilde{K}(\omega_p^{[3]})$  and therefore permutation independent, as discussed before Equation (23). Since  $G^{[123]} = G^{222}$  implies  $k_p = 222$  and consequently  $[\hat{\eta}_1\hat{\eta}_2\hat{\eta}_3] = [123]$  for any permutation, the kernel for  $G^{[123]} - G^{[3]}$  reads

$$K^{[123]}(\omega_p) - K^{[3]}(\omega_p) = \tilde{K}(\omega_p^{[1]}) - \tilde{K}(\omega_p^{[2]}) + \tilde{K}(\omega_p^{[3]}) - \tilde{K}(\omega_p^{[3]}) \quad (\text{C32})$$

and therefore the effect of subtracting  $G^{[3]}$  is permutation dependent.

We first consider permutation  $p = (123)$ , for which the difference of kernels simplifies to

$$\begin{aligned} K^{[123]}(\omega_{(123)}) - K^{[3]}(\omega_{(123)}) &= \tilde{K}(\omega_{(123)}^{[1]}) - \tilde{K}(\omega_{(123)}^{[2]}) \\ &= \frac{1}{\omega_1^{[1]}\omega_{12}^{[1]}} - \frac{1}{\omega_1^{[2]}\omega_{12}^{[2]}} = \hat{\delta}(\omega_1)\frac{1}{\omega_2^+} \end{aligned} \quad (\text{C33})$$

In the last step, we were able to use Equation (58) again, set  $\omega_{12}^{[1]} = \omega_{12}^{[2]} = \omega_{12}^+$ , and reduced  $\omega_{12} = \omega_2$  due to the  $\delta$ -function. For the comparison to kernels of other permutations, it is convenient to additionally add and subtract  $\hat{\delta}(\omega_1)/\omega_2^-$  to obtain

$$K^{[123]}(\omega_{(123)}) - K^{[3]}(\omega_{(123)}) = \hat{\delta}(\omega_1)\hat{\delta}(\omega_2) + \hat{\delta}(\omega_1)\frac{1}{\omega_2^-} \quad (\text{C34})$$

For permutation  $p = (132)$ , Equation (C32) yields

$$\begin{aligned} \tilde{K}(\omega_{(132)}^{[1]}) - \tilde{K}(\omega_{(132)}^{[3]}) + \tilde{K}(\omega_{(132)}^{[2]}) - \tilde{K}(\omega_{(132)}^{[3]}) \\ = \hat{\delta}(\omega_1)\frac{1}{\omega_3^+} - \hat{\delta}(\omega_{13})\frac{1}{\omega_1^-} \end{aligned} \quad (\text{C35})$$

Using  $\omega_3^+ = -\omega_2^-$  due to energy conservation and the  $\delta$ -function, the first term matches the second term in Equation (C34). Therefore, PSFs of permutations  $p = (123), (132)$  can be expressed through PSF (anti)commutators as in the previous section, motivating the manipulation from Equation (C33) to (C34).

A summary of the kernels for all permutations is given in Table C2. In these kernels, a total of three unique terms occur, given by  $\hat{\delta}(\omega_1)\hat{\delta}(\omega_2)$ ,  $\hat{\delta}(\omega_1)/\omega_2^-$ , or  $\hat{\delta}(\omega_2)/\omega_1^-$ . Collecting all PSFs convoluted with the same expressions gives Equation (81), with the PSF (anti)commutators evaluating to

$$\begin{aligned} S_{[[1,2]_+,3]_+}(\epsilon_1, \epsilon_2) &= (1 + N_{\epsilon_1}N_{\epsilon_2})\tilde{G}^{\epsilon_2, \epsilon_1} + N_{\epsilon_{12}}N_{\epsilon_1}\tilde{G}^{\epsilon_{12}, \epsilon_1} \\ &\quad - 2\hat{\delta}(\epsilon_1)N_{\epsilon_2}\hat{G}_1^{\Delta; \epsilon_2} - 2\hat{\delta}(\epsilon_2)N_{\epsilon_1}\hat{G}_2^{\Delta; \epsilon_1} \\ &\quad - 2\hat{\delta}(\epsilon_{12})N_{\epsilon_1}\hat{G}_3^{\Delta; \epsilon_1} + 4\hat{\delta}(\epsilon_1)\hat{\delta}(\epsilon_2)\hat{G}_{1,2}, \end{aligned}$$

$$\begin{aligned} S_{[1,[2,3]_-]}(\epsilon_1, \epsilon_2) &= \tilde{G}^{\epsilon_1, \epsilon_2}, \\ S_{[2,[1,3]_-]}(\epsilon_2, \epsilon_1) &= \tilde{G}^{\epsilon_2, \epsilon_1} \end{aligned} \quad (\text{C36})$$

This concludes our appendix on additional computations for the analytic continuation of 3p correlators.

## Appendix D: Partial MF 4p Correlators

In this appendix, we discuss purely fermionic partial MF 4p correlators. However, we do not display explicit calculations here. Rather, we introduce an iterative procedure to derive the structure of 4p PSFs from 3p PSFs, based on our insights from 2p and 3p calculations. For a general fermionic MF 4p correlator, only the sums of two fermionic frequencies result in bosonic frequencies, which, in turn, might lead to anomalous terms. According to Equation (A5), the general form of the correlator thus reads

$$\begin{aligned} G_{i\omega_1, i\omega_2, i\omega_3} &= \tilde{G}_{i\omega_1, i\omega_2, i\omega_3} + \beta\delta_{i\omega_{12}}\hat{G}_{12; i\omega_1, i\omega_3} \\ &\quad + \beta\delta_{i\omega_{13}}\hat{G}_{13; i\omega_1, i\omega_2} + \beta\delta_{i\omega_{23}}\hat{G}_{23; i\omega_1, i\omega_2} \end{aligned} \quad (\text{D1})$$

### D.1. Regular Contributions

Step 1. *Matsubara summation through contour integration*: To derive partial MF 4p correlators, we insert Equation (D1) and the singularity-free 4p kernel (Equation (A2c)) into Equation (31):

$$\tilde{G}_{(1234)}(i\omega_{(1234)}) + \mathcal{O}\left(\frac{1}{\beta}\right) = [K \star G](i\omega_{(1234)}) \quad (\text{D2})$$

Here, we again consider the permutation  $p = (1234)$  first, before obtaining the general result by replacing all indices  $i \rightarrow \bar{i}$ . By repeated use of the identities in Equations (C4) and (C5), together with the analogously proven new identity

$$\frac{1}{(-\beta)^3} \sum_{i\omega'} \Delta_{i\omega-i\omega'}^3 \tilde{f}(i\omega') = \mathcal{O}\left(\frac{1}{\beta}\right) \quad (\text{D3})$$

the imaginary-frequency convolution can again be expressed through contour integrals. Focusing on the regular contribution to the correlator,  $\tilde{G}$ , first, we indeed recover Equation (39) for  $\ell = 4$ :

$$\begin{aligned} \tilde{G}_{(1234)}^r(i\omega_{(1234)}) + \mathcal{O}\left(\frac{1}{\beta}\right) &= [K \star \tilde{G}](i\omega_{(1234)}) \\ &= \oint_{z_1} \oint_{z_{12}} \oint_{z_{123}} \frac{n_{z_1} n_{z_{12}} n_{z_{123}} \tilde{G}_{z_1, z_{12}, z_{123}}}{(i\omega_1 - z_1)(i\omega_{12} - z_{12})(i\omega_{123} - z_{123})} \end{aligned} \quad (\text{D4})$$

Step 2. *Extraction of PSFs*: For the deformation of the contour, it is instructive to recapitulate the 2p and 3p results for the regular contributions to the PSFs. As a function of complex frequencies, a general 2p MF correlator  $\tilde{G}_{z_1} = \tilde{G}(z_1, -z_1)$  has one possible branch cut defined by  $\text{Im}(z_1) = 0$ , resulting in

$$(2\pi i)S_{(12)}^r(\epsilon_1) = n_{\epsilon_1}\tilde{G}^{\epsilon_1} \quad (\text{D5})$$

In the 3p case, the additional frequency dependence of  $\tilde{G}_{z_1, z_{12}} = \tilde{G}(z_1, z_{12} - z_1, -z_{12})$  introduces two further branch cuts at  $\text{Im}(z_{12}) = 0$  and  $\text{Im}(z_{12} - z_1) = 0$ , additionally to  $\text{Im}(z_1) = 0$ . According to Equation (C10), the contour of  $\tilde{G}_{z_1, z_{12}}^r$  is deformed first, taking account of the latter two out of the three branch cuts. This yields a sum of the discontinuities  $\tilde{G}_{z_1}^{\epsilon_{12}}$  and  $\tilde{G}_{z_1}^{\epsilon_2}$ , multiplied with the respective MWFs (Equation (C12)). The

subsequent contour deformation of  $\oint_{z_1}$  reduces to an effective 2p calculation, i.e., only the branch cut at  $\text{Im}(z_1) = 0$  remains, resulting in

$$(2\pi i)^2 S_{(123)}^r(\varepsilon_1, \varepsilon_2) = n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_2, \varepsilon_1} + n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{12}, \varepsilon_1} \quad (D6)$$

with the discontinuity in  $\varepsilon_1$  to the right of  $\varepsilon_2$  and  $\varepsilon_{12}$ .

In the 4p case, the new frequency  $z_{123}$  generates four additional branch cuts (see discussion in Section 4.1), defined by vanishing  $\text{Im}(z_{123})$ ,  $\text{Im}(z_{123} - z_1)$ ,  $\text{Im}(z_{123} - z_{12})$  or  $\text{Im}(z_{123} - z_{12} + z_1)$ , yielding a total of seven possible branch cuts together with  $\text{Im}(z_{12}) = 0$ ,  $\text{Im}(z_{12} - z_1) = 0$ , and  $\text{Im}(z_1) = 0$  from the 3p case. Since  $\oint_{z_{123}}$  is deformed first according to Equation (D4), the four new branch cuts are taken into account via a sum of the discontinuities  $\tilde{G}_{z_{12}, z_1}^{\varepsilon_3}$ ,  $\tilde{G}_{z_{12}, z_1}^{\varepsilon_{123}}$ ,  $\tilde{G}_{z_{12}, z_1}^{\varepsilon_{13}}$ , and  $\tilde{G}_{z_{12}, z_1}^{\varepsilon_{23}}$ , multiplied with the respective MWFs. For each of these discontinuities, the subsequent contour deformations of  $\oint_{z_{12}}$  and  $\oint_{z_1}$  reduces to an effective 3p calculation. Consequently, we obtain

$$(2\pi i)^3 S_{(1234)}^r(\varepsilon_1, \varepsilon_2, \varepsilon_3) = n_{\varepsilon_3} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_3, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{123}} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{123}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{13}} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{13}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{23}} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{23}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_3} n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_3, \varepsilon_{12}, \varepsilon_1} + n_{\varepsilon_{123}} n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{123}, \varepsilon_{12}, \varepsilon_1} + n_{\varepsilon_{13}} n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{13}, \varepsilon_{12}, \varepsilon_1} + n_{\varepsilon_{23}} n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{23}, \varepsilon_{12}, \varepsilon_1} \quad (D7)$$

We have also checked this result by explicit contour deformations in Equation (D4). There, the poles of the denominators can be ignored since they only contribute at order  $\mathcal{O}(\frac{1}{\beta})$ , similarly to Equation (C17) in the 3p case. To further simplify Equation (D7), we note that, for fermionic 4p correlators, two consecutive bosonic discontinuities have to vanish, i.e.,  $\tilde{G}^{\varepsilon_{13}, \varepsilon_{12}, \varepsilon_1} = \tilde{G}^{\varepsilon_{23}, \varepsilon_{12}, \varepsilon_1} = 0$ , since their kernels carry one bosonic argument only (see Appendix E.1 for further details).

## D.2. Anomalous Contributions

We do not present the derivations of the anomalous contributions of  $G$  to Equation (D2) explicitly here, as these correspond to 3p calculations. There is one crucial difference, however. The anomalous kernel in Equation (A4c) for the fermionic 4p case reduces to

$$\hat{K}_p^{\text{alt}}(\mathbf{Q}_p) = -\frac{\beta}{2} \delta_{i\omega_1 - \varepsilon_{12}} \frac{1}{(i\omega_1 - \varepsilon_1)(i\omega_3 - \varepsilon_3)} \quad (D8)$$

and thus only depends on fermionic Matsubara frequencies. Therefore, anomalous terms such as  $\hat{G}_{13; i\omega_1, i\omega_2}$  only depend on the frequencies  $i\omega_1$  and  $i\omega_2$  separately, but not on their sum  $i\omega_{12}$ . In the complex frequency plain, this implies that  $\hat{G}_{13; z_1, z_2}$  has branch cuts only for  $\text{Im}(z_1) = 0$  and  $\text{Im}(z_2) = 0$ , but not for  $\text{Im}(z_{12}) = 0$ , in contrast to the regular 3p case. Additionally, since the denominators in Equation (D8) are non-singular due to the fermionic Matsubara frequencies, we need not distinguish the anomalous contributions by factors of  $\Delta_{i\omega}$ , e.g., splitting  $\hat{G}_{13}$  into  $\hat{G}_{13}^{\Delta}$  and  $\hat{G}_{13}^{\Delta}$  terms, as was the case for 3p functions (Equation (C2)).

## D.3. Final Result

Finally, the fermionic partial 4p correlators for general permutations  $p$  is obtained from the full correlator via

$$\tilde{G}_p(i\omega_p) = \int_{\varepsilon_1, \varepsilon_2, \varepsilon_3} \frac{(2\pi i)^3 S_p(\varepsilon_1, \varepsilon_2, \varepsilon_3)}{(i\omega_1 - \varepsilon_1)(i\omega_2 - \varepsilon_2)(i\omega_3 - \varepsilon_3)} \quad (D9)$$

with the PSFs given by

$$(2\pi i)^3 S_p(\varepsilon_1, \varepsilon_2, \varepsilon_3) = n_{\varepsilon_3} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_3, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{123}} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{123}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{13}} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{13}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{23}} n_{\varepsilon_2} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{23}, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_3} n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_3, \varepsilon_{12}, \varepsilon_1} + n_{\varepsilon_{123}} n_{\varepsilon_{12}} n_{\varepsilon_1} \tilde{G}^{\varepsilon_{123}, \varepsilon_{12}, \varepsilon_1} + n_{\varepsilon_3} n_{\varepsilon_1} \delta(\varepsilon_{12}) \hat{G}_{12}^{\varepsilon_3, \varepsilon_1} + n_{\varepsilon_2} n_{\varepsilon_1} \delta(\varepsilon_{13}) \hat{G}_{13}^{\varepsilon_2, \varepsilon_1} + n_{\varepsilon_2} n_{\varepsilon_1} \delta(\varepsilon_{23}) \hat{G}_{23}^{\varepsilon_2, \varepsilon_1} \quad (D10)$$

For the anomalous parts, the order of discontinuities does not matter, as, e.g.,  $\hat{G}_{12}^{\varepsilon_3, \varepsilon_1} = \hat{G}_{12}^{\varepsilon_1, \varepsilon_3}$ .

For completeness, we express the discontinuities in Equation (D10) in terms of analytic regions according to their definition in Section 6.1. This gives

$$\tilde{C}^{\varepsilon_1, \varepsilon_2, \varepsilon_3} = -\tilde{C}^{\varepsilon_{234}, \varepsilon_2, \varepsilon_3} = -\tilde{C}^{\varepsilon_1, \varepsilon_2, \varepsilon_4} = \tilde{C}^{\varepsilon_{234}, \varepsilon_2, \varepsilon_4} = -\tilde{C}^{\varepsilon_1, \varepsilon_34, \varepsilon_3} = \tilde{C}^{\varepsilon_{234}, \varepsilon_34, \varepsilon_3} = \tilde{C}^{\varepsilon_1, \varepsilon_34, \varepsilon_4} = -\tilde{C}^{\varepsilon_{234}, \varepsilon_34, \varepsilon_4} = C^{(3)} - C^{(4)} + C^{(123)} - C^{(124)} - C_{||}^{(13)} + C_{||}^{(14)} - C_{||}^{(23)} + C_{||}^{(24)} \quad (D11a)$$

$$\tilde{C}^{\varepsilon_1, \varepsilon_3, \varepsilon_2} = -\tilde{C}^{\varepsilon_{234}, \varepsilon_3, \varepsilon_2} = -\tilde{C}^{\varepsilon_1, \varepsilon_3, \varepsilon_4} = \tilde{C}^{\varepsilon_{234}, \varepsilon_3, \varepsilon_4} = -\tilde{C}^{\varepsilon_1, \varepsilon_24, \varepsilon_2} = \tilde{C}^{\varepsilon_{234}, \varepsilon_24, \varepsilon_2} = \tilde{C}^{\varepsilon_1, \varepsilon_24, \varepsilon_4} = -\tilde{C}^{\varepsilon_{234}, \varepsilon_24, \varepsilon_4} = C^{(2)} - C^{(4)} + C^{(123)} - C^{(134)} - C_{||}^{(12)} + C_{||}^{(14)} - C_{||}^{(23)} + C_{||}^{(34)} \quad (D11b)$$

$$\tilde{C}^{\varepsilon_1, \varepsilon_4, \varepsilon_2} = -\tilde{C}^{\varepsilon_{234}, \varepsilon_4, \varepsilon_2} = -\tilde{C}^{\varepsilon_1, \varepsilon_4, \varepsilon_3} = \tilde{C}^{\varepsilon_{234}, \varepsilon_4, \varepsilon_3} = -\tilde{C}^{\varepsilon_1, \varepsilon_23, \varepsilon_2} = \tilde{C}^{\varepsilon_{234}, \varepsilon_23, \varepsilon_2} = \tilde{C}^{\varepsilon_1, \varepsilon_23, \varepsilon_3} = -\tilde{C}^{\varepsilon_{234}, \varepsilon_23, \varepsilon_3} = C^{(2)} - C^{(3)} + C^{(124)} - C^{(134)} - C_{||}^{(12)} + C_{||}^{(13)} - C_{||}^{(24)} + C_{||}^{(34)} \quad (D11c)$$

$$\tilde{C}^{\varepsilon_2, \varepsilon_1, \varepsilon_3} = -\tilde{C}^{\varepsilon_{134}, \varepsilon_1, \varepsilon_3} = -\tilde{C}^{\varepsilon_2, \varepsilon_1, \varepsilon_4} = \tilde{C}^{\varepsilon_{134}, \varepsilon_1, \varepsilon_4} = -\tilde{C}^{\varepsilon_2, \varepsilon_34, \varepsilon_3} = \tilde{C}^{\varepsilon_{134}, \varepsilon_34, \varepsilon_3} = \tilde{C}^{\varepsilon_2, \varepsilon_34, \varepsilon_4} = -\tilde{C}^{\varepsilon_{134}, \varepsilon_34, \varepsilon_4} = C^{(3)} - C^{(4)} + C^{(123)} - C^{(124)} - C_{||}^{(12)} + C_{||}^{(14)} - C_{||}^{(23)} + C_{||}^{(24)} \quad (D11d)$$

$$\tilde{C}^{\varepsilon_3, \varepsilon_1, \varepsilon_2} = -\tilde{C}^{\varepsilon_{124}, \varepsilon_1, \varepsilon_2} = -\tilde{C}^{\varepsilon_3, \varepsilon_1, \varepsilon_4} = \tilde{C}^{\varepsilon_{124}, \varepsilon_1, \varepsilon_4} = -\tilde{C}^{\varepsilon_3, \varepsilon_24, \varepsilon_2} = \tilde{C}^{\varepsilon_{124}, \varepsilon_24, \varepsilon_2} = \tilde{C}^{\varepsilon_3, \varepsilon_24, \varepsilon_4} = -\tilde{C}^{\varepsilon_{124}, \varepsilon_24, \varepsilon_4} = C^{(2)} - C^{(4)} + C^{(123)} - C^{(134)} - C_{||}^{(12)} + C_{||}^{(14)} + C_{||}^{(34)} - C_{||}^{(23)} \quad (D11e)$$

$$\tilde{C}^{\varepsilon_4, \varepsilon_1, \varepsilon_2} = -\tilde{C}^{\varepsilon_{123}, \varepsilon_1, \varepsilon_2} = -\tilde{C}^{\varepsilon_4, \varepsilon_1, \varepsilon_3} = \tilde{C}^{\varepsilon_{123}, \varepsilon_1, \varepsilon_3} = -\tilde{C}^{\varepsilon_4, \varepsilon_23, \varepsilon_2} = \tilde{C}^{\varepsilon_{123}, \varepsilon_23, \varepsilon_2} = \tilde{C}^{\varepsilon_4, \varepsilon_23, \varepsilon_3} = -\tilde{C}^{\varepsilon_{123}, \varepsilon_23, \varepsilon_3} = C^{(2)} - C^{(3)} + C^{(124)} - C^{(134)} - C_{||}^{(12)} + C_{||}^{(13)} - C_{||}^{(24)} + C_{||}^{(34)} \quad (D11f)$$

$$\tilde{C}^{\varepsilon_2, \varepsilon_3, \varepsilon_1} = -\tilde{C}^{\varepsilon_{134}, \varepsilon_3, \varepsilon_1} = -\tilde{C}^{\varepsilon_2, \varepsilon_3, \varepsilon_4} = \tilde{C}^{\varepsilon_{134}, \varepsilon_3, \varepsilon_4} = -\tilde{C}^{\varepsilon_2, \varepsilon_14, \varepsilon_1} = \tilde{C}^{\varepsilon_{134}, \varepsilon_14, \varepsilon_1} = \tilde{C}^{\varepsilon_2, \varepsilon_14, \varepsilon_4} = -\tilde{C}^{\varepsilon_{134}, \varepsilon_14, \varepsilon_4} = C^{(1)} - C^{(4)} + C^{(123)} - C^{(234)} - C_{||}^{(12)} + C_{||}^{(34)} - C_{||}^{(13)} + C_{||}^{(24)} \quad (D11g)$$



The discontinuities in the anomalous parts Equation (D10) read

$$\hat{G}_{12}^{\varepsilon_1, \varepsilon_3} = -\hat{G}_{12}^{\varepsilon_2, \varepsilon_3} = -\hat{G}_{12}^{\varepsilon_1, \varepsilon_4} = \hat{G}_{12}^{\varepsilon_2, \varepsilon_4} = \hat{C}_{12}^{(13)} - \hat{C}_{12}^{(14)} - \hat{C}_{12}^{(23)} + \hat{C}_{12}^{(24)} \quad (\text{D13a})$$

$$\hat{G}_{13}^{\varepsilon_1, \varepsilon_2} = -\hat{G}_{13}^{\varepsilon_3, \varepsilon_2} = -\hat{G}_{13}^{\varepsilon_1, \varepsilon_4} = \hat{G}_{13}^{\varepsilon_3, \varepsilon_4} = \hat{C}_{13}^{(12)} - \hat{C}_{13}^{(14)} - \hat{C}_{13}^{(23)} + \hat{C}_{13}^{(34)} \quad (\text{D13b})$$

$$\hat{G}_{14}^{\varepsilon_1, \varepsilon_2} = -\hat{G}_{14}^{\varepsilon_4, \varepsilon_2} = -\hat{G}_{14}^{\varepsilon_1, \varepsilon_3} = \hat{G}_{14}^{\varepsilon_4, \varepsilon_3} = \hat{C}_{14}^{(12)} - \hat{C}_{14}^{(13)} - \hat{C}_{14}^{(24)} + \hat{C}_{14}^{(34)} \quad (\text{D13c})$$

with

$$\begin{aligned} \hat{C}_{12}^{(13)} &= \hat{G}_{12}(\varepsilon_1^+, \varepsilon_2^-, \varepsilon_3^+, \varepsilon_4^-), & \hat{C}_{12}^{(24)} &= \hat{G}_{12}(\varepsilon_1^-, \varepsilon_2^+, \varepsilon_3^-, \varepsilon_4^+), \\ \hat{C}_{12}^{(14)} &= \hat{G}_{12}(\varepsilon_1^+, \varepsilon_2^-, \varepsilon_3^-, \varepsilon_4^+), & \hat{C}_{12}^{(23)} &= \hat{G}_{12}(\varepsilon_1^-, \varepsilon_2^+, \varepsilon_3^+, \varepsilon_4^-), \\ \hat{C}_{13}^{(12)} &= \hat{G}_{13}(\varepsilon_1^+, \varepsilon_2^+, \varepsilon_3^-, \varepsilon_4^-), & \hat{C}_{13}^{(34)} &= \hat{G}_{13}(\varepsilon_1^-, \varepsilon_2^-, \varepsilon_3^+, \varepsilon_4^+), \\ \hat{C}_{13}^{(14)} &= \hat{G}_{13}(\varepsilon_1^+, \varepsilon_2^-, \varepsilon_3^-, \varepsilon_4^+), & \hat{C}_{13}^{(23)} &= \hat{G}_{13}(\varepsilon_1^-, \varepsilon_2^+, \varepsilon_3^+, \varepsilon_4^-), \\ \hat{C}_{14}^{(12)} &= \hat{G}_{14}(\varepsilon_1^+, \varepsilon_2^+, \varepsilon_3^-, \varepsilon_4^-), & \hat{C}_{14}^{(34)} &= \hat{G}_{14}(\varepsilon_1^-, \varepsilon_2^-, \varepsilon_3^+, \varepsilon_4^+), \\ \hat{C}_{14}^{(13)} &= \hat{G}_{14}(\varepsilon_1^+, \varepsilon_2^-, \varepsilon_3^+, \varepsilon_4^-), & \hat{C}_{14}^{(24)} &= \hat{G}_{14}(\varepsilon_1^-, \varepsilon_2^+, \varepsilon_3^-, \varepsilon_4^+) \end{aligned} \quad (\text{D14})$$

The remaining terms follow from  $\hat{C}_{34} = \hat{G}_{12}$ ,  $\hat{G}_{24} = \hat{G}_{13}$ , and  $\hat{G}_{23} = \hat{G}_{14}$ .

## Appendix E: Additional Spectral Representations

In this appendix, we derive spectral representations for discontinuities (Appendix E.1) and for anomalous parts (Appendix E.2) for general  $\ell$ . These are used in Appendix F.2 to relate Keldysh components  $G^{[n_1 n_2]}$  to discontinuities of regular parts and analytic continuations of anomalous parts, resulting in Equation (95) in Section 6.2.1. Additionally, they serve as a key ingredient in Appendix G for consistency checks performed on our results for the 2p, 3p, and 4p PSFs, where we express all occurring discontinuities through PSF (anti)commutators. We use the notation introduced in the beginning of Section 6.2 throughout this appendix.

### E.1. Spectral Representation of Discontinuities

Here, we focus on the discontinuities of the regular MF correlator  $\tilde{G}$ , as introduced in Section 4. The results carry over to anomalous contributions  $\hat{G}$ , as presented in Appendix E.2. We first consider discontinuities of 3p correlators (Appendix E.1.1) and then their generalization to arbitrary  $\ell$  (Appendix E.1.2).

#### E.1.1. Example for $\ell = 3$

Let us consider the discontinuity in Equation (69) as an example for  $\ell = 3$ . Inserting the spectral representation in Equations (14) yields

$$\begin{aligned} \frac{1}{(2\pi i)^2} \tilde{G}_{\omega_1^+}^{\omega_2} &= \frac{1}{(2\pi i)^2} \left( \tilde{G}_{\omega_2^+, \omega_1^+} - \tilde{G}_{\omega_2^-, \omega_1^+} \right) \\ &= \int_{\varepsilon_1} \int_{\varepsilon_2} \int_{\varepsilon_3} \delta(\varepsilon_{123}) \\ &\quad \times \frac{1}{\omega_1^+ - \varepsilon_1} \left[ \frac{1}{\omega_{13}^- - \varepsilon_{13}} - \frac{1}{\omega_{13}^+ - \varepsilon_{13}} \right] S_{(132)}(\varepsilon_1, \varepsilon_3) \end{aligned}$$

$$\begin{aligned} &+ \frac{1}{\omega_{12}^+ - \varepsilon_{12}} \left[ \frac{1}{\omega_2^+ - \varepsilon_2} - \frac{1}{\omega_2^- - \varepsilon_2} \right] S_{(213)}(\varepsilon_2, \varepsilon_1) \\ &+ \frac{1}{\omega_{23}^- - \varepsilon_{23}} \left[ \frac{1}{\omega_2^+ - \varepsilon_2} - \frac{1}{\omega_2^- - \varepsilon_2} \right] S_{(231)}(\varepsilon_2, \varepsilon_3) \\ &+ \frac{1}{\omega_3^- - \varepsilon_3} \left[ \frac{1}{\omega_{13}^- - \varepsilon_{13}} - \frac{1}{\omega_{13}^+ - \varepsilon_{13}} \right] S_{(312)}(\varepsilon_3, \varepsilon_1) \\ &= \int_{\varepsilon_1} \int_{\varepsilon_2} \int_{\varepsilon_3} \delta(\varepsilon_{123}) \left[ \hat{\delta}(\omega_2 - \varepsilon_2) \frac{1}{\omega_1^+ - \varepsilon_1} S_{[2,13]_-}(\varepsilon_1, \varepsilon_2, \varepsilon_3) \right. \\ &\quad \left. + \hat{\delta}(\omega_2 - \varepsilon_2) \frac{1}{\omega_3^- - \varepsilon_3} S_{[2,31]_-}(\varepsilon_1, \varepsilon_2, \varepsilon_3) \right] \\ &= - \int_{\varepsilon_1} \frac{1}{\omega_1^+ - \varepsilon_1} S_{[2,[1,3]_-]_-}(\varepsilon_1, \omega_2, -\varepsilon_1 - \omega_2) \quad (\text{E1}) \end{aligned}$$

where we used the identity (58) and energy conservation. The permutations  $p = (123)$ ,  $(321)$  do not contribute to the discontinuity as their kernels only depend on the external frequencies  $\omega_1^+$  and  $\omega_3^-$  with imaginary parts independent of  $\omega_2^\pm$ .

For the discontinuity  $\tilde{G}^{\omega_2, \omega_1} = \tilde{G}_{\omega_1^+}^{\omega_2} - \tilde{G}_{\omega_1^-}^{\omega_2}$ , Equation (E1) yields

$$\begin{aligned} \tilde{G}^{\omega_2, \omega_1} &= (2\pi i)^2 S_{[2,[1,3]_-]_-}(\omega), \\ \tilde{G}^{\omega_{12}, \omega_1} &= (2\pi i)^2 S_{[[1,2]_-, 3]_-}(\omega) \end{aligned} \quad (\text{E2})$$

The second identity for  $\tilde{G}^{\omega_{12}, \omega_1}$  follows from a similar derivation as for  $\tilde{G}^{\omega_2, \omega_1}$ . Note that the above relations hold for permuted indices as well (see Equation (G11)). Thus, consecutive discontinuities eventually give a (nested) commutator of PSFs. For  $\ell = 2$ , this corresponds to the standard spectral function,  $-\tilde{G}^{\omega_1} = (2\pi i) S_{[1,2]_-} = (2\pi i) S^{\text{std}}$ .

#### E.1.2. Generalization to Arbitrary $\ell$

For general  $\ell$ p functions, the discontinuity in Equation (67) can be computed analogously by inserting the spectral representation. Then, only those permutations survive the difference for which the frequency combinations  $\omega_l$  or  $\omega_{l^c}$  appear in the kernel  $\tilde{K}(z_p)$ , leading to

$$\tilde{G}_{z'}^{\omega_l} = \tilde{G}_{\omega_l^+, z'} - \tilde{G}_{\omega_l^-, z'} = \sum_{\vec{l}|\vec{l}'} [\tilde{K}_{\vec{l}|\vec{l}'} \diamond S_{\vec{l}|\vec{l}'}] (z_{\vec{l}|\vec{l}'}(\omega_l, z')) \quad (\text{E3a})$$

$$\begin{aligned} \tilde{K}_{\vec{l}|\vec{l}'}(z_{\vec{l}|\vec{l}'}(\omega_l, z')) &= \tilde{K}(z_{\vec{l}|\vec{l}'}(\omega_l^+, z')) - \tilde{K}(z_{\vec{l}|\vec{l}'}(\omega_l^-, z')) \\ &= \hat{\delta}(\omega_l) \tilde{K}(z_{\vec{l}|\vec{l}'}(z')) \tilde{K}(z_{\vec{l}|\vec{l}'}(z')) \end{aligned} \quad (\text{E3b})$$

$$\tilde{K}(z_l) = \prod_{i=1}^{|\ell|-1} \frac{1}{\omega_{l_1 \dots l_i}} \quad (\text{E3c})$$

The set  $l^c = L \setminus l$  is complementary to  $l$ . Here,  $z_p(\omega_l, z')$  expresses the permuted vector  $z_p$  in terms of  $\omega_l$  and the remaining  $\ell - 2$  independent frequencies  $z'$ , and similarly  $z_{\vec{l}|\vec{l}'}$  for the subtuple  $z_{\vec{l}}$ . Equation (E3c) defines a regular kernel for the subtuple  $z_{\vec{l}}$ . In Equation (E3b), the difference of regular kernels leads to the Dirac delta factor due to  $1/\omega_l^+ - 1/\omega_l^- = \hat{\delta}(\omega_l)$  and  $1/\omega_{l^c}^+ - 1/\omega_{l^c}^- = -\hat{\delta}(\omega_l)$  (using Equation (58)). The definition of the regular product kernel in Equation (E3b) implies  $\tilde{K}_{\vec{l}|\vec{l}'} = \tilde{K}_{\vec{l}'|\vec{l}}$ ; thus, the corresponding PSFs from permutations  $\vec{l}|\vec{l}'$  and  $\vec{l}'|\vec{l}$  have been combined in a PSF commutator in Equation (E3a).

Consider, e.g., the 3p discontinuity  $\tilde{G}_{\omega_1^+}^{\omega_2}$  from Appendix E.1.1, where the sets in Equation (E3) are given by  $l = \{2\}$ ,  $l^c = \{1, 3\}$ , and  $z' = \omega_1^+$ . Then,

the sum over permutations  $p = \bar{l}|l^c$  includes  $\bar{l}|l^c \in \{2|13, 2|31\}$ , and we obtain the PSF commutator contribution  $S_{[2,13]_-}$  in Equation (E1) from Equation (E3).

For  $\ell = 4$ , let us consider  $\tilde{G}_{z_1, z_2}^{\omega_{13}}$  as an example. Then, the sets  $l = \{1, 3\}$  and  $l^c = \{2, 4\}$  yield the permutations  $\{13|24, 13|42, 31|24, 31|42\}$ , resulting in

$$\tilde{G}_{z_1, z_2}^{\omega_{13}} = \int d^4 \epsilon \frac{\delta(\epsilon_{1234}) \delta(\epsilon_{13})}{(z_1 - \epsilon_1)(z_2 - \epsilon_2)} S_{[[1,3]_-|[2,4]_-]}(\epsilon) \quad (\text{E4})$$

where we summarized all terms with the same kernels.

To compute consecutive discontinuities, such as  $\tilde{G}^{\omega_2, \omega_1}$  (see Equation (E2)), we can iterate the above procedure: By analyzing the spectral representation of the first discontinuity, we determine the branch cuts which lead to non-vanishing second discontinuities, and then compute these second discontinuities by use of identity (58). For fermionic 4p correlators, this iterative procedure implies that double bosonic discontinuities must vanish, e.g.,  $\tilde{G}_{\omega_+}^{\omega_{13}, \omega_{14}} = 0$ . This follows from the spectral representation of  $\tilde{G}_{z_1, z_2}^{\omega_{13}}$  in Equation (E4), where the kernels only depend on fermionic frequencies  $z_1, z_2$  in the denominators. Hence, there is no  $\text{Im}z_{14} = 0$  branch cut, and therefore  $\tilde{G}_{\omega_+}^{\omega_{13}, \omega_{14}}$  must vanish.

## E.2. Spectral Representation of Anomalous Parts

In this appendix, we focus on the spectral representation for contributions to the MF correlator anomalous w.r.t. one frequency. We again start with an example for  $\ell = 3$  (Appendix E.2.1), before generalizing to arbitrary  $\ell$  (Appendix E.2.2).

### E.2.1. Example for $\ell = 3$

Consider  $\beta \delta_{i\omega_1} \hat{G}_1(i\omega)$  for  $\ell = 3$ . Only those terms in the 3p kernel Equation (A4b) proportional to  $\delta_{\Omega_1} = \delta_{\omega_1} \delta_{\epsilon_1}$  and  $\delta_{\Omega_{23}} = \delta_{\omega_{23}} \delta_{\epsilon_{23}} = \delta_{\omega_1} \delta_{\epsilon_1}$  can contribute to  $\hat{G}_1$ . Hence, the anomalous PSFs  $S_p$  must contain factors  $\delta(\epsilon_1)$ , i.e.,

$$\begin{aligned} & \beta \delta_{i\omega_1} \hat{G}_1(i\omega) \\ &= -\frac{1}{2} \beta \delta_{i\omega_1} \int d^3 \epsilon \delta(\epsilon_{123}) \left[ \delta_{\epsilon_1} S_{(123)}(\epsilon_1, \epsilon_2) \Delta_{i\omega_{12} - \epsilon_{12}} \right. \\ & \quad + \delta_{\epsilon_1} S_{(132)}(\epsilon_1, \epsilon_3) \Delta_{i\omega_{13} - \epsilon_{13}} + \delta_{\epsilon_{23}} S_{(231)}(\epsilon_2, \epsilon_3) \Delta_{i\omega_2 - \epsilon_2} \\ & \quad \left. + \delta_{\epsilon_{23}} S_{(321)}(\epsilon_3, \epsilon_2) \Delta_{i\omega_3 - \epsilon_3} \right] \\ &= -\frac{1}{2} \beta \delta_{i\omega_1} \int d^3 \epsilon \delta(\epsilon_{123}) \left[ \delta_{\epsilon_1} S_{[1,23]_+}(\epsilon_1, \epsilon_2, \epsilon_3) \Delta_{i\omega_2 - \epsilon_2} \right. \\ & \quad \left. + \delta_{\epsilon_1} S_{[1,32]_+}(\epsilon_1, \epsilon_2, \epsilon_3) \Delta_{i\omega_3 - \epsilon_3} \right] \\ &= -\frac{1}{2} \beta \delta_{i\omega_1} \int d^3 \epsilon \delta(\epsilon_{123}) \delta_{\epsilon_1} S_{[1, [2,3]_-]_+}(\epsilon_1, \epsilon_2, \epsilon_3) \Delta_{i\omega_2 - \epsilon_2} \quad (\text{E5}) \end{aligned}$$

where we used the symbolic Kronecker notation from Appendix B.1. The remaining contributions  $p = (213), (312)$  can only contribute to the anomalous terms  $\hat{G}_2$  and  $\hat{G}_3$ , as they are not proportional to  $\delta_{i\omega_1}$ .

Note that, in the spectral representation (E5), the decomposition of  $\hat{G}_{1; i\omega_2} = \hat{G}_{1; i\omega_2}^{\Delta} + \Delta_{i\omega_2} \hat{G}_{1,2}^{\Delta}$  follows from the PSF decomposition. Only PSF terms proportional to  $\delta(\epsilon_2)$ ,  $\delta_{\epsilon_1} \delta_{\epsilon_2} S_{[1, [2,3]_-]_+}$ , contribute to  $\hat{G}_{1,2}^{\Delta}$ . In the absence of such  $\delta(\epsilon_2)$  contributions, we can evaluate  $\Delta_{i\omega_2 - \epsilon_2} \rightarrow 1/(i\omega_2 -$

$\epsilon_2)$  and compute the discontinuity  $\hat{G}_1^{\Delta; \omega_2} = \hat{G}_{1; \omega_2^+}^{\Delta} - \hat{G}_{1; \omega_2^-}^{\Delta}$ :

$$\begin{aligned} \delta(\omega_1) \delta(\omega_2) \hat{G}_{1,2}^{\Delta} &= -\delta_{\omega_1} \delta_{\omega_2} S_{[1, [2,3]_-]}(\omega_1, \omega_2, -\omega_{12}), \\ \delta(\omega_1) \hat{G}_1^{\Delta; \omega_2} &= (2\pi i) \delta_{\omega_1} (1 - \delta_{\omega_2}) S_{[1, [2,3]_-]}(\omega_1, \omega_2, -\omega_{12}) \quad (\text{E6}) \end{aligned}$$

Here, we used  $\delta_{\omega_1} S_{[1, [2,3]_-]_+} = 2\delta_{\omega_1} S_{[1, [2,3]_-]}$  due to the equilibrium condition (4). These commutator representations will be used for the 3p consistency check in Appendix G.2.2.

### E.2.2. Generalization to Arbitrary $\ell$

Now, we generalize the insights from the  $\ell = 3$  example to arbitrary  $\ell$ . The result will be used in Appendix F to provide a general formula for the construction of KF components  $G^{[l_1 l_2]}$  from MF functions.

In the  $\beta\delta$  expansion of the MF kernel  $K = \tilde{K} + \hat{K}^{\beta\delta} + \mathcal{O}(\delta^2)$ , the  $\beta\delta$  term reads (see Equation (45) in ref. [23])

$$\beta \hat{K}^{\beta}(\Omega_p) = -\frac{\beta}{2} \sum_{i=1}^{\ell-1} \delta_{\Omega_{\tau \dots i}} \prod_{\substack{j=1 \\ j \neq i}}^{\ell-1} \Delta_{\Omega_{\tau \dots j}} \quad (\text{E7})$$

which was originally derived for  $\ell \leq 4$ , but can be extended to arbitrary  $\ell$  with the same line of arguments, starting from the results in ref. [30]. For general  $\ell$ p functions and terms anomalous w.r.t. the frequency  $i\omega_l = 0$ , with  $l \subset L = \{1, \dots, \ell\}$ , only permutations of the form  $p = \bar{l}|l^c$  and  $p = \bar{l}^c|l$ , with  $l^c = L \setminus l$  again the complementary set to  $l$ , can lead to the  $\beta\delta_{i\omega_l}$  factor coming from the anomalous kernel in Equation (E7), yielding

$$\begin{aligned} & \beta \delta_{i\omega_l} \hat{G}_l(i\omega) \\ &= -\frac{1}{2} \beta \delta_{i\omega_l} \sum_{\bar{l}|l^c} \int d^\ell \epsilon_p \delta(\epsilon_{1 \dots \ell}) \prod_{i=1}^{|\bar{l}|-1} \Delta_{\Omega_{\tau \dots i}} \prod_{i=1}^{|l^c|-1} \Delta_{\Omega_{\tau \dots i}} \\ & \quad \times \delta_{\epsilon_{\tau}} S_{[\bar{l}, l^c]_+}(\epsilon_{\tau}) \quad (\text{E8}) \end{aligned}$$

Equation (E5) is a direct application of this formula for  $\ell = 3, l = \{1\}$ , and  $l^c = \{2, 3\}$ , where the permutations  $p = \bar{l}|l^c$  run over  $\bar{l}|l^c \in \{1|23, 1|32\}$ .

To make the connection to Keldysh correlators in the next appendix, we replace any  $\Delta_{i\omega} \rightarrow 1/(i\omega)$  in the final expression for  $\hat{G}_l$ , which amounts to replacing  $\Delta_{\Omega} \rightarrow 1/\Omega$  in the kernels, such that

$$\begin{aligned} \hat{G}_{l; \tilde{z}^{\ell}} &\equiv [\hat{G}_l(i\omega)]_{\Delta_{i\omega} \rightarrow \frac{1}{i\omega}, i\omega \rightarrow z(\tilde{z}^{\ell})} \\ &= -\frac{1}{2} \sum_{\bar{l}|l^c} \int d^\ell \epsilon_p \delta(\epsilon_{1 \dots \ell}) \tilde{K}(z_{\tau}(\tilde{z}^{\ell}) - \epsilon_{\tau}) \\ & \quad \times \tilde{K}(z_{\tau}(\tilde{z}^{\ell}) - \epsilon_{\tau}) \delta_{\epsilon_{\tau}} S_{[\bar{l}, l^c]_+}(\epsilon_{\tau}) \quad (\text{E9}) \end{aligned}$$

where we identified a product of regular kernels (see Equation (E3c)). The subscript  $\tilde{z}^{\ell}$  again denotes  $\ell - 2$  independent frequencies parametrizing the  $\ell - 1$  arguments  $z$  of  $\hat{G}_l(z(\tilde{z}^{\ell})) = \hat{G}_{l; \tilde{z}^{\ell}}$ , with  $z$  independent of the anomalous frequency  $\omega_l$ .

The anomalous parts  $\hat{G}_l$  typically enter the Keldysh components with prefactors depending on  $4\pi i \delta(\omega_l)$ . Including this factor, the spectral representation turns out to be particularly convenient, as we can make use of

the definition in Equation (90a), leading to

$$\begin{aligned} 4\pi i \delta(\omega_l) \hat{G}_{l,z^r} &= -2 \hat{\delta}(\omega_l) \hat{G}_{l,z^r} \\ &= \sum_{\bar{l}|\bar{\ell}} \int d^\ell \varepsilon_p \delta(\varepsilon_{\bar{l} \dots \bar{\ell}}) \hat{\delta}(\omega_{\bar{l}} - \varepsilon_{\bar{l}}) \tilde{K}(\mathbf{z}_{\bar{l}}(\mathbf{z}^r) - \varepsilon_{\bar{l}}) \tilde{K}(\mathbf{z}_{\bar{\ell}}(\mathbf{z}^r) - \varepsilon_{\bar{\ell}}) \\ &\times \delta_{\varepsilon_{\bar{l}} \dots \varepsilon_{\bar{\ell}}}(\varepsilon_{\bar{l}|\bar{\ell}}) \\ &= \sum_{\bar{l}|\bar{\ell}} \int d^\ell \varepsilon_p \delta(\varepsilon_{\bar{l} \dots \bar{\ell}}) \tilde{K}_{\bar{l}|\bar{\ell}}(\mathbf{z}_{\bar{l}|\bar{\ell}}(\omega_l, \mathbf{z}^r) - \varepsilon_{\bar{l}|\bar{\ell}}) \delta_{\varepsilon_{\bar{l}} \dots \varepsilon_{\bar{\ell}}}(\varepsilon_{\bar{l}|\bar{\ell}}). \end{aligned} \quad (\text{E10})$$

In the second step, we used  $\omega_l = \omega_{\bar{l}}$  and

$$\delta_{\varepsilon_{\bar{l}} \dots \varepsilon_{\bar{\ell}}}(\varepsilon_{\bar{l}|\bar{\ell}}) \hat{\delta}(\omega_l) = \delta_{\varepsilon_{\bar{l}} \dots \varepsilon_{\bar{\ell}}}(\varepsilon_{\bar{l}|\bar{\ell}}) \hat{\delta}(\omega_{\bar{l}} - \varepsilon_{\bar{l}}) \quad (\text{E11})$$

In the last line, we inserted the definition of the regular product kernel (E3b). Equation (E10) is the representation needed in Equation (F10) to express Keldysh components  $G^{[\eta_1 \eta_2]}$  in terms of analytically continued anomalous parts of MF correlators.

## Appendix F: Simplifications for KF Correlators

In this appendix, we derive reformulations of the spectral representation of KF components, presented in Sections 6.2.1 and 6.2.2, which are amenable to finding relations between KF correlators and analytically continued MF correlators. First, we derive a convenient identity for particular KF kernels for general  $\ell$ p correlators in Appendix F.1. This identity is then applied in Appendix F.2 to obtain an alternative representation of KF components  $G^{[\eta_1 \eta_2]}$ , yielding a general analytic continuation formula (Equation (F10)) for these components (using the results from Appendix E). This constitutes a generalization of Equation (23) for  $G^{[\eta_1]}$  ( $\alpha = 1$ ) to  $\alpha = 2$ . An analogous procedure is then applied to KF components  $G^{[\eta_1 \dots \eta_\alpha]}$  for  $\alpha = 3$  and  $\alpha = 4$  in Appendices F.3 and F.4, respectively (see Equations (98) and (F16)). In the following, we will use the notation introduced in the beginning of Section 6.2 repeatedly.

### F.1. Identity for $K^{[\hat{\eta}_1 \hat{\eta}_2]}$ for General $\ell$ p Correlators

For  $\alpha = 2$ , Keldysh correlators  $G^{[\eta_1 \eta_2]}$  are determined by the KF kernel  $K^{[\hat{\eta}_1 \hat{\eta}_2]} = K^{[\hat{\eta}_1]} - K^{[\hat{\eta}_2]}$  in Equation (19d). For  $\alpha \geq 2$ , such differences of fully retarded kernels occur repeatedly in the spectral representation. In the following, we therefore derive a convenient identity for the kernel  $K^{[\hat{\eta}_1 \hat{\eta}_2]}$ .

According to Equations (19c) and (22), the kernel  $K^{[\hat{\eta}_1 \hat{\eta}_2]}$  takes the form

$$K^{[\hat{\eta}_1 \hat{\eta}_2]}(\omega_p) = K^{[\hat{\eta}_1]}(\omega_p) - K^{[\hat{\eta}_2]}(\omega_p) = \tilde{K}(\omega_p^{\bar{\eta}_1}) - \tilde{K}(\omega_p^{\bar{\eta}_2}) \quad (\text{F1})$$

Note that  $\hat{\eta}_1 < \hat{\eta}_2$ , which holds by definition, does not imply  $\bar{\eta}_1 < \bar{\eta}_2$ .

For simplicity, we rename  $\mu = \hat{\eta}_1$  and  $\nu = \hat{\eta}_2$ . Using Equations (19d) and (21), the retarded kernels generally read

$$K^{[\mu]}(\omega_p) = \left( \prod_{i=1}^{\mu-1} \frac{1}{\omega_{\bar{l} \dots \bar{i}}} \right) \left( \prod_{i=\mu}^{\ell-1} \frac{1}{\omega_{\bar{l} \dots \bar{i}}} \right) = K_{\bar{l} \mu}^- K_{\mu \bar{\ell}}^+$$

$$K_{xy}^\pm = \prod_{i=x}^{y-1} \frac{1}{\omega_{\bar{l} \dots \bar{i}}} \quad (\text{F2})$$

From this definition of  $K_{xy}^\pm$ , the identities

$$K_{xy}^\pm K_{yz}^\pm = K_{xz}^\pm, \quad K_{xx}^\pm = 1, \quad K^{[\mu]} = K_{\bar{l} \mu}^- K_{\mu \bar{\ell}}^+ \quad (\text{F3})$$

directly follow, which allow us to rewrite  $K^{[\mu\nu]}(\omega_p)$  as

$$\begin{aligned} K^{[\mu\nu]} &= K^{[\mu]} - K^{[\nu]} = K_{\bar{l} \mu}^- (K_{\mu \bar{\ell}}^+ - K_{\nu \bar{\ell}}^-) K_{\nu \bar{\ell}}^+ \\ &= \sum_{\gamma=\mu}^{\nu-1} K_{\bar{l} \mu}^- (K_{\mu \gamma+1}^+ K_{\gamma+1 \nu}^- - K_{\mu \gamma}^+ K_{\gamma \nu}^-) K_{\nu \bar{\ell}}^+ \\ &= \sum_{\gamma=\mu}^{\nu-1} K_{\bar{l} \mu}^- K_{\mu \gamma}^+ \left( \frac{1}{\omega_{\bar{l} \dots \bar{\gamma}}} - \frac{1}{\omega_{\bar{l} \dots \bar{\gamma}}} \right) K_{\gamma+1 \nu}^- K_{\nu \bar{\ell}}^+ \\ &= \hat{\delta}(\omega_{\bar{l} \dots \bar{\gamma}}) \end{aligned} \quad (\text{F4})$$

In the second line, the terms  $\gamma = \mu$  and  $\gamma = \nu - 1$  represent the first line, the remaining contributions  $\mu < \gamma < \nu - 1$  cancel pairwise. In the last line, we used identity (58) to obtain  $\hat{\delta}(\omega_{\bar{l} \dots \bar{\gamma}})$ , enforcing  $\omega_{\bar{l} \dots \bar{i}}^\pm = \omega_{\bar{l} \dots \bar{i}}^\pm$  for  $i > \gamma$ .

Inserting this identity into the arguments of  $K_{\gamma+1 \nu}^- K_{\nu \bar{\ell}}^+$  yields

$$\begin{aligned} K^{[\mu\nu]}(\omega_p) &= \sum_{\gamma=\mu}^{\nu-1} K^{[\mu]}(\omega_{\bar{l} \dots \bar{\gamma}}) \hat{\delta}(\omega_{\bar{l} \dots \bar{\gamma}}) K^{[\nu]}(\omega_{\bar{l} \dots \bar{\ell}}) \\ &= \sum_{\gamma=\mu}^{\nu-1} \tilde{K}(\omega_{\bar{l} \dots \bar{\gamma}}^{\bar{\mu}}) \hat{\delta}(\omega_{\bar{l} \dots \bar{\gamma}}) \tilde{K}(\omega_{\bar{l} \dots \bar{\ell}}^{\bar{\nu}}) \\ &= \sum_{\gamma=\mu}^{\nu-1} \tilde{K}_{\bar{l} \dots \bar{\gamma}|\bar{\gamma}+1 \dots \bar{\ell}}(\omega_{\bar{l} \dots \bar{\gamma}|\bar{\gamma}+1 \dots \bar{\ell}}^{\bar{\mu}|\bar{\nu}}) \end{aligned} \quad (\text{F5})$$

The last equality follows from the definition (90a), with  $\alpha = 2$ ,  $\eta_1 = \bar{\mu}$ ,  $\eta_2 = \bar{\nu}$ ,  $\bar{l} = \bar{l} \dots \bar{\gamma}$ , and  $\bar{l} = \bar{\gamma} + 1 \dots \bar{\ell}$ . Note that, for  $\ell = 3$ , Equation (F5) readily yields the results of Table C1.

### F.2. Simplifications for $G^{[\eta_1 \eta_2]}$ for $\ell$ p Correlators

After the preparations in Appendices E and F.1, we can now derive an alternative representation of the Keldysh correlators  $G^{[\eta_1 \eta_2]}$ , equivalent to the spectral representation in Equation (19b) but more convenient for the analytic continuation. This generalizes the concepts of Section C.3.1 from  $\ell = 3$  to arbitrary  $\ell$ .

We start by inserting Equation (F5) into the spectral representation in Equation (19b),

$$\begin{aligned} G^{[\eta_1 \eta_2]}(\omega) &= \sum_p [K^{[\hat{\eta}_1 \hat{\eta}_2]} * S_p](\omega_p) \\ &= \sum_p \sum_{\gamma=\hat{\eta}_1}^{\hat{\eta}_2-1} \left( \tilde{K}_{\bar{l} \dots \bar{\gamma}|\bar{\gamma}+1 \dots \bar{\ell}} * S_p \right) (\omega_{\bar{l} \dots \bar{\gamma}|\bar{\gamma}+1 \dots \bar{\ell}}^{\bar{\eta}_1|\bar{\eta}_2}) \end{aligned} \quad (\text{F6})$$

Since  $\hat{\eta}_1 \leq \gamma < \hat{\eta}_2$ , the subtuples  $\bar{l} = (\bar{l} \dots \bar{\gamma})$  and  $\bar{l} = (\bar{\gamma} + 1 \dots \bar{\ell})$  always contain  $\hat{\eta}_1$  and  $\hat{\eta}_2$ , respectively. Each of these in turn equals either  $\eta_1$  or  $\eta_2$ , since  $\hat{\eta}_i \in \{p^{-1}(\eta_1), p^{-1}(\eta_2)\}$ , hence  $\bar{\eta}_i \in \{\eta_1, \eta_2\}$ . Correspondingly, we will denote the subtuple containing  $\eta_1$  as  $\bar{l}^1$ , and that containing  $\eta_2$  as  $\bar{l}^2$ . The sum over  $\gamma$  can then be interpreted as a sum over all possible partitions of  $(\bar{l}, \dots, \bar{\ell})$  for which each of the two subtuples contains either  $\eta_1$  or  $\eta_2$ . Defining  $\mathcal{I}^{12} = \{(\bar{l}^1, \bar{l}^2) | \eta_1 \in \bar{l}^1, \eta_2 \in \bar{l}^2, \bar{l}^1 \cup \bar{l}^2 = L, \bar{l}^1 \cap \bar{l}^2 = \emptyset\}$  as the set of all possibilities to partition  $L = \{1, \dots, \ell\}$  into subsets  $\bar{l}^1$  and  $\bar{l}^2$  containing  $\eta_1$  and  $\eta_2$ , respectively, we find

$$\begin{aligned} G^{[\eta_1 \eta_2]}(\omega) &= \sum_{(\bar{l}^1, \bar{l}^2) \in \mathcal{I}^{12}} \left[ \sum_{\bar{l}^1 \bar{l}^2} \left( \tilde{K}_{\bar{l}^1 \bar{l}^2} \diamond S_{\bar{l}^1 \bar{l}^2} \right) (\omega_{\bar{l}^1 \bar{l}^2}^{[\eta_1][\eta_2]}) \right. \\ &\quad \left. + \sum_{\bar{l}^1 \bar{l}^2} \left( \tilde{K}_{\bar{l}^2 \bar{l}^1} \diamond S_{\bar{l}^2 \bar{l}^1} \right) (\omega_{\bar{l}^2 \bar{l}^1}^{[\eta_2][\eta_1]}) \right] \end{aligned} \quad (\text{F7})$$

**Table F1.** Keldysh kernel of  $G^{[\eta_1 \eta_2 \eta_3]} - G^{[\eta_3]}$  (Equation (F11)) for different permutation classes depending on the order of the  $\mu_i = p^{-1}(\eta_i)$ . Manipulations similar to Equations (F12) and (F13) result in the alternative spectral representation in the third column, which can be further rewritten as Equation (98) using Equation (F14) (and equivalent identities).

$p$	$K^{[\eta_1 \eta_2 \eta_3]} - K^{[\mu_3]}$	$(G^{[\eta_1 \eta_2 \eta_3]} - G^{[\eta_3]})(\omega) = \sum_p [(K^{[\eta_1 \eta_2 \eta_3]} - K^{[\mu_3]}) * S_p](\omega_p)$
$\mu_1 < \mu_2 < \mu_3$	$K^{[\mu_1 \mu_2]}$	$= \sum_{(l^1, l^2, l^3) \in I^{123}} \{ \tilde{K}_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]} (\omega_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]}) + (\tilde{K}_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]} \diamond S_{l^1 l^2 l^3}) (\omega_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]}) \}$
$\mu_1 < \mu_3 < \mu_2$	$K^{[\mu_1 \mu_3]} - K^{[\mu_3 \mu_2]}$	$+ \sum_{l^1 l^3 l^2} [(\tilde{K}_{l^1 l^3 l^2}^{[\eta_1 \eta_3 \eta_2]} \diamond S_{l^1 l^3 l^2}) (\omega_{l^1 l^3 l^2}^{[\eta_1 \eta_3 \eta_2]}) + (\tilde{K}_{l^1 l^3 l^2}^{[\eta_1 \eta_3 \eta_2]} \diamond S_{l^1 l^3 l^2}) (\omega_{l^1 l^3 l^2}^{[\eta_3 \eta_2 \eta_1]})]$
$\mu_2 < \mu_1 < \mu_3$	$K^{[\mu_2 \mu_1]}$	$+ \sum_{l^2 l^1 l^3} [(\tilde{K}_{l^2 l^1 l^3}^{[\eta_2 \eta_1 \eta_3]} \diamond S_{l^2 l^1 l^3}) (\omega_{l^2 l^1 l^3}^{[\eta_2 \eta_1 \eta_3]}) + (\tilde{K}_{l^2 l^1 l^3}^{[\eta_2 \eta_1 \eta_3]} \diamond S_{l^2 l^1 l^3}) (\omega_{l^2 l^1 l^3}^{[\eta_3 \eta_1 \eta_2]})]$
$\mu_2 < \mu_3 < \mu_1$	$K^{[\mu_2 \mu_3]} - K^{[\mu_3 \mu_1]}$	$+ \sum_{l^2 l^3 l^1} [(\tilde{K}_{l^2 l^3 l^1}^{[\eta_2 \eta_3 \eta_1]} \diamond S_{l^2 l^3 l^1}) (\omega_{l^2 l^3 l^1}^{[\eta_2 \eta_3 \eta_1]}) + (\tilde{K}_{l^2 l^3 l^1}^{[\eta_2 \eta_3 \eta_1]} \diamond S_{l^2 l^3 l^1}) (\omega_{l^2 l^3 l^1}^{[\eta_3 \eta_1 \eta_2]})]$
$\mu_3 < \mu_1 < \mu_2$	$-K^{[\mu_1 \mu_2]}$	$+ \sum_{l^3 l^1 l^2} [(\tilde{K}_{l^3 l^1 l^2}^{[\eta_3 \eta_1 \eta_2]} \diamond S_{l^3 l^1 l^2}) (\omega_{l^3 l^1 l^2}^{[\eta_3 \eta_1 \eta_2]}) - (\tilde{K}_{l^3 l^1 l^2}^{[\eta_3 \eta_1 \eta_2]} \diamond S_{l^3 l^1 l^2}) (\omega_{l^3 l^1 l^2}^{[\eta_3 \eta_2 \eta_1]})]$
$\mu_3 < \mu_2 < \mu_1$	$-K^{[\mu_2 \mu_1]}$	$+ \sum_{l^3 l^2 l^1} [(\tilde{K}_{l^3 l^2 l^1}^{[\eta_3 \eta_2 \eta_1]} \diamond S_{l^3 l^2 l^1}) (\omega_{l^3 l^2 l^1}^{[\eta_3 \eta_2 \eta_1]}) - (\tilde{K}_{l^3 l^2 l^1}^{[\eta_3 \eta_2 \eta_1]} \diamond S_{l^3 l^2 l^1}) (\omega_{l^3 l^2 l^1}^{[\eta_3 \eta_1 \eta_2]})]$

Here, we collected all terms in Equation (F6) proportional to  $\hat{\delta}(\omega_{\bar{l}})$  and summed over all allowed partitions. Using the symmetry of the kernels (90a) and the (anti)commutator notation from Equation (92), we finally obtain

$$G^{[\eta_1 \eta_2]}(\omega) = \sum_{(l^1, l^2) \in I^{12}} \sum_{l^1 l^2} \left( \tilde{K}_{l^1 l^2}^{[\eta_1 \eta_2]} \diamond S_{l^1 l^2} \right) (\omega_{l^1 l^2}^{[\eta_1 \eta_2]}) \quad (\text{F8})$$

Building on this expression, the KF component can be related to MF functions for arbitrary  $\ell$ . For this purpose, we use the equilibrium condition to replace PSF commutators with anticommutators,

$$S_{[\bar{l}, \bar{l}]}^{\zeta \bar{l}}(\epsilon_{\bar{l}}) = N_{\epsilon_{\bar{l}}} S_{[\bar{l}, \bar{l}]}^{\zeta \bar{l}}(\epsilon_{\bar{l}}) + \delta_{\epsilon_{\bar{l}}} S_{[\bar{l}, \bar{l}]}^{\zeta \bar{l}}(\epsilon_{\bar{l}}) \quad (\text{F9})$$

$$N_{\epsilon_{\bar{l}}} = \frac{\zeta^{\bar{l}} e^{\beta \epsilon_{\bar{l}}} + 1}{\zeta^{\bar{l}} e^{\beta \epsilon_{\bar{l}}} - 1} = \coth(\beta \epsilon_{\bar{l}} / 2)^{\zeta \bar{l}}$$

where  $N_{\epsilon_{\bar{l}}}$  is identical to the statistical factor in Equation (60), and we used the symbolic Kronecker notation from Appendix B.1. The sign factor is given by  $\zeta^{\bar{l}} = \pm 1$  for an even/odd number of fermionic operators in the set  $\bar{l}$ . Inserting Equation (F9) into the representation (F8), we thus obtain

$$G^{[\eta_1 \eta_2]}(\omega) = \sum_{(l^1, l^2) \in I^{12}} \sum_{l^1 l^2} \int d^\ell \epsilon \tilde{K}_{l^1 l^2}^{[\eta_1 \eta_2]} (\omega_{l^1 l^2}^{[\eta_1 \eta_2]} - \epsilon_{l^1 l^2})$$

$$\times \left( N_{\epsilon_{\bar{l}}} S_{[\bar{l}, \bar{l}]}^{\zeta \bar{l}}(\epsilon_{\bar{l}}) + \delta_{\epsilon_{\bar{l}}} S_{[\bar{l}, \bar{l}]}^{\zeta \bar{l}}(\epsilon_{\bar{l}}) \right) \hat{\delta}(\epsilon_{1\dots\ell})$$

$$= \sum_{(l^1, l^2) \in I^{12}} \left( N_{\omega_{l^1}} \tilde{G}_{\bar{z}}^{\omega_{l^1}} + 4\pi i \delta(\omega_{l^1}) \hat{G}_{l^1, \bar{z}} \right)$$

$$\text{with } \bar{z} = \{\omega_{\bar{l}}^{-1} | i \neq \eta_1, i \neq \eta_2\} \quad (\text{F10})$$

This remarkable formula generalizes Equation (23) for  $G^{[\eta_1]}$ , i.e. for  $\alpha = 1$  and arbitrary  $\ell$ , to  $G^{[\eta_1 \eta_2]}$  ( $\alpha = 2$ ). To obtain its final form, we used that the retarded product kernel (Equation (90a)) in the second line is proportional to  $\hat{\delta}(\omega_{l^1} - \epsilon_{l^1})$  and thereby sets  $N_{\epsilon_{l^1}} = N_{\omega_{l^1}} = N_{\omega_{l^1}}$  independent of the integration variables. In the second step, we then identified the spectral representations of discontinuities of the regular MF correlator  $\tilde{G}_{\bar{z}}^{\omega_{l^1}}$  (Equation (E3)) and of the anomalous contribution  $\hat{G}_{l^1, \bar{z}}$  (Equation (E10)). Note that the retarded product kernel coincides with the kernel (E3b) with a suitably continued  $\bar{z}$ . In Equation (F10), the  $\ell - 2$  frequencies in  $\bar{z}$  carry negative imaginary shifts, in accordance with the definition of  $\omega_{l^1 l^2}^{[\eta_1 \eta_2]}$ .

### F.3. Simplifications for $G^{[\eta_1 \eta_2 \eta_3]}$ for $\ell$ p Correlators

The calculation in Appendix C.3.2, too, can be generalized to arbitrary  $\ell$  p correlators, in particular for the spectral representation of  $G^{[\eta_1 \eta_2 \eta_3]} - G^{[\eta_3]}$ . The Keldysh kernel for  $G^{[\mu_3]}$  is given by  $\tilde{K}(\omega_p^{[\mu_3]}) = K^{[\mu_3]}(\omega_p)$  for arbitrary permutations  $p$ , with  $\mu_3 = p^{-1}(\eta_3)$ . Then, the corresponding Keldysh kernel for  $G^{[\eta_1 \eta_2 \eta_3]} - G^{[\eta_3]}$  reads

$$K^{[\eta_1 \eta_2 \eta_3]} - K^{[\mu_3]} = K^{[\eta_1]} - K^{[\eta_2]} + K^{[\eta_3]} - K^{[\mu_3]} \quad (\text{F11})$$

such that the effect of subtracting  $K^{[\mu_3]}$  depends on the permutation. The permutations can be divided into six categories, depending on the order in which the  $\mu_j = p^{-1}(\eta_j)$  occur, see Table F1. This is important since placing the  $\mu_j$  in increasing order yields  $[\eta_1 \eta_2 \eta_3]$ , see discussion before Equations (19).

Here, we focus on the key steps in rewriting permutations with  $\mu_1 < \mu_2 < \mu_3$ , denoted by  $\sum_{p | \mu_1 < \mu_2 < \mu_3}$ . Defining  $I^{123} = \{(l^1, l^2, l^3) | \eta_1 \in l^1, \eta_2 \in l^2, \eta_3 \in l^3, l^b \cap l^{b'} = \emptyset \text{ for } b \neq b'\}$  as the set of all possibilities to partition  $L = \{1, \dots, \ell\}$  into three blocks, each of which contains one of the indices  $\eta_j \in \bar{l}$ , we have

$$\sum_{p | \mu_1 < \mu_2 < \mu_3} [(K^{[\eta_1 \eta_2 \eta_3]} - K^{[\mu_3]}) * S_p](\omega_p)$$

$$= \sum_{p | \mu_1 < \mu_2 < \mu_3} (K^{[\mu_1 \mu_2]} * S_p)(\omega_p)$$

$$= \sum_{p | \mu_1 < \mu_2 < \mu_3} \sum_{\gamma = \mu_1}^{\mu_2 - 1} \left( \tilde{K}_{\bar{l} \dots \bar{\gamma} | \bar{\gamma} + 1 \dots \bar{\ell}}^{[\eta_1 \eta_2]} * S_p \right) (\omega_{\bar{l} \dots \bar{\gamma} | \bar{\gamma} + 1 \dots \bar{\ell}}^{[\eta_1 \eta_2]})$$

$$= \sum_{(l^1, l^2, l^3) \in I^{123}} \sum_{l^1 l^2 l^3} \left( \tilde{K}_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]} \diamond S_{l^1 l^2 l^3} \right) (\omega_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]}) \quad (\text{F12})$$

In the first step, we used that  $[\eta_1 \eta_2 \eta_3] = [\mu_1 \mu_2 \mu_3]$ . In the second step, we inserted the kernel expansion Equation (F5) with  $\bar{\mu}_j = \eta_j$ . In the third step, we identified the sum over  $\gamma$  as a sum over all possibilities to subdivide the permutations into the form  $p = \bar{l} | \bar{l}^2 | \bar{l}^3$  (which guarantees  $\mu_1 < \mu_2 < \mu_3$ ), with the concatenation of  $\bar{l}^2$  and  $\bar{l}^3$  denoted by  $\bar{l}^{23} = \bar{l}_1 \dots \bar{l}_{|\bar{l}^2|} \bar{l}_1 \dots \bar{l}_{|\bar{l}^3|}$ .

Further, we use

$$\sum_{(l^1, l^2, l^3) \in I^{123}} \sum_{l^1 l^2 l^3} \left( \tilde{K}_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]} \diamond S_{l^1 l^2 l^3} \right) (\omega_{l^1 l^2 l^3}^{[\eta_1 \eta_2 \eta_3]})$$

$$\begin{aligned}
 & - \sum_{(i^1, i^2, i^3) \in \mathcal{I}^{123}} \sum_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \left( \tilde{K}_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \diamond S_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \right) (\omega_{\bar{i}^1 \bar{i}^2 \bar{i}^3}^{[i^1][i^2][i^3]}) \\
 & = \sum_{(i^1, i^2, i^3) \in \mathcal{I}^{123}} \sum_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \left( \tilde{K}_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \diamond S_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \right) (\omega_{\bar{i}^1 \bar{i}^2 \bar{i}^3}^{[i^1][i^2][i^3]}) \quad (F13)
 \end{aligned}$$

which again follows by inserting Equation (F5), to arrive at the result in Table F1.

Contributions of different permutations can be further simplified, e.g., the second term of  $p|\mu_1 < \mu_2 < \mu_3$  and the first term of  $p|\mu_1 < \mu_3 < \mu_2$  can be collected, yielding

$$\begin{aligned}
 & \sum_{(i^1, i^2, i^3) \in \mathcal{I}^{123}} \sum_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \left( \tilde{K}_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \diamond S_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \right) (\omega_{\bar{i}^1 \bar{i}^2 \bar{i}^3}^{[i^1][i^2][i^3]}) \\
 & + \sum_{(i^1, i^2, i^3) \in \mathcal{I}^{123}} \sum_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \left( \tilde{K}_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \diamond S_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \right) (\omega_{\bar{i}^1 \bar{i}^2 \bar{i}^3}^{[i^1][i^2][i^3]}) \\
 & = \sum_{(i^1, i^2, i^3) \in \mathcal{I}^{123}} \sum_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \left[ \tilde{K}_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \diamond S_{\bar{i}^1 \bar{i}^2 \bar{i}^3} \right] (\omega_{\bar{i}^1 \bar{i}^2 \bar{i}^3}^{[i^1][i^2][i^3]}) \quad (F14)
 \end{aligned}$$

with  $\mathcal{I}^{123}$  defined in Equation (99a). Using the symmetry of retarded product kernels, e.g.,  $\tilde{K}_{\bar{i}^1 \bar{i}^2 \bar{i}^3} = \tilde{K}_{\bar{i}^2 \bar{i}^1 \bar{i}^3}$ , the spectral representation of  $G^{[i^1 i^2 i^3]} - G^{[i^3 i^2 i^1]}$  finally results in Equation (98). Unlike for  $\alpha = 2$  we don't have a general formula for the analytic continuation to  $G^{[i^1 i^2 i^3]}$ .

Equation (100) shows an example for  $\ell = 4$ . Inserting Equation (88) into the PSF (anti)commutators and abbreviating  $S'_p = (2\pi i)^3 S_p$ , we obtain the following relations:

$$\begin{aligned}
 S'_{[[\bar{1}, \bar{2}], \bar{3}], \bar{4}]_+} & = -N_4 \left( N_3 \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} + N_{12} \tilde{G}^{\varepsilon_2 \varepsilon_1 \varepsilon_3 \varepsilon_4} - 2\hat{\delta}(\varepsilon_{12}) \hat{G}_{12}^{\varepsilon_3 \varepsilon_4} \right), \\
 S'_{[[\bar{1}, \bar{2}], \bar{3}], \bar{4}]_+} & = N_{12} \left( N_4 \tilde{G}^{\varepsilon_4 \varepsilon_3 \varepsilon_2 \varepsilon_1} + N_3 \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} \right) - 2\hat{\delta}(\varepsilon_{12}) N_3 \hat{G}_{12}^{\varepsilon_3 \varepsilon_4} \quad (F15)
 \end{aligned}$$

Inserting these into the alternative spectral representation (98), we can evaluate the convolution integrals and obtain the relations in Equations (101g)-(101j), which express KF components in terms of MF functions and MWFs.

#### F.4. Simplifications for $G^{[1234]}$ for $\ell = 4$

For  $\alpha = 4$ , we can directly apply Equation (F5) on the Keldysh kernel, and a straightforward calculation gives

$$\begin{aligned}
 G^{[1234]}(\omega) & = \sum_{234} [\tilde{K}_{234|1} \diamond S_{[234, 1]_+}] (\omega_{234|1}^{[4][1]}) \\
 & + \sum_{134} [\tilde{K}_{134|2} \diamond S_{[134, 2]_+}] (\omega_{134|2}^{[4][2]}) \\
 & + \sum_{124} [\tilde{K}_{124|3} \diamond S_{[124, 3]_+}] (\omega_{124|3}^{[2][3]}) \\
 & + \sum_{123} [\tilde{K}_{123|4} \diamond S_{[123, 4]_+}] (\omega_{123|4}^{[3][4]}) \\
 & + [\tilde{K}_{4|12|3} \diamond S_{[[4, 1, 2], \dots, 3]_+}] (\omega_{4|12|3}^{[4][2][3]}) \\
 & + [\tilde{K}_{3|14|2} \diamond S_{[[3, 1, 4], \dots, 2]_+}] (\omega_{3|14|2}^{[3][1][2]})
 \end{aligned}$$

$$\begin{aligned}
 & + [\tilde{K}_{1|23|4} \diamond S_{[[1, 2, 3], \dots, 4]_+}] (\omega_{1|23|4}^{[1][3][4]}) \\
 & + [\tilde{K}_{2|34|1} \diamond S_{[[2, 3, 4], \dots, 1]_+}] (\omega_{2|34|1}^{[2][4][1]}) \\
 & + [\tilde{K}_{4|2|13} \diamond S_{[[4, 2], \dots, [1, 3], \dots]_+}] (\omega_{4|2|13}^{[4][2][3]}) \\
 & + [\tilde{K}_{1|3|24} \diamond S_{[[1, 3], \dots, [2, 4], \dots]_+}] (\omega_{1|3|24}^{[1][3][4]}) \\
 & + (-2\pi i)^3 \left( S_{[[2, 3], \dots, 1]_+} + S_{[[4, 2], \dots, 1]_+} \right. \\
 & \left. - S_{[[3, 4], \dots, 2]_+} - S_{[[4, 1], \dots, 3]_+} + S_{[[2, 4], \dots, [1, 3], \dots]_+} \right) (\omega) \quad (F16)
 \end{aligned}$$

where  $\sum_I$  denotes a sum over permutations of the subset  $I \subset \{1, \dots, \ell\}$ . All occurring PSF (anti)commutators can be identified with one of the following four forms,

$$S'_{[[\bar{1}, \bar{2}], \bar{3}], \bar{4}]_+} = N_4 \tilde{G}^{\varepsilon_4 \varepsilon_3 \varepsilon_2 \varepsilon_1} \quad (F17a)$$

$$S'_{[[\bar{1}, \bar{2}], \bar{3}], \bar{4}]_+} = N_4 \tilde{G}^{\varepsilon_4 \varepsilon_3 \varepsilon_2 \varepsilon_1} + N_3 \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} \quad (F17b)$$

$$\begin{aligned}
 S'_{[[\bar{1}, \bar{2}], \bar{3}], \bar{4}]_+} & = N_1 \tilde{G}^{\varepsilon_2 \varepsilon_1 \varepsilon_4 \varepsilon_3} + N_2 \tilde{G}^{\varepsilon_1 \varepsilon_4 \varepsilon_3 \varepsilon_2} + N_{13} \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} \\
 & + N_{14} \tilde{G}^{\varepsilon_4 \varepsilon_3 \varepsilon_2 \varepsilon_1} - 2\hat{\delta}(\varepsilon_{13}) \hat{G}_{13}^{\varepsilon_2 \varepsilon_4} - 2\hat{\delta}(\varepsilon_{14}) \hat{G}_{14}^{\varepsilon_2 \varepsilon_3} \quad (F17c)
 \end{aligned}$$

$$\begin{aligned}
 S'_{[[\bar{1}, \bar{2}], \bar{3}], \bar{4}]_+} & = N_1 N_3 \hat{G}_{12}^{\varepsilon_1 \varepsilon_3} - (1 + N_1 N_2) (\hat{G}_{13}^{\varepsilon_1 \varepsilon_2} + \hat{G}_{14}^{\varepsilon_1 \varepsilon_2}) \\
 & - (1 + N_1 N_2) (N_3 \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} + N_4 \tilde{G}^{\varepsilon_4 \varepsilon_3 \varepsilon_2 \varepsilon_1}) \\
 & + N_{13} \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} + N_{23} \tilde{G}^{\varepsilon_2 \varepsilon_1 \varepsilon_4 \varepsilon_3} \\
 & - N_1 N_{12} (N_3 \tilde{G}^{\varepsilon_3 \varepsilon_2 \varepsilon_1 \varepsilon_4} + N_4 \tilde{G}^{\varepsilon_4 \varepsilon_3 \varepsilon_2 \varepsilon_1}) \quad (F17d)
 \end{aligned}$$

where we abbreviated  $S'_p = (2\pi i)^3 S_p$  and  $N_i = N_{e_i}$ , and we used Equation (88) to evaluate above expressions. Inserting these into Equation (F16) and after application of Cauchy's integral formula, one obtains Equation (101k).

## Appendix G: Consistency Checks

In Equations (47), (74), and (88), we expressed the 2p, 3p and 4p PSFs in terms of analytically continued MF functions. While the derivation of these important results extends over several pages, some consistency checks can be presented compactly. In Appendix G.1, we first show that our formulas fulfill the equilibrium condition (4). Since this was not explicitly imposed during the derivations, it serves as a strong test for our results. In Appendix G.2, we further show, for  $\ell = 2, 3, 4$ , that our formulas for  $S_p[G]$ , when expressing that  $G$  through PSFs, recover the input PSFs.

### G.1. Fulfillment of the Equilibrium Condition

Here, we show that the results in (74) and (88) fulfill the equilibrium condition (4) (for the 2p case, this was already demonstrated in (50)). It suffices to show that they are fulfilled for  $p_\lambda$  with  $\lambda = 2$ , i.e., that for  $p = (\bar{1} \dots \bar{\ell})$  we have

$$S_{(\bar{1} \dots \bar{\ell})}(\varepsilon_{(\bar{1} \dots \bar{\ell})}) = \varepsilon^{\bar{1}} e^{\beta \varepsilon^{\bar{1}}} S_{(\bar{2} \dots \bar{\ell})}(\varepsilon_{(\bar{2} \dots \bar{\ell})}) \quad (G1)$$

The result for general  $\lambda$  follows by induction.

We start with  $\ell = 3$  and separate the contributions to the PSFs in Equation (74) from the regular  $\tilde{G}$  (denoted by  $S'_p$ ) and the anomalous  $\hat{G}$  terms

(denoted by  $S_p^a$ ,  $S_p = S_p^r + S_p^a$ . Inserting Equation (74) into Equation (G1) first yields

$$\begin{aligned} & \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} (2\pi i)^2 S_{(23\bar{1})}^r \\ &= \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} \left[ n_{\varepsilon_{\bar{2}}} n_{\varepsilon_{\bar{3}}} \tilde{G}^{\varepsilon_{\bar{3}}, \varepsilon_{\bar{2}}} + n_{\varepsilon_{\bar{2}}} n_{\varepsilon_{\bar{2}\bar{3}}} \tilde{G}^{\varepsilon_{\bar{2}\bar{3}}, \varepsilon_{\bar{2}}} \right] \\ &= \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} \left[ n_{\varepsilon_{\bar{2}}} (n_{\varepsilon_{\bar{3}}} - n_{\varepsilon_{\bar{2}\bar{3}}}) \tilde{G}^{\varepsilon_{\bar{3}}, \varepsilon_{\bar{2}}} - n_{\varepsilon_{\bar{2}}} n_{\varepsilon_{\bar{2}\bar{3}}} \tilde{G}^{\varepsilon_{\bar{2}\bar{3}}, \varepsilon_{\bar{2}}} \right] \\ &= \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} \left[ -n_{\varepsilon_{\bar{2}}} n_{-\varepsilon_{\bar{1}}} \tilde{G}^{\varepsilon_{\bar{2}}, \varepsilon_{\bar{1}}} - n_{\varepsilon_{\bar{2}}} n_{-\varepsilon_{\bar{1}}} \tilde{G}^{\varepsilon_{\bar{2}\bar{3}}, \varepsilon_{\bar{1}}} \right] \\ &= (2\pi i)^2 S_{(12\bar{3})}^r \end{aligned} \quad (\text{G2})$$

where we used in the second line  $\tilde{G}^{\varepsilon_{\bar{2}\bar{3}}, \varepsilon_{\bar{2}}} = -\tilde{G}^{\varepsilon_{\bar{3}}, \varepsilon_{\bar{2}}} - \tilde{G}^{\varepsilon_{\bar{2}}, \varepsilon_{\bar{1}}}$  (following from Equations (C26)), in the third line  $n_{\varepsilon_{\bar{2}}} (n_{\varepsilon_{\bar{3}}} - n_{\varepsilon_{\bar{2}\bar{3}}}) = -n_{\varepsilon_{\bar{2}}} n_{-\varepsilon_{\bar{1}}}$ , and in the fourth line

$$\zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} n_{-\varepsilon_{\bar{1}}} = \frac{\zeta^{-1} e^{\beta \varepsilon_{\bar{1}}}}{\zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} - 1} = -n_{\varepsilon_{\bar{1}}} \quad (\text{G3})$$

For the  $\hat{G}$  terms, we similarly obtain

$$\begin{aligned} & \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} (2\pi i)^2 S_{(23\bar{1})}^a \\ &= \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} \left[ \hat{\delta}(\varepsilon_{\bar{2}}) n_{\varepsilon_{\bar{3}}} \hat{G}_{\bar{2}}^{\Delta; \varepsilon_{\bar{3}}} + \hat{\delta}(\varepsilon_{\bar{3}}) n_{\varepsilon_{\bar{2}}} \hat{G}_{\bar{3}}^{\Delta; \varepsilon_{\bar{2}}} \right. \\ & \quad \left. + \hat{\delta}(\varepsilon_{\bar{1}}) n_{\varepsilon_{\bar{2}}} \hat{G}_{\bar{1}}^{\Delta; \varepsilon_{\bar{2}}} + \hat{\delta}(\varepsilon_{\bar{2}}) \hat{\delta}(\varepsilon_{\bar{3}}) \left( \hat{G}_{\bar{2}\bar{3}}^{\Delta} - \frac{1}{2} \hat{G}_{\bar{1}\bar{2}}^{\Delta} \right) \right] \\ &= \zeta^{-1} e^{\beta \varepsilon_{\bar{1}}} \left[ -\hat{\delta}(\varepsilon_{\bar{2}}) n_{-\varepsilon_{\bar{1}}} \hat{G}_{\bar{2}}^{\Delta; \varepsilon_{\bar{1}}} - \hat{\delta}(\varepsilon_{\bar{3}}) n_{-\varepsilon_{\bar{1}}} \hat{G}_{\bar{3}}^{\Delta; \varepsilon_{\bar{1}}} \right. \\ & \quad \left. + \hat{\delta}(\varepsilon_{\bar{1}}) n_{\varepsilon_{\bar{2}}} \hat{G}_{\bar{1}}^{\Delta; \varepsilon_{\bar{2}}} + \hat{\delta}(\varepsilon_{\bar{1}}) \hat{\delta}(\varepsilon_{\bar{2}}) \left( \hat{G}_{\bar{1}\bar{2}}^{\Delta} - \frac{1}{2} \hat{G}_{\bar{3}\bar{1}}^{\Delta} \right) \right] \\ &= (2\pi i)^2 S_{(12\bar{3})}^a \end{aligned} \quad (\text{G4})$$

In the last step, we used that  $\hat{G}_{\bar{1}}^{\Delta} \neq 0$  and  $\hat{G}_{\bar{1}\bar{2}}^{\Delta} \neq 0$  imply  $\zeta^{-1} = +1$ . Thus, we find that our 3p formula (74) indeed fulfills the equilibrium condition.

For 4p PSFs, we confirmed the fulfillment of the equilibrium condition by inserting the analytic regions (D11) for the discontinuities and by comparing the coefficients.

## G.2. Full Recovery of Spectral Information

Equations (47), (74), and (88) contain formulas for PSFs,  $S_p[G]$ , as functionals of the MF correlator  $G$  for  $\ell = 2, 3, 4$ . In this section, we explicitly perform the following consistency check: given an arbitrary set of PSFs  $S_p$  as input, compute the MF correlator  $G = \sum_p K * S_p$  and verify that  $S_p[G]$  correctly recovers the input PSFs. To this end, we insert results from Appendix E to express the discontinuities in the formulas via PSF (anti)commutators. From the resulting expressions, we then show  $S_p[G] = S_p$  by use of the equilibrium condition (4).

### G.2.1. For $\ell = 2$

We first examine the relations between the MF correlator and the PSF contributions. Using the decomposition of PSFs from Appendix B.1, the standard spectral function reads

$$S_{\text{std}}(\varepsilon_1) = S_{[1,2]_{-}}(\varepsilon_1, -\varepsilon_1) = \tilde{S}_{[1,2]_{-}}(\varepsilon_1, -\varepsilon_1) \quad (\text{G5})$$

For bosonic functions,  $\zeta = +1$ , there may be anomalous contributions  $\delta(\varepsilon_{\bar{1}}) \tilde{S}_{p, \bar{1}}$ . However, the equilibrium condition implies  $\tilde{S}_{(12), 1} = \tilde{S}_{(21), 2}$ , so that the anomalous contributions cancel in the PSF commutator. Instead, they solely enter the anomalous correlator,  $\hat{G}(i\omega_1) = \beta \delta_{i\omega_1} \hat{G}_1$ , via the spectral representation with kernel (A4a), yielding

$$\hat{G}_1 = -\tilde{S}_{(12), 1} \quad (\text{G6})$$

Now, we can show that Equation (47) recovers the input PSFs from the MF correlator. Inserting  $\tilde{G}^{\varepsilon_1} = -\tilde{G}^{\varepsilon_2} = (-2\pi i) S_{\text{std}}^{\text{std}}(\varepsilon_1)$  (Equation (51)) and Equation (G6) into Equation (47) yields

$$S_p[G] = \frac{1}{2\pi i} \left[ n_{\varepsilon_{\bar{1}}} \tilde{G}^{\varepsilon_{\bar{1}}} + \hat{\delta}(\varepsilon_{\bar{1}}) \hat{G}_{\bar{1}} \right] = -n_{\varepsilon_{\bar{1}}} \tilde{S}_{[\bar{1}, \bar{2}]_{-}} + \delta_{\varepsilon_{\bar{1}}} S_{(\bar{1}\bar{2})} \quad (\text{G7})$$

(Here and in the following, we suppress frequency arguments of PSFs.) To simplify the PSF commutator, we can use the equilibrium condition (4) to obtain

$$\begin{aligned} -n_{\varepsilon_{\bar{1}}} \tilde{S}_{[\bar{1}, \bar{2}]_{-}} &= \frac{-1}{\zeta^{-1} e^{-\beta \varepsilon_{\bar{1}}} - 1} [\tilde{S}_{(\bar{1}\bar{2})} - \zeta^{-1} e^{-\beta \varepsilon_{\bar{1}}} \tilde{S}_{(\bar{1}\bar{2})}] \\ &= \tilde{S}_{(\bar{1}\bar{2})} = (1 - \delta_{\varepsilon_{\bar{1}}}) S_{(\bar{1}\bar{2})} \end{aligned} \quad (\text{G8})$$

For bosonic 2p functions, the MWF  $n_{\varepsilon_{\bar{1}}}$  is undefined for  $\varepsilon_{\bar{1}} = 0$ . But since  $\tilde{S}_p$  then has no  $\delta(\varepsilon_{\bar{1}})$  contribution, the left and right side of Equation (47) can only differ by zero spectral weight. We can nevertheless recover the correct value for  $\tilde{S}_p(\varepsilon_{\bar{1}})$  at  $\varepsilon_{\bar{1}} = 0$  if we demand that continuum contributions are (piece-wise) continuous. Then, the correct value at  $\varepsilon_{\bar{1}} = 0$  is obtained from the formula in Equation (47) by taking the appropriate limit.

Inserting Equation (G8) into Equation (G7) results in

$$S_p[G] = (1 - \delta_{\varepsilon_{\bar{1}}}) S_{(\bar{1}\bar{2})} + \delta_{\varepsilon_{\bar{1}}} S_{(\bar{1}\bar{2})} = S_{(\bar{1}\bar{2})} \quad (\text{G9})$$

concluding our proof.

### G.2.2. For $\ell = 3$

Following the line of argument for  $\ell = 2$  from the previous section, we now check that the formula  $S_p[G]$  recovers the input PSF  $S_p$  also for  $\ell = 3$ . Analogously to Equation (G8), the MWFs can be eliminated using the identity (suppressing frequency arguments)

$$S_{(\bar{1}\bar{2}\bar{3})} = -n_{\varepsilon_{\bar{1}}} S_{[\bar{1}, \bar{2}\bar{3}]_{-}} + \delta_{\varepsilon_{\bar{1}}} S_{(\bar{1}\bar{2}\bar{3})} \quad (\text{G10a})$$

$$S_{(\bar{2}\bar{3}\bar{1})} = n_{-\varepsilon_{\bar{1}}} S_{[\bar{1}, \bar{2}\bar{3}]_{-}} + \delta_{\varepsilon_{\bar{1}}} S_{(\bar{2}\bar{3}\bar{1})} \quad (\text{G10b})$$

Note that  $\delta(\varepsilon_{\bar{1}})$  contributions cancel in  $S_{[\bar{1}, \bar{2}\bar{3}]_{-}}$  for  $\zeta^{-1} = +$  due to the equilibrium condition (as before), i.e.,  $S_{[\bar{1}, \bar{2}\bar{3}]_{-}} = (1 - \delta_{\varepsilon_{\bar{1}}}) S_{[\bar{1}, \bar{2}\bar{3}]_{-}}$ . Hence, such terms must be treated separately to obtain the PSF on the left.

In Appendix E.1, we have already shown that the discontinuities in the 3p PSF are proportional to nested PSF commutators. Analogously to the derivations for Equations (B8a), (E6), and (E2), we obtain the following relations:

$$\hat{\delta}(\varepsilon_{\bar{1}}) \hat{\delta}(\varepsilon_{\bar{2}}) \hat{G}_{\bar{1}\bar{2}}^{\Delta} = (2\pi i)^2 \frac{1}{2} \delta_{\varepsilon_{\bar{1}}} \delta_{\varepsilon_{\bar{2}}} S_{[\bar{1}, \bar{2}, \bar{3}]_{+}}$$

$$\hat{\delta}(\varepsilon_{\bar{1}}) \hat{\delta}(\varepsilon_{\bar{2}}) \hat{G}_{\bar{3}\bar{1}}^{\Delta} = -(2\pi i)^2 \delta_{\varepsilon_{\bar{1}}} \delta_{\varepsilon_{\bar{2}}} S_{[\bar{1}, \bar{2}, \bar{3}]_{-}}$$

$$\hat{\delta}(\varepsilon_{\bar{1}}) \hat{G}_{\bar{1}}^{\Delta; \varepsilon_{\bar{2}}} = -(2\pi i)^2 \delta_{\varepsilon_{\bar{1}}} (1 - \delta_{\varepsilon_{\bar{2}}}) S_{[\bar{1}, \bar{2}, \bar{3}]_{-}}$$

$$\hat{\delta}(\varepsilon_{\bar{2}}) \hat{G}_{\bar{2}}^{\Delta; \varepsilon_{\bar{1}}} = -(2\pi i)^2 \delta_{\varepsilon_{\bar{2}}} (1 - \delta_{\varepsilon_{\bar{1}}}) S_{[\bar{1}, \bar{2}, \bar{3}]_{-}}$$

$$\hat{\delta}(\varepsilon_{\bar{3}}) \hat{G}_{\bar{3}}^{\Delta; \varepsilon_{\bar{1}}} = -(2\pi i)^2 \delta_{\varepsilon_{\bar{3}}} (1 - \delta_{\varepsilon_{\bar{1}}}) S_{[\bar{1}, \bar{2}, \bar{3}]_{-}}$$

$$\begin{aligned}\tilde{G}^{\varepsilon_2, \varepsilon_1} &= (2\pi i)^2 S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-}, \\ \tilde{G}^{\varepsilon_1, \varepsilon_2} &= -(2\pi i)^2 S_{[\bar{3}, [\bar{1}, \bar{2}]_-, ]_-}\end{aligned}\quad (\text{G11})$$

Inserting these into Equation (74) yields

$$\begin{aligned}S_p[G] &= \left[ n_{\varepsilon_1} \left( n_{\varepsilon_2} \tilde{G}^{\varepsilon_2, \varepsilon_1} + \hat{\delta}(\varepsilon_2) \hat{G}_2^{\Delta, \varepsilon_1} + n_{\varepsilon_{12}} \tilde{G}^{\varepsilon_1, \varepsilon_2} + \hat{\delta}(\varepsilon_3) \hat{G}_3^{\Delta, \varepsilon_1} \right) \right. \\ &\quad \left. + \hat{\delta}(\varepsilon_1) n_{\varepsilon_2} \hat{G}_1^{\Delta, \varepsilon_2} - \frac{1}{2} \hat{\delta}(\varepsilon_1) \hat{\delta}(\varepsilon_2) \left( \hat{G}_{3,1}^{\Delta} - 2\hat{G}_{1,2}^{\Delta} \right) \right] \frac{1}{(2\pi i)^2} \quad (\text{G12a}) \\ &= n_{\varepsilon_1} \left( n_{\varepsilon_2} S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} - \delta_{\varepsilon_2} (1 - \delta_{\varepsilon_1}) S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} - n_{\varepsilon_{12}} S_{[\bar{3}, [\bar{1}, \bar{2}]_-, ]_-} \right. \\ &\quad \left. - \delta_{\varepsilon_3} (1 - \delta_{\varepsilon_1}) S_{[\bar{1}, \bar{2}]_-, \bar{3}]_-} \right) - n_{\varepsilon_2} \delta_{\varepsilon_1} (1 - \delta_{\varepsilon_2}) S_{[\bar{1}, \bar{2}]_-, \bar{3}]_-} \\ &\quad + \delta_{\varepsilon_1} \delta_{\varepsilon_2} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \quad (\text{G12b})\end{aligned}$$

We can now check whether Equation (G12b) reproduces the full PSF,  $S_{[\bar{1}, \bar{2}, \bar{3}]_-}$ , by repeated application of Equations (G10). For this purpose, we use the PSF decomposition in Appendix B.1 to separately consider the contributions in the PSF proportional to  $\delta(\varepsilon_1)$ , and those which are not. Note that  $S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-}$  and  $S_{[\bar{1}, \bar{2}]_-, \bar{3}]_-}$  in the first line of Equation (G12b) contribute to both of these cases.

For PSF contributions not proportional to  $\delta(\varepsilon_1)$ , the last line of Equation (G12b) can be omitted (due to  $\delta_{\varepsilon_1}$ ), so that

$$\begin{aligned}(1 - \delta_{\varepsilon_1}) S_p[G] &= -(1 - \delta_{\varepsilon_1}) n_{\varepsilon_1} \left( -n_{\varepsilon_2} S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} + \delta_{\varepsilon_2} S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} \right. \\ &\quad \left. + n_{\varepsilon_3} S_{[\bar{3}, [\bar{1}, \bar{2}]_-, ]_-} + \delta_{\varepsilon_3} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \right) \\ &= -(1 - \delta_{\varepsilon_1}) n_{\varepsilon_1} \left( S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} + S_{[\bar{1}, \bar{2}, \bar{3}]_-} \right) \\ &= -(1 - \delta_{\varepsilon_1}) n_{\varepsilon_1} S_{[\bar{1}, \bar{2}, \bar{3}]_-} = (1 - \delta_{\varepsilon_1}) S_{[\bar{1}, \bar{2}, \bar{3}]_-} \quad (\text{G13})\end{aligned}$$

Here, we used Equations (G10) in the first and third step.

For PSF contributions proportional to  $\delta(\varepsilon_1)$ , the MWF  $n_{\varepsilon_1}$  multiplying  $S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-}$  and  $S_{[\bar{1}, \bar{2}]_-, \bar{3}]_-}$  in Equation (G12b) seems to diverge in the bosonic case. This issue was already discussed in Equation (C28) (for unpermuted indices): There,  $\tilde{G}^{\varepsilon_1, \varepsilon_2} = (2\pi i)^2 S_{[\bar{1}, \bar{2}, \bar{3}]_-}$  does not contain factors  $\delta(\varepsilon_1)$  due to the equilibrium condition, and therefore only the first term, expressed as  $-n_{\varepsilon_{12}} n_{\varepsilon_2} S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-}$ , needs to be considered. As this PSF commutator does not contain factors  $\delta(\varepsilon_2)$  due to the equilibrium condition, we obtain (using  $n_{\varepsilon_2} = n_{\varepsilon_{12}} = n_{\varepsilon_3}$  and  $\delta_{\varepsilon_2} = \delta_{\varepsilon_{12}} = \delta_{\varepsilon_3}$  due to  $\delta_{\varepsilon_1}$ )

$$\begin{aligned}\delta_{\varepsilon_1} S_p[G] &= \delta_{\varepsilon_1} \left( -n_{\varepsilon_2} n_{\varepsilon_2} S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} - n_{\varepsilon_{12}} (1 - \delta_{\varepsilon_2}) S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-} + \delta_{\varepsilon_2} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \right) \\ &= \delta_{\varepsilon_1} \left( -n_{\varepsilon_2} (1 - \delta_{\varepsilon_2}) S_{[\bar{1}, \bar{3}]_-, \bar{2}]_-} - n_{\varepsilon_{12}} (1 - \delta_{\varepsilon_2}) S_{[\bar{1}, \bar{2}, \bar{3}]_-} + \delta_{\varepsilon_2} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \right) \\ &= \delta_{\varepsilon_1} \left( n_{\varepsilon_3} (1 - \delta_{\varepsilon_3}) S_{[\bar{3}, [\bar{1}, \bar{2}]_-, ]_-} + \delta_{\varepsilon_3} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \right) \\ &= \delta_{\varepsilon_1} \left( (1 - \delta_{\varepsilon_3}) S_{[\bar{1}, \bar{2}, \bar{3}]_-} + \delta_{\varepsilon_3} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \right) \\ &= \delta_{\varepsilon_1} S_{[\bar{1}, \bar{2}, \bar{3}]_-} \quad (\text{G14})\end{aligned}$$

Here, Equation (G10b) was applied in the first and the third step.

Therefore, we conclude that Equation (G12b) indeed recovers the input PSF  $S_{[\bar{1}, \bar{2}, \bar{3}]_-}$ , including terms proportional to  $\delta(\varepsilon_1)$  in Equation (G14) and those which are not in Equation (G13).

### G.2.3. For $\ell = 4$

Now, the same consistency check can be performed for fermionic 4p correlators. Similarly to Equation (G10), for 4p PSFs, we have

$$S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} = -n_{\varepsilon_1} S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} \quad (\text{G15a})$$

$$S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} = -n_{\varepsilon_{12}} S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} + \delta_{\varepsilon_{12}} S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} \quad (\text{G15b})$$

Here, the symbolic Kronecker  $\delta$  only arises in the latter case, since  $\varepsilon_1$  is the energy difference for a fermionic operator. Starting from the formula in Equation (88), we obtain

$$\begin{aligned}S_p[G] &= \frac{n_{\varepsilon_1}}{(2\pi i)^3} \left[ n_{\varepsilon_2} \left( n_{\varepsilon_3} \tilde{G}^{\varepsilon_3, \varepsilon_2, \varepsilon_1} + n_{\varepsilon_{123}} \tilde{G}^{\varepsilon_1, \varepsilon_2, \varepsilon_3} + n_{\varepsilon_{13}} \tilde{G}^{\varepsilon_3, \varepsilon_2, \varepsilon_1} \right) \right. \\ &\quad \left. + n_{\varepsilon_{23}} \tilde{G}^{\varepsilon_2, \varepsilon_3, \varepsilon_1} \right] + n_{\varepsilon_{12}} \left( n_{\varepsilon_3} \tilde{G}^{\varepsilon_3, \varepsilon_1, \varepsilon_2} + n_{\varepsilon_{123}} \tilde{G}^{\varepsilon_1, \varepsilon_2, \varepsilon_3} \right) \\ &\quad + n_{\varepsilon_3} \hat{\delta}(\varepsilon_{12}) \hat{G}_{12}^{\varepsilon_3, \varepsilon_1} + n_{\varepsilon_2} \hat{\delta}(\varepsilon_{13}) \hat{G}_{13}^{\varepsilon_2, \varepsilon_1} + n_{\varepsilon_2} \hat{\delta}(\varepsilon_{23}) \hat{G}_{23}^{\varepsilon_2, \varepsilon_1} \\ &= -n_{\varepsilon_1} \left[ n_{\varepsilon_2} \left( n_{\varepsilon_3} S_{[\bar{3}, [\bar{2}, [\bar{1}, \bar{4}]_-, ]_-} + n_{\varepsilon_{123}} S_{[[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-, \bar{4}]_-} \right. \right. \\ &\quad \left. \left. + n_{\varepsilon_{13}} S_{[[\bar{1}, \bar{3}]_-, [\bar{2}, \bar{4}]_-, ]_-} - \delta_{\varepsilon_{13}} S_{[\bar{1}, \bar{3}]_-, [\bar{2}, \bar{4}]_-, ]_-} \right) \right. \\ &\quad \left. + n_{\varepsilon_{23}} S_{[[\bar{2}, \bar{3}]_-, [\bar{1}, \bar{4}]_-, ]_-} - \delta_{\varepsilon_{23}} S_{[\bar{1}, \bar{4}]_-, [\bar{2}, \bar{3}]_-, ]_-} \right) \\ &\quad \left. + n_{\varepsilon_{12}} \left( n_{\varepsilon_3} S_{[\bar{3}, [[\bar{1}, \bar{2}]_-, \bar{4}]_-, ]_-} + n_{\varepsilon_{123}} S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-} \right) - n_{\varepsilon_3} \delta_{\varepsilon_{12}} S_{[\bar{1}, \bar{2}]_-, [\bar{3}, \bar{4}]_-, ]_-} \right] \\ &= n_{\varepsilon_1} \left[ n_{\varepsilon_2} \left( S_{[\bar{3}, [\bar{2}, [\bar{1}, \bar{4}]_-, ]_-} + S_{[\bar{2}, [\bar{1}, \bar{3}]_-, ]_-, \bar{4}]_-} + S_{[\bar{1}, \bar{3}]_-, [\bar{2}, \bar{4}]_-, ]_-} \right. \right. \\ &\quad \left. \left. + S_{[\bar{2}, \bar{3}]_-, [\bar{1}, \bar{4}]_-, ]_-} \right) + n_{\varepsilon_{12}} (1 - \delta_{\varepsilon_{12}}) \left( S_{[\bar{3}, [[\bar{1}, \bar{2}]_-, \bar{4}]_-, ]_-} + S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-} \right) \right. \\ &\quad \left. - n_{\varepsilon_3} \delta_{\varepsilon_{12}} \left( S_{[\bar{4}, [[\bar{1}, \bar{2}]_-, \bar{3}]_-, ]_-} - S_{[\bar{1}, \bar{2}]_-, [\bar{3}, \bar{4}]_-, ]_-} \right) \right] \\ &= n_{\varepsilon_1} \left[ n_{\varepsilon_2} S_{[\bar{3}, [\bar{2}, [\bar{1}, \bar{4}]_-, ]_-} + n_{\varepsilon_{12}} S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-} - \delta_{\varepsilon_{12}} S_{[\bar{1}, \bar{2}]_-, \bar{3}, \bar{4}]_-} \right] \\ &= -n_{\varepsilon_1} S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} \\ &= S_{[\bar{1}, \bar{2}, \bar{3}, \bar{4}]_-} \quad (\text{G16})\end{aligned}$$

In the first step, we inserted expressions for the discontinuities, derived analogously to Equations (B8a), (E6), and (E2). We apply relations (G15) to eliminate the MWFs in the remaining steps. For the second step, we note that  $S_{[\bar{3}, [[\bar{1}, \bar{2}]_-, \bar{4}]_-, ]_-}$  and  $S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-}$  contain terms with and without  $\delta(\varepsilon_{12})$  factor. For the  $\delta(\varepsilon_{12})$  terms, the prefactor of  $n_{\varepsilon_{12}}$  is undefined at  $\varepsilon_{12}$ . Analogously to the 3p calculation, we evaluate Equation (G16) using  $\delta_{\varepsilon_{12}} (S_{[\bar{3}, [[\bar{1}, \bar{2}]_-, \bar{4}]_-, ]_-} + S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-}) = 0$  and  $n_{\varepsilon_{34}} (-n_{\varepsilon_3} + n_{\varepsilon_4}) = n_{\varepsilon_3} n_{\varepsilon_4}$ :

$$\begin{aligned}n_{\varepsilon_{12}} \left( n_{\varepsilon_3} S_{[\bar{3}, [[\bar{1}, \bar{2}]_-, \bar{4}]_-, ]_-} + n_{\varepsilon_{123}} S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-} \right) \\ = n_{\varepsilon_{12}} (1 - \delta_{\varepsilon_{12}}) \left( n_{\varepsilon_3} S_{[\bar{3}, [[\bar{1}, \bar{2}]_-, \bar{4}]_-, ]_-} + n_{\varepsilon_{123}} S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-} \right) \\ + \delta_{\varepsilon_{12}} n_{\varepsilon_3} n_{\varepsilon_4} S_{[[\bar{1}, \bar{2}]_-, \bar{3}]_-, \bar{4}]_-} \quad (\text{G17})\end{aligned}$$

To simplify the  $\delta_{\varepsilon_{12}}$  terms in the third step, remember that the Kronecker symbol extracts those PSF contributions proportional to a  $\delta(\varepsilon_{12})$ , such that the equilibrium condition allows for manipulations like  $\delta_{\varepsilon_{12}} S_{(1234)} = \delta_{\varepsilon_{12}} S_{(3412)}$ . Finally, Equation (G17) shows that the formula in Equation (88) fully recovers the input PSFs from 4p MF correlators.

## Appendix H: Additional Hubbard Atom Material

### H.1. Useful Identities

In this section, we prove the identities given in Equations (107a) and (107b). The first identity follows from

$$\begin{aligned} & \lim_{\gamma_0 \rightarrow 0^+} \left( \frac{\omega + i\gamma_0}{(\omega + i\gamma_0)^2 - u^2} - \frac{\omega - i\gamma_0}{(\omega - i\gamma_0)^2 - u^2} \right) \\ &= -i \lim_{\gamma_0 \rightarrow 0^+} \left( \frac{\gamma_0}{(\omega + u)^2 + \gamma_0^2} + \frac{\gamma_0}{(\omega - u)^2 + \gamma_0^2} \right) \\ &= -i\pi [\delta(\omega + u) + \delta(\omega - u)] \end{aligned} \quad (\text{H1})$$

where we used Equation (58). Identity (107b) is derived via

$$\begin{aligned} & \lim_{\gamma_0 \rightarrow 0^+} \left( \frac{1}{(\omega + i\gamma_0)^2 - u^2} - \frac{1}{(\omega - i\gamma_0)^2 - u^2} \right) \\ &= \frac{i}{u} \lim_{\gamma_0 \rightarrow 0^+} \left( \frac{\gamma_0}{(\omega + u)^2 + \gamma_0^2} - \frac{\gamma_0}{(\omega - u)^2 + \gamma_0^2} \right) \\ &= \frac{i\pi}{u} [\delta(\omega + u) - \delta(\omega - u)]. \end{aligned} \quad (\text{H2})$$

### H.2. Simplifications for 3p Electron-Density Correlator

In Section 7.2.1, we introduced the 3p electron-density correlator with regular and anomalous parts

$$\begin{aligned} \tilde{C}(i\omega_1, i\omega_2) &= \frac{u^2 - i\omega_1 i\omega_2}{[(i\omega_1)^2 - u^2][(i\omega_2)^2 - u^2]} \\ \hat{C}_3(i\omega_1) &= \frac{u}{2} \frac{1}{(i\omega_1)^2 - u^2} \end{aligned} \quad (\text{H3})$$

Here, we derive the explicit expression  $G'^{[2]} - G^{[3]}$  given in Equation (114),

$$\begin{aligned} G'^{[2]} - G^{[3]} &= \tilde{C}(\omega_1^+, \omega_2^-) - \tilde{C}(\omega_1^-, \omega_2^-) \\ &= \frac{u^2}{(\omega_2^-)^2 - u^2} \left( \frac{1}{(\omega_1^+)^2 - u^2} - \frac{1}{(\omega_1^-)^2 - u^2} \right) \\ &\quad - \frac{\omega_2^-}{(\omega_2^-)^2 - u^2} \left( \frac{\omega_1^+}{(\omega_1^+)^2 - u^2} - \frac{\omega_1^-}{(\omega_1^-)^2 - u^2} \right) \end{aligned} \quad (\text{H4})$$

Using both identities (H1) and (H2), this expression can be further simplified to

$$G'^{[2]} - G^{[3]} = \pi i \frac{u + \omega_2^-}{(\omega_2^-)^2 - u^2} \delta(\omega_1 + u) + \pi i \frac{\omega_2^- - u}{(\omega_2^-)^2 - u^2} \delta(\omega_1 - u) \quad (\text{H5})$$

Additionally multiplying both sides with  $N_1 = N_{\omega_1}$  and using  $N_{-\omega_1} = -N_{\omega_1}$ , we recover the first term in the second line of Equation (114),

$$N_1 (G'^{[2]} - G^{[3]}) = \pi i t \left[ \frac{\delta(\omega_1 - u)}{\omega_2^- + u} - \frac{\delta(\omega_1 + u)}{\omega_2^- - u} \right] \quad (\text{H6})$$

Next, we consider the Keldysh component  $G_{d_1 d_1^\dagger n_1}^{[123]}$ . Since the regular part in Equation (H3) is independent of  $i\omega_3$ , we can set  $G'^{[1]} = G^{[2]}$  and  $G'^{[2]} = G^{[1]}$  (see Figure 6b). Additionally using Equation (83) as well as  $\hat{C}_1 = \hat{C}_2$  for the 3p electron-density correlator, the last FDR in Equation (84) reduces to

$$\begin{aligned} G_{d_1 d_1^\dagger n_1}^{[123]} &= G'^{[3]} + N_1 N_2 (G'^{[3]} - G^{[2]} - G^{[1]} + G^{[3]}) \\ &\quad + 4\pi i \delta(\omega_{12}) N_1 (\hat{C}_3^{[1]} - \hat{C}_3^{[2]}) \end{aligned} \quad (\text{H7})$$

Here, we show that all terms except  $G'^{[3]}$  cancel out. To this end, we can reuse Equation (H5) to obtain

$$\begin{aligned} & G'^{[3]} - G^{[2]} - G^{[1]} + G^{[3]} \\ &= \tilde{C}(\omega_1^+, \omega_2^+, \omega_3^-) - \tilde{C}(\omega_1^-, \omega_2^+, \omega_3^-) - \tilde{C}(\omega_1^+, \omega_2^-, \omega_3^-) + \tilde{C}(\omega_1^-, \omega_2^-, \omega_3^-) \\ &= \pi i \delta(\omega_1 + u) \left( \frac{1}{\omega_2^+ - u} - \frac{1}{\omega_2^- - u} \right) \\ &\quad + \pi i \delta(\omega_1 - u) \left( \frac{1}{\omega_2^+ + u} - \frac{1}{\omega_2^- + u} \right) \\ &= 2\pi^2 [\delta(\omega_1 + u) \delta(\omega_2 - u) + \delta(\omega_1 - u) \delta(\omega_2 + u)] \\ &= 2\pi^2 \delta(\omega_{12}) [\delta(\omega_1 + u) + \delta(\omega_1 - u)] \end{aligned} \quad (\text{H8})$$

The discontinuity of  $\hat{C}_3$  is easily evaluated with identity (H2)

$$\begin{aligned} \hat{C}_3^{[1]} - \hat{C}_3^{[2]} &= \frac{u}{2} \left( \frac{1}{(\omega_1^+)^2 - u^2} - \frac{1}{(\omega_1^-)^2 - u^2} \right) \\ &= \pi i \frac{1}{2} [\delta(\omega_1 + u) - \delta(\omega_1 - u)] \end{aligned} \quad (\text{H9})$$

Inserting all terms (except  $G'^{[3]}$ ) in Equation (H7) and using again  $N_i = N_{\omega_i} = -N_{-\omega_i}$ , we find

$$\begin{aligned} & N_1 N_2 (G'^{[3]} - G^{[2]} - G^{[1]} + G^{[3]}) + 4\pi i \delta(\omega_{12}) N_1 \sqrt{2} (\hat{C}_3^{[1]} - \hat{C}_3^{[2]}) \\ &= -2\pi^2 t^2 \delta(\omega_{12}) [\delta(\omega_1 + u) + \delta(\omega_1 - u)] \\ &\quad + 2\pi^2 t^2 \delta(\omega_{12}) [\delta(\omega_1 + u) + \delta(\omega_1 - u)] = 0 \end{aligned} \quad (\text{H10})$$

Thus, Equation (H7) reduces to

$$G_{d_1 d_1^\dagger n_1}^{[123]} = G'^{[3]} \quad (\text{H11})$$

corresponding to the last equality in Equation (115).

### H.3. Simplifications for Fermionic 4p Correlator

In this section, we present the steps needed to obtain the Keldysh component  $G_{\uparrow\downarrow}^{[12]}$  in Section 7.3. The discontinuities can be easily evaluated after rewriting the regular part in terms of general complex frequencies as

$$\begin{aligned} \tilde{G}(z) = & -\frac{u}{z^2 - u^2} \left[ \frac{1}{z_1 + u} \left( \frac{1}{z_3 - u} + \frac{1}{z_4 - u} \right) \right. \\ & \left. + \frac{1}{z_3 + u} \left( \frac{1}{z_1 - u} + \frac{1}{z_4 - u} \right) + \frac{1}{z_4 + u} \left( \frac{1}{z_1 - u} + \frac{1}{z_3 - u} \right) \right] \quad (\text{H12}) \end{aligned}$$

The discontinuity  $C_{\text{III}}^{(12)} - C^{(2)}$  in Equation (120) then reduces to

$$\begin{aligned} C_{\text{III}}^{(12)} - C^{(2)} = & \tilde{G}(\omega_1^+, \omega_2^+, \omega_3^-, \omega_4^-) - \tilde{G}(\omega_1^-, \omega_2^+, \omega_3^-, \omega_4^-) \\ = & \frac{2\pi i u}{(\omega_2^+)^2 - u^2} \left[ \delta(\omega_1 + u) \left( \frac{1}{\omega_3^- - u} + \frac{1}{\omega_4^- - u} \right) \right. \\ & \left. + \delta(\omega_1 - u) \left( \frac{1}{\omega_3^- + u} + \frac{1}{\omega_4^- + u} \right) \right] \quad (\text{H13}) \end{aligned}$$

The second discontinuity  $C_{\text{I}}^{(12)} - C^{(1)}$  follows by exchanging  $\omega_1 \rightarrow \omega_2$ . Using the  $\delta$ -functions to replace  $u$  by  $\omega_1$  and multiplying with  $N_1$ , the Keldysh component  $G_{\uparrow\downarrow}^{[12]}$  takes the form

$$\begin{aligned} G_{\uparrow\downarrow}^{[12]} = & \frac{2\pi i u t}{(\omega_2^+)^2 - u^2} [\delta(\omega_1 - u) - \delta(\omega_1 + u)] \left( \frac{1}{\omega_{13}^-} + \frac{1}{\omega_{14}^-} \right) \\ & + \frac{2\pi i u t}{(\omega_1^+)^2 - u^2} [\delta(\omega_2 - u) - \delta(\omega_2 + u)] \left( \frac{1}{\omega_{23}^-} + \frac{1}{\omega_{24}^-} \right) \\ & + 4\pi i u^2 \frac{\delta(\omega_{13})(t-1) + \delta(\omega_{14})(t+1)}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]} \quad (\text{H14}) \end{aligned}$$

Collecting terms proportional to  $t$  and replacing the  $\delta$ -functions of its coefficient using the identities in Equations (58) and (H2) yields

$$G_{\uparrow\downarrow}^{\text{II}}(\omega) = 0 \quad (\text{H18a})$$

$$G_{\uparrow\downarrow}^{\text{I}}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^+, \omega_2^-, \omega_3^-, \omega_4^-) \quad (\text{H18b})$$

$$G_{\uparrow\downarrow}^{\text{II}}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^+, \omega_3^-, \omega_4^-) \quad (\text{H18c})$$

$$G_{\uparrow\downarrow}^{\text{III}}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^-, \omega_3^+, \omega_4^-) \quad (\text{H18d})$$

$$G_{\uparrow\downarrow}^{\text{IV}}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^-, \omega_3^-, \omega_4^+) \quad (\text{H18e})$$

$$G_{\uparrow\downarrow}^{\text{IV}}(\omega) = \frac{2\pi i u^2 [\delta(\omega_{14}) - \delta(\omega_{13})]}{[(\omega_1^-)^2 - u^2][(\omega_2^-)^2 - u^2]} + u^2 t \left[ \frac{1}{[(\omega_3^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \left( \frac{1}{\omega_{24}^-} + \frac{1}{\omega_{14}^-} \right) - \text{c.c.} \right] \quad (\text{H18f})$$

$$G_{\uparrow\downarrow}^{\text{IV}}(\omega) = \frac{2\pi i u^2 \delta(\omega_{14})}{[(\omega_1^-)^2 - u^2][(\omega_3^-)^2 - u^2]} + u^2 t \left[ \frac{1}{[(\omega_2^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \left( \frac{1}{\omega_{34}^-} + \frac{1}{\omega_{14}^-} \right) - \text{c.c.} \right] \quad (\text{H18g})$$

$$\begin{aligned} G_{\uparrow\downarrow}^{[12]} = & \frac{4\pi i u^2 [\delta(\omega_{14}) - \delta(\omega_{13})]}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]} \\ & - 2u^2 t \left[ \frac{1}{(\omega_2^+)^2 - u^2} \left( \frac{1}{(\omega_1^+)^2 - u^2} - \frac{1}{(\omega_1^-)^2 - u^2} \right) \left( \frac{1}{\omega_{13}^-} + \frac{1}{\omega_{14}^-} \right) \right. \\ & + \frac{1}{(\omega_1^+)^2 - u^2} \left( \frac{1}{(\omega_2^+)^2 - u^2} - \frac{1}{(\omega_2^-)^2 - u^2} \right) \left( \frac{1}{\omega_{23}^-} + \frac{1}{\omega_{24}^-} \right) \\ & \left. + \frac{1}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]} \left( \frac{1}{\omega_{13}^+} - \frac{1}{\omega_{13}^-} + \frac{1}{\omega_{14}^+} - \frac{1}{\omega_{14}^-} \right) \right] \quad (\text{H15}) \end{aligned}$$

By energy conservation,  $\omega_{1234} = 0$ , many terms in the bracket cancel, and we obtain the final result

$$\begin{aligned} G_{\uparrow\downarrow}^{[12]} = & \frac{4\pi i u^2 [\delta(\omega_{14}) - \delta(\omega_{13})]}{[(\omega_1^+)^2 - u^2][(\omega_2^+)^2 - u^2]} \\ & + 2u^2 t \left[ \frac{1}{[(\omega_1^+)^2 - u^2][(\omega_2^-)^2 - u^2]} \left( \frac{1}{\omega_{23}^-} + \frac{1}{\omega_{24}^-} \right) - \text{c.c.} \right] \quad (\text{H16}) \end{aligned}$$

where c.c. denotes the complex conjugate.

### H.4. Results for Fermionic 4p Correlator

In this section, we summarize results for all Keldysh components of the four-electron correlator for both the  $G_{\uparrow\downarrow}$  and  $G_{\uparrow\uparrow}$  component. They can be derived following similar calculations presented in the previous section. Defining

$$\tilde{G}_{\uparrow\downarrow}(z) = \frac{2u \prod_{i=1}^4 (z_i) + u^3 \sum_{i=1}^4 (z_i)^2 - 6u^5}{\prod_{i=1}^4 [(z_i)^2 - u^2]} \quad (\text{H17})$$

the results for  $G_{\uparrow\downarrow}$  read

$$G_{\uparrow\downarrow}^{[23]}(\omega) = \frac{-2\pi i u^2 \delta(\omega_{13})}{[(\omega_1^-)^2 - u^2][(\omega_4^-)^2 - u^2]} + u^2 t \left[ \frac{1}{[(\omega_2^+)^2 - u^2][(\omega_3^-)^2 - u^2]} \left( \frac{1}{\omega_{34}^-} + \frac{1}{\omega_{13}^-} \right) - \text{c.c.} \right] \quad (\text{H18h})$$

$$G_{\uparrow\downarrow}^{[14]}(\omega) = \frac{-2\pi i u^2 \delta(\omega_{13})}{[(\omega_2^-)^2 - u^2][(\omega_3^-)^2 - u^2]} + u^2 t \left[ \frac{1}{[(\omega_1^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \left( \frac{1}{\omega_{34}^-} + \frac{1}{\omega_{24}^-} \right) - \text{c.c.} \right] \quad (\text{H18i})$$

$$G_{\uparrow\downarrow}^{[13]}(\omega) = \frac{2\pi i u^2 \delta(\omega_{14})}{[(\omega_2^-)^2 - u^2][(\omega_4^-)^2 - u^2]} + u^2 t \left[ \frac{1}{[(\omega_1^+)^2 - u^2][(\omega_3^-)^2 - u^2]} \left( \frac{1}{\omega_{34}^-} + \frac{1}{\omega_{23}^-} \right) - \text{c.c.} \right] \quad (\text{H18j})$$

$$G_{\uparrow\downarrow}^{[12]}(\omega) = \frac{2\pi i u^2 [\delta(\omega_{14}) - \delta(\omega_{13})]}{[(\omega_3^-)^2 - u^2][(\omega_4^-)^2 - u^2]} + u^2 t \left[ \frac{1}{[(\omega_1^+)^2 - u^2][(\omega_2^-)^2 - u^2]} \left( \frac{1}{\omega_{24}^-} + \frac{1}{\omega_{23}^-} \right) - \text{c.c.} \right] \quad (\text{H18k})$$

$$G_{\uparrow\downarrow}^{[234]}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^+, \omega_3^+, \omega_4^+) + 2\pi^2 u t [\delta(\omega_2 - u) + \delta(\omega_2 + u)] [\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{(\omega_1^-)^2 - u^2} \quad (\text{H18l})$$

$$G_{\uparrow\downarrow}^{[134]}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^+, \omega_2^-, \omega_3^+, \omega_4^+) + 2\pi^2 u t [\delta(\omega_1 - u) + \delta(\omega_1 + u)] [\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{(\omega_2^-)^2 - u^2} \quad (\text{H18m})$$

$$G_{\uparrow\downarrow}^{[124]}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^+, \omega_2^+, \omega_3^-, \omega_4^+) + 2\pi^2 u t [\delta(\omega_4 - u) + \delta(\omega_4 + u)] [\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{(\omega_3^-)^2 - u^2} \quad (\text{H18n})$$

$$G_{\uparrow\downarrow}^{[123]}(\omega) = \tilde{G}_{\uparrow\downarrow}(\omega_1^+, \omega_2^+, \omega_3^+, \omega_4^-) + 2\pi^2 u t [\delta(\omega_3 - u) + \delta(\omega_3 + u)] [\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{(\omega_4^-)^2 - u^2} \quad (\text{H18o})$$

$$G_{\uparrow\downarrow}^{[1234]}(\omega) = \frac{t}{u} [\omega_1^+ \tilde{G}_{\uparrow\downarrow}(\omega_1^+, \omega_2^-, \omega_3^-, \omega_4^-) + \omega_2^+ \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^+, \omega_3^-, \omega_4^-) + \omega_3^+ \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^-, \omega_3^+, \omega_4^-) + \omega_4^+ \tilde{G}_{\uparrow\downarrow}(\omega_1^-, \omega_2^-, \omega_3^-, \omega_4^+)] \\ - 4\pi^3 i t^2 \delta(\omega_{12}) [\delta(u + \omega_1) - \delta(u - \omega_1)] [\delta(u + \omega_3) - \delta(u - \omega_3)] \quad (\text{H18p})$$

The same-spin correlator in the MF turns out to be purely anomalous

$$G_{\uparrow\uparrow}(i\omega) = \frac{u^2 (\beta \delta_{i\omega_{14}} - \beta \delta_{i\omega_{12}})}{\prod_{i=1}^4 (i\omega_i) - u} \quad (\text{H19})$$

Therefore, the derivation of the corresponding Keldysh correlators is straightforward and yields

$$G_{\uparrow\uparrow}^{[0]}(\omega) = G_{\uparrow\uparrow}^{[1]}(\omega) = G_{\uparrow\uparrow}^{[2]}(\omega) = G_{\uparrow\uparrow}^{[3]}(\omega) = G_{\uparrow\uparrow}^{[4]}(\omega) = 0 \quad (\text{H20a})$$

$$G_{\uparrow\uparrow}^{[34]}(\omega) = 2\pi i u^2 \frac{\delta(\omega_{14})}{[(\omega_2^-)^2 - u^2][(\omega_4^+)^2 - u^2]} \quad (\text{H20b})$$

$$G_{\uparrow\uparrow}^{[24]}(\omega) = 2\pi i u^2 \frac{\delta(\omega_{14}) - \delta(\omega_{12})}{[(\omega_2^+)^2 - u^2][(\omega_4^+)^2 - u^2]} \quad (\text{H20c})$$

$$G_{\uparrow\uparrow}^{[23]}(\omega) = 2\pi i u^2 \frac{-\delta(\omega_{12})}{[(\omega_2^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \quad (\text{H20d})$$

$$G_{\uparrow\uparrow}^{[14]}(\omega) = 2\pi i u^2 \frac{-\delta(\omega_{12})}{[(\omega_2^-)^2 - u^2][(\omega_4^+)^2 - u^2]} \quad (\text{H20e})$$

$$G_{\uparrow\uparrow}^{[13]}(\omega) = 2\pi i u^2 \frac{\delta(\omega_{14}) - \delta(\omega_{12})}{[(\omega_2^-)^2 - u^2][(\omega_4^-)^2 - u^2]} \quad (\text{H20f})$$

$$G_{\uparrow\uparrow}^{[12]}(\omega) = 2\pi i u^2 \frac{\delta(\omega_{14})}{[(\omega_2^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \quad (\text{H20g})$$

$$G_{\uparrow\uparrow}^{[234]}(\omega) = 2\pi^2 u t \frac{1}{(\omega_1^-)^2 - u^2} [\delta(\omega_3 - u) + \delta(\omega_3 + u)] [\delta(\omega_{14}) - \delta(\omega_{12})] \quad (\text{H20h})$$

$$G_{\uparrow\uparrow}^{[134]}(\omega) = 2\pi^2 u t \frac{1}{(\omega_2^-)^2 - u^2} [\delta(\omega_4 - u) + \delta(\omega_4 + u)] [\delta(\omega_{14}) - \delta(\omega_{12})] \quad (\text{H20i})$$

$$G_{\uparrow\uparrow}^{[124]}(\omega) = 2\pi^2 u t \frac{1}{(\omega_3^-)^2 - u^2} [\delta(\omega_1 - u) + \delta(\omega_1 + u)] [\delta(\omega_{14}) - \delta(\omega_{12})] \quad (\text{H20j})$$

$$G_{\uparrow\uparrow}^{[123]}(\omega) = 2\pi^2 u t \frac{1}{(\omega_4^-)^2 - u^2} [\delta(\omega_2 - u) + \delta(\omega_2 + u)] [\delta(\omega_{14}) - \delta(\omega_{12})] \quad (\text{H20k})$$

$$G_{\uparrow\uparrow}^{[1234]}(\omega) = -4\pi^3 i t^2 [\delta(\omega_{12}) - \delta(\omega_{14})] [\delta(\omega_1 + u) - \delta(\omega_1 - u)] [\delta(\omega_3 + u) - \delta(\omega_3 - u)]. \quad (\text{H20l})$$

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## Conflict of Interest

The authors declare no conflict of interest.

## Data Availability Statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

## Keywords

analytic continuation, Keldysh formalism, multipoint correlation functions, thermal field theory

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