Analytic Continuation of Correlators from the Matsubara to the Keldysh Formalism

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Abstract

Conceptually, the Matsubara formalism (MF) and the Keldysh formalism (KF) give equivalent results for equilibrium systems which are invariant under time translations. However, while the MF is more convenient for compact analytical calculations, the computation of physical observables requires to continue functions from imaginary to real frequencies. The latter is highly challenging in numerics. The KF, already formulated in real frequencies, circumvents this problem at the cost of higher complexity. It is therefore desirable to construct the various components of a KF function starting from an analytic result for a MF function. In this thesis we show how one can construct the components of a KF correlator with analytic continuations of the MF correlator, dubbed AC functions. We thereby extend the work of other authors (Evans, Weldon, Baym and Mermin) and provide formulas (AC formulas) for the analytic continuation of three-point and four-point functions. However, most of our results actually hold for any multi-point correlator.

To obtain general results without any further assumptions than total energy conservation and equilibrium, we use the spectral representation derived by Kugler, Lee and von Delft. This representation divides the correlator into *formalism-independent* partial spectral functions and *formalism-specific* kernels facilitating the search for relations between MF and KF correlators. Thereby we easily reproduce the familiar correspondence of *retarded* KF correlators to certain AC functions. To express the remaining KF correlators we have to expand them in a suitable way. This allows us to relate them to linear combinations of AC functions by use of the equilibrium condition.

We then apply our AC formulas in various contexts. Due to the close relation of four-point correlators to susceptibilities, the work done by Eliashberg and Oguri is particularly interesting. They used the analytic continuation method in the MF to convert Matsubara sums into contour integrals. Out of numerous vertex contributions that arise they identified a single contribution which is in fact relevant for the susceptibility of their physical model under consideration. We show that each of their vertex contributions has a counterpart in the KF which is proportional to a single KF component in the R/A basis. For the Hubbard atom we explicitly compute the vertex function in the KF. This exactly solvable model can be used as benchmark for numerical works.

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Contents

Chapter 1

Introduction

Multi-point correlation functions are central objects of investigation in the field of many-body physics. The one-particle correlator describes the propagation of a single particle, containing information on the spectrum of single-particle excitations. Here we focus on higher-point functions such as the two-particle correlator. The two-particle or four-point (4p) correlator is associated with the effective interaction between two particles. Interesting observables, such as the optical and magnetic response function, can be computed from it. Moreover the closely related vertex function is an essential ingredient in numerous many-body methods such as the functional renormalization group [1], the parquet formalism [2] and diagrammatic extensions of dynamical mean field theory [3].

The most common formalism for the study of equilibrium systems at finite-temperature $T = 1/\beta$ is the imaginary-time Matsubara formalism (MF) [4,5]. It exploits the cyclicity of the trace and the fact that the statistical weight of a thermal state $e^{-\beta\mathcal{H}}$ corresponds to a time-evolution $e^{-i\mathcal{H}t}$ along the imaginary axis of the time argument. After a Wick rotation $t \to -i\tau$ the correlators are (anti-)periodic functions of imaginary times with period β. Due to the periodicity the Fourier transform of a MF correlator is a function which has to be evaluated on a discrete set of imaginary frequencies. To obtain a correlator of real times or real frequencies one has to "unwind" the Wick rotation by performing a suitable analytic continuation. However, numerically the analytic continuation to real frequencies is a highly challenging problem [6, 7].

The Keldysh formalism (KF) is another well-established theoretical framework. Unlike the MF it is not restricted to equilibrium systems. Additionally, it directly works with real times and frequencies obviating the need for an analytic continuation. However, this comes at the cost of increased complexity: the KF is formulated on a doubled time contour, and an ℓ-point (ℓp) function involves 2^ℓ components [8, 9]. By contrast, every MF correlator involves just one function.

On purely analytical grounds both MF and KF are expected to provide identical results in equilibrium. Following the philosophy that, irrespective of the formalism, any function should contain the same information we wish to transition from one formalism to the other. This would allow us to "cherry-pick" advantages from either formalism. In this thesis we show how to obtain a KF correlator by analytic continuation of a MF correlator.

This procedure is well-known for two-point (2p) functions which effectively depend on a single time or frequency argument, see e.g. Refs. [5, 10, 11]. For higher-point functions the analytic continuation becomes increasingly complicated. Nevertheless, it is always possible analytically if the functional dependence on the imaginary frequencies is known explicitly in closed form. We show this in the main part of this thesis in chapter 2. Thereby we derive explicit formulas for the analytic continuation in some relevant cases.

Our analysis finally provides relations, not only between functions in the MF and the KF, but also between different Keldysh components of the KF function. As an application of the results we derive the generalized fluctuation dissipation relations (FDRs) for 3p and 4p functions. Our results reproduce those of Wang and Heinz [12], but go beyond theirs in that we additionally identify the terms which cannot be reconstructed from FDRs. Moreover, our results are not restricted to real operators or to systems with specific assumptions such as time-reversal symmetry.

We further apply our results on "translating" formulas from the MF to the KF: In fact, already within the MF the analytic continuation is a common method for converting Matsubara sums into contour integrals. This method has been successfully applied by Eliashberg and Oguri to compute real-frequency susceptibilities from 4p MF functions [13, 14]. While the analytic continuation initially produces several vertex contributions, they identified a single one which is actually relevant for the linear response function of the system under consideration. Later on, Heyder et al. derived Oguri's formula by an independent line of argument for the KF [15]. We close the gap between the MF and the KF approach by directly "translating" Eliashberg's and Oguri's formulas to the KF. We find that each MF vertex contribution by Eliashberg is proportional to a KF component in the so-called R/A basis.

As a more specific example we present the 4p correlator of the Hubbard atom in chapter 5 which is already known in MF [16–20]. The Hubbard atom is exactly solvable and follows from other models in the atomic limit. For these models it can be used as numerical benchmark. We first compute the correlators directly in a spectral representation. Afterwards we show that the result obtained by analytic continuation is equivalent. The Hubbard atom is also a good example for a model where the MF correlators contain contributions with Kronecker symbols (anomalous contributions). The analytic continuation of such a symbol is not unique in the first place. However, we will argue that it can be "continued" to real frequencies by an appropriate substitution. In chapter 6 we then summarize and reflect on the presented results.

Chapter 2

Preparations for the analytic continuation

Our goal is to obtain relations between ℓ-point correlators in the imaginary-time MF and the KF. For this purpose we first introduce the theoretical frameworks in Sec. 2.1. Since we seek general results, not limited to particular systems, our strategy will be to use the spectral representations derived in Ref. [21] by Kugler, Lee and von Delft (KLD). They serve as an analytically exact starting point which is fit to describe any equilibrium system with time translation symmetry. Since the equilibrium condition is an assumption which is not formalism-inherent in the KF, it is expected to be important for the search for relations to MF correlators. In Sec. 2.2 we briefly present a consequence of the equilibrium condition in the KF. The analytic continuation of Matsubara correlators is then investigated in Sec. 2.3.

2.1 Spectral representation

In this section, we review the major results on the spectral representations derived by KLD. In these representations ℓp correlators are expressed interms of kernel functions and partial spectral functions (PSFs). The PSFs contain all system-specific spectral properties, while the kernel functions encode the respective time-ordering conventions of the MF and KF. This representation is especially suited for investigating analytic continuations because in both MF and KF the very same PSFs are being used. By comparison, other representations for KF correlators, involving Keldysh-rotated partial spectral functions and time-ordered kernels [22–26], somewhat obfuscate the relations between correlators in MF and KF (cf. Sec. 5.1.4 for the alternative spectral representation).

2.1.1 Definition of ℓ-point correlators

We begin by defining the objects of interest, adopting the notation of KLD. Consider a tuple $\boldsymbol{\mathcal{O}} = (\mathcal{O}^1, \dots, \mathcal{O}^\ell)$ of ℓ operators, time-evolving as $\mathcal{O}^i(t_i) = e^{\mathrm{i}\mathcal{H}t_i}\mathcal{O}^i e^{-\mathrm{i}\mathcal{H}t_i}$. They can

be fermionic (e.g. for vertex functions), bosonic (for susceptibilities) or mixed (for fermion-boson vertices).

In the MF, ℓp correlators are defined as

$$\mathcal{G}(\boldsymbol{\tau}) = (-1)^{\ell-1}\langle \mathcal{T}\prod_{i=1}^{\ell}\mathcal{O}^i(-\mathrm{i}\tau_i)\rangle, \tag{2.1.1}$$

where $\boldsymbol{\tau} = (\tau_1, ..., \tau_\ell)$ is a tuple of time arguments, each $\tau_i \in (0, \beta)$ and $\mathcal{T}$ denotes imaginary-time ordering[1]. Moreover, $\langle\mathcal{O}\rangle = \mathrm{Tr}[\varrho\,\mathcal{O}]$ denotes thermal averaging, with density matrix $\varrho = e^{-\beta\mathcal{H}}/Z$ and inverse temperature β.

KF correlators in the contour basis, $\mathcal{G}^{\boldsymbol{c}}$, are defined as

$$\mathcal{G}^{\boldsymbol{c}}(\boldsymbol{t}) = (-\mathrm{i})^{\ell-1}\langle \mathcal{T}_{\mathrm{c}}\prod_{i=1}^{\ell}\mathcal{O}^i(t_i^{c_i})\rangle, \tag{2.1.2}$$

where $\boldsymbol{t} = (t_1, ..., t_\ell)$, $t_i^{c_i} \in \mathbb{R}$, and $\mathcal{T}_{\mathrm{c}}$ denotes contour ordering. They carry a tuple of contour indices $\boldsymbol{c} = c_1\cdots c_\ell$, with $c_i = -$ or $+$ if operator $\mathcal{O}^i$ resides on the forward or backward branch of the Keldysh contour, respectively.

KF correlators in the Keldysh basis, $\mathcal{G}^{\boldsymbol{k}}$, carry a tuple $\boldsymbol{k} = k_1\cdots k_\ell$ of Keldysh indices $k_i \in \{1, 2\}$. They are obtained from those in the contour basis by applying a linear transformation, D, to each contour index [8],

$$\mathcal{G}^{\boldsymbol{k}}(\boldsymbol{t}) = \sum_{c_1\ldots c_\ell}\prod_{i=1}^{\ell}\Big[D^{k_i,c_i}\Big]\mathcal{G}^{\boldsymbol{c}}(\boldsymbol{t}), \qquad\qquad D^{k_i,\mp} = (\pm 1)^{k_i}/\sqrt{2}. \tag{2.1.3}$$

Time-dependent correlators are invariant under global shifts of all ℓ time arguments because they only depend on the relative times. This time-translational invariance leads to total frequency conservation. The discrete (MF) or continuous (KF) Fourier transforms of the above correlators have the following forms, respectively:

$$\mathcal{G}(\mathrm{i}\boldsymbol{\omega}) = \int_0^\beta \mathrm{d}^\ell\tau\,\mathcal{G}(\boldsymbol{\tau})\,e^{\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{\tau}} = \beta\delta_{\omega_{1\cdots\ell},0}\,G(\mathrm{i}\boldsymbol{\omega}), \tag{2.1.4}$$

$$\mathcal{G}^{\boldsymbol{k}}(\boldsymbol{\omega}) = \int_{-\infty}^{\infty} \mathrm{d}^\ell t\,\mathcal{G}^{\boldsymbol{k}}(\boldsymbol{t})\,e^{\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{t}} = 2\pi\delta(\omega_{1\cdots\ell})\,G^{\boldsymbol{k}}(\boldsymbol{\omega}). \tag{2.1.5}$$

Here we have used the following notational conventions: Depending on context, $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_\ell)$ denotes a set of discrete Matsubara frequencies (MF) or continuous real frequencies (KF). Moreover, $\boldsymbol{\omega}\cdot\boldsymbol{\tau} = \sum_{i=1}^{\ell}\omega_i\tau_i$ and $\mathrm{d}^\ell\tau = \prod_{i=1}^{\ell}\mathrm{d}\tau_i$. We use the shorthand $\omega_{i\cdots i'} = \sum_{j=i}^{i'}\omega_j$ for a sum over frequencies. The discrete Kronecker symbol $\delta_{\omega_{1\cdots\ell},0}$ (for MF) and the Dirac $\delta(\omega_{1\cdots\ell})$ (for KF) implement the *frequency-conservation relations*

$$\omega_{1\cdots\ell} = 0, \qquad \omega_{1\cdots i} = -\omega_{i+1\cdots\ell}. \tag{2.1.6}$$

[1]Note that operators in the MF are evolved in the imaginary time direction $\mathcal{O}^i(-\mathrm{i}\tau_i) = e^{\mathcal{H}\tau_i}\mathcal{O}^i e^{-\mathcal{H}\tau_i}$.

We use calligraphic symbols, $\mathcal{G}$, $\mathcal{K}$, $\mathcal{S}$, for functions of all ℓ arguments, and roman symbols, G, K, S, for functions of $\ell-1$ independent arguments. We nevertheless write the latter as $G(\mathrm{i}\boldsymbol{\omega})$ or $G^{\boldsymbol{k}}(\boldsymbol{\omega})$, with $\boldsymbol{\omega}$ containing ℓ components, it being understood that these satisfy frequency conservation, $\omega_{1\ldots\ell}=0$. This convention leads to particularly compact formulas.

2.1.2 Spectral representation of MF correlators

The spectral representations derived by KLD involve sums over permutations of ordered ℓ-tuples, generated by the time-ordering prescription. We adopt KLD's notation for these permutations. A permutation of an ordered tuple such as $\boldsymbol{\omega}=(\omega_1,\ldots,\omega_\ell)$ is denoted $\boldsymbol{\omega}_p=(\omega_{\overline{1}},\ldots,\omega_{\overline{\ell}})$, where the index permutation $p(12\ldots\ell)=(\overline{12}\ldots\overline{\ell})$ (or $p=(\overline{12}\ldots\overline{\ell})$ for short) acts on the index tuple $(12\ldots\ell)$ by replacing i by $p(i)=\bar{\imath}$ at position i. Note that p moves i to position $j=p^{-1}(i)$, replacing j by $p(j)=i$. For example, if $p=(312)$, then $(\omega_1,\omega_2,\omega_3)_p=(\omega_3,\omega_1,\omega_2)$. The sum $\sum_p$ runs over all such permutations.

The spectral representation for MF correlators found by KLD exploits the following observation: the time-ordered correlator $\mathcal{G}(\boldsymbol{\tau})$ of Eq. (2.1.1) can be expressed as a sum over permutations yielding all possible operator orderings,

$$\mathcal{G}(\boldsymbol{\tau})=\sum_p \boldsymbol{\zeta}^p\langle\mathcal{O}^{\overline{1}}(-\mathrm{i}\tau_{\overline{1}})\ldots\mathcal{O}^{\overline{\ell}}(-\mathrm{i}\tau_{\overline{\ell}})\rangle\,\mathcal{K}(\boldsymbol{\tau}_p), \tag{2.1.7}$$

where the *kernel* $\mathcal{K}(\boldsymbol{\tau}_p)=\prod_{i=1}^{\ell-1}\big[-\theta(\tau_{\bar{\imath}}-\tau_{\overline{i+1}})\big]$ is nonzero only if the permuted times $\boldsymbol{\tau}_p=(\tau_{\overline{1}},\ldots,\tau_{\overline{\ell}})$ satisfy $\tau_{\bar{\imath}}>\tau_{\overline{i+1}}$. The sign $\boldsymbol{\zeta}^p$ is $+1$ or -1 if the permuted tuple $\boldsymbol{\mathcal{O}}_p=(\mathcal{O}_{\overline{1}},\ldots\mathcal{O}_{\overline{\ell}})$ differs from $\boldsymbol{\mathcal{O}}$ by an even or odd number of transpositions of fermionic operators, respectively.

The multiplicative structure of Eq. (2.1.7) gives rise to a convolution in the Fourier domain. Exploiting time translational invariance and the resulting frequency conservation conditions, $G(\mathrm{i}\boldsymbol{\omega})$ can be expressed as an $(\ell-1)$-fold convolution of the form (for details, see [21]):

$$G(\mathrm{i}\boldsymbol{\omega})=\sum_p\big(S_p*K\big)(\mathrm{i}\boldsymbol{\omega}_p)=\sum_p\int\mathrm{d}^{\ell-1}\omega'_p\,S_p(\boldsymbol{\omega}'_p)K(\mathrm{i}\boldsymbol{\omega}_p-\boldsymbol{\omega}'_p)\ . \tag{2.1.8}$$

Here, $\boldsymbol{\omega}=(\omega_1,\ldots,\omega_\ell)$ are Matsubara frequencies and $\boldsymbol{\omega}'=(\omega'_1,\ldots,\omega'_\ell)$ real frequencies. Both tuples are understood to satisfy frequency conservation, $\omega_{1\ldots\ell}=0$ and $\omega'_{1\ldots\ell}=0$, implying the same for all permuted versions $\boldsymbol{\omega}_p$ and $\boldsymbol{\omega}'_p$, $\omega_{\overline{1}\ldots\overline{\ell}}=0$ and $\omega'_{\overline{1}\ldots\overline{\ell}}=0$. Thus, G, K and S each have only $\ell-1$ independent arguments, and the integral is over $\ell-1$ independent components of $\boldsymbol{\omega}'_p$.

The *partial spectral functions* (PSFs) S_p, obtained by Fourier transforming the permuted operator product in Eq. (2.1.7), have Lehmann representations of the form

$$S_p(\boldsymbol{\omega}'_p)=\boldsymbol{\zeta}^p\sum_{\underline{1},\ldots,\underline{\ell}}\rho_{\underline{1}}\prod_{i=1}^{\ell-1}\Big[O^{\bar{\imath}}_{\underline{i}\,\underline{i+1}}\,\delta(\omega'_{\overline{1}\ldots\bar{\imath}}-E_{\underline{i+1}\,\underline{1}})\Big]O^{\overline{\ell}}_{\underline{\ell}\underline{1}}. \tag{2.1.9}$$

Here, each underlined summation index $\underline{i}$ enumerates a complete set of many-particle eigenstates $|\underline{i}\rangle$ of $\mathcal{H}$, with eigenenergies $E_{\underline{i}}$, energy differences $E_{\underline{j}\underline{i}} = E_{\underline{j}} - E_{\underline{i}}$, and matrix elements $O_{\underline{i}\underline{j}} = \langle \underline{i}|\mathcal{O}|\underline{j}\rangle$, $\rho_{\underline{1}} = e^{-\beta E_{\underline{1}}}/Z$. Note that, different from KLD, we have included the sign factor $\boldsymbol{\zeta}^p$ in the definition of the PSF for notational convenience. In later sections we can thereby write formulas without special consideration of the exchange symmetry of the operators.

The MF kernel K is obtained by Fourier transforming $\mathcal{K}(\boldsymbol{\tau}_p)$. It can be written as a sum, $K = \widetilde{K} + \widehat{K}$, of *regular* and *anomalous* contributions. Expressed through $\boldsymbol{\Omega}_p = \mathrm{i}\boldsymbol{\omega}_p - \boldsymbol{\omega}'_p$, the regular contribution reads

$$\widetilde{K}(\boldsymbol{\Omega}_p) = \prod_{i=1}^{\ell-1} \frac{1}{\Omega_{\overline{1}\cdots\overline{i}}}\,. \tag{2.1.10}$$

It is an analytic function of its arguments $\Omega_{\overline{i}}$ on certain regions of the complex plane (see Sec. 2.3). It diverges if $\Omega_{\overline{1}\cdots\overline{j}} \to 0$ for some j. However, then also $\Omega_{\overline{i+1}\cdots\overline{\ell}} \to 0$ (because $\Omega_{\overline{1}\cdots\overline{\ell}} = 0$), and the $1/\Omega_{\overline{1}\cdots\overline{i}}$ divergence turns out to be canceled by a $-1/\Omega_{\overline{i+1}\cdots\overline{\ell}}$ divergence stemming from a cyclically related permutation in the sum $\sum_p$ in Eq. (2.1.8). Their cancellation can be tracked by a limiting procedure which treats these denominators as infinitesimals [21].

Each denominator $1/\Omega_{\overline{1}\cdots\overline{i}}$ in $\widetilde{K}$ originates from an integral of the form $-\int_0^\beta \mathrm{d}\tau_{\overline{1}} e^{\tau_{\overline{1}}\Omega_{\overline{1}\cdots\overline{i}}}$, arising when Fourier transforming $\mathcal{K}$. If $\Omega_{\overline{1}\cdots\overline{j}} = 0$ for some $j < \ell$, this integral yields $-\beta$ instead. All such contributions are collected in the anomalous part of the kernel $\widehat{K}$. We will only consider the case that for each $\boldsymbol{\Omega}_p$ at most one denominator vanishes. Examples are bosonic 2p functions, or ℓp functions of fermionic operators with $\ell \leq 4$, such that $\omega_{\overline{1}\cdots\overline{i}}$, with $i < \ell$, produces at most one bosonic frequency. Then, $\widehat{K}$ has the form [16, 21, 27, 28]

$$\widehat{K}(\boldsymbol{\Omega}_p) = \sum_{j=1}^{\ell-1} \widehat{K}_{\overline{1}\cdots\overline{j}}(\boldsymbol{\Omega}_p), \tag{2.1.11a}$$

$$\widehat{K}_{\overline{1}\cdots\overline{j}}(\boldsymbol{\Omega}_p) = -\delta_{\Omega_{\overline{1}\cdots\overline{j}},0} \frac{\beta}{2} \prod_{\substack{i=1 \\ i\neq j}}^{\ell-1} \frac{1}{\Omega_{\overline{1}\cdots\overline{i}}}. \tag{2.1.11b}$$

Here, $\delta_{\Omega_{\overline{1}\cdots\overline{j}},0}$ is symbolic notation indicating that this term contributes only if $\Omega_{\overline{1}\cdots\overline{j}} = 0$, i.e. if both $\omega_{\overline{1}\cdots\overline{j}} = 0$ and $\omega'_{\overline{1}\cdots\overline{j}} = 0$. The latter happens if the spectrum has a degeneracy, $E_{\underline{j+1}} = E_{\underline{1}}$, since then the integral (2.1.8) over the factor $\delta(\omega'_{\overline{1}\cdots\overline{j}} - E_{\underline{j+1}\underline{1}})$ in $S_p(\boldsymbol{\omega}'_p)$ sets $\omega'_{\overline{1}\cdots\overline{j}}$ to zero.

Equations (2.1.8) to (2.1.11) give the spectral representation for MF ℓp correlators derived by KLD. For the purposes of analytic continuation, the main topic of this thesis, we note that the regular part $\widetilde{K}$ can readily be continued to a rational function. By contrast, the anomalous part $\widehat{K}$ contains Kronecker symbols and hence needs to be considered separately.

To prepare the ground for that discussion (presented in Sec. 3.1.3), we introduce compact notation reflecting the structure of Eqs. (2.1.11) for $\widehat{K}$. For a given permutation $p = (\overline{1}..\overline{\ell})$ and a specified term j, we express the permutation as $p = \overline{I}\,\overline{I}^c$, where $\overline{I} = (\overline{1}..\overline{j})$ and $\overline{I}^c = (\overline{j+1}..\overline{\ell})$ are the complementary subtuples formed from the first j or last $\ell-j$ entries of p, respectively. Since the Kronecker symbol in Eq. (2.1.11b) enforces $\Omega_{\overline{I}} = \Omega_I = 0$, implying $\Omega_{\overline{1}\cdots\overline{i}} = \Omega_{\overline{j+1}\cdots\overline{i}}$ for the factors with $i > j$, we may express $\widehat{K}_{\overline{1}\cdots\overline{j}}$ as

$$\widehat{K}_{\overline{I}}(\mathbf{\Omega}_{\overline{I}\,\overline{I}^c}) = -\delta_{\Omega_I,0}\frac{\beta}{2}\widetilde{K}(\mathbf{\Omega}_{\overline{I}})\widetilde{K}(\mathbf{\Omega}_{\overline{I}^c}), \tag{2.1.12}$$

where the argument $\mathbf{\Omega}_{\overline{I}} = (\Omega_{\overline{1}},...\Omega_{\overline{j}})$ contains the first j entries of the permuted tuple $\mathbf{\Omega}_p = (\Omega_{\overline{1}},...\Omega_{\overline{\ell}})$; similarly $\mathbf{\Omega}_{\overline{I}^c}$ contains the last $\ell-j$ entries. Here $\widetilde{K}(\mathbf{\Omega}_{\overline{I}})$ and $\widetilde{K}(\mathbf{\Omega}_{\overline{I}^c})$ both have the form (2.1.10), with the product there involving $j-1$ or $\ell-j-1$ factors, respectively. Now consider the permutation $\overline{I}^c\overline{I}$, built from the same subtuples as $\overline{I}\,\overline{I}^c$, concatenated in opposite order. The identity $\delta_{\Omega_{\overline{I}^c},0} = \delta_{\Omega_{\overline{I}},0}$ (ensured by frequency conservation) and the product form of Eq. (2.1.12) imply

$$\widehat{K}_{\overline{I}^c}(\mathbf{\Omega}_{\overline{I}^c\overline{I}}) = \widehat{K}_{\overline{I}}(\mathbf{\Omega}_{\overline{I}\,\overline{I}^c})\,. \tag{2.1.13}$$

2.1.3 Notation for restricted permutations

In Eq. (2.1.12) we encountered a kernel which factorizes into several kernels, each taking a subtuple of the frequencies $\mathbf{\Omega}_p$ as arguments. The notation introduced in the last section will be needed in a broader context. Given an ℓ-tuple, say $\boldsymbol{\omega}_p$, subtuples thereof will be identified using notation such as $\boldsymbol{\omega}_{(\overline{\lambda}\cdots\overline{\lambda'})} = (\omega_{\overline{\lambda}},\dots,\omega_{\overline{\lambda'}})$, with $\lambda < \lambda'$. For example, $\boldsymbol{\omega}_p = (\boldsymbol{\omega}_{(\overline{1}\cdots\overline{\lambda})}, \boldsymbol{\omega}_{(\overline{\lambda+1}\cdots\overline{\ell})})$ and $(\omega_1,\omega_4,\omega_3,\omega_2) = (\boldsymbol{\omega}_{(14)},\boldsymbol{\omega}_{(32)})$. Similarly for more than two subtuples, $(\omega_4,\omega_3,\omega_5,\omega_1,\omega_2) = (\boldsymbol{\omega}_{(4)},\boldsymbol{\omega}_{(35)},\boldsymbol{\omega}_{(12)})$.

We will also consider permutations with a restricted substructure. Let $L = \{1,\dots\ell\}$ be the set of all indices, and let $I \subsetneq L$ and $I^c = L\backslash I$ be two complementary index subsets, containing $|I|$ and $\ell - |I|$ elements, respectively, where $|I|$ denotes the number of elements in I. Any index tuple of length $|I|$ or $\ell-|I|$, built from elements of I or I^c, will be denoted by $\overline{I}$ or $\overline{I}^c$, respectively. Then $\sum_{p_{I|I^c}}$ denotes a sum over all permutations with the concatenated structure $p = \overline{I}\,\overline{I}^c$, containing the entries of $\overline{I} = (\overline{1},\cdots\overline{j})$ followed by those of $\overline{I}^c = (\overline{j+1},\cdots\overline{\ell})$. For example, if for $\ell = 4$ we choose $I = \{1,4\}$ and $I^c = \{2,3\}$ as complementary subsets, with subtuples $\overline{I} = (14)$ or (41) and $\overline{I}^c = (23)$ or (32), then $\sum_{p_{I|I^c}} = \sum_{p_{\{1,4\}|\{2,3\}}}$ runs over (1423), (1432), (4123), and (4132). Similarly, let $I_1 \cup I_2 \cup I_3 = L$ be three complementary index sets, then $\sum_{p_{I_1|I_2|I_3}}$ denotes a sum over all permutations with the structure $p = \overline{I}_1\overline{I}_2\overline{I}_3$.

For any function with p-dependent arguments the sum over all p can be organized in terms of permutations within all pairs of complementary subsets,

$$\sum_p F_p = \sum_{I\subsetneq L}\sum_{p_{I|I^c}} F_{\overline{I}\,\overline{I}^c} = \sum_{I\subsetneq L}\sum_{p_{I|I^c}} \frac{1}{2}\big[F_{\overline{I}\,\overline{I}^c} + F_{\overline{I}^c\overline{I}}\big]. \tag{2.1.14}$$

The sum is over all subsets I of L, and for each I over all concatenations $\overline{I}\,\overline{I^c}$ of subtuples built from I and I^c; on the right, the factor $1/2$ compensates for double counting.

Finally, we write $\omega_{\overline{I}} = \sum_{\bar{i}\in\overline{I}} \omega_{\bar{i}}$ for a sum over the components of the subtuple $\boldsymbol{\omega}_{\overline{I}}$. Note that $\omega_{\overline{I}} = \omega_I$. If $\boldsymbol{\omega}$ satisfies frequency conservation, $\omega_L = 0$, then any permutation of its components, expressed through two complementary index subtuples as $\boldsymbol{\omega}_p = (\boldsymbol{\omega}_{\overline{I}}, \boldsymbol{\omega}_{\overline{I^c}})$, satisfies $\omega_{\overline{I}} = -\omega_{\overline{I^c}}$. For example, $\omega_{1\cdots 4} = 0$ implies $\omega_{14} = -\omega_{23}$.

2.1.4 Compact notation for the MF correlator

The MF kernel decomposition $K = \widetilde{K} + \widehat{K}$ into regular and anomalous parts implies a corresponding decomposition for the MF correlator, $G = \widetilde{G} + \widehat{G}$, with[2]

$$\widetilde{G}(\mathrm{i}\boldsymbol{\omega}) = \sum_p \big(S_p * \widetilde{K}\big)(\mathrm{i}\boldsymbol{\omega}_p), \tag{2.1.15}$$

$$\widehat{G}(\mathrm{i}\boldsymbol{\omega}) = \sum_p \big(S_p * \widehat{K}\big)(\mathrm{i}\boldsymbol{\omega}_p) = \frac{1}{2}\sum_{I\subsetneq L} \widehat{G}_I(\mathrm{i}\boldsymbol{\omega})\,. \tag{2.1.16}$$

On the right, we evoked Eq. (2.1.14) to express the permutation sum through a sum over subsets $I \subsetneq L$ of indices, with

$$\begin{aligned}\widehat{G}_I(\mathrm{i}\boldsymbol{\omega}) \quad &= \sum_{p_{I|I^c}} \Big[\big(S_{\overline{I}\,\overline{I^c}} * \widehat{K}_{\overline{I}\,\overline{I^c}}\big)(\mathrm{i}\boldsymbol{\omega}_{\overline{I}\,\overline{I^c}}) + \big(S_{\overline{I^c}\,\overline{I}} * \widehat{K}_{\overline{I^c}\,\overline{I}}\big)(\mathrm{i}\boldsymbol{\omega}_{\overline{I^c}\,\overline{I}})\Big] \\ &= \sum_{p_{I|I^c}} \big(S_{[\overline{I};\overline{I^c}]_+} * \widehat{K}_{\overline{I}}\big)(\mathrm{i}\boldsymbol{\omega}_{\overline{I}\,\overline{I^c}}).\end{aligned} \tag{2.1.17}$$

For the last step, we recalled Eq. (2.1.13) to factor out a common kernel $\widehat{K}_{\overline{I}}(\boldsymbol{\Omega}_{\overline{I}\,\overline{I^c}})$, collecting the remaining combination of PSFs using the PSF (anti-)commutator[3] shorthand

$$S_{[\overline{I};\overline{I^c}]_\pm}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I^c}}) = S_{\overline{I}\,\overline{I^c}}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I^c}}) \pm S_{\overline{I^c}\,\overline{I}}(\boldsymbol{\omega}'_{\overline{I^c}\,\overline{I}})\,. \tag{2.1.18}$$

Each $\widehat{K}_{\overline{I}}$ in the sum (2.1.17) for $\widehat{G}_I$ contains a $\delta_{\Omega_I,0}$, thus $\widehat{G}_I$ is proportional to $\delta_{\omega_I,0}$. This may be regarded as its defining property. The fate of this Kronecker symbol during analytical continuation will be discussed in Sec. 3.1.3.

Example: To demonstrate the notation we consider a 4p correlator of fermionic operators. Anomalous contributions arise for the composite bosonic frequencies $\mathrm{i}\omega_{12}$, $\mathrm{i}\omega_{13}$ and $\mathrm{i}\omega_{14}$. The contribution proportional to $\delta_{0,\omega_{13}}$ is

$$\widehat{G}_{13}(\mathrm{i}\boldsymbol{\omega}) = \sum_{p_{\{1,3\}|\{2,4\}}} \Big(S_{[(\overline{1}\,\overline{2});(\overline{3}\,\overline{4})]_+} * \widehat{K}_{(\overline{1}\,\overline{2})}\Big)\,(\mathrm{i}\boldsymbol{\omega}_{(\overline{12})}, \mathrm{i}\boldsymbol{\omega}_{(\overline{34})}). \tag{2.1.19}$$

[2]For a correlator which hosts both regular and anomalous contributions, see e.g. the 4p correlator $G_{\uparrow\downarrow}$ of the Hubbard atom in Eq. (5.1.23).

[3]Henceforth we denote with "PSF commutator" ("PSF anti-commutator") a linear combination of the partial spectral functions $S_{[\overline{I};\overline{I^c}]_-}$ ($S_{[\overline{I};\overline{I^c}]_+}$), irrespective of the actual exchange symmetry of the operators.

The summation is performed over all orderings of $\{1,3\}$, giving (13) or (31), and all orderings of $\{2,4\}$ giving (24) and (42). In total the sum runs over the permutations (1324), (1342), (3124) and (3142). The PSF anti-commutator automatically produces the further orderings (2413), (4213), (2431) and (4231). To be explicit $\widehat{G}_{13}$ is thus expressed as follows (suppressing frequency arguments for brevity):

$$\widehat{G}_{13} = S_{[(13);(24)]_+} * \widehat{K}_{(13)} + S_{[(13);(42)]_+} * \widehat{K}_{(13)} + S_{[(31);(24)]_+} * \widehat{K}_{(31)} + S_{[(31);(42)]_+} * \widehat{K}_{(31)}.$$

2.1.5 Spectral representation of KF correlators

We now turn to the spectral representation of Keldysh correlators in the Keldysh basis, $\mathcal{G}^{\boldsymbol{k}}$. KLD obtained it via a permutation expansion of $\mathcal{G}^{\boldsymbol{k}}(\boldsymbol{t})$ analogous to Eq. (2.1.7).

The results depend on the number and placement of 2's (2-indices) in the Keldysh tuple $\boldsymbol{k} = k_1 \cdots k_\ell$. It is therefore convenient to specify the latter through the ordered list $\boldsymbol{k} = [\eta_1 \cdots \eta_\alpha]$, where η_j denotes the position of the j-th 2-index in $k_1 \cdots k_\ell$, with $\eta_j < \eta_{j+1}$, e.g. $1111 = [\,]$, $1221 = [23]$. Correspondingly, a permuted Keldysh tuple can be specified as $\boldsymbol{k}_p = [\hat{\eta}_1 \ldots \hat{\eta}_\alpha]$, where $\hat{\eta}_j$ denotes the position of the j-th 2-index in $k_{\overline{1}} \cdots k_{\overline{\ell}}$, with $\hat{\eta}_j < \hat{\eta}_{j+1}$. To find the $\hat{\eta}_j$'s describing $\boldsymbol{k}_p$ given the η_j's describing $\boldsymbol{k}$, note that p moves a 2-index from position η_j in $\boldsymbol{k}$ to position $\mu_j = p^{-1}(\eta_j)$ in $\boldsymbol{k}_p$. The sequence $[\mu_1 \ldots \mu_\alpha]$ lists the new positions of the 2-indices'; putting its elements in increasing order yields $[\hat{\eta}_1 \ldots \hat{\eta}_\alpha]$. For example, if $\boldsymbol{k} = 1221 = [23]$, then $p = (3412)$ yields $[\mu_1 \mu_2] = [41]$ and $\boldsymbol{k}_p = 2112 = [14]$.

KLD's spectral representation for $G^{\boldsymbol{k}}(\boldsymbol{\omega})$ has the following form, written first in compact, then explicit notation:

$$G^{\boldsymbol{k}}(\boldsymbol{\omega}) = \frac{2}{2^{\ell/2}} \sum_p \big(S_p * K^{\boldsymbol{k}_p}\big)(\boldsymbol{\omega}_p), \tag{2.1.20}$$

$$G^{[\eta_1 \ldots \eta_\alpha]}(\boldsymbol{\omega}) = \frac{2}{2^{\ell/2}} \sum_p \int \mathrm{d}^{\ell-1}\omega'_p S_p(\boldsymbol{\omega}'_p) K^{[\hat{\eta}_1 \ldots \hat{\eta}_\alpha]}(\boldsymbol{\omega}_p - \boldsymbol{\omega}'_p).$$

The frequencies $\boldsymbol{\omega}$ and $\boldsymbol{\omega}'$ are real, with $\omega_{1\ldots\ell} = 0$ and $\omega'_{1\ldots\ell} = 0$. The PSFs S_p are again given by Eq. (2.1.9). The KF kernel is given by $K^{[\,]} = 0$ if $\alpha = 0$, and for $1 < \alpha \leq \ell$,

$$K^{[\hat{\eta}_1 \ldots \hat{\eta}_\alpha]}(\boldsymbol{\omega}_p) = \sum_{j=1}^{\alpha} (-1)^{j-1} K^{[\hat{\eta}_j]}(\boldsymbol{\omega}_p)\,, \tag{2.1.21}$$

where the $K^{[\hat{\eta}_j]}$ are *retarded* kernels, having the following form (stated for superscript η in the following definition; in (2.1.21), replace it by $\hat{\eta}_j$):

$$K^{[\eta]}(\boldsymbol{\omega}_p) = \widetilde{K}(\boldsymbol{\omega}_p^{[\overline{\eta}]}) \overset{(2.1.10)}{=} \prod_{i=1}^{\ell-1} \frac{1}{\omega^{[\overline{\eta}]}_{\overline{1}\ldots\overline{i}}}\,. \tag{2.1.22}$$

Here $\widetilde{K}$ actually is the MF kernel from Eq. (2.1.10). Remarkably, the retarded Keldysh

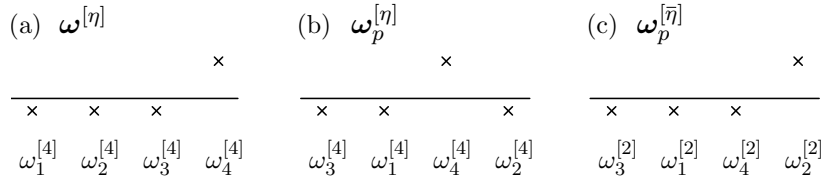

Figure 2.1: Complex frequency tuples, for $\ell = 4$, $\eta = 4$, $p = (3142)$, in which case $p^{-1} = (2413)$, $\mu = p^{-1}(\eta) = 3$, $\overline{\eta} = p(\eta) = 2$. (Reprinted from Ref. [21].)

kernel $K^{[\eta]}$ has the same functional form, just containing different arguments. The complex frequency tuple $\boldsymbol{\omega}^{[\eta]}$ is defined to be the real tuple $\boldsymbol{\omega}$ with its components shifted by the imaginary parts $\boldsymbol{\gamma}^{[\eta]}$. These shifts are defined as follows (see Fig. 2.1(a)):

$$\omega_i \to \omega_i^{[\eta]} = \omega_i + \mathrm{i}\gamma_i^{[\eta]}, \qquad \gamma_{i\neq\eta}^{[\eta]} < 0, \qquad \gamma_\eta^{[\eta]} = \sum_{\substack{i\in L\\ i\neq\eta}} |\gamma_i^{[\eta]}|. \tag{2.1.23}$$

This assigns a positive imaginary part to $\omega_\eta^{[\eta]}$ while the remaining complex frequencies $\omega_{i\neq\eta}^{[\eta]}$ have a negative imaginary part. The shifts are thus determined by the superscript η. By construction $\gamma_{1\cdots\ell}^{[\eta]} = 0$ holds. An explicit choice is $\gamma_{i\neq\eta}^{[\eta]} = -\gamma_0$ and $\gamma_\eta^{[\eta]} = (\ell-1)\gamma_0$ where $\gamma_0 > 0$ is infinitesimal (or small but finite for numerics). The tuple $\boldsymbol{\omega}_p^{[\eta]} = (\omega_{\overline{1}}^{[\eta]}, ..., \omega_{\overline{\ell}}^{[\eta]})$, is obtained by permuting the components of $\boldsymbol{\omega}^{[\eta]}$ according to p, including their imaginary parts (see Fig. 2.1(b)). This moves $\omega_\eta^{[\eta]}$, the component with positive imaginary part, to the position $\mu = p^{-1}(\eta)$. The complex frequency tuple $\boldsymbol{\omega}_p^{[\bar{\eta}]}$ in the definition of the retarded kernel in Eq. (2.1.22) is then obtained by inserting the superscript $\overline{\eta} = p(\eta)$, which gives the needed imaginary shifts for the kernel (see Fig. 2.1(c)): the imaginary part of the frequency sum $\omega_{\overline{1}\cdots\overline{i}}^{[\overline{\eta}]}$ is negative for $1 \leq i < \mu$ and positive for $\mu \leq i < \ell$. Thus Eq. (2.1.22) becomes[4]

$$K^{[\eta]}(\boldsymbol{\omega}_p) = \prod_{i=1}^{\eta-1} \left(\omega_{\overline{1}\cdots\overline{i}}^{-}\right)^{-1} \prod_{i=\eta}^{\ell-1} \left(\omega_{\overline{1}\cdots\overline{i}}^{+}\right)^{-1}, \tag{2.1.24}$$

where the superscript in $\omega_{\overline{1}\cdots\overline{i}}^{\pm} = \omega_{\overline{1}\cdots\overline{i}} \pm \mathrm{i}0^+$ denotes whether the frequency sum has a positive or negative (infinitesimal) imaginary part. As usual, a product over an empty set, with lower limit larger than upper limit, is defined to equal unity. $K^{[\eta]}(\boldsymbol{\omega}_p)$ is called retarded since its inverse Fourier transform, $\mathcal{K}^{[\eta]}(\boldsymbol{t}_p)$, is retarded with respect to $t_{\overline{\eta}}$, i.e., nonzero only for $t_{\overline{i}} < t_{\overline{\eta}}$, $i \neq \eta$ [21]. Equations (2.1.9) and (2.1.20) to (2.1.24) give the

[4]To see that this is indeed equivalent to the retarded kernel defined by KLD [21] in the time domain,

$$\mathcal{K}^{[\eta]}(\boldsymbol{t}_p) = \prod_{i=1}^{\eta-1} \left[\mathrm{i}\theta(t_{\overline{i+1}} - t_{\overline{i}})\right] \prod_{i=\eta}^{\ell-1} \left[-\mathrm{i}\theta(t_{\overline{i}} - t_{\overline{i+1}})\right],$$

use that a step functions are retrieved via inverse Fourier transforms according to Eq. (2.3.5) below.

spectral representation for KF ℓp correlators. Note that, by definition of the complex frequency tuple $\boldsymbol{\omega}^{[\overline{\eta}]}$, the kernels $K^{[\eta]}(\boldsymbol{\omega}_p)$ and $\widetilde{K}(\boldsymbol{\omega}_p^{[\overline{\eta}]})$ are equivalent and can in fact be used interchangeably. We use either of these depending on the convenience of notation.

Leaving a detailed discussion of the analytic structure to Sec. 2.3, we here just discuss how the above relations reproduce well-known results for the correlators $G^{[\eta_{1\cdots}\eta_\alpha]}$ with $\alpha=0$ or 1. For $\alpha=0$, where $K^{[]}=0$, we have $G^{[]}=G^{1\cdots1}=0$. For $\alpha=1$ there is only one η, hence $\hat{\eta}=\mu=p^{-1}(\eta)$ and $\overline{\hat{\eta}}=\eta$. Thus the permutation expansion for $G^{[\eta]}$ involves just a single complex tuple $\boldsymbol{\omega}^{[\eta]}$:

$$G^{[\eta]}(\boldsymbol{\omega}) = \frac{2}{2^{\ell/2}}\sum_p \int \mathrm{d}^{\ell-1}\omega'_p\, S_p(\boldsymbol{\omega}'_p)\widetilde{K}(\boldsymbol{\omega}_p^{[\eta]}-\boldsymbol{\omega}'_p). \tag{2.1.25}$$

Moreover, $G^{[\eta]}(\boldsymbol{\omega})$ is an analytic function of the variable ω_η in the upper half-plane. To see this, note that $\widetilde{K}$ is a product of denominators of the for $(\omega^{[\eta]}_{\overline{1}\cdots\bar{i}}-\omega'_{\overline{1}\cdots\bar{i}})^{-1}$. Whenever one of these denominators contains $\omega^{[\eta]}_\eta=\omega_\eta+\mathrm{i}\gamma^{[\eta]}_\eta$ as a term in the sum $\omega^{[\eta]}_{\overline{1}\cdots\bar{i}}$ (i.e. whenever $\eta\in\{\overline{1},...,\bar{i}\}$), the latter has the form $(\omega_\eta+\mathrm{i}\gamma^{[\eta]}_{\overline{1}\cdots\bar{i}}+\text{real frequencies})^{-1}$, with a positive imaginary part, $\gamma^{[\eta]}_{\overline{1}\cdots\bar{i}}>0$. Therefore ω_η can be analytically continued into the upper half of the complex plane without encountering any singularities.

Accordingly, in the time domain $G^{[\eta]}(\boldsymbol{t})$ is fully retarded with respect to t_η (i.e. nonzero only for $t_i<t_\eta$, $i\neq\eta$) [29, 30].

Comparing Eq. (2.1.25) for the KF correlator to the spectral representation (2.1.15) of the regular MF kernel

$$\widetilde{G}(\mathrm{i}\boldsymbol{\omega}) = \sum_p \int \mathrm{d}^{\ell-1}\omega'_p\, S_p(\boldsymbol{\omega}'_p)\widetilde{K}(\mathrm{i}\boldsymbol{\omega}_p-\boldsymbol{\omega}'_p), \tag{2.1.26}$$

we see that they are related by the analytic continuation

$$2^{\ell/2-1}G^{[\eta]}(\boldsymbol{\omega}) = \widetilde{G}(\mathrm{i}\boldsymbol{\omega})\big|_{\mathrm{i}\boldsymbol{\omega}\to\boldsymbol{\omega}^{[\eta]}}. \tag{2.1.27}$$

Compactly encapsulating results known from Refs. [23, 26, 30, 31], this relation generalizes the well known 2p relation $G^{21/12}(\omega_1)=\widetilde{G}(\mathrm{i}\omega_1\to\omega_1^\pm)$ (where we used conventional notation, dropping the second argument, $\omega_2=-\omega_1$).

Keldysh correlators with multiple 2-indices ($\alpha>1$) cannot be obtained from MF ones by *direct* analytic continuation. The reason is that their kernels in Eq. (2.1.21) involve two or more complex frequency tuples $\boldsymbol{\omega}^{[\eta_1]}$, $\boldsymbol{\omega}^{[\eta_2]}$, etc., having *different* imaginary parts. They therefore do not have any well-defined region of analyticity in the space of complex frequencies. We will discuss their properties in detail in Sec. 2.3-3.2.

For later use we define a *primed correlator* (cf. Eq. (3.16) of Ref. [32]):

$$G'^{\boldsymbol{k}}(\boldsymbol{\omega}) = 2^{1-\ell/2}\sum_p \big[S_p * (K^{\boldsymbol{k}_p})^*\big](\boldsymbol{\omega}_p)\,. \tag{2.1.28}$$

It differs from $G^{\boldsymbol{k}}(\boldsymbol{\omega})$ of Eq. (2.1.21) by the complex conjugation of the kernel $(K^{\boldsymbol{k}_p})^*$ such that $\omega^{\pm} \to \omega^{\mp}$ in Eq. (2.1.24). In the time domain this corresponds to using a reversed time-order on the Keldysh contour. For systems with special behavior under time-reversal $G'^{\boldsymbol{k}} = (G^{\boldsymbol{k}})^*$ holds [33]. Since we are mostly interested in correlators of creation and annihilation operators, a relevant case is covered by Hamiltonians which are real functions of creation and annihilation operators. Since all matrix elements in the occupation number basis are real [11, 19], all PSFs are real and hence $G'^{\boldsymbol{k}} = (G^{\boldsymbol{k}})^*$.

Clarification of the notation for products of kernels

We conclude this section by clarifying the notation for products of kernels. Above we have summarized the spectral representation for general ℓp correlators. (All functions are well-defined for any ℓ.) In the course of later sections we construct functions which have "substructures". We will encounter kernels consisting of the product of regular MF kernels or the product of retarded KF kernels. Each of these kernels takes a subtuple $\boldsymbol{\omega}_{\overline{I}}$ as arguments. For these substructures, the above formulas for regular and retarded kernels can be used analogously by restricting the set $L = \{1, ..., \ell\}$ to a subset I. However, to avoid obscurities we clarify the notation here.

In fact, with the anomalous kernel in Eq. (2.1.12) we have already encountered a kernel with such substructures: It involves the product of two regular MF kernels $\widetilde{K}(\boldsymbol{\Omega}_{\overline{I}}) \times \widetilde{K}(\boldsymbol{\Omega}_{\overline{I}^c})$. The arguments of the regular kernels are the frequency tuples $\boldsymbol{\Omega}_{\overline{I}}$ and $\boldsymbol{\Omega}_{\overline{I}^c}$ having j and $(\ell - j)$ components, respectively. Correspondingly, we have to use the definition of the regular kernel $\widetilde{K}$ in Eq. (2.1.10) for jp and $(\ell - j)$p functions. For example, writing out the regular kernel on the subtuple (432) gives $\widetilde{K}(\boldsymbol{\Omega}_{(432)}) = \widetilde{K}(\Omega_4, \Omega_3, \Omega_2) = 1/(\Omega_4 \Omega_{43})$.

In Sec. 3.1.3 we show that the anomalous kernels have to be continued to a product of retarded ones. Since the regular MF kernel is defined for subtuples so is the retarded kernel: analogous to Eq. (2.1.22) the retarded kernel of a subtuple $\boldsymbol{\omega}_{\overline{I}}$ is defined as

$$K^{[\eta]}(\boldsymbol{\omega}_{\overline{I}}) = \widetilde{K}\left(\boldsymbol{\omega}_{\overline{I}}^{[\overline{\eta}]}\right). \tag{2.1.29}$$

The superscript on $K^{[\eta]}(\boldsymbol{\omega}_{\overline{I}})$ indicates that this kernel is retarded with respect to the η-th component of the subtuple $\boldsymbol{\omega}_{\overline{I}}$. The η-th component of the subtuple $\overline{I}$ is $\overline{\eta}$ and the complex frequency tuple $\boldsymbol{\omega}_{\overline{I}}^{[\overline{\eta}]}$ is defined according to Eq. (2.1.23) with the indices $L = \{1,...\ell\}$ restricted to those in $\overline{I}$. For example,

$$K^{[2]}(\boldsymbol{\omega}_{(432)}) = \widetilde{K}(\boldsymbol{\omega}_{(432)}^{[3]}) = \widetilde{K}(\omega_4 - \mathrm{i}\gamma_0, \omega_3 + \mathrm{i}2\gamma_0, \omega_2 - \mathrm{i}\gamma_0)$$

with infinitesimal $\gamma_0 > 0$. Note that, for a fixed ν, the set of components $\{\, \omega_i^{[\nu]} \mid i \in I \,\}$ is fixed, while the order in which the elements of I appear in a tuple $\overline{I}$ determines the order in which they appear in $\boldsymbol{\omega}_{\overline{I}}^{[\nu]}$. Having defined the complex frequency tuples $\boldsymbol{\omega}_{\overline{I}}^{[\overline{\eta}]}$, the two notations for the retarded kernel $K^{[\eta]}(\boldsymbol{\omega}_{\overline{I}})$ and $\widetilde{K}\left(\boldsymbol{\omega}_{\overline{I}}^{[\overline{\eta}]}\right)$ can again be used interchangeably.

The *retarded product kernel* will be particularly useful. Using the abbreviation

$$\hat{\delta}(\cdot) = -2\pi \mathrm{i}\delta(\cdot),$$

the retarded product kernel is defined as

$$K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\ldots\overline{I}_\alpha^{[\eta_\alpha]}}(\boldsymbol{\omega}_{\overline{I}_1\overline{I}_2\ldots\overline{I}_\alpha}) = \prod_{j=1}^{\alpha-1}\left[\hat{\delta}(\omega_{I_j})\right]\prod_{j=1}^{\alpha}\left[\widetilde{K}\big(\boldsymbol{\omega}_{\overline{I}_j}^{[\eta_j]}\big)\right] \tag{2.1.30}$$

for permutations of the type $p = \overline{I}_1\overline{I}_2\ldots\overline{I}_\alpha$ with complementary subsets I_j and $\eta_j \in I_j$ $(1 \leq j \leq \alpha)$. The functions $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}_j}^{[\eta_j]})$ are retarded kernels and defined according to Eq. (2.1.29). For example,

$$K_{(13)^{[3]}(42)^{[4]}}(\boldsymbol{\omega}_{(1342)}) = \hat{\delta}(\omega_{13})\widetilde{K}(\boldsymbol{\omega}_{(13)}^{[3]})\widetilde{K}(\boldsymbol{\omega}_{(42)}^{[4]}) = \hat{\delta}(\omega_{13})K^{[2]}(\boldsymbol{\omega}_{(13)})K^{[1]}(\boldsymbol{\omega}_{(42)}).$$

Observe that, due to its product structure, retarded product kernels remain unchanged under interchanging the subtuples, i.e. $K_{(13)^{[3]}(42)^{[4]}}(\boldsymbol{\omega}_{(1342)}) = K_{(42)^{[4]}(13)^{[3]}}(\boldsymbol{\omega}_{(4213)})$.

2.2 Consequences of the equilibrium condition in the Keldysh formalism

While the MF is inherently a formalism for equilibrium, the KF is more general. The equilibrium condition enters the KF via the density matrix within the PSFs which is chosen to be the normalized Boltzmann factor $\varrho = e^{-\beta\mathcal{H}}/Z$. By cyclicity of the trace the PSFs in Eq. (2.1.9) are related under cyclic permutations. Let $\overline{I}$ and $\overline{I}^c$ be tuples built from the elements of the complementary sets I and I^c. Denoting two cyclically related permutations by $\overline{I}\,\overline{I}^c$ and $\overline{I}^c\overline{I}$ the corresponding PSFs are related by

$$S_{\overline{I}\,\overline{I}^c}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I}^c}) = \boldsymbol{\zeta}_I e^{\beta\omega'_I}\, S_{\overline{I}^c\overline{I}}(\boldsymbol{\omega}'_{\overline{I}^c\overline{I}}), \tag{2.2.1}$$

where the sign factor

$$\boldsymbol{\zeta}_I = \boldsymbol{\zeta}^{\overline{I}\,\overline{I}^c}/\boldsymbol{\zeta}^{\overline{I}^c\overline{I}} \tag{2.2.2}$$

only depends on the number of fermionic operators in the two sets I and I^c.[5] Therefore $\boldsymbol{\zeta}_I$ is already unambiguously labeled by the index set I. The prime in $e^{\beta\omega'_I}$ can be dropped when these PSFs are multiplied with $\delta(\omega_I - \omega'_I)$. The Eqs. (2.2.1) and (2.1.18) imply the relation

$$S_{[\overline{I};\overline{I}^c]_\pm}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I}^c}) = (\boldsymbol{\zeta}_I e^{\beta\omega'_I} \pm 1)S_{\overline{I}^c\overline{I}}(\boldsymbol{\omega}'_{\overline{I}^c\overline{I}}). \tag{2.2.3}$$

[5] Amongst the operators $\mathcal{O}$ there has to be an even number of fermionic ones. Therefore the sign factor $\boldsymbol{\zeta}_I$ is $+1$ (-1) if I contains an even (uneven) number of fermionic operators.

By means of the statistical factor

$$N_I = \frac{\boldsymbol{\zeta}_I e^{\beta\omega_I}+1}{\boldsymbol{\zeta}_I e^{\beta\omega_I}-1} = \begin{cases} \tanh(\beta\omega_I/2), & \text{for } \zeta_I=-1, \\ \coth(\beta\omega_I/2), & \text{for } \zeta_I=+1, \end{cases} \tag{2.2.4}$$

PSF commutators and PSF anti-commutators are therefore related by

$$S_{[\overline{I};\overline{I}^c]_+}(\boldsymbol{\omega'})\,\delta(\omega_I-\omega_I') = N_I\, S_{[\overline{I};\overline{I}^c]_-}(\boldsymbol{\omega'})\,\delta(\omega_I-\omega_I'), \tag{2.2.5}$$

provided that N_I does not diverge. It does diverge for $\zeta_I=+1$ and $\omega_I=0$. So, if the spectral function has a non-vanishing weight at $\omega_I'=0$ it has to be considered with special care. In this case one has to exclude the points with $\omega_I=0$ from the application of Eq. (2.2.5). However, this special case can be ignored for the major part of our discussion. It will be treated in Sec. 3.1.3 where we find that it can be recovered by the analytic continuation of the anomalous part of the MF correlator.

So, for a kernel of the form $K(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) \propto \delta(\omega_I)$, Eq. (2.2.5) can also be used on the level of correlators, implying for non-divergent N_I

$$\big(S_{[\overline{I};\overline{I}^c]_+} * K\big)(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) = N_I\big(S_{[\overline{I};\overline{I}^c]_-} * K\big)(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}). \tag{2.2.6}$$

Before we can apply this relation we need a function with the corresponding PSF (anti-)commutator structure. We obtain it if the following conditions are fulfilled: Two index orderings are related by cyclic permutation, i.e. they can be written as $\overline{I}\,\overline{I}^c$ and $\overline{I}^c\overline{I}$, respectively. The two corresponding kernels K_1 and K_2 contain a suitable $\delta(\omega_I)$ and are equal (up to a minus sign). Under these conditions we can collect the contributions in an PSF (anti-)commutator, i.e.

$$K_1(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) = \pm K_2(\boldsymbol{\omega}_{\overline{I}^c\overline{I}}) \propto \delta(\omega_I) \quad \Rightarrow \quad S_{\overline{I}\,\overline{I}^c} * K_1 + S_{\overline{I}^c\overline{I}} * K_2 = S_{[\overline{I};\overline{I}^c]_\pm} * K_1, \tag{2.2.7}$$

for which the relation in Eq. (2.2.5) can now be applied. Indeed we find in the following sections that certain linear combinations of analytically continued MF functions (AC functions) can be written as (nested) PSF commutators convolved with kernels which equal retarded product kernels (up to a minus sign). Our strategy will thus be to express the KF correlators through (nested) PSF (anti-)commutators and then to use the equilibrium condition via Eq. (2.2.6) to express KF correlators in terms of AC functions.

2.3 Analytic structure of Matsubara correlators

In the following we investigate the analytic continuation of MF correlators. While doing so, we solely consider the regular part of the MF kernel $\widetilde{K}$, which is a rational function and can thus be continued to complex frequencies. According to Eq. (2.1.12) the anomalous part of the MF kernel $\widehat{K}$ contains Kronecker symbols which do not have a unique "analytic

continuation"[6]. However, the kernel $\widehat{K}$ contains products of regular kernels $\widetilde{K}$ for which the considerations in this section can be applied again.

The analytic continuation of 2p correlators has been thoroughly studied by Baym and Mermin [10], who proved the uniqueness of the analytic continuation and its relation to retarded and advanced correlators. Later on Evans generalized their ideas to ℓp correlators [23]. He identified analytic continuations of the MF correlator (AC functions), $\Phi(\boldsymbol{z})$, which directly recover certain components (*retarded correlators*) in the KF, and *advanced* correlators which are related to the retarded ones by conjugation of all complex frequencies, $\omega + \mathrm{i}\gamma \to \omega - \mathrm{i}\gamma$. He however found that there is no simple generalization of the well-known results on 2p functions to higher-point functions. For $\ell \geq 4$ he found that there exist AC functions which are neither retarded nor advanced. We will call them *non-causal* functions. In fact, Weldon proved that these non-causal functions cannot be written in terms of a linear combination of KF correlators [31]. We will show that the non-causal AC functions are nevertheless needed to recover all KF components via analytic continuation from a single MF correlator.

In the following we first summarize the known results which are relevant for the goal of this thesis. (For a comprehensive presentation of the above-mentioned work we refer to the literature [10, 13, 23].) We then extend Weldon's work [26] and show that the discontinuities of $\Phi(\boldsymbol{z})$ along branch cuts can be expressed in terms of PSF commutators in the sense of Eq. (2.2.7). (These discontinuities are linear combinations of AC functions.) Such a discontinuity is a function of ℓ complex frequencies again. We find that it has two lower-dimensional substructures whose analytic properties can be regarded independently. In anticipation of later results we use this property to identify linear combinations of AC functions which are needed for the construction of KF correlators.

2.3.1 Regions of analyticity and AC functions

In Eq. (2.1.27) we have already stated the known analytic continuation of $\widetilde{G}$ to the retarded correlators $G^{[\eta]}$ [10, 23, 30]. One has to replace the tuple of imaginary frequencies $\mathrm{i}\boldsymbol{\omega}$ by a suitable complex frequency tuple $\boldsymbol{\omega}^{[\eta]}$. For a general analytic continuation we continue the imaginary frequencies to complex ones by replacing

$$\mathrm{i}\omega_i \to z_i = \omega_i + \mathrm{i}\gamma_i \quad (\omega_i, \gamma_i \in \mathbb{R}), \tag{2.3.1}$$

thereby obtaining the analytically continued function of complex frequencies

$$\Phi(\boldsymbol{z}) = \widetilde{G}(\mathrm{i}\boldsymbol{\omega})\Big|_{\mathrm{i}\boldsymbol{\omega}\to\boldsymbol{z}}. \tag{2.3.2}$$

[6] See Sec. 3.1.3 for the resolution of this issue. There we argue that the factor $\beta\delta_\omega$ needs to be replaced by $4\pi\mathrm{i}\delta(\omega)$ to obtain a contribution to certain KF correlators.

Writing out this function in the permutation expansion we obtain

$$\begin{aligned}\Phi(\boldsymbol{z}) &= \sum_p \int \mathrm{d}^{\ell-1}\omega'_p\, S_p(\boldsymbol{\omega}'_p)\widetilde{K}(\boldsymbol{z}_p - \boldsymbol{\omega}'_p) \\ &= \sum_p \int \mathrm{d}^{\ell-1}\omega'_p\, S_p(\boldsymbol{\omega}'_p)\prod_{i=1}^{\ell-1}\frac{1}{z_{\overline{1}\cdots\overline{i}} - \omega'_{\overline{1}\cdots\overline{i}}}.\end{aligned} \tag{2.3.3}$$

The regular kernel is a rational function and thereby analytic on certain regions. The integral over $\boldsymbol{\omega}'$ inserts poles (or branch cuts for a continuous spectrum) along the real axis, more precisely, at the positions where $S_p(\boldsymbol{\omega}'_p)$ has finite weight according to Eq. (2.1.9). We see that the branch cuts of the function $\Phi(\boldsymbol{z})$ lie along all those points for which a sum of complex frequencies z_I in the denominators of Eq. (2.3.3) is real,

$$\{\boldsymbol{z}|\, z_I \in \mathbb{R} \quad \text{for some } I \subsetneq L\,\}. \tag{2.3.4}$$

Outside of this set $\Phi(\boldsymbol{z})$ is analytic. Equivalently, each subset $I \subsetneq L$ defines a branch cut, to be denoted $\mathcal{B}_I$, along which $\gamma_I = 0$.

Ultimately we want to regard $\Phi(\boldsymbol{z})$ as a function of real frequencies $\boldsymbol{\omega}$ and, making repeated use of the formula for the inverse Fourier transformation

$$\lim_{\gamma\searrow 0}\int_{\mathbb{R}} \frac{\mathrm{d}\omega}{2\pi}\frac{e^{-\mathrm{i}\omega t}}{\omega \pm \mathrm{i}\gamma} = \pm(-\mathrm{i})\theta(\pm t), \tag{2.3.5}$$

we indeed recover products of step functions θ in the real time domain. (Remember that step functions are used to explicitly implement the contour ordering for KF correlators [21].) For this reason the imaginary parts γ_i of the complex frequencies z_i will henceforth be regarded as infinitesimals. The limits $\gamma_i \to 0$ have to be taken in a careful way. To illustrate the issue, we regard $z = \omega \pm \mathrm{i}\gamma$ as a complex variable again, then the left side of Eq. (2.3.5) corresponds to a contour integral along a path parallel to the real axis, shifted along the imaginary axis by $\pm\gamma$. In this sense, the limit $\gamma \searrow 0$ deforms the contour while staying within a region of analyticity. Analogously, also for $\Phi(\boldsymbol{z})$ the limits $\boldsymbol{\gamma} \to 0$ have to be taken while staying in one region of analyticity. So, each of these regions corresponds to a different analytically continued function (*AC function*) of real frequencies $\boldsymbol{\omega}$,

$$C^{\boldsymbol{\gamma}}(\boldsymbol{\omega}) = \Phi(\boldsymbol{z})|_{\boldsymbol{z}=\boldsymbol{\omega}+\mathrm{i}\boldsymbol{\gamma}}\,, \tag{2.3.6}$$

with the infinitesimals $\boldsymbol{\gamma}$ determining the corresponding region of analyticity. The label $\boldsymbol{\gamma}$ on $C^{\boldsymbol{\gamma}}$ serves to identify this region; since the components γ_i are infinitesimal the identification is fully determined by their signs.

We remark that the imaginary part $\boldsymbol{\gamma}$ underlies the constraint $\gamma_{1\cdots\ell} = 0$. The tuple of complex frequencies $\boldsymbol{z}$ thus has only $\ell - 1$ independent components, as expected for the analytic continuation of a function of $\mathrm{i}\boldsymbol{\omega}$ with only $\ell - 1$ independent frequency arguments.

To visualize the regions on which $\Phi(\boldsymbol{z})$ is analytic we use diagrams whose construction we exemplify for the cases $\ell = 3$ and $\ell = 4$. In Fig. 2.2 we illustrate the case for $\ell = 3$,

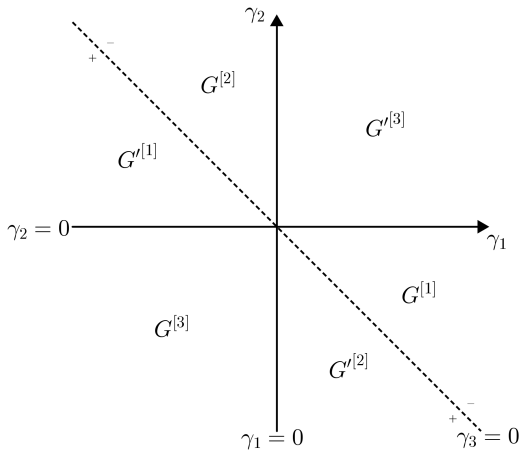

Figure 2.2: Regions of analyticity of three-point correlators (adapted from Ref. [23]): The regions are distinguished by the imaginary parts of the complex frequencies $\gamma_i = \mathrm{Im}(z_i)$. In this diagram the parameters γ_1 and γ_2 are used as coordinate system. The branch cuts $\mathcal{B}_I$ are given by the points for which $\gamma_I = 0$ with $I \subsetneq \{1, 2, 3\}$. There are three of them: The vertical solid line $\mathcal{B}_1$ where $\gamma_1 = -\gamma_{23} = 0$; the horizontal solid line $\mathcal{B}_2$ where $\gamma_2 = -\gamma_{13} = 0$; and the diagonal dashed line $\mathcal{B}_3$ where $\gamma_3 = -\gamma_{12} = 0$, i.e. where $\gamma_2 = -\gamma_1$. They divide the γ_1-γ_2 plane into six distinct regions. Each such region is associated with that retarded or advanced correlator $G^{[\eta]}$ or $G'^{[\eta]}$, respectively, functions of the complex frequencies $\boldsymbol{\omega}^{[\eta]}$ or $(\boldsymbol{\omega}^{[\eta]})^*$, respectively, for which the imaginary parts $\boldsymbol{\gamma}^{[\eta]}$ or $-\boldsymbol{\gamma}^{[\eta]}$ have signs matching those of $\boldsymbol{\gamma}$ in the corresponding region.

using γ_1 and γ_2 as independent variables which define the coordinate axes, while $\gamma_3 = -\gamma_{12}$ is fixed by the choice of a point in this plane. There are three branch cuts $\mathcal{B}_1$, $\mathcal{B}_2$ and $\mathcal{B}_3$ along which $\gamma_1 = -\gamma_{23} = 0$ or $\gamma_2 = -\gamma_{13} = 0$ or $\gamma_3 = -\gamma_{12} = 0$, respectively. These branch cuts divide the plane into six separate regions, each associated with one of the three retarded or advanced correlators, $G^{[\eta]}$ or $G'^{[\eta]}$. These are functions of the complex frequencies $\boldsymbol{\omega}^{[\eta]} = \boldsymbol{\omega} \pm \mathrm{i}\boldsymbol{\gamma}^{[\eta]}$, respectively. Each correlator is associated with that region for which the signs of all $\gamma_i^{[\eta]}$ (or $-\gamma_i^{[\eta]}$), the imaginary parts of its frequency arguments, match the signs of all γ_i in the corresponding region. For example, $G^{[1]}$ requires a complex frequency tuple $\boldsymbol{\omega}^{[1]}$ with $\gamma_1 > 0$, $\gamma_2 < 0$ and $\gamma_{12} > 0$, i.e. the region labeled $G^{[1]}$ in Fig. 2.2. Similarly, $G'^{[2]}$ requires a complex frequency tuple $(\boldsymbol{\omega}^{[1]})^*$ with $\gamma_1 > 0$, $\gamma_2 < 0$ and $\gamma_{12} < 0$, i.e. the region labeled $G'^{[1]}$ in Fig. 2.2.

The construction of the diagram proceeds analogously for $\ell = 4$ in Fig. 2.3. Here the parameters γ_1, γ_4 and γ_{12} are chosen to be the coordinates. (The third dimension is for γ_{12}.) In each of the two diagrams of Fig. 2.3 we can assume a fixed $\gamma_{12} \lesseqgtr 0$ and draw the remaining branch cuts. Due to $\gamma_{1\ldots4} = 0$ there are only 7 independent branch cuts, namely for $\gamma_1 = 0$, $\gamma_2 = 0$, $\gamma_3 = 0$, $\gamma_4 = 0$, $\gamma_{12} = 0$, $\gamma_{13} = 0$ and $\gamma_{14} = 0$. Having drawn all the branch cuts one then sees in Fig. 2.3 the 32 connected regions of analyticity of 4p

correlators (16 for each γ_{12}).

In Fig. 2.3 the regions of analyticity are labeled by arabic numbers for the rectangular sections. Roman numbers are used to differentiate regions which are separated by the branch cuts $\mathcal{B}_{12}$, $\mathcal{B}_{13}$ or $\mathcal{B}_{14}$ at $\gamma_{12} = 0$, $\gamma_{13} = 0$ or $\gamma_{14} = 0$. The AC functions $C^{\boldsymbol{\gamma}}$ are labeled correspondingly, e.g. $C^{\mathrm{I}}_{2,2}$. Some regions can be identified with the retarded correlators $G^{[\eta]}$. Their parametrization is given in the definition of the complex frequency tuple $\boldsymbol{\omega}^{[\eta]}$ in Eq. (2.1.23). The regions for the advanced correlators $G'^{[\eta]}$ are the complex conjugates of the retarded ones.

2.3.2 Discontinuities of AC functions

In our example with $\ell = 4$ only 8 out of the 32 regions of analyticity are associated with retarded or advanced correlators. So, there are 24 left whose significance have not been clarified yet. Weldon proved that the retarded and advanced correlators are the only KF correlators that can be directly expressed through AC functions $C^{\boldsymbol{\gamma}}(\boldsymbol{\omega})$ [31]. We conclude that it is at least necessary to combine different AC functions for the construction of the remaining KF correlators. In Ref. [26] Weldon investigates, for $\ell = 4$, the discontinuities of Φ at branch cuts and computes explicit formulas. In the following we generalize the discussion and give formulas for the functions which are relevant for the analytic continuation to KF correlators. As we will see in later sections, the discontinuities $C^{\boldsymbol{\gamma}^{[I,+]}}(\boldsymbol{\omega}) - C^{\boldsymbol{\gamma}^{[I,-]}}(\boldsymbol{\omega})$ between two neighboring regions of analyticity separated by a branch cut $\mathcal{B}_I$ are of great importance for the construction of KF correlators.

To quantify these discontinuities we consider two arbitrary regions which are separated by the branch cut $\mathcal{B}_I$ where $\gamma_I = 0$ ($I \subsetneq L$). The corresponding AC functions on either side of the branch cut are $C^{\boldsymbol{\gamma}^{[I,+]}}(\boldsymbol{\omega})$ and $C^{\boldsymbol{\gamma}^{[I,-]}}(\boldsymbol{\omega})$, with tuples $\boldsymbol{\gamma}^{[I,+]}$ and $\boldsymbol{\gamma}^{[I,-]}$ representing the two regions such that the sums $\gamma_I^{[I,\pm]} \gtrless 0$ are positive or negative on the respective side of the branch cut $\mathcal{B}_I$. The discontinuity at the branch cut $\mathcal{B}_I$ is defined as

$$\Delta C^{\boldsymbol{\gamma}}_I(\boldsymbol{\omega}) = C^{\boldsymbol{\gamma}^{[I,+]}}(\boldsymbol{\omega}) - C^{\boldsymbol{\gamma}^{[I,-]}}(\boldsymbol{\omega}). \tag{2.3.7}$$

Here the subscript in $\Delta C_I^{\boldsymbol{\gamma}^{[I,\pm]}}$ indicates that this discontinuity is at the branch cut $\mathcal{B}_I$. In App. A.1 we prove that the kernel of the discontinuity $\Delta C_I^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega})$ is non-zero only for permutations of the type $\overline{I}\,\overline{I}^c$ and $\overline{I}^c\overline{I}$.[7] Denoting the two complex frequencies on either side of and infinitesimally close to the branch cut by $\boldsymbol{z}^{[I,\pm]} = \boldsymbol{\omega} + \mathrm{i}\boldsymbol{\gamma}^{[I,\pm]}$, the discontinuity kernel is given by

$$\Delta\widetilde{K}_I^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega}_p) = \widetilde{K}(\boldsymbol{z}_p^{[I,+]}) - \widetilde{K}(\boldsymbol{z}_p^{[I,-]}) = \begin{Bmatrix} +\hat{\delta}(\omega_I), \\ -\hat{\delta}(\omega_I), \\ 0, \end{Bmatrix} \widetilde{K}(\boldsymbol{z}_{\overline{I}})\widetilde{K}(\boldsymbol{z}_{\overline{I}^c}) \begin{Bmatrix} \text{for } p = \overline{I}\,\overline{I}^c, \\ \text{for } p = \overline{I}^c\overline{I}, \\ \text{else.} \end{Bmatrix}, \tag{2.3.8}$$

[7] It follows that any discontinuity at the branch cut $\mathcal{B}_I$ splits the indices L into two complementary subsets I and I^c.

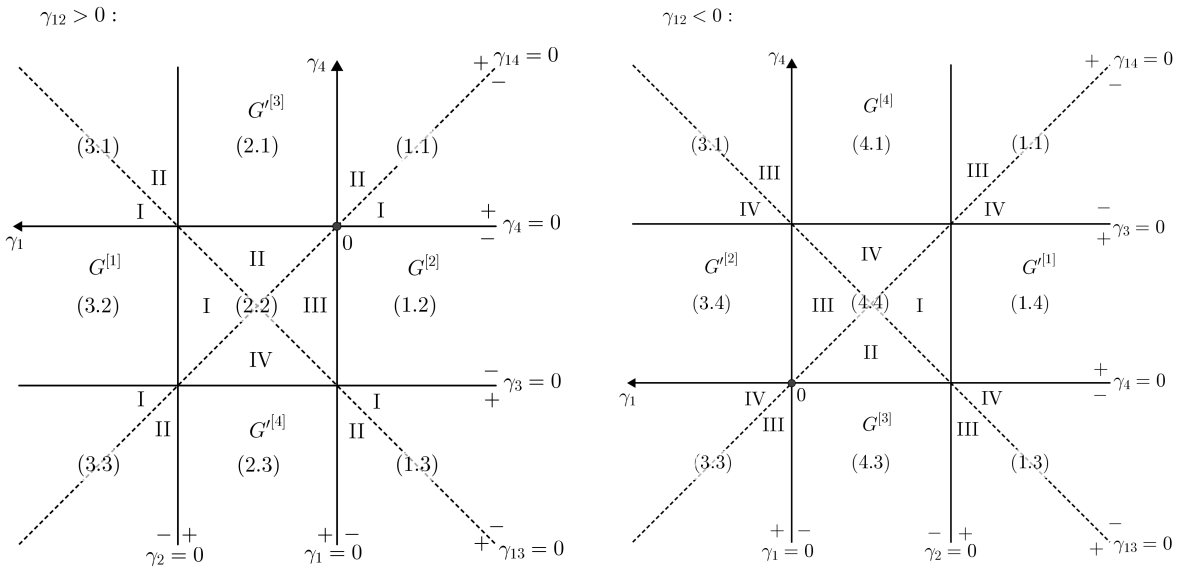

Figure 2.3: Regions of analyticity for 4p correlators (adapted from Ref. [13]): The independent imaginary parts of the frequencies γ_1, γ_4 and γ_{12} are used as coordinate system (thick lines with arrows). Thick and dotted lines indicate the branch cuts. Regions have been marked which directly correspond to retarded and advanced Green's functions. The inscriptions at the bottom and the right edge of each diagram are reading aids: the "$\gamma_I = 0$" next to a line indicates the corresponding branch cut. The $-/+$ sign distinguishes on which side of the line one has $\gamma_I \lessgtr 0$. Each region is labeled by arabic and roman numbers.
Let us explain the construction of these diagrams for the left one. Here $\gamma_{12} > 0$ is fixed to a positive value. Consider $\gamma_2 = \gamma_{12} - \gamma_1$. For fixed $\gamma_{12} > 0$, γ_1 has to be a positive constant if $\gamma_2 = 0$. So, the line $\gamma_2 = 0$ runs parallel to and left of $\gamma_1 = 0$. To the left/right of this line, γ_2 is negative/positive. Similarly, one considers $\gamma_3 = -\gamma_{12} - \gamma_4$. The line $\gamma_3 = 0$ runs parallel and below the line $\gamma_4 = 0$. Next, consider $\gamma_{14} = -\gamma_{23}$. This equals zero along the line $\gamma_1 = -\gamma_4$, or equivalently, along $\gamma_2 = -\gamma_3$, i.e. a diagonal intersecting the points $\gamma_1 = \gamma_4 = 0$ and $\gamma_2 = \gamma_3 = 0$.

where the delta function $\hat{\delta}(\cdot) = -2\pi\mathrm{i}\delta(\cdot)$, and the regular kernel $\widetilde{K}$ on the right depend on subtuples of the complex argument evaluated *on* the branch cut, $\boldsymbol{z}_p = \boldsymbol{\omega}_p + \mathrm{i}\boldsymbol{\gamma}_p\big|_{\gamma_I=0} = \boldsymbol{z}_{\overline{I}\,\overline{I}^c} = (\boldsymbol{z}_{\overline{I}}, \boldsymbol{z}_{\overline{I}^c})$.

The discontinuity $\Delta C_I^\gamma(\boldsymbol{\omega})$ is obtained by collecting all contributions from the permutation expansion, giving

$$\Delta C_I^\gamma(\boldsymbol{\omega}) = \sum_{p_{I|I^c}} \big(S_{\overline{I}\,\overline{I}^c} * \Delta\widetilde{K}_I^\gamma\big)(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) + \sum_{p_{I^c|I}} \big(S_{\overline{I}^c\overline{I}} * \Delta\widetilde{K}_I^\gamma\big)(\boldsymbol{\omega}_{\overline{I}^c\overline{I}}).$$

Collecting the PSFs contributing with kernels differing only by a sign (see Eq. (2.2.7)), we obtain

$$\Delta C_I^\gamma(\boldsymbol{\omega}) = \sum_{p_{I|I^c}} \big([S_{\overline{I}\,\overline{I}^c} - S_{\overline{I}^c\overline{I}}] * \Delta\widetilde{K}_I^\gamma\big)(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) = \sum_{p_{I|I^c}} \big(S_{[\overline{I};\overline{I}^c]_-} * \Delta\widetilde{K}_I^\gamma\big)(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}). \tag{2.3.9}$$

The discontinuity has two independent substructures. For every permutation the kernel of the discontinuity $\Delta\widetilde{K}_I^\gamma(\boldsymbol{z}_p)$ factorizes into two regular kernels, $\widetilde{K}(\boldsymbol{z}_{\overline{I}})$ and $\widetilde{K}(\boldsymbol{z}_{\overline{I}^c})$, which only depend on the complex frequencies of a single subtuple $\widetilde{K}(\boldsymbol{z}_{\overline{I}})$ and $\widetilde{K}(\boldsymbol{z}_{\overline{I}^c})$, which only depend on the complex frequencies of a single subtuple, $\boldsymbol{z}_{\overline{I}}$ or $\boldsymbol{z}_{\overline{I}^c}$. The analytic structure of the two lower-dimensional substructures on the respective sets I and I^c can now be considered independently. This has two important consequences. Firstly, the kernels $\widetilde{K}(\boldsymbol{z}_{\overline{I}})$ and $\widetilde{K}(\boldsymbol{z}_{\overline{I}^c})$ can be analytically continued to retarded kernels by a suitable choice of $\boldsymbol{\gamma}_{\overline{I}}$ and $\boldsymbol{\gamma}_{\overline{I}^c}$ (see below). Secondly, the above arguments may be used repeatedly for subdividing one of the two sets (I or I^c) into smaller sets by considering discontinuities of ΔC_I^γ as function of $\boldsymbol{z}_I$ and $\boldsymbol{z}_{I^c}$. Both of these possibilities will be used later on to obtain suitable AC functions for the construction of KF correlators (see Secs. 3.1.2 and 3.2).

In anticipation of the needs in the next sections we now define the notation for certain discontinuities. For complementary subsets $I_1 \cup I_2 = \{1, ..., \ell\}$ we can pick an element $\eta_1 \in I_1$ and $\eta_2 \in I_2$ from each subset. Exploiting the fact that the discontinuity kernel $\Delta\widetilde{K}_I^\gamma$, factorizes into two kernels $\widetilde{K}(\boldsymbol{z}_{\overline{I}_1})$ and $\widetilde{K}(\boldsymbol{z}_{\overline{I}_2})$ (see Eq. (2.3.8)), we can pick the imaginary parts of $\boldsymbol{z}_{\overline{I}_j}$ as $\boldsymbol{\gamma}_{\overline{I}_j} = \boldsymbol{z}_{\overline{I}_j}^{[\eta_j]}$ for $j = 1, 2$, thereby ensuring that these are *retarded*, kernels $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}_1}^{[\eta_1]})$ and $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}_2}^{[\eta_2]})$. Recall that the imaginary parts in $\boldsymbol{\omega}_{\overline{I}_1}^{[\eta_1]}$ are fixed by the choice of the set I_1 and η_1. The order of the elements in $\overline{I}_1$ only determines the order of the components in the complex frequency tuple. Then $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}_1}^{[\eta_1]})$ is retarded with respect to ω_{η_1} for any permutation of $\overline{I}_1$ (and likewise for $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}_2}^{[\eta_2]})$). With this choice of imaginary parts, the discontinuity (2.3.9) can be expressed through a retarded product kernel of the form (2.1.30) denoted as

$$\Delta C_{I_1}^{[\eta_1][\eta_2]} = \sum_{p_{I_1|I_2}} S_{[\overline{I}_1;\overline{I}_2]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}}. \tag{2.3.10}$$

The subscript to $\Delta C_{I_1}^{[\eta_1][\eta_2]}$ indicate that this is a discontinuity at the branch cut $\mathcal{B}_{I_1}$, with an AC function with $\gamma_{I_1} < 0$ being subtracted from one with $\gamma_{I_1} > 0$. The superscript

indicates that the kernels on the two subtuples are retarded with respect to η_1 and η_2, respectively. We have thereby proven that such functions can be obtained by taking linear combinations of AC functions.

A remaining task is the identification of the AC functions involved in a discontinuity. Let us consider two examples: For $\ell = 4$, Weldon has studied the discontinuity

$$\sum_{p_{\{2\}|\{1,3,4\}}} S_{[(2);(\overline{2}\,\overline{3}\,\overline{4})]_-} * K_{(\overline{1})^{[2]}(\overline{2}\,\overline{3}\,\overline{4})^{[1]}},$$

and by direct computation found an expression for it given by Eq. (4.15) of Ref. [26]. Since the subtuples $\overline{I}_1$ and $\overline{I}_2$ are composed of the sets $\{2\}$ and $\{1,3,4\}$, it is a discontinuity at the branch cut $\mathcal{B}_2$. For a retarded kernel the complex frequency subtuple is $\boldsymbol{\omega}^{[1]}_{(134)} = (\omega_1 + \mathrm{i}2\gamma_0, \omega_3 - \mathrm{i}\gamma_0, \omega_4 - \mathrm{i}\gamma_0)$, implying $\gamma_1 > 0$, $\gamma_{13} > 0$, $\gamma_{14} > 0$, $\gamma_2 = -\gamma_{134} = 0$ which is only compatible with that part of the branch cut separating the regions $C_{3.2}$ and $C^{\mathrm{I}}_{2.2}$ in Fig. 2.3. We hence conclude that the above function is

$$\Delta C_2^{[2][1]} = \sum_{p_{\{2\}|\{1,3,4\}}} S_{[(2);(\overline{2}\,\overline{3}\,\overline{4})]_-} * K_{(\overline{1})^{[2]}(\overline{2}\,\overline{3}\,\overline{4})^{[1]}} = C^{\mathrm{I}}_{2.2} - C_{3.2}, \tag{2.3.11}$$

which matches the Eq. (4.15) in Ref. [26].

Now consider the discontinuity

$$\sum_{p_{\{2,3\}|\{1,4\}}} S_{[(\overline{1}\,\overline{2});(\overline{3}\,\overline{4})]_-} * K_{(\overline{1}\,\overline{2})^{[2]}(\overline{3}\,\overline{4})^{[1]}}.$$

This is a discontinuity at the branch cut $\mathcal{B}_{23} = \mathcal{B}_{14}$. The complex frequency tuples $\boldsymbol{\omega}^{[2]}_{(23)} = (\omega_2 + \mathrm{i}\gamma_0, \omega_3 - \mathrm{i}\gamma_0)$ and $\boldsymbol{\omega}^{[1]}_{(14)} = (\omega_1 + \mathrm{i}\gamma_0, \omega_4 - \mathrm{i}\gamma_0)$ having $\gamma_2 > 0$, $\gamma_3 < 0$, $\gamma_1 > 0$, $\gamma_4 < 0$, only compatible with the region $C_{2.2}$. So we have identified

$$\Delta C_{23}^{[2][1]} = \sum_{p_{\{2,3\}|\{1,4\}}} S_{[(\overline{1}\,\overline{2});(\overline{3}\,\overline{4})]_-} * K_{(\overline{1}\,\overline{2})^{[2]}(\overline{3}\,\overline{4})^{[1]}} = C^{\mathrm{IV}}_{2.2} - C^{\mathrm{I}}_{2.2} = C^{\mathrm{III}}_{2.2} - C^{\mathrm{II}}_{2.2}, \tag{2.3.12}$$

with the parts where $\gamma_{23} = -\gamma_{14}$ is negative being subtracted from those where it is positive. This matches Eq. (4.16) in Ref. [26] obtained by Weldon. Note that in this case the involved regions are not unique. The discontinuity can be expressed in two ways. Once the discontinuity along $\gamma_{23} = 0$ is computed for $\gamma_{13} > 0$ and once for $\gamma_{13} < 0$. This can be explained on the basis of the regular kernel $\widetilde{K}$: the factors $(\Omega_{13})^{-1}$ and $(\Omega_{23})^{-1}$ cannot occur in the regular kernel in the same permutation. Hence, the parameter $\gamma_{13} \gtrless 0$ has no influence on a discontinuity at $\gamma_{23} = 0$.

In this section we have found that the discontinuities of AC functions ΔC^{γ}_I in Eq. (2.3.9) have a PSF commutator structure which fulfills the condition in Eq. (2.2.7). Due to the factorization of the kernel, the analytic structure of a discontinuity is independent of the two complementary subsets of complex frequencies $\{z_i \,|\, i \in I\}$ and $\{z_i \,|\, i \in I^c\}$. In Sec. 3.2

we take this process a step further by computing discontinuities of discontinuities, thereby producing nested PSF commutators. In the following chapter we express KF components like $G^{[\eta_1\eta_2]}$ in terms of nested PSF (anti-)commutators. Recalling that Eq. (2.2.6) relates PSF commutators to PSF anti-commutators, we then express KF correlators in terms of AC functions and statistical factors N_I.

Chapter 3

Construction of KF correlators via the analytic continuation method

In this chapter we derive how one can construct KF correlators from MF correlators, assuming that the exact functional dependence on the frequency arguments of the latter is known. We have seen that the retarded correlators $G^{[\eta]}$ can be directly obtained from the regular MF correlator by analytic continuation to certain regions of analyticity [cf. Eq. (2.1.27)]. However, for the other KF components this simple prescription is not applicable anymore. We find that the construction of KF correlators becomes increasingly complicated with the number of 2-indices. Therefore we begin this chapter with the reconstruction of those with only two 2-indices: the correlators $G^{[\eta_1\eta_2]}$.

3.1 Construction of $G^{[\eta_1\eta_2]}$ from AC functions

The exact expression (2.1.20) for the correlator $G^{[\eta_1\eta_2]}$ reads

$$G^{[\eta_1\eta_2]}(\boldsymbol{\omega}) = \frac{2}{2^{\ell/2}} \sum_p \left(S_p * K^{[\hat{\eta}_1\hat{\eta}_2]}\right)(\boldsymbol{\omega}_p), \tag{3.1.1}$$

with $\hat{\eta}_j \in \{p^{-1}(\eta_1), p^{-1}(\eta_2)\}$. This expression can be expanded into functions for which the equilibrium condition can be used via Eqs. (2.2.5) and (2.2.7). Thereby the correlator $G^{[\eta_1\eta_2]}$ can be related to AC functions. In fact, we find that $G^{[\eta_1\eta_2]}$ is a linear combination of the discontinuities ΔC_I^γ which make up the difference $G^{[\eta_1]} - G^{[\eta_2]}$.

For simplicity we will first disregard divergencies of the factor N_I for which the relation in Eq. (2.2.5) is ill-defined. These are separately treated in Sec. 3.1.3. There we show that these problematic parts are in fact obtained by analytic continuation of the anomalous parts of the MF correlators $\widehat{K}_I$.

3.1.1 Expansion of $G^{[\eta_1\eta_2]}$

Consider a certain permutation $p = (\overline{1}, ..., \overline{\ell})$ and the corresponding kernel $K^{[\hat{\eta}_1\hat{\eta}_2]}(\boldsymbol{\omega}_p)$. As we show in App. A.2, we can expand the kernel as

$$K^{[\hat{\eta}_1\hat{\eta}_2]}(\boldsymbol{\omega}_p) = \sum_{y=\hat{\eta}_1}^{\hat{\eta}_2-1} K_{(\overline{1}\cdots\overline{y})^{[\overline{\hat{\eta}}_1]}(\overline{y+1}\cdots\overline{\ell})^{[\overline{\hat{\eta}}_2]}}(\boldsymbol{\omega}_p), \tag{3.1.2}$$

where the sum is over a range of y values, each yielding a different split-up of the same permutation into left and right subtuples $p = \overline{I}\,\overline{I}^c$, with $\overline{I} = (\overline{1}..\overline{y})$ and $\overline{I}^c = (\overline{y+1}..\overline{\ell})$, and the range of y values depends on p, since $\hat{\eta}_1$ and $\hat{\eta}_2$ do. The retarded product kernel is defined according to Eq. (2.1.30),

$$K_{\overline{I}^{[\mu]}\overline{I}^{c\,[\nu]}}(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) = \hat{\delta}(\omega_I)\widetilde{K}(\boldsymbol{\omega}_{\overline{I}}^{[\mu]})\widetilde{K}(\boldsymbol{\omega}_{\overline{I}^c}^{[\nu]}). \tag{3.1.3}$$

with μ and ν shorthands for $\overline{\hat{\eta}}_1$ and $\overline{\hat{\eta}}_2$. Furthermore, the kernel $K_{\overline{I}^{[\mu]}\overline{I}^{c\,[\nu]}}$ factorizes into two retarded kernels, $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}}^{[\mu]})$ and $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}^c}^{[\nu]})$, with frequency arguments $\boldsymbol{\omega}_{\overline{I}}^{[\mu]}$ or $\boldsymbol{\omega}_{\overline{I}^c}^{[\nu]}$. So, if the kernel expansion for a given permutation p contains the split-up $p = \overline{I}\,\overline{I}^c$, giving the kernel $K_{\overline{I}^{[\mu]}\overline{I}^{c\,[\nu]}}$, then there exists another cyclically related permutation p', whose kernel expansion contains the split-up $p' = \overline{I}^c\overline{I}$, giving the kernel $K_{\overline{I}^{c\,[\nu]}\overline{I}^{[\mu]}}$. These two kernels are equal and fulfill the condition to form an PSF anti-commutator according to Eq. (2.2.7). Since the variable y governing the split $p = \overline{I}\,\overline{I}^c$ satisfies $\hat{\eta}_1 \leq y < \hat{\eta}_2$, the subtuples $\overline{I}$ and $\overline{I}^c$ always contain $\overline{\hat{\eta}}_1$ and $\overline{\hat{\eta}}_2$, respectively. Each of these in turn equals either η_1 or η_2, since $\hat{\eta}_i \in \{p^{-1}(\eta_1), p^{-1}(\eta_2)\}$ hence $\overline{\hat{\eta}}_1 \in \{\eta_1, \eta_2\}$. Therefore, the subtuples $\overline{I}$ and $\overline{I}^c$ contain either η_1 or η_2, respectively. Correspondingly, we will denote the one containing η_1 by I_1, and that containing η_2 by I_2, respectively. The expansion of the kernel $K^{[\hat{\eta}_1\hat{\eta}_2]}$ into several contributions yields a corresponding expansion of the correlator $G^{[\eta_1\eta_2]}$.

$$G^{[\eta_1\eta_2]}(\boldsymbol{\omega}) = \frac{2}{2^{\ell/2}}\sum_p\sum_{y=\hat{\eta}_1}^{\hat{\eta}_2} S_p * K_{(\overline{1}\cdots\overline{y})^{[\overline{\hat{\eta}}_1]}(\overline{y+1}\cdots\overline{\ell})^{[\overline{\hat{\eta}}_2]}}(\boldsymbol{\omega}_p), \tag{3.1.4}$$

From this sum we wish to collect all terms proportional to the same delta functions $\hat{\delta}(\omega_{I_1}) = \hat{\delta}(\omega_{I_2})$, involving complementary subsets $I_1 \subsetneq L$ and $I_2 = L\backslash I_1$ containing η_1 and η_2, respectively. For each such pair of subsets I_1 and I_2 all permutations of the type $\overline{I}_1\overline{I}_2$ and $\overline{I}_2\overline{I}_1$ yield contributions proportional to $\hat{\delta}(\omega_{I_1})$, hence it is convenient to combine these in an object defined as

$$\begin{aligned} 2^{\ell/2-1}\, G_{I_1}^{[\eta_1\eta_2]}(\boldsymbol{\omega}) &= \sum_{p_{I_1|I_2}} \left(S_{\overline{I}_1\overline{I}_2} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}}\right)(\boldsymbol{\omega}_{\overline{I}_1\overline{I}_2}) + \sum_{p_{I_2|I_1}} \left(S_{\overline{I}_2\overline{I}_1} * K_{\overline{I}_2^{[\eta_2]}\overline{I}_1^{[\eta_1]}}\right)(\boldsymbol{\omega}_{\overline{I}_2\overline{I}_1}) \\ &= \sum_{p_{I_1|I_2}} \left(S_{[\overline{I}_1;\overline{I}_2]_+} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}}\right)(\boldsymbol{\omega}_{\overline{I}_1\overline{I}_2}), \end{aligned} \tag{3.1.5}$$

p	$\boldsymbol{k}_p$	$[\hat\eta_1\hat\eta_2]$	$[\overline{\hat\eta}_1\overline{\hat\eta}_2]$	y	$K_{\overline{I}_1^{[\overline{\hat\eta}_1]}\overline{I}_2^{[\overline{\hat\eta}_2]}}$	$\overline{I}_1$	$\overline{I}_2$	$I_1=\{1\}$ $I_2=\{2,3\}$	$I_1=\{1,2\}$ $I_2=\{3\}$
(123)	(212)	[13]	[13]	1	$K_{(1)^{[1]}(23)^{[3]}}$	(1)	(23)	x	
				2	$K_{(12)^{[1]}(3)^{[3]}}$	(12)	(3)		x
(132)	(221)	[12]	[13]	1	$K_{(1)^{[1]}(32)^{[3]}}$	(1)	(32)	x	
(213)	(122)	[23]	[13]	2	$K_{(21)^{[1]}(3)^{[3]}}$	(21)	(3)		x
(231)	(122)	[23]	[31]	2	$K_{(23)^{[3]}(1)^{[1]}}$	(1)	(23)	x	
(312)	(221)	[12]	[31]	1	$K_{(3)^{[3]}(12)^{[1]}}$	(12)	(3)		x
(321)	(212)	[13]	[31]	1	$K_{(3)^{[3]}(21)^{[1]}}$	(21)	(3)		x
				2	$K_{(32)^{[3]}(1)^{[1]}}$	(1)	(32)	x	
					$\sum_p = G^{212}$			$\sum_p = G_1^{212}$	$\sum_p = G_{12}^{212}$

Table 3.1: Expansion of G^{212} according to Eq. (3.1.6): The indices $[\hat\eta_1\hat\eta_2]$ are the positions of the 2-indices in $\boldsymbol{k}_p$, and y is the summation variable in Eq. (3.1.4). The various summands from the expansions of $K^{[\hat\eta_1\hat\eta_2]}$ contribute either to G_1^{212} or to G_{12}^{212} as indicated in the lowest row. The latter two functions are related to different AC functions.

see Eq. (2.2.7). Finally, the KF correlator $G^{[\eta_1\eta_2]}$ is obtained by summing all contributions $G_I^{[\eta_1\eta_2]}$ which result from the kernel expansion. To identify these, recall that the split-up into two subtuples is performed in all possible ways for which each of the two subtuples contains either η_1 or η_2. Since $G_{I_1}^{[\eta_1\eta_2]}$ accounts for both $\overline{I}_1\overline{I}_2$ and $\overline{I}_2\overline{I}_1$, the full correlator is given by

$$G^{[\eta_1\eta_2]}(\boldsymbol{\omega}) = \sum_{I_1\in\mathcal{I}_1} G_{I_1}^{[\eta_1\eta_2]}(\boldsymbol{\omega}), \tag{3.1.6}$$

where $\mathcal{I}_1 = \{I_1 \subsetneq L | \eta_1 \in I_1, \eta_2 \notin I_1\}$ is the set of all subtuples of L containing η_1 but not η_2. Accordingly, for each of these I_1 the complementary set I_2 contains η_2. The sums over I_1 in (3.1.6) and $p_{(I_1|I_2)}$ in (3.1.5) together generate the same terms as the sums over p and y in (3.1.4), but packaged in more convenient combinations.

In Table 3.1 we exemplify the kernel expansion of Eq. (3.1.4) for G^{212}. Then $[\eta_1\eta_2] = [13]$, hence there are only two possible choices of I_1, namely $\{1\}$ with $I_2 = \{2,3\}$, or $\{1,2\}$ with $I_2 = \{3\}$. For example, $p = (123)$ yields

$$K^{[13]}(\boldsymbol{\omega}_{(123)}) = K_{(1)^{[1]}(23)^{[3]}}(\boldsymbol{\omega}_{(123)}) + K_{(12)^{[1]}(3)^{[3]}}(\boldsymbol{\omega}_{(123)}).$$

The first term corresponds to the tuples $\overline{I} = (1)$ and $\overline{I}^c = (23)$ yielding the original permutation $p = (123)$. The second term corresponds to the tuples $\overline{I} = (12)$ and $\overline{I}^c = (3)$ again yielding the original permutation $p = (123)$. However, since the first and the second term are proportional to $\hat\delta(\omega_1)$ and $\hat\delta(\omega_2)$, they belong to G_1^{212} and G_{12}^{212}, respectively, and these are related to different AC functions. the first term belongs to the function G_1^{212} which will be related to a different AC function than the second one (which belongs to G_{12}^{212}). The other rows are generated analogously, enumerating all six possible permutations

$p = (\overline{123})$, the terms contributing to G_{12}^{212} have an "x" in the rightmost column. We have contributions from the permutations $p \in \{(123), (213), (312), (321)\}$. These can be written as combinations of permutations over the set $I_1 = \{1, 2\}$ giving $\overline{I}_1 = (12)$ or (21), and permutations over the set $I_2 \in \{3\}$ giving $\overline{I}_2 = (3)$. To obtain all contributions we construct the permutations $\overline{I}_1\overline{I}_2 \in \{(123), (213)\}$ and $\overline{I}_2\overline{I}_1 \in \{(312), (321)\}$. Together, they give the needed permutations $p \in \{(123), (213), (312), (321)\}$. Note that, for any permutation of the type $\overline{I}_1\overline{I}_2$ there is also the permutation $\overline{I}_2\overline{I}_1$ with interchanged order of the subtuples. The corresponding kernels $K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}}$ and $K_{\overline{I}_2^{[\eta_2]}\overline{I}_1^{[\eta_1]}}$ are equal, allowing us to combine the corresponding PSFs into an PSF anti-commutator according to Eq. (3.1.5).

Altogether, we have (for $\ell = 3$)

$$G^{212} = G_1^{212} + G_{12}^{212} \tag{3.1.7}$$

$$G_1^{212} = 2^{-\frac{1}{2}} \sum_{p_{\{1\}|\{2,3\}}} S_{[(1);(\overline{2}\,\overline{3})]_+} * K_{(1)^{[1]}(\overline{2}\,\overline{3})^{[3]}} \tag{3.1.8}$$

$$G_{12}^{212} = 2^{-\frac{1}{2}} \sum_{p_{\{1,2\}|\{3\}}} S_{[(\overline{1}\,\overline{2});(3)]_+} * K_{(\overline{1}\,\overline{2})^{[1]}(3)^{[3]}}. \tag{3.1.9}$$

3.1.2 Relation of $G^{[\eta_1\eta_2]}$ to AC functions

In the previous section we have expanded the correlator $G^{[\eta_1\eta_2]}$ into several contributions $G_{I_1}^{[\eta_1\eta_2]}$ each involving a PSF anti-commutator see (3.1.5). The latter can be converted into a PSF commutator using Eq. (2.2.5), thereby expressing $G_{I_1}^{[\eta_1\eta_2]}$ in terms of discontinuities $\Delta C_{I_1}^{[\eta_1\eta_2]}$ [cf. Eq. (2.3.10)]. Temporarily neglecting the caveat due to diverging statistical factors N_I we obtain

$$\begin{aligned} 2^{\ell/2-1}\, G_{I_1}^{[\eta_1\eta_2]}(\boldsymbol{\omega}) &= N_{I_1} \sum_{p_{I_1|I_2}} \left(S_{[\overline{I}_1;\overline{I}_2]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}} \right)(\boldsymbol{\omega}_{\overline{I}_1\overline{I}_2}) \\ &= N_{I_1}\, \Delta C_{I_1}^{[\eta_1][\eta_2]}(\boldsymbol{\omega}). \end{aligned} \tag{3.1.10}$$

The full correlator is thereby now a linear combination of AC functions

$$G^{[\eta_1\eta_2]}(\boldsymbol{\omega}) = \sum_{I_1 \in \mathcal{I}_1} G_{I_1}^{[\eta_1\eta_2]}(\boldsymbol{\omega}) = 2^{1-\ell/2} \sum_{I_1 \in \mathcal{I}_1} N_{I_1}\, \Delta C_{I_1}^{[\eta_1][\eta_2]}(\boldsymbol{\omega}). \tag{3.1.11}$$

It is also helpful to explicitly identify the needed discontinuities and the involved regions of analyticity. Due to the prescription for retarded kernels in Eq. (2.1.23) at least one of the two regions involved in the discontinuity $\Delta C^{\gamma^{[I,\pm]}} = C^{\gamma^+} - C^{\gamma^-}$ fulfills

$$\gamma_{\eta_1} > 0, \quad \gamma_{\eta_2} > 0, \quad \gamma_{j\neq\eta_i} < 0. \tag{3.1.12}$$

The only exception is $\ell = 2$, where there is no such region. However, the needed regions for $\ell = 2$ are trivial, such that we can disregard $\ell = 2$ for the present discussion. So,

these regions and adjacent discontinuities are needed for the construction of the correlator $G^{[\eta_1\eta_2]}$. For the 4-point correlator $G^{[12]}$ these are the central regions with arabic number (2.2) and neighboring regions in the second diagram of Fig. 2.3.

The very same AC functions $\Delta C_I^{[\eta_1][\eta_2]}$ which are needed in Eq. (3.1.11) are obtained by a kernel expansion of the combination $G^{[\eta_1]} - G^{[\eta_2]}$, following a derivation analogous to Sec. 3.1.1. This expansion leads to the relation

$$G^{[\eta_1]} - G^{[\eta_2]} = \sum_{I_1 \in \mathcal{I}_1} \Delta C_{I_1}^{[\eta_1][\eta_2]}(\boldsymbol{\omega}). \tag{3.1.13}$$

For 4p functions, this reproduces relation (4.20) given in Ref. [26]. Hence, we can understand the discontinuities $\Delta C_I^{[\eta_1][\eta_2]}$ to be the ones lying between the regions which correspond to $G^{[\eta_1]}$ and $G^{[\eta_2]}$.

The observations in Eqs. (3.1.11) to (3.1.13) allow us to give a simple prescription for obtaining the AC functions needed for $G^{[\eta_1\eta_2]}$:

1. First, identify the needed regions of analyticity. These are the regions for the retarded correlators $G^{[\eta_1]}$ and $G^{[\eta_2]}$ and the regions which fulfill Eq. (3.1.12).

2. Collect every discontinuity ΔC_I^{γ} between the regions for $G^{[\eta_1]}$ and $G^{[\eta_2]}$ and multiply them with the appropriate prefactor N_I. (Recall that the discontinuities are defined as $\Delta C_I^{\gamma} = C^{\gamma}|_{\gamma_I>0} - C^{\gamma}|_{\gamma_I<0}$.)

Example: Assuming that the MF correlator contains no anomalous parts, we next identify the AC functions which are needed for the construction of $G^{2211} = G^{[12]}$ (for $\ell = 4$). The possible choices for I_1, including $\eta_1 = 1$ but excluding $\eta_2 = 2$ are $\{\,1\,\}$, $\{\,13\,\}$, $\{\,14\,\}$ and $\{\,134\,\}$. Evaluating the sum in Eq. (3.1.11) gives

$$\begin{aligned} 2\,G^{[12]} &= N_1 \Delta C_1^{[1][2]} + N_{13} \Delta C_{13}^{[1][2]} + N_{14} \Delta C_{14}^{[1][2]} + N_{134} \Delta C_{134}^{[1][2]} \\ &= N_1 (C_{2.2}^{\mathrm{III}} - C_{1.2}) + N_{13} (C_{2.2}^{\mathrm{I}} - C_{2.2}^{\mathrm{II}}) + N_{14} (C_{2.2}^{\mathrm{II}} - C_{2.2}^{\mathrm{III}}) + N_{134} (C_{3.2} - C_{2.2}^{\mathrm{I}}). \end{aligned} \tag{3.1.14}$$

The needed AC functions are obtained according to the explanation at the end of Sec. 2.3.2. In total we can write the correlator $G^{[12]}$ (for $\ell = 4$) as a linear combination of AC functions with explicit labels for the regions according to Fig. 2.3.

3.1.3 Caveat: Analytic continuation of anomalous parts of the MF correlator

In the previous section we used the equilibrium condition via Eq. (2.2.5) allowing us to rewrite PSF anti-commutators in terms of PSF commutators. This enabled us to express the function $G_I^{[\mu\nu]}$ in terms of AC functions. However, we neglected a pathological case: the possible divergence of a statistical factor N_I for $\omega_I = 0$ and $\boldsymbol{\zeta}_I = 1$. Now we revisit the

proof for Eq. (2.2.5) and focus on the pathological case by considering a PSF proportional to $\delta(\omega_I')$, i.e. $S_{\overline{I}\,\overline{I}^c}(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c})' \propto \delta(\omega_I')$ and $\boldsymbol{\zeta}_I = 1$.

In this case we have to exclude the frequencies for which N_I diverges and we obtain the exact expression

$$S_{[\overline{I};\overline{I}^c]_+}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I}^c}) \times \delta(\omega_I - \omega_I') = \begin{cases} N_I S_{[\overline{I};\overline{I}^c]_-}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I}^c}) \times \delta(\omega_I - \omega_I'), & \text{for } \omega_I \neq 0, \\ S_{[\overline{I};\overline{I}^c]_+}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I}^c}) \times \delta(\omega_I - \omega_I'), & \text{for } \omega_I = 0. \end{cases}$$

The first line can be constructed from the regular part of the MF correlator according to the previous section. The second line cannot be obtained on the same way since the discontinuity yields zero. To obtain the second line one needs to remember that for $\boldsymbol{\zeta}_I = 1$ and $S_{\overline{I}\,\overline{I}^c}(\boldsymbol{\omega}'_{\overline{I}\,\overline{I}^c}) \propto \delta(\omega_I')$ the MF correlator additionally contains an anomalous part $\widehat{G}_I$ which was explicitly computed for $\ell = 3$ and $\ell = 4$. Its permutation expansion involves all permutations of the type $p = \overline{I}\,\overline{I}^c$ and $p = \overline{I}^c\overline{I}$. For both $p = \overline{I}\,\overline{I}^c$ and $p = \overline{I}^c\overline{I}$ the anomalous part of the MF kernel (see Eq. (2.1.12)) gives

$$\widehat{K}_{\overline{I}}(\boldsymbol{\Omega}_{\overline{I}\,\overline{I}^c}) = \widehat{K}_{\overline{I}^c}(\boldsymbol{\Omega}_{\overline{I}^c\overline{I}}) = -\frac{\beta}{2}\delta_{\Omega_I,0}\widetilde{K}(\boldsymbol{\Omega}_{\overline{I}})\widetilde{K}(\boldsymbol{\Omega}_{\overline{I}^c}),$$

with the abbreviation $\Omega_i = \mathrm{i}\omega_i - \omega_i'$. On the other hand, for the same permutations the KF kernel of $G_I^{[\mu\nu]}$ is (see Eq. (3.1.3))

$$K_{\overline{I}^{[\mu]}\overline{I}^{c\,[\nu]}}(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) = K_{\overline{I}^{c\,[\nu]}\overline{I}^{[\mu]}}(\boldsymbol{\omega}_{\overline{I}^c\overline{I}}) = -2\pi\mathrm{i}\delta(\omega_I)\widetilde{K}(\boldsymbol{\omega}_{\overline{I}}^{[\mu]})\widetilde{K}(\boldsymbol{\omega}_{\overline{I}^c}^{[\nu]}),$$

where the kernels $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}}^{[\mu]})$ and $\widetilde{K}(\boldsymbol{\omega}_{\overline{I}^c}^{[\nu]})$ are retarded with respect to μ and ν respectively. We conclude that the problematic terms of the KF correlator can be directly obtained from the corresponding anomalous MF correlator $\widehat{G}_{I_1}(\mathrm{i}\boldsymbol{\omega})$ by the replacement[1]

$$\beta\delta_{\omega_I,0} \quad \to \quad 4\pi\mathrm{i}\delta(\omega_I) \tag{3.1.15}$$

and analytic continuation of the kernels $\widetilde{K}(\boldsymbol{\Omega}_{\overline{I}})$ and $\overline{K}(\boldsymbol{\Omega}_{\overline{I}^c})$ to retarded kernels according to Eq. (2.1.29), yielding

$$\mathrm{i}\boldsymbol{\omega}_{\overline{I}} \to \boldsymbol{\omega}_{\overline{I}}^{[\mu]}, \quad \mathrm{i}\boldsymbol{\omega}_{\overline{I}^c} \to \boldsymbol{\omega}_{\overline{I}^c}^{[\nu]}. \tag{3.1.16}$$

Thereby we obtain a suitable analytic continuation of the anomalous part of the MF correlator

$$\widehat{G}_I(\mathrm{i}\boldsymbol{\omega}) \to \widehat{\Phi}_I(\boldsymbol{z}), \tag{3.1.17}$$

which has to be added to recover the full KF correlator. Hence, our previous result in Eq. (3.1.10) needs to be supplemented and the full formula for the construction of the KF function is

$$2^{\ell/2-1}\, G_{I_1}^{[\eta_1\eta_2]}(\boldsymbol{\omega}) = N_{I_1}\, \Delta C_{I_1}^{[\eta_1][\eta_2]}(\boldsymbol{\omega}) + \widehat{\Phi}_{I_1}(\hat{\boldsymbol{z}}), \tag{3.1.18}$$

where $\hat{\boldsymbol{z}}$ are the complex frequencies given by the analytic continuation according to Eq. (3.1.16). For some relevant cases ($\ell \in \{3, 4\}$) we have summarized in App. B for which correlators the analytic continuations of anomalous parts have to be included.

[1]This replacement might be surprising since a unity on the time domain yields $\beta\delta_{0,\omega}$ and $2\pi\mathrm{i}\delta(\omega)$ in the space of imaginary- and real-frequencies.

3.2 Construction of further functions

In previous sections we have seen that certain AC functions, namely analytic continuations of the regular part of the MF correlator C^γ and its discontinuities ΔC^γ_I, are used to construct the KF correlators $G^{[\eta_1\cdots\eta_\alpha]}$ with $\alpha \leq 2$. Now we want to provide more AC functions which are useful for the construction of KF correlators $G^{[\eta_1\cdots\eta_\alpha]}$ with $\alpha \leq 4$

The construction of these AC functions works by the very same principle as for ΔC^γ_I. In Sec. 2.3.2 we considered an arbitrary discontinuity at a branch cut $\mathcal{B}_I$ which divides the set $\{1,...,\ell\}$ in in two complementary subsets I and I^c. We found that we only have to consider permutations of the type $\overline{I}\,\overline{I^c}$ by summarizing the PSFs $S_{\overline{I}\,\overline{I}^c}$ and $S_{\overline{I}^c\overline{I}}$ with a PSF commutator $S_{[\overline{I};\overline{I}^c]_-}$. This works because the kernels for these permutations are equal up to a minus sign. Furthermore, the kernels factorize in two functions which can be analytically continued independently on I and I^c according to the prescription for retarded correlators.

Due to the factorization of the kernel (see Eq. (2.3.8)) in two functions that depend on complex frequencies of a single set (I or I^c) any discontinuity of ΔC^γ_I can only occur along a branch cut $\mathcal{B}_{I'}$ with either $I' \subsetneq I$ or $I' \subsetneq I^c$. For this discontinuity one can use the very same steps as in Eqs. (2.3.7)-(2.3.9). Thus, computing the discontinuity of ΔC^γ_I splits one of the sets I or I^c in smaller subsets. The kernel now factorizes in three regular kernels $\widetilde{K}(\boldsymbol{z}_{\overline{I}_b})$, with $b \in \{1,2,3\}$, which only depend on frequency arguments of the subset I_b and therefore can be analytically continued independently again. The PSFs can be summarized by a nested PSF commutator, e.g. $S_{[[\overline{I}_1;\overline{I}_2]_-;\overline{I}_3]_-}$, such that one only has to sum over permutations of the type $p = \overline{I}_1\overline{I}_2\overline{I}_3$. From each set I_b we can pick one index $\eta_b \in I_b$ and follow the prescription for analytic continuation to retarded kernels according to Eq. (2.1.29) such that on every subtuple $\overline{I}_b$ we obtain a retarded kernel $\overline{K}(\boldsymbol{\omega}^{[\eta_b]}_{\overline{I}_b})$.

Starting from $\alpha \geq 3$ it matters in which order the branch cuts are considered. Correspondingly, in the following definition of the discontinuities the order of the subscripts is important. We first exemplify this for $\alpha = 3$ and pick three complementary sets I_1, I_2 and I_3 with $\eta_b \in I_b$. Then we can construct the AC function

$$\Delta C^{[\eta_1][\eta_2][\eta_3]}_{I_1\cup I_2, I_1} = \sum_{p_{I_1|I_2|I_3}} S_{[[\overline{I}_1;\overline{I}_2]_-;\hat{I}_3]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}} \tag{3.2.1}$$

by first computing $\Delta C^\gamma_{I_1\cup I_2}$, then computing its discontinuities along $\mathcal{B}_{I_1}$ and lastly continuing each subtuple according to Eq. (2.1.29). Here the super-script $[\eta_1][\eta_2][\eta_3]$ makes it explicit that these are chosen as the $\eta_b \in I_b$ with respect to which the kernels $\widetilde{K}(\boldsymbol{\omega}^{[\eta_b]}_{\overline{I}_b})$ are retarded. The subscript $I_1 \cup I_2, I_1$ states in which order the branch cuts have to be considered. We can also construct

$$\Delta C^{[\eta_1][\eta_2][\eta_3]}_{I_1, I_2} = \sum_{p_{I_1|I_2|I_3}} S_{[\overline{I}_1;[\overline{I}_2;\overline{I}_3]_-]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}} \tag{3.2.2}$$

by first considering the branch cut $\mathcal{B}_{I_1}$ and then $\mathcal{B}_{I_2}$.

For these discontinuities it is again possible to make use of Eq. (2.2.5). Thereby, nested PSF anti-commutators can be turned into nested PSF commutators for $\alpha = 3$ by

$$\begin{aligned} S_{[\overline{I}_3;[\overline{I}_1;\overline{I}_2]_+]_+} * K &= N_{I_3} \cdot S_{[\overline{I}_3;[\overline{I}_1;\overline{I}_2]_+]_-} * K \\ &= -N_{I_3} \cdot \left(S_{[\overline{I}_2;[\overline{I}_1;\overline{I}_3]_-]_+} + S_{[\overline{I}_1;[\overline{I}_2;\overline{I}_3]_-]_+} \right) * K \\ &= -N_{I_3} \cdot \left(N_{I_2} \cdot S_{[\overline{I}_2;[\overline{I}_1;\overline{I}_3]_-]_-} + N_{I_1} \cdot S_{[\overline{I}_1;[\overline{I}_2;\overline{I}_3]_-]_-} \right) * K \\ &= -N_{I_3} \left(N_{I_2} \cdot \Delta C^{[\eta_2][\eta_1][\eta_3]}_{I_2,I_1} + N_{I_1} \cdot \Delta C^{[\eta_1][\eta_2][\eta_3]}_{I_1,I_2} \right) * K, \end{aligned} \tag{3.2.3}$$

where the kernels K are all equal to the retarded product kernel $K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}}(\boldsymbol{\omega}_{\overline{I}_1\overline{I}_2\overline{I}_3})$ defined in Eq. (2.1.30). For the second line one needs to make use of an (anti-)commutator identity which is easily checked by unfolding the nested (anti-)commutator. In the last line we expressed the nested PSF commutators in terms of AC functions Eq. (3.2.2).

For $\alpha = 4$ we e.g. obtain the discontinuities

$$\Delta C^{[\eta_1][\eta_2][\eta_3][\eta_4]}_{I_1,I_2,I_3} = \sum_{p_{I_1|I_2|I_3|I_4}} S_{[\overline{I}_1;[\overline{I}_2;[\overline{I}_3;\overline{I}_4]_-]_-]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}\overline{I}_4^{[\eta_4]}} \tag{3.2.4}$$

or

$$\Delta C^{[\eta_1][\eta_2][\eta_3][\eta_4]}_{I_1\cup I_2,I_1,I_3} = \sum_{p_{I_1|I_2|I_3|I_4}} S_{[[\overline{I}_1;I_2]_-;[\overline{I}_3;\overline{I}_4]_-]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}\overline{I}_4^{[\eta_4]}}. \tag{3.2.5}$$

We identify the regions of analyticity which correspond to certain discontinuities and exemplify this for $\ell = 3$ for which the regions of analyticity are depicted in Fig. 2.2. The function $\Delta C_1^{[1][3]}$ is a discontinuity along $\mathcal{B}_1$. There are two possible discontinuities along this branch cut. To pick the correct one, one needs to remember that e.g. $\Delta C_1^{[1][3]}$ splits the set $\{\omega_1, \omega_2, \omega_3\}$ into $\{\omega_1\}$ and $\{\omega_2, \omega_3\}$. For the subtuples (ω_2, ω_3) and (ω_3, ω_2) we need a kernel which is retarded with respect to ω_3. The corresponding complex frequency tuple is given by Eq. (2.1.29). Thus the two regions of analyticity must have a negative imaginary part for $\gamma_2 < 0$ and and a positive one for $\gamma_3 > 0$ which gives

$$\Delta C_1^{[1][3]} = G'^{[2]} - G^{[3]}.$$

For $\ell = 3$, the function $\Delta C_{1,2}^{[1][2][3]}$ is a discontinuity of ΔC_1^{γ} along $\mathcal{B}_2$. Thus we have to subtract the following discontinuities, yielding

$$\Delta C_{1,2}^{[1][2][3]} = \Delta C_1^{\gamma}|_{\gamma_2>0} - \Delta C_1^{\gamma}|_{\gamma_2<0} = G'^{[3]} - G^{[2]} + G^{[3]} - G'^{[2]}. \tag{3.2.6}$$

3.2.1 Construction of $G^{[\eta_1\eta_2\eta_3]}$

The correlators $G^{[\eta_1\eta_2\eta_3]}$ can be written in terms of AC functions, too. We pursue a similar strategy as for $G^{[\eta_1\eta_2]}$ by expanding the $G^{[\eta_1\eta_2\eta_3]}$ in terms of nested PSF (anti-)commutators with suitable kernels. By use of the equilibrium condition via Eq. (2.2.5) these can be related to nested PSF commutators which can be identified with AC functions. In

		kernel of $G^{[\eta_1\eta_2\eta_3]} - G^{[\eta_3]}$	
a)	$\mu_1 < \mu_2 < \mu_3$	$K^{[\hat{\eta}_1]} - K^{[\hat{\eta}_2]}$	$= K^{[\hat{\eta}_1\hat{\eta}_2]}$
b)	$\mu_3 < \mu_1 < \mu_2$	$-K^{[\hat{\eta}_2]} + K^{[\hat{\eta}_3]}$	$= -K^{[\hat{\eta}_2\hat{\eta}_3]}$
c)	$\mu_2 < \mu_3 < \mu_1$	$K^{[\hat{\eta}_1]} - 2K^{[\hat{\eta}_2]} + K^{[\hat{\eta}_3]}$	$= K^{[\hat{\eta}_1\hat{\eta}_2]} - K^{[\hat{\eta}_2\hat{\eta}_3]}$
d)	$\mu_2 < \mu_1 < \mu_3$	$K^{[\hat{\eta}_1]} - K^{[\hat{\eta}_2]}$	$= K^{[\hat{\eta}_1\hat{\eta}_2]}$
e)	$\mu_3 < \mu_2 < \mu_1$	$-K^{[\hat{\eta}_2]} + K^{[\hat{\eta}_3]}$	$= -K^{[\hat{\eta}_2\hat{\eta}_3]}$
f)	$\mu_1 < \mu_3 < \mu_2$	$K^{[\hat{\eta}_1]} - 2K^{[\hat{\eta}_2]} + K^{[\hat{\eta}_3]}$	$= K^{[\hat{\eta}_1\hat{\eta}_2]} - K^{[\hat{\eta}_2\hat{\eta}_3]}$

Table 3.2: General kernels of $G^{[\eta_1\eta_2\eta_3]} - G^{[\eta_3]}$ for different permutations. The indices $\mu_b = p^{-1}(\eta_b)$ are the positions of the indices η_b. Depending on their order we differentiate between six cases.

	p	kernel of $G^{222} - G^{112}$	
a)	(123)	$K^{[12]}$	$= +K_{(1)^{[1]}(23)^{[2]}}$
b)	(312)	$-K^{[23]}$	$= -K_{(31)^{[1]}(2)^{[2]}}$
c)	(231)	$K^{[12]} - K^{[23]}$	$= +K_{(2)^{[2]}(31)^{[3]}} - K_{(23)^{[3]}(1)^{[1]}}$
d)	(213)	$K^{[12]}$	$= +K_{(2)^{[2]}(13)^{[1]}}$
e)	(321)	$-K^{[23]}$	$= -K_{(32)^{[2]}(1)^{[1]}}$
f)	(132)	$K^{[12]} - K^{[23]}$	$= +K_{(1)^{[1]}(32)^{[3]}} - K_{(13)^{[3]}(2)^{[2]}}$

Table 3.3: Contributions to $G^{[123]} - G^{[3]}$ for different permutations.

the following we make repeated use of the kernel expansion (3.1.2). Due to the kernel expansion the problem is mostly reduced to the analytic continuation of 3p functions. The generalization to arbirary ℓp functions is explained at the end of this section.

Firstly, recall that the Keldysh kernels in Eq. (2.1.20) give

$$K^{[\hat{\eta}_1\hat{\eta}_2\hat{\eta}_3]} = K^{[\hat{\eta}_1]} - K^{[\hat{\eta}_2]} + K^{[\hat{\eta}_3]},$$

where we have $\hat{\eta}_1 < \hat{\eta}_2 < \hat{\eta}_3$ by definition. The indices $\mu_b = p^{-1}(\eta_b)$ are the positions of the indices η_b. To reuse the kernel expansion $K^{[\mu\nu]}$ according to Eq. (3.1.2) we have to subtract a retarded correlator from $G^{[\eta_1\eta_2\eta_3]}$. This is not problematic for the process of analytic continuation since a retarded correlator itself can be expressed as an AC function. In the following we choose to subtract $G^{[\eta_3]}$. The kernel of $G^{[\eta_3]}$ equals one of the kernels $K^{[\hat{\eta}_1]}, K^{[\hat{\eta}_2]}$ or $K^{[\hat{\eta}_3]}$. On the level of kernels, the effect of subtracting $G^{[\eta_3]}$ depends on the permutation. For instance, assume that in a permutation the indices appear in the order $\mu_1 < \mu_2 < \mu_3$. Then $\hat{\eta}_3$ is the position of η_3, such that for this permutation the function $G^{[\eta_1\eta_2\eta_3]} - G^{[\eta_3]}$ has the kernel $K^{[\hat{\eta}_1]} - K^{[\hat{\eta}_2]} = K^{[\hat{\eta}_1\hat{\eta}_2]}$. For the five remaining cases we have summarized the kernels in Table 3.2.

For these kernels we can now perform the split-up according to Eq. (3.1.2). Before we continue with the general construction, we first show the basic steps using the example of the 3p correlator G^{222}. Here each of the cases a)–f) exactly corresponds to one permutation of the three indices. We obtain the contributions in Table 3.3 .

	p	kernel of $G^{[123]} - G^{[3]}$
a)	(123)	$+K_{(1)^{[1]}(2)^{[2]}(3)^{[3]}} + K_{(1)^{[1]}(23)^{[3]}}$
b)	(312)	$+K_{(3)^{[3]}(1)^{[1]}(2)^{[2]}} - K_{(31)^{[3]}(2)^{[2]}}$
c)	(231)	$+K_{(2)^{[2]}(31)^{[3]}} + K_{(23)^{[3]}(1)^{[1]}}$
d)	(213)	$+K_{(2)^{[2]}(1)^{[1]}(3)^{[3]}} + K_{(2)^{[2]}(13)^{[3]}}$
e)	(321)	$+K_{(3)^{[3]}(2)^{[2]}(1)^{[1]}} - K_{(32)^{[3]}(1)^{[1]}}$
f)	(132)	$+K_{(1)^{[1]}(32)^{[3]}} - K_{(13)^{[3]}(2)^{[2]}}$

Table 3.4: Final version of contributions to $G^{[123]} - G^{[3]}$ for different permutations.

The contributions

$$S_{(123)} * K_{(1)^{[1]}(23)^{[2]}} + S_{(132)} * K_{(1)^{[1]}(32)^{[3]}} - S_{(231)} * K_{(23)^{[3]}(1)^{[1]}} - S_{(321)} * K_{(32)^{[2]}(1)^{[1]}}$$

are almost identical to an AC function[2]. To equate this with a discontinuity it would be necessary that the kernels taking frequencies from the subset $\{\omega_2, \omega_3\}$ are retarded with respect to the same frequency throughout all permutations, e.g. $\widetilde{K}(\boldsymbol{\omega}^{[3]}_{(23)})$. In the following we choose retardation with respect to index 3. To adjust the kernel for the permutation $p = (123)$ we expand the kernel

$$S_{(123)} * K_{(1)^{[1]}(23)^{[2]}} = S_{(123)} * \Bigg(\underbrace{K_{(1)^{[1]}(23)^{[2]}} - K_{(1)^{[1]}(23)^{[3]}}}_{\hat{\delta}(\omega_1)\widetilde{K}(\boldsymbol{\omega}^{[1]}_{(1)}) \times K^{[12]}(\boldsymbol{\omega}_{23})} + K_{(1)^{[1]}(23)^{[3]}} \Bigg),$$

where for $K^{[12]}(\boldsymbol{\omega}_{23})$ we can use the kernel expansion according to Eq. (3.1.2) yielding

$$S_{(123)} * K_{(1)^{[1]}(23)^{[2]}} = S_{(123)} * \Bigg(K_{(1)^{[1]}(2)^{[2]}(3)^{[3]}} + K_{(1)^{[1]}(23)^{[3]}} \Bigg).$$

By performing analogous manipulations for the other cases we obtain the result in Table 3.4. Now we can collect the contributions[2] for the AC function $\Delta C_1^{[1][3]}$ and for $\Delta C_2^{[2][3]}$. The remaining contributions form the nested PSF anti-commutator

$$\begin{aligned} &S_{(123)} * K_{(1)^{[1]}(2)^{[2]}(3)^{[3]}} + S_{(312)} * K_{(3)^{[3]}(1)^{[1]}(2)^{[2]}} + S_{(213)} * K_{(2)^{[2]}(1)^{[1]}(3)^{[3]}} + S_{(321)} * K_{(3)^{[3]}(2)^{[2]}(1)^{[1]}} \\ &= S_{[[[1;2]_+;3]_+} * K_{(1)^{[1]}(2)^{[2]}(3)^{[3]}}. \end{aligned}$$

In total, this yields the result

$$\begin{aligned} \sqrt{2}(G^{222} - G^{112}) = &\sum_{p_{\{1\}|\{2,3\}}} S_{[(1);(\overline{2}\,\overline{3})]_-} * K_{(1)^{[1]}(\overline{2}\,\overline{3})^{[3]}} + \sum_{p_{2|1,3}} S_{[(2);(\overline{2}\,\overline{3})]_-} * K_{(2)^{[2]}(\overline{2}\,\overline{3})^{[3]}} \\ &+ S_{[[[1;2]_+;3]_+} * K_{(1)^{[1]}(2)^{[2]}(3)^{[3]}}. \end{aligned} \tag{3.2.7}$$

[2]Compare with the discontinuity

$$\begin{aligned} \Delta C_1^{[1][3]} &= \sum_{p_{\{1\}|\{2,3\}}} S_{[(1);(\overline{2}\,\overline{3})]} * K_{(1)^{[1]}(\overline{2}\,\overline{3})^{[3]}} \\ &= S_{(123)} * K_{(1)^{[1]}(23)^{[3]}} + S_{(132)} * K_{(1)^{[1]}(3)^{[3]}} - S_{(231)} * K_{(23)^{[3]}(1)^{[1]}} - S_{(321)} * K_{(32)^{[3]}(1)^{[1]}}. \end{aligned}$$

Using the identity (3.2.3) one can express the last line in terms of AC functions (up to divergencies of statistical factors)

$$\sqrt{2}(G^{222} - G^{112}) = -N_3(N_1 \Delta C_{1,2}^{[1][2][3]} + N_2 \Delta C_{2,1}^{[2][1][3]}) + \Delta C_1^{[1][3]} + \Delta C_2^{[2][3]}. \tag{3.2.8}$$

Let us return to general ℓ. The only additional complication arises due to the further possibilities to split up the indices $\{1, ..., \ell\}$ in subsets according to the kernel expansion in Eq. (3.1.2). Performing steps analogous to those for $\ell = 3$ one obtains the general result

$$\begin{aligned} 2^{\ell/2-1} \left(G^{[\eta_1\eta_2\eta_3]} - G^{[\eta_3]}\right) = & \sum_{(I_1,I_2,I_3)\in\mathcal{I}_{123}} \sum_{p_{I_1|I_2|I_3}} S_{[[\overline{I}_1;\overline{I}_2]_+;\overline{I}_3]_+} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}} \\ & + \sum_{(I_1,I_3)\in\mathcal{I}_{13}} \sum_{p_{I_1|I_3}} S_{[\overline{I}_1;\overline{I}_3]_-} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_3^{[\eta_3]}} \\ & + \sum_{(I_2,I_3)\in\mathcal{I}_{23}} \sum_{p_{I_2|I_3}} S_{[\overline{I}_2;\overline{I}_3]_-} * K_{\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}} \end{aligned} \tag{3.2.9}$$

with $\mathcal{I}_{123} = \{(I_1, I_2, I_3) |\, \eta_1 \in I_1, \eta_2 \in I_2, \eta_3 \in I_3, I_b \cap I_{b'} = \emptyset \text{ for } b \neq b'\}$ being the set of all possibilities to split $\{1, ..., \ell\}$ into three sets, each of which contains one of the indices $\eta_b \in I_b$. The sets $\mathcal{I}_{13} = \{(I_1, I_3) |\, \eta_1 \in I_1,\ \eta_2, \eta_3 \in I_3,\ I_1 \cap I_3 = \emptyset\}$ and $\mathcal{I}_{23} = \{(I_2, I_3) |\, \eta_2 \in I_2,\ \eta_1, \eta_3 \in I_3,\ I_2 \cap I_3 = \emptyset\}$ are defined analogously.

The last two lines in Eq. (3.2.9) involve a PSF commutator and can thus be identified with the AC functions $\Delta C_{I_1}^{[\eta_1][\eta_3]}$ and $\Delta C_{I_2}^{[\eta_2][\eta_3]}$. The nested PSF anti-commutators in Eq. (3.2.9) have to be rewritten according to Eq. (3.2.3) to relate it to AC functions, giving

$$\sum_{p_{I_1|I_2|I_3}} S_{[[\overline{I}_1;\overline{I}_2]_+;\overline{I}_3]_+} * K_{\overline{I}_1^{[\eta_1]}\overline{I}_2^{[\eta_2]}\overline{I}_3^{[\eta_3]}} = -N_{I_3} \left(N_{I_1} \cdot \Delta C_{I_1,I_2}^{[\eta_1][\eta_2][\eta_3]} + N_{I_2} \cdot \Delta C_{I_2,I_1}^{[\eta_2][\eta_1][\eta_3]}\right). \tag{3.2.10}$$

The general result in Eq. (3.2.9) can be obtained by repeating the same steps as for $\ell = 3$. Another way to derive it is by repeatedly "inserting" additional arguments in the correlator. Including an additional argument with Keldysh index 1 does not fundamentally change the structure of the formula. In fact, one can infer the formula for $\ell+1$ arguments from the one for ℓ arguments. Permutations over $\ell+1$ arguments can be inferred from the permutations $(\overline{1}, ..., \overline{\ell})$ by inserting the new argument at any of the $\ell+1$ positions. For instance consider $\ell = 3$. The final version of the contributions to $G^{222} - G^{112}$ is in Table 3.4. Consider the contribution

$$S_{(123)} * K_{(1)^{[1]}(23)^{[3]}}.$$

We can systematically infer the corresponding contributions for $\ell = 4$ by inserting the 4 at any position. Due to the way in which index sets are split up by the kernel expansion according to Eq. (3.1.2) the contributions for permutations (4123), (1243) and (1234) are

$$S_{(4123)} * K_{(41)^{[1]}(23)^{[3]}} \quad + S_{(1243)} * K_{(1)^{[1]}(243)^{[3]}} \quad + S_{(1234)} * K_{(1)^{[1]}(234)^{[3]}},$$

such that the new contribution is simply the old one with the new index inserted corresponding to its position in the permutation. Only when the new index 4 is inserted at the *boundary* between two subtuples, i.e. in this case for (1423), one obtains two contributions,

$$S_{(1423)} * \Big(K_{(14)^{[1]}(23)^{[3]}} + K_{(1)^{[1]}(423)^{[3]}} \Big)$$

one for inserting 4 in the left subtuple and one for inserting it in the right subtuple. In total one obtains the above five contributions for $\ell = 4$. To infer the formula for $\ell + 1$ from the one for ℓ, we sum over all possibilities for inserting the new index into existing subtuples, above (1) and (23), and each subtuple is augmented by the new index 4 by inserting it at any possible position. (This holds for an arbitrary number of subtuples.) Now recall how permutations over $\ell + 1$ indices can be inferred from permutations over ℓ indices. Thereby, we obtain Eq. (3.2.9) for arbitrary ℓ by induction.

3.2.2 Construction of $G^{[\eta_1\eta_2\eta_3\eta_4]}$

Rewriting $G^{[\eta_1\eta_2\eta_3\eta_4]}$ follows the very same principles as for $G^{[\eta_1\eta_2\eta_3]}$. For the sake of brevity we only present the result for the most relevant case of $\ell = 4$. The generalization to $\ell > 4$ can be achieved analogously to the previous section. The result for $\ell = 4$ is

$$\begin{aligned}
2\,G^{2222} = &\sum_{p_{\{2,3,4\}|\{1\}}} S_{[(\overline{1}\,\overline{2}\,\overline{3});(1)]_+} * K_{(\overline{1}\,\overline{2}\,\overline{3})^{[4]}(1)^{[1]}} + \sum_{p_{\{1,3,4\}|\{2\}}} S_{[(\overline{1}\,\overline{2}\,\overline{3});(2)]_+} * K_{(\overline{1}\,\overline{2}\,\overline{3})^{[4]}(2)^{[2]}} \\
&+ \sum_{p_{\{1,2,4\}|\{3\}}} S_{[(\overline{1}\,\overline{2}\,\overline{3});(3)]_+} * K_{(\overline{1}\,\overline{2}\,\overline{3})^{[2]}(3)^{[3]}} + \sum_{p_{\{3,1,2\}|\{4\}}} S_{[(\overline{1}\,\overline{2}\,\overline{3});(4)]_+} * K_{(\overline{1}\,\overline{2}\,\overline{3})^{[3]}(4)^{[4]}} \\
&+ \sum_{p_{\{4\}|\{1,2\}|\{3\}}} S_{[[(4);(\overline{2}\,\overline{3})]_-;(3)]_+} * K_{(4)^{[4]}(\overline{2}\,\overline{3})^{[2]}(3)^{[3]}} + \sum_{p_{\{3\}|\{4,1\}|\{2\}}} S_{[[(3);(\overline{2}\,\overline{3})]_-;(2)]_+} * K_{(3)^{[3]}(\overline{2}\,\overline{3})^{[1]}(2)^{[2]}} \\
&+ \sum_{p_{\{1\}|\{2,3\}|\{4\}}} S_{[[(1);(\overline{2}\,\overline{3})]_-;(4)]_+} * K_{(1)^{[1]}(\overline{2}\,\overline{3})^{[3]}(4)^{[4]}} + \sum_{p_{\{2\}|\{3,4\}|\{1\}}} S_{[[(2);(\overline{2}\,\overline{3})]_-;(1)]_+} * K_{(2)^{[2]}(\overline{2}\,\overline{3})^{[4]}(1)^{[1]}} \\
&+ \sum_{p_{\{4\}|\{2\}|\{1,3\}}} S_{[[(4);(2)]_+;(\overline{3}\,\overline{4})]_-} * K_{(4)^{[4]}(2)^{[2]}(\overline{3}\,\overline{4})^{[3]}} + \sum_{p_{\{1\}|\{3\}|\{2,4\}}} S_{[[(1);(3)]_+;(\overline{3}\,\overline{4})]_-} * K_{(1)^{[1]}(3)^{[3]}(\overline{3}\,\overline{4})^{[4]}} \\
&+ \frac{(-2\pi\mathrm{i})^3}{2}\Big(S_{[[[1;2]_+;4]_-;3]_-} - S_{[[[1;2]_-;4]_-;3]_+} + S_{[[[4;1]_+;3]_-;2]_-} - S_{[[[4;1]_-;3]_-;2]_+} \\
&+ S_{[[[2;3]_+;1]_-;4]_-} - S_{[[[2;3]_-;1]_-;4]_+} + S_{[[[3;4]_+;2]_-;1]_-} - S_{[[[3;4]_-;2]_-;1]_+} \\
&+ S_{[[4;2]_+;[1;3]_+]_+} + S_{[[4;2]_+;[1;3]_-]_-} + S_{[[1;3]_+;[2;4]_+]_+} + S_{[[1;3]_+;[2;4]_-]_-} \Big).
\end{aligned} \tag{3.2.11}$$

For the expression in round brackets we evaluated the convolution with the kernel $K_{(1)^{[1]}(2)^{[2]}(3)^{[3]}} = \prod_{j=1}^{3} \hat{\delta}(\omega_j)$ for the sake of brevity. One can now rewrite the above expressions in terms

of AC functions which only contain nested PSF commutators. To do so one can use the following relations which are obtained by (anti-)commutator relations and repeated use of Eq. (2.2.5)

$$\begin{aligned} S_{[[[A;B]_+;C]_-;D]_-} =& S_{[[[A;C]_-;D]_-;B]_+} + S_{[[[B;C]_-;D]_-;A]_+} + S_{[[A;C]_-;[B;D]_-]_+} + S_{[[A;D]_-;[B;C]_-]_+} \\ =& - N_B S_{[[[A;C]_-;D]_-;B]_-} - N_A S_{[[[B;C]_-;D]_-;A]_-} \\ & + N_{AC} S_{[[A;C]_-;[B;D]_-]_-} + N_{AD} S_{[[A;D]_-;[B;C]_-]_-}, \end{aligned} \tag{3.2.12}$$

$$\begin{aligned} S_{[[A;B]_-;[C;D]_+]_-} =& S_{[[[A;B]_-;C]_-;D]_+} + S_{[[[A;B]_-;D]_-;C]_+} \\ =& - N_D S_{[[[A;B]_-;C]_-;D]_-} - N_C S_{[[[A;B]_-;D]_-;C]_-}, \end{aligned} \tag{3.2.13}$$

$$\begin{aligned} S_{[[A;B]_+;[C;D]_+]_+} =& N_{AB} \Big(S_{[[[A;B]_-;C]_-;D]_-} + S_{[[[A;B]_-;D]_-;C]_-} \\ & - 2 \cdot S_{[[[A;C]_-;B]_-;D]_-} - 2 \cdot S_{[[[A;D]_-;B]_-;C]_-} \\ & + N_{AC} S_{[[A;C]_-;[B;D]_+]_-} + N_{AD} S_{[[A;D]_-;[B;C]_+]_-} \\ & + N_{BC} S_{[[B;C]_-;[A;D]_+]_-} + N_{BD} S_{[[B;D]_-;[A;C]_+]_-} \Big). \end{aligned} \tag{3.2.14}$$

where $A, B, C, D \in \{1, ..., 4\}$. These (anti-)commutator relations can be checked explicitly by unfolding the the (anti-)commutators. Using the PSFs S_p as basis vectors the search for these relations is basically a problem which can be solved with linear algebra.

3.2.3 Caveat: Anomalous parts

Also for $\alpha = 3$ and $\alpha = 4$ we need to pay attention to the divergencies of the factors N_I. Similar to the case in Sec. 3.1.3 the divergencies indicate that these contributions can only be recovered by $\widehat{\Phi}_I$, the analytic continuation of the anomalous part $\widehat{G}_I$ of the MF correlator. There are different ways to expand the correlators which are all equivalent for the continuation of the regular MF correlator. However, for the anomalous parts we need to be cautious as we illustrate in the following example.

With Eq. (3.2.7) we have derived a formula to construct the function $G^{222} - G^{112}$ via analytic continuation. However, rewriting $S_{[[1,2]_+,3]_+}$ in terms of AC functions is problematic if $\mathcal{O}^3$ is a bosonic operator. When we apply Eq. (2.2.5) we have to exclude the point for which N_3 diverges and get

$$S_{[[1,2]_+,3]_+} = \begin{cases} -N_3 S_{[[1,2]_+,3]_-}, & \text{for } \omega_3 \neq 0, \\ S_{[[1,2]_+,3]_+}, & \text{for } \omega_3 = 0. \end{cases} \tag{3.2.15}$$

Using the AC function $\widehat{\Phi}_3$ we cannot reconstruct the second line since the discontinuities of AC functions only produce (nested) PSF commutators. This problem does not arise

if, instead, $\mathcal{O}^1$ is a bosonic operator. Then the divergence of N_1 in Eq. (3.2.7) has to be avoided and we get

$$S_{[1,[2,3]_-]_+} = \begin{cases} N_1 S_{[1,[2,3]_-]_-}, & \text{for } \omega_1 \neq 0, \\ S_{[1,[2,3]_-]_+}, & \text{for } \omega_1 = 0. \end{cases} \tag{3.2.16}$$

Here the second line can be constructed with $\widehat{\Phi}_1$, making use of the fact that the discontinuity of AC functions produces PSF commutators.

In the following section we see that the various Keldysh components of a correlator are not independent. For instance 4p correlators can all be expressed in terms of correlators $G^{[\eta_1 \cdots \eta_\alpha]}$ with $\alpha \leq 2$. Hence, the easiest way to obtain all Keldysh components of a 3p or 4p correlator via analytic continuation is by use of the continuation formulas for $\alpha \leq 2$ and then computing the remaining correlators via the fluctuation dissipation relations.

Chapter 4

Applications of the analytic continuation formula

In the previous chapter we have shown how KF correlators can be constructed from AC functions. Thereby we have derived formulas for particularly relevant cases of 3p and 4p functions. Our results do not rely on any assumptions about the nature of the operators or about the physical system (apart from equilibrium and time-translational invariance). In this chapter we apply the formulas to various cases. At first we use the known relations between KF correlators and AC functions to derive relations between the KF correlators, known as generalized fluctuation-dissipation relations (FDRs). In Sec. 4.2 we then transfer the known results to vertex functions. These describe the effective interaction between two particles and are obtained from certain 4p correlators. For this purpose we transform the correlators to the R/A basis [34] and use the previously found FDRs. Lastly, in Sec. 4.3 we consider the vertex contributions to susceptibilities. The computation of real-frequency susceptibilities has been analyzed by Eliashberg [13] who used the analytic continuation method to convert Matsubara sums into contour integrals. We then identify the KF functions which correspond to his vertex contributions and thereby enable transfering Eliashberg's arguments to the KF.

4.1 Generalized fluctuation-dissipation relations

Due to the double-contour technique an ℓ-point correlator in KF can carry 2^ℓ different tuples of Keldysh indices $\boldsymbol{k}$ (with $k_i \in \{1, 2\}$). One of them, $G^{[]} = 0$, is known to be always zero. Due to the equilibrium condition also the remaining correlators may not be independent. For $\ell = 2$ the corresponding relation is known as Fluctuation-Dissipation theorem. Generalized fluctuations-dissipation relations (FDRs) have been derived for $\ell \leq 4$ (see Refs. [12,33]) by employing further assumptions additional to the equilibrium condition and invariance under time-translation.

In the following we derive the FDRs for $\ell \leq 4$ without invoking additional assumptions. We deduce relations between Keldysh correlators $G^{\boldsymbol{k}}$ and the primed correlators $G'^{\boldsymbol{k}}$ defined

in Eq. (3.2.8). Thereby we reproduce the relations derived in Ref. [12], using that the primed is equal to the complex conjugated correlator for bosonic operators, i.e. $G'^{\boldsymbol{k}} = (G^{\boldsymbol{k}})^*$.[1] To find the analogous relation for fermionic operators one simply has to redefine the prefactors N_i according to Eq. (2.2.4). The FDRs hold for any correlator of bosonic and fermionic operators. The exchange symmetry is fully respected via the definition of the statistical factors N_I according to Eq. (2.2.4).

Our derivation of the FDRs makes use of the fact that KF correlators and primed KF correlators can be written as a linear combination of AC functions. For $\ell \leq 3$ the derivation of the FDRs is particularly simple because all regions of analyticity can be identified with retarded or advanced correlators (see Fig. 2.2). For $\ell \geq 4$ further regions of analyticity exist which do not directly correspond to KF correlators. In this case one needs to solve a set of linear equations to obtain the FDRs.

For the derivation of the FDRs we temporarily neglect the parts of the KF correlators which are retrieved from the anomalous part of the MF correlator (see Sec. 3.1.3). One can however include them afterwards and check that the FDRs still hold. One can also plug the spectral representation of the KF correlators into the FDR and check explicitly that they hold exactly up to frequencies for which the factors N_i in the FDR diverge. (This is a lengthy calculation which involves the use of the equilibrium condition according to Eq. (2.2.1) and has already been done by Haehl et al. in Ref. [24].) For the important case of 4p correlators with only fermionic operators there are no such divergencies since all N_i in the FDRs are tanh functions. For 2p correlators with bosonic operators or 3p correlators with one bosonic and two fermionic operators we can add the appropriate functions to obtain exact relations between the correlators. These are the analytic continuations of the anomalous parts $\widehat{\Phi}_I$. In App. B we have summarized the corresponding formulas for 3p and 4p correlators.

In the following we use some relations for the statistical factors N_I (see definition in Eq. (2.2.4)). The sum rules for tanh and coth give the relation

$$N_{ij} = \frac{1 + N_i N_j}{N_i + N_j}.$$

Together with frequency conservation, this leads to the relation

$$\prod_{i=1}^{\ell} (N_i + 1) = \prod_{i=1}^{\ell} (N_i - 1)$$

which can be proven iteratively [24].

4.1.1 FDRs for three-point functions

For 3p functions all AC functions correspond to retarded or advanced correlators, see Fig. 2.2. The correlators $G^{[\eta_1 \eta_2]}$ are expressed in terms of discontinuities by Eq. (3.1.11).

[1] As remarked after Eq. (2.1.28), another important case for which $G' = G^*$ holds, are Hamiltonians which are real functions of creation and annihilation operators or systems with special behavior under time reversal [33].

At the end of Sec. 2.3.2 we have explained how to identify the corresponding AC functions. This gives

$$G^{[12]} = N_{13}(G^{[1]} - G'^{[3]}) + N_1(G'^{[3]} - G^{[2]}), \tag{4.1.1}$$

$$G^{[13]} = N_3(G'^{[2]} - G^{[1]}) + N_1(G'^{[2]} - G^{[3]}), \tag{4.1.2}$$

$$G^{[23]} = N_3(G'^{[1]} - G^{[2]}) + N_2(G'^{[1]} - G^{[3]}). \tag{4.1.3}$$

Furthermore, we have expressed the correlator $G^{[123]}$ in terms of discontinuities in Eq. (3.2.8), giving

$$\begin{aligned} G^{[123]} - G^{[3]} &= \Delta C_1^{[1][3]} + \Delta C_2^{[2][3]} - N_3(N_1 \Delta C_{1,2}^{[1][2][3]} + N_2 \Delta C_{2,1}^{[2][1][3]}) \\ &= G'^{[2]} - G^{[3]} + G'^{[1]} - G^{[3]} \\ &\quad - N_3\big[N_1(G'^{[3]} - G^{[2]} + G^{[3]} - G'^{[2]}) + N_2(G'^{[3]} - G^{[1]} + G^{[3]} - G'^{[1]})\big] \\ &= (1 + N_2N_3)G'^{[1]} + (1 + N_1N_3)G'^{[2]} + (1 + N_1N_2)G'^{[3]} + N_2N_3G^{[1]} + N_1N_3G^{[2]} \\ &\quad + (N_1N_2 - 1)G^{[3]} \end{aligned} \tag{4.1.4}$$

In the second line we identified the AC functions which make up the discontinuities. This process has been exemplified in Eq. (3.2.6). In the last step we used the relation

$$1 + N_1N_2 + N_1N_3 + N_2N_3 = 0,$$

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

4.1.2 FDRs for four-point functions

For 4-point correlators there are several regions of analyticity which cannot be identified with a KF correlator. Unlike for $\ell \leq 3$ we thus cannot simply express any KF correlator in terms of retarded and advanced correlators. Our strategy for $\ell = 4$ relies on the comparison of the AC functions with which KF correlators can be constructed. By writing a correlator as a linear combination of AC functions it can be represented by a vector for which the AC functions serve as the basis vectors $\hat{\mathbf{e}}_i$. Thereby we are able to find relations between KF correlators by solving linear equations. We demonstrate this method with the example of the KF correlators $G^{[12]}$, $G^{[123]}$ and $G^{[1234]}$. The FDRs for 4p correlators of fermionic operators are summarized in Eqs. (B.2.3) and (B.2.3).

It is sufficient to choose the discontinuities of AC functions ΔC_I^{γ} as basis vectors since the construction of all correlators (except for $G^{[\eta]}$ and $G'^{[\eta]}$) has been performed with the discontinuities ΔC_I^{γ}. In Fig. 4.1 we depict the discontinuities with short arrows which are enumerated according to the basis vectors $\hat{\mathbf{e}}_i$, such that e.g. $\hat{\mathbf{e}}_1 = \Delta C_{124}^{[2][3]}$. Note that every region of analyticity and hence every AC function ΔC_I^{γ} has a counterpart which is related to it by conjugation of the complex frequencies $\Delta C'^{\gamma}_I = -\Delta C_I^{-\gamma}$.

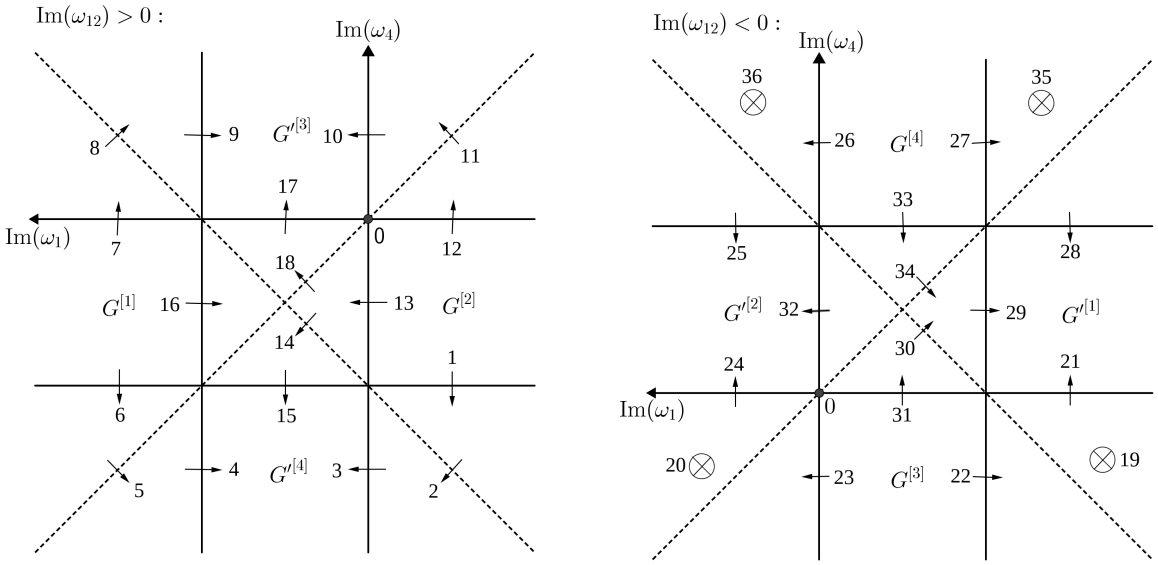

Figure 4.1: Regions of analyticity of four-point correlators: The 36 distinct discontinuities ΔC_I^γ are indicated by short arrows. For the derivation of FDRs they are used as basis vectors $\hat{\mathbf{e}}_i$ with $1 \leq i \leq 36$. In the diagram the index i for $\hat{\mathbf{e}}_i$ is placed next to the corresponding discontinuity.

We exemplify the derivation of an FDR first with $G^{[12]}$. By Eq. (3.1.14) we have

$$\begin{aligned} G^{[12]} &= N_1 \Delta C_1^{[1][2]} + N_{13} \Delta C_{13}^{[1][2]} + N_{14} \Delta C_{14}^{[1][2]} + N_{134} \Delta C_{134}^{[1][2]} \\ &= -N_1 \hat{\mathbf{e}}_{13} - N_{13} \hat{\mathbf{e}}_{14} - N_{14} \hat{\mathbf{e}}_{18} - N_2 \hat{\mathbf{e}}_{16}. \end{aligned} \tag{4.1.5}$$

These discontinuities are the ones adjacent to the regions labeled by the arabic numbers (2.2) in Fig. 2.3. Thus, we may expect to find a relation to the correlator $G'^{[34]}$ since the regions labeled by (4.4) are the complex conjugates to these. We find

$$\begin{aligned} G'^{[34]} &= N_3 \Delta C'^{[3][4]}_3 + N_{31} \Delta C'^{[3][4]}_{31} + N_{32} \Delta C'^{[3][4]}_{32} + N_{321} \Delta C'^{[3][4]}_{321} \\ &= N_3 \Delta C'^{[3][4]}_3 - N_{31} \Delta C_{31}^{[1][2]} + N_{32} \Delta C_{14}^{[1][2]} + N_{321} \Delta C'^{[3][4]}_{321} \\ &= N_3 \hat{\mathbf{e}}_{15} + N_{13} \hat{\mathbf{e}}_{14} + N_{14} \hat{\mathbf{e}}_{18} + N_4 \hat{\mathbf{e}}_{17}. \end{aligned} \tag{4.1.6}$$

The retarded and advanced correlators are represented by the basis ΔC_I^γ via

$$\begin{aligned} G^{[1]} - G'^{[3]} &= -\hat{\mathbf{e}}_{14} + \hat{\mathbf{e}}_{16} + \hat{\mathbf{e}}_{17}, \\ G^{[1]} - G'^{[4]} &= \hat{\mathbf{e}}_{15} + \hat{\mathbf{e}}_{16} - \hat{\mathbf{e}}_{18}, \\ G^{[2]} - G'^{[3]} &= \hat{\mathbf{e}}_{13} + \hat{\mathbf{e}}_{17} + \hat{\mathbf{e}}_{18}. \end{aligned}$$

Thus the problem is reduced to the linear algebra problem of finding a solution $\boldsymbol{x}$ to

$$\begin{pmatrix} -N_1 \\ -N_{13} \\ 0 \\ -N_2 \\ 0 \\ -N_{14} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ N_{13} & -1 & 0 & 0 \\ N_3 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ N_4 & 1 & 0 & 1 \\ N_{14} & 0 & -1 & 1 \end{pmatrix} \boldsymbol{x},$$

where the vector on the left represents $G^{[12]}$ according to Eq. (4.1.5) and the columns of the matrix represent the functions $\widetilde{G}^{[34]}$, $G^{[1]} - G'^{[3]}$, $G^{[1]} - G'^{[4]}$ and $G^{[2]} - G'^{[3]}$. One finds the solution

$$\boldsymbol{x}^T = \left(N^{(12)}_{(34)}, N^{(12)}_{(34)} N_3 - N_2, -N^{(12)}_{(34)} N_3, -N_1 \right)$$

with $N^{(ij)}_{(kl)} = \frac{N_i + N_j}{N_k + N_l}$. To see that this is indeed a solution one has to convince oneself that the equations

$$N_{13} = N^{(12)}_{(34)}(-N_{13} + N_3) - N_2, \qquad \text{and} \qquad N_{14} = N^{(12)}_{(34)}(-N_{14} - N_3) + N_1,$$

hold which can be checked using the properties of hyperbolic functions and frequency conservation. After regrouping the prefactors one obtains

$$G^{[12]} = -N_2 G^{[1]} - N_1 G^{[2]} + N^{(12)}_{(34)} \left(N_4 G'^{[3]} + N_3 G'^{[4]} + G'^{[34]} \right),$$

which agrees with the result in [12].

To obtain FDRs for $G^{[234]} - G^{[2]}$ or $G^{[1234]}$ we can again write them in terms of discontinuities ΔC^{γ}_I, yielding the rather lengthy expressions

$$\begin{aligned} G^{[234]} - G^{[2]} = &-\hat{\mathbf{e}}_1 - \hat{\mathbf{e}}_2 - \hat{\mathbf{e}}_{12} - \hat{\mathbf{e}}_{11} + N_{12}[N_3(\hat{\mathbf{e}}_{28} - \hat{\mathbf{e}}_1) + N_4(\hat{\mathbf{e}}_{21} - \hat{\mathbf{e}}_{12})] \\ &+ N_2[N_{13}(-\hat{\mathbf{e}}_2 - \hat{\mathbf{e}}_{30}) + N_4(-\hat{\mathbf{e}}_{21} + \hat{\mathbf{e}}_{31})] + N_2[N_3(\hat{\mathbf{e}}_{33} - \hat{\mathbf{e}}_{28}) + N_{14}(-\hat{\mathbf{e}}_{34} - \hat{\mathbf{e}}_{11})], \end{aligned}$$

and

$$\begin{aligned} &G^{[1234]} \\ &= [N_{13}(1 + N_{12}N_3)]\hat{\mathbf{e}}_1 + [N_{13} - N_1(1 + N_{12}N_{13})]\hat{\mathbf{e}}_3 + [N_{13}(-N_{12} + N_{14})N_2]\hat{\mathbf{e}}_4 - [N_{14}]\hat{\mathbf{e}}_5 \\ &\quad + [N_3 - N_{13}(2 + N_{12}N_3 + N_{14}N_3)]\hat{\mathbf{e}}_6 - [N_{12}N_{13}N_4]\hat{\mathbf{e}}_7 + [N_2(-1 + N_{12}N_{13})]\hat{\mathbf{e}}_9 \\ &\quad + [N_{13}(-2 + N_1(N_{12} + N_{14}))]\hat{\mathbf{e}}_{10} + [N_{14}]\hat{\mathbf{e}}_{11} + [N_4(1 + N_{12}N_{13} - N_{13}N_{14})]\hat{\mathbf{e}}_{12} \\ &\quad + [N_{13} - N_1 N_{13} N_{14}]\hat{\mathbf{e}}_{13} + [N_{13} - N_3 + N_{13}N_{14}N_3]\hat{\mathbf{e}}_{15} - [N_{13}N_{14}N_2]\hat{\mathbf{e}}_{16} \\ &\quad + [N_4(-1 + N_{13}N_{14})]\hat{\mathbf{e}}_{17} - [N_{14}]\hat{\mathbf{e}}_{18} + [N_{12}]\hat{\mathbf{e}}_{19} - [N_{12}]\hat{\mathbf{e}}_{20} - [N_4(1 + N_{12}N_{13})]\hat{\mathbf{e}}_{21} \\ &\quad + [N_{12}N_{13}N_2]\hat{\mathbf{e}}_{22} + [N_1 - 2N_{13} + N_{13}N_1(N_{12} + N_{14})]\hat{\mathbf{e}}_{23} + [N_{13}N_4(N_{12} - N_{14})]\hat{\mathbf{e}}_{24} \\ &\quad + [-N_3 + N_{13}(1 + N_{12}N_3)]\hat{\mathbf{e}}_{25} + [N_{13} - N_1 N_{12} N_{13}]\hat{\mathbf{e}}_{26} + [N_2(1 - N_{12}N_{13} + N_{13}N_{14})]\hat{\mathbf{e}}_{27} \\ &\quad - [N_{13}(2 + N_{12}N_3 + N_{14}N_3)]\hat{\mathbf{e}}_{28} - [N_2(1 + N_{13}N_{14})]\hat{\mathbf{e}}_{29} + [N_{13}N_{14}N_4]\hat{\mathbf{e}}_{31} \\ &\quad + [N_{13} - N_1(1 + N_{13}N_{14})]\hat{\mathbf{e}}_{32} + [N_{13}(1 + N_{14}N_3)]\hat{\mathbf{e}}_{33} + N_{14}\hat{\mathbf{e}}_{34} - N_{12}\hat{\mathbf{e}}_{35} + N_{12}\hat{\mathbf{e}}_{36}. \end{aligned}$$

These can be expressed in terms of $G^{[\eta_1\eta_2]}$ and $(G^{[\eta_1]} - G'^{[\eta_2]})$. Note that the latter objects each have different representations in terms of $\hat{\mathbf{e}}_i$ (corresponding to different paths between $G^{[\eta_1]}$ and $G'^{[\eta_2]}$). We can hence set up a matrix equation analogously to the one for $G^{[12]}$, using

$$\begin{aligned}
G^{[1]} - G'^{[2]} &= \hat{\mathbf{e}}_6 + \hat{\mathbf{e}}_{20} + \hat{\mathbf{e}}_{24} = \hat{\mathbf{e}}_7 + \hat{\mathbf{e}}_{36} + \hat{\mathbf{e}}_{25},\\
G^{[1]} - G'^{[3]} &= -\hat{\mathbf{e}}_{14} + \hat{\mathbf{e}}_{16} + \hat{\mathbf{e}}_{17} = \hat{\mathbf{e}}_7 + \hat{\mathbf{e}}_8 + \hat{\mathbf{e}}_9,\\
G^{[1]} - G'^{[4]} &= \hat{\mathbf{e}}_{15} + \hat{\mathbf{e}}_{16} - \hat{\mathbf{e}}_{18} = \hat{\mathbf{e}}_4 + \hat{\mathbf{e}}_5 + \hat{\mathbf{e}}_6,\\
G^{[2]} - G'^{[1]} &= \hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_{19} + \hat{\mathbf{e}}_{21} = \hat{\mathbf{e}}_{12} + \hat{\mathbf{e}}_{35} + \hat{\mathbf{e}}_{28},\\
G^{[2]} - G'^{[3]} &= \hat{\mathbf{e}}_{13} + \hat{\mathbf{e}}_{17} + \hat{\mathbf{e}}_{18} = \hat{\mathbf{e}}_{10} + \hat{\mathbf{e}}_{11} + \hat{\mathbf{e}}_{12},\\
G^{[2]} - G'^{[4]} &= \hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2 + \hat{\mathbf{e}}_3 = \hat{\mathbf{e}}_{13} + \hat{\mathbf{e}}_{14} + \hat{\mathbf{e}}_{15},\\
G^{[3]} - G'^{[1]} &= \hat{\mathbf{e}}_{22} - \hat{\mathbf{e}}_2 + \hat{\mathbf{e}}_{21} = \hat{\mathbf{e}}_{31} + \hat{\mathbf{e}}_{30} + \hat{\mathbf{e}}_{29},\\
G^{[3]} - G'^{[2]} &= \hat{\mathbf{e}}_{23} - \hat{\mathbf{e}}_5 + \hat{\mathbf{e}}_{24} = \hat{\mathbf{e}}_{31} - \hat{\mathbf{e}}_{34} + \hat{\mathbf{e}}_{32},\\
G^{[3]} - G'^{[4]} &= \hat{\mathbf{e}}_{22} - \hat{\mathbf{e}}_{19} + \hat{\mathbf{e}}_3 = \hat{\mathbf{e}}_{23} - \hat{\mathbf{e}}_{20} + \hat{\mathbf{e}}_4,\\
G^{[4]} - G'^{[1]} &= -\hat{\mathbf{e}}_{11} + \hat{\mathbf{e}}_{27} + \hat{\mathbf{e}}_{28} = \hat{\mathbf{e}}_{29} + \hat{\mathbf{e}}_{33} + \hat{\mathbf{e}}_{34},\\
G^{[4]} - G'^{[2]} &= \hat{\mathbf{e}}_{26} - \hat{\mathbf{e}}_8 + \hat{\mathbf{e}}_{25} = \hat{\mathbf{e}}_{33} - \hat{\mathbf{e}}_{30} + \hat{\mathbf{e}}_{32},\\
G^{[4]} - G'^{[3]} &= \hat{\mathbf{e}}_{27} - \hat{\mathbf{e}}_{35} + \hat{\mathbf{e}}_{10} = \hat{\mathbf{e}}_{26} - \hat{\mathbf{e}}_{36} + \hat{\mathbf{e}}_9,\\
G^{[12]} &= -N_1\hat{\mathbf{e}}_{13} - N_{13}\hat{\mathbf{e}}_{14} - N_{14}\hat{\mathbf{e}}_{18} - N_2\hat{\mathbf{e}}_{16},\\
G^{[34]} &= -N_4\hat{\mathbf{e}}_{31} - N_3\hat{\mathbf{e}}_{33} + N_{13}\hat{\mathbf{e}}_{30} + N_{14}\hat{\mathbf{e}}_{34},\\
G^{[13]} &= -N_3\hat{\mathbf{e}}_6 - N_1\hat{\mathbf{e}}_{23} + N_{14}\hat{\mathbf{e}}_5 + N_{12}\hat{\mathbf{e}}_{20},\\
G^{[24]} &= -N_4\hat{\mathbf{e}}_{12} - N_2\hat{\mathbf{e}}_{27} - N_{14}\hat{\mathbf{e}}_{11} + N_{12}\hat{\mathbf{e}}_{35},\\
G^{[14]} &= -N_4\hat{\mathbf{e}}_7 - N_1\hat{\mathbf{e}}_{26} + N_{13}\hat{\mathbf{e}}_8 + N_{12}\hat{\mathbf{e}}_{36},\\
G^{[23]} &= -N_3\hat{\mathbf{e}}_1 - N_2\hat{\mathbf{e}}_{22} - N_{13}\hat{\mathbf{e}}_2 + N_{12}\hat{\mathbf{e}}_{19}.
\end{aligned}$$

This linear algebra problem can be solved to find

$$\begin{aligned}
G^{[234]} = (1 + N_2N_4 + N_2N_3 + N_3N_4)G'^{[1]} - N_3N_4G^{[2]}\\
- N_2N_4G^{[3]} - N_2N_3G^{[4]} - N_4G^{[23]} - N_3G^{[24]} - N_2G^{[34]}
\end{aligned}$$

and

$$\begin{aligned}
G^{[1234]} = {} & 2N_2N_3N_4G^{[1]} + (N_2N_3N_4 + N_2 + N_3 + N_4)G'^{[1]}\\
& + 2N_1N_3N_4G^{[2]} + (N_1N_3N_4 + N_1 + N_3 + N_4)G'^{[2]}\\
& + 2N_1N_2N_4G^{[3]} + (N_1N_2N_4 + N_1 + N_2 + N_4)G'^{[3]}\\
& + 2N_2N_3N_4G^{[4]} + (N_1N_2N_3 + N_1 + N_2 + N_3)G'^{[4]}\\
& + N_3N_4G^{[12]} + N_2N_4G^{[13]} + N_2N_3G^{[14]} + N_1N_4G^{[23]} + N_1N_3G^{[24]} + N_1N_2G^{[34]},
\end{aligned}$$

which agrees with the result in Ref. [12].

4.2 Vertex functions and the R/A basis

So far we have never specified the operators $\boldsymbol{\mathcal{O}} = (\mathcal{O}^1, ..., \mathcal{O}^\ell)$ in the correlators. In this section we choose them to be creation and annihilation operators and focus on vertex functions F which describe the effective interaction between two particles. Based on our knowledge about 2p and 4p correlators we can now infer the formulas for the analytic continuation of vertex functions. We find that vertex functions have the same regions of analyticity as correlators, the same FDRs and the Keldysh components can be constructed with the same linear combinations of AC functions as for correlators. We find that for KF functions the R/A basis, derived in Refs. [34, 35], is particularly convenient to work with. In this basis every component can be expressed with a small number of AC functions.

The propagation of a single particle is described by the 2p correlator (*propagator*) defined by

$$G_\sigma^{k_1 k_2}(t_1, t_2) = -\mathrm{i}\langle \mathcal{T}_c d_\sigma(t_1^{k_1}) d_\sigma^\dagger(t_2^{k_2})\rangle. \tag{4.2.1}$$

where the operators $d_\sigma^\dagger$ and d_σ are creation and annihilation operators specified by the index σ. Typically σ is a spin ($\uparrow$ or $\downarrow$) as e.g. in our calculations on the Hubbard atom in Sec. 5, and position or momentum. In the following we first focus on 4p functions with solely outgoing particles[2] defined by

$$G_{\sigma_1\sigma_2\sigma_3\sigma_4}^{k_1 k_2 k_3 k_4}(\boldsymbol{t}) = (-\mathrm{i})^3 \langle \mathcal{T}_c d_{\sigma_1}(t_1^{k_1}) d_{\sigma_2}(t_2^{k_2}) d_{\sigma_3}(t_3^{k_3}) d_{\sigma_4}(t_4^{k_4})\rangle. \tag{4.2.2}$$

It consists of a disconnected and a connected part, $G = G_{\mathrm{dis}} + G_{\mathrm{con}}$. The disconnected part $G_{\mathrm{dis}}^{\boldsymbol{k}}$ contains all the "factorizations" of the 4p correlator in propagators such as $(-\mathrm{i})^3 \langle \mathcal{T}_c d_{\sigma_1}(t_1^{k_1}) d_{\sigma_2}(t_2^{k_2})\rangle \langle \mathcal{T}_c d_{\sigma_3}(t_3^{k_3}) d_{\sigma_4}(t_4^{k_4})\rangle$ as they are obtained by Wick's theorem for non-interacting particles. It corresponds to the independent propagation of particles without mutual scattering. Note that the disconnected part contributes to the anomalous part in the MF. It can be analytically continued to the KF, based on the well-known continuation of 2p functions.

The connected part of the 4p correlator G_{con} is associated with the effective two-particle interaction. The corresponding vertex function F is given by factorizing out four propagators [11] (henceforth hiding the indices σ_i again)

$$G_{\mathrm{con}}^{k_1 k_2 k_3 k_4}(\boldsymbol{\omega}) = \left[\prod_{i=1}^{4} G^{k_i k_i'}(\omega_i)\right] F^{k_1' k_2' k_3' k_4'}(\boldsymbol{\omega}), \tag{4.2.3}$$

where summation over the doubly occurring indices k_i' is implied. These four propagators $G^{k_i k_i'}(\omega_i)$ are called *external legs* in a diagrammatic language.[3] For solely outgoing legs they are all on the left of the vertex function.

[2] see below for incoming particles

[3] We denote the 2-point correlators $G^{k_i k_i'}(\omega_i)$ solely by the frequency argument of the first operator. See Fig. 5.1 for a diagrammatic representation of the disconnected and connected part of the 4p correlator of the Hubbard atom.

Since we concentrate on outgoing legs, all 2-point correlators $G^{k_i k_i'}$ are on the left of F. The Keldysh components are summarized in the matrix

$$G(\omega) = \begin{pmatrix} 0 & G^A(\omega) \\ G^R(\omega) & G^K(\omega) \end{pmatrix} = \begin{pmatrix} G^{11}(\omega) & G^{12}(\omega) \\ G^{21}(\omega) & G^{22}(\omega) \end{pmatrix}, \tag{4.2.4}$$

where the retarded and advanced correlators (G^R and G^A) can be obtained from the MF correlator by

$$G^{R/A}(\omega_i) = G(\mathrm{i}\omega_i)|_{\mathrm{i}\omega_i \to \omega_i \pm \mathrm{i}0^+}, \qquad G^K(\omega_i) = N_i[G^R(\omega_i) - G^A(\omega_i)].$$

The FDT for the Keldysh component holds true up to an anomalous contribution in MF. It has to be considered for bosonic operators and corresponds to a constant in the time domain. However, for fermionic creation and annihilation operators such an anomalous part cannot exist.

To obtain the vertex function from the connected part of the correlator $G^{\boldsymbol{k}}_{\mathrm{con}}$ one has to amputate the external legs, i.e. the latter needs to be multiplied with the inverse of the propagators $G^{k_i k_i'}$. Since the propagator is a non-diagonal matrix, this can yield an abundance of summands for certain vertex components in the Keldysh basis. It is therefore convenient to switch to the R/A basis according to Refs. [34,35] in which the 2p correlator in KF assumes a diagonal form

$$Q(\omega_i)G(\omega_i)P^{-1}(\omega_i) = \begin{pmatrix} N_i & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & G^A \\ G^R & G^K \end{pmatrix} \begin{pmatrix} 1 & N_i \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} G^R & 0 \\ 0 & G^A \end{pmatrix} (\omega_i). \tag{4.2.5}$$

Correspondingly, the transformation into the R/A basis with $\Lambda_i \in \{R, A\}$ is performed with the matrices $Q(\omega_i)$ for correlators and with $P(\omega_i)$ for vertex functions by

$$G^{\boldsymbol{\Lambda}} = \sum_{\boldsymbol{k}} \left[\prod_{i=1}^{\ell} Q^{\Lambda_i k_i}(\omega_i) \right] G^{\boldsymbol{k}}, \tag{4.2.6}$$

$$F^{\boldsymbol{\Lambda}} = \sum_{\boldsymbol{k}} \left[\prod_{i=1}^{\ell} P^{\Lambda_i k_i}(\omega_i) \right] F^{\boldsymbol{k}}. \tag{4.2.7}$$

Some correlators in the R/A basis are e.g.

$$G^{AAAA} = 0, \tag{4.2.8}$$

$$G^{RAAA} = -G^{[1]}, \tag{4.2.9}$$

$$G^{RRAA} = G^{[12]} + N_1 G^{[2]} + N_2 G^{[1]}, \tag{4.2.10}$$

$$G^{RRRA} = -G^{[123]} - N_1 G^{[23]} - N_2 G^{[13]} - N_3 G^{[12]} - N_1 N_2 G^{[3]} - N_1 N_3 G^{[2]} - N_2 N_3 G^{[1]} \tag{4.2.11}$$

Wang et al. explicitly showed in Ref. [12] that the FDRs for $\ell \leq 4$ are equivalent to the relation

$$G^{\boldsymbol{\Lambda}} = G'^{\overline{\boldsymbol{\Lambda}}} \cdot \frac{\prod\limits_{\Lambda_i = R} (N_i + 1)}{\prod\limits_{\Lambda_i = A} (N_i - 1)} (-1)^{\ell - 1}, \tag{4.2.12}$$

which was derived in Ref. [35] on the basis of diagrammatic rules. Here the bar over $\overline{\mathbf{\Lambda}}$ indicates conjugation of the R/A index, such that $\overline{R} = A$ and vice versa. From this, it follows that $G^{RRRR} \propto G^{AAAA} = 0$. Moreover, the expression for the component

$$G^{RRRA} = (1 + N_1N_2 + N_1N_3 + N_2N_3)G'^{AAAR} = -(1 + N_1N_2 + N_1N_3 + N_2N_3)G'^{[4]} \tag{4.2.13}$$

simplifies tremendously. It can be expressed in terms of the advanced correlator $G'^{[4]}$ which directly corresponds to an AC function. For the correlators with two R's and two A's, consider for instance the correlator G^{RRAA} which we expressed in the Keldysh basis in Eq. (4.2.10). By construction of $G^{[12]}$ (see Eq. (3.1.14)) the AC functions $C_{2.2}^{\text{I-IV}}$, $C_{3.2}$ and $C_{1.2}$ are involved. The latter two correspond to the correlators $G^{[1]}$ and $G^{[2]}$ and are exactly canceled in G^{RRAA}, giving

$$G^{RRAA} = N_4(C_{2.2}^{\text{II}}) + N_{23}(C_{2.2}^{\text{II}} - C_{2.2}^{\text{III}}) + N_{13}(C_{2.2}^{\text{III}} - C_{2.2}^{\text{IV}}) + N_3(C_{2.2}^{\text{IV}}),$$

where we left out the anomalous parts for brevity[4]. Hence, this KF component can be expressed with three AC functions (plus anomalous parts). Other KF compoents can be expressed with a single AC function [see Eqs. (4.2.9) and (4.2.13)]. For comparison, in the Keldysh basis the correlators $G^{[\eta_1\cdots\eta_\alpha]}$ with $\alpha \geq 3$ involve a complicated linear combination of AC functions.

Observe that in the R/A basis the involved regions of analyticity of the 4p correlator $G^{\Lambda_1\Lambda_2\Lambda_3\Lambda_4}$ are consistent with the analytic continuation of the external legs. By choice of a KF component in the R/A basis the analytic continuation of the external legs $G^{\Lambda_i}(\omega_i)$ is fixed. For example, for G^{RRAA} the imaginary parts of ω_1^+ and ω_2^+ are positive while those of ω_3^- and ω_4^- are negative. In Fig. 2.3 the signs of the imaginary parts of $\omega_i^\pm$ are constant within the rectangular sections labeled by the same arabic numbers. So, by ignoring the branch cuts $\mathcal{B}_{12} = 0$, $\mathcal{B}_{13} = 0$ and $\mathcal{B}_{14} = 0$ one finds the regions of the diagram which are consistent with a certain choice of the external legs.

The consistency with the external legs follows immediately for $G^{AAAA} = 0 = G^{RRRR}$, and also for a correlator like G^{RAAA} (which is proportional to the retarded correlator $G^{[1]}$) and a correlator like G^{RRRA} (which is proportional to the advanced correlator $G'^{[4]}$ according to Eq. (4.2.12)). For G^{RRAA} note that all involved AC functions are labeled by the same arabic numbers, namely (2.2).

Every non-vanishing KF component in the R/A basis corresponds to a rectangular region carrying a label with the same arabic numbers.

Due to the diagonal form of the propagators in the R/A basis it is easy to compute the vertex functions from the correlators. For instance we get $F^{AARR} = [G^AG^AG^RG^R]^{-1}G_{\text{con}}^{AARR}$. Since the FDRs according to Eq. (4.2.12) hold for the disconnected part G_{dis} and since the analytic continuation of the external legs is consistent with the analytic continuation of

[4]See App. B for the anomalous parts in a 4p correlator of fermionic operators.

the 4p correlator, we infer that the same FDRs

$$F^{\mathbf{\Lambda}} = F'^{\overline{\mathbf{\Lambda}}} \cdot \frac{\prod\limits_{\Lambda_i=R}(N_i+1)}{\prod\limits_{\Lambda_i=A}(N_i-1)}(-1)^{\ell-1} \tag{4.2.14}$$

hold for the vertex functions due to $G'^R = G^A$. From the consistency of the analytic continuation of the external legs and of the vertex function we furthermore deduce that the vertex function is analytic in the same regions as already found in Ref. [13]. Hence they can be constructed from the very same linear combination of AC functions as for correlators. In the Keldysh basis the meaning of the Keldysh indices 1 and 2 interchange for vertex functions, such that e.g. a retarded vertex function is given by $F^{[1]} = F^{1222}$. This is due to the fact that the transformation matrices are related by $P^{-1} = \sigma_x Q^{-1}$ where σ_x is the Pauli matrix

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The R/A basis for *incoming* legs: For completeness, we also give the corresponding matrices for the transformation from the Keldysh to the R/A basis for *incoming* legs. The correlator and the vertex are then related by

$$G^{k_1k_2k_3k_4}_{\text{con}}(\boldsymbol{\omega}) = F^{k_1'k_2'k_3'k_4'}(\boldsymbol{\omega}) \left[\prod_{i=1}^{4} G^{k_i'k_i}(-\omega_i)\right], \tag{4.2.15}$$

where summation over k_i' is implied. The transformation to the R/A basis is then given by

$$G^{\mathbf{\Lambda}} = \sum_{\boldsymbol{k}} G^{\boldsymbol{k}} \left[\prod_{i=1}^{\ell} [P^{-1}(-\omega_i)]^{k_i\Lambda_i}\right], \tag{4.2.16}$$

$$F^{\mathbf{\Lambda}} = \sum_{\boldsymbol{k}} F^{\boldsymbol{k}} \left[\prod_{i=1}^{\ell} [Q^{-1}(-\omega_i)]^{k_i\Lambda_i}\right]. \tag{4.2.17}$$

These transformation matrices are related to the ones for *outgoing* legs by

$$[P^{-1}(-\omega_i)]^T = \begin{pmatrix} 1 & 0 \\ -N_i & -1 \end{pmatrix} = -\sigma_x Q(\omega_i), \tag{4.2.18}$$

$$[Q^{-1}(-\omega_i)]^T = \begin{pmatrix} 0 & 1 \\ -1 & -N_i \end{pmatrix} = -\sigma_x P(\omega_i). \tag{4.2.19}$$

Hence, reverting the direction of a leg implies interchanging the labels R and A and multiplication by a global factor of (-1). In general, one has both in- and outgoing legs. The corresponding formulas are obtained from those for solely outgoing legs by reverting the direction of legs.

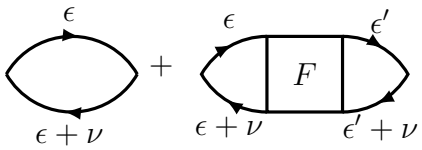

Figure 4.2: Diagrammatic representation of the susceptibility consisting of a bare bubble and a vertex contribution.

4.3 Computation of susceptibilities in KF and MF

In the following we compare the computation of real-frequency susceptibilities in the KF and in the MF. On the part of the MF we review a method introduced by Eliashberg [13]. He performed the analytic continuation of a 4p function to convert Matsubara sums into contour integrals. Thereby he obtained a formula with various vertex contributions (linear combinations of AC functions). Working with Eliashberg's method Oguri found that, out of the many vertex contributions, only one is relevant for the particular response function under his consideration [14].

We then translate the individual vertex contributions from Eliashberg's method to the KF. With these relations we are able to immediately convert Oguri's formula to the KF. In fact, Oguri's formula has been reproduced in the KF already [15]. However in a completely different line of argument. With the result in this section we are hence able to close a gap between the two formalisms. A very convenient stepping stone for this purpose is the R/A basis for the KF functions.

We first review Eliashberg's formula in Ref. [13] where he considered the susceptibility of a fermionic system. He obtained the retarded correlator $K^R(\nu) = K^{21}(\nu)$ via the well-known analytic continuation for the 2p function $K(\mathrm{i}\nu) \overset{\mathrm{i}\nu\to\nu+\mathrm{i}0^+}{\longrightarrow} K^R(\nu)$. The retarded correlator is defined via

$$K^{k_1k_2}(\nu) = \int_{\mathbb{R}} \mathrm{d}t\, e^{\mathrm{i}\nu t} \big\langle \mathcal{T}_c \big(d^\dagger_{\sigma_1} d_{\sigma_2}\big)^{k_1}(t) \big(d^\dagger_{\sigma_3} d_{\sigma_4}\big)^{k_2}(0) \big\rangle \tag{4.3.1}$$

with $d^\dagger_\sigma$ and d_σ being fermionic creation and annihilation operators specified by σ (in Eliashberg's case σ is a momentum). The composite operators $(d^\dagger d)$ each carry a time argument and a Keldysh index. Note that writing the contour index as a superscript to the operator $\mathcal{O}^c(t)$ is equivalent to the previous notation $\mathcal{O}^c(t) = \mathcal{O}(t^c)$. In this section we denote the contour indices by $\mathcal{O}^c$ to define operators in the Keldysh basis $\sqrt{2}\mathcal{O}^k = \mathcal{O}^- + (-1)^k \mathcal{O}^+$ as linear combinations of those in the contour basis. Similarly, operators in the R/A basis $\mathcal{O}^\Lambda$ are defined by a linear combination, i.e.

$$\mathcal{O}^1 = -\mathcal{O}^A, \quad \mathcal{O}^2 = N\mathcal{O}^A + \mathcal{O}^R, \tag{4.3.2}$$

where N is the statistical factor from the transformation matrix $Q(\omega)$ in Eq. (4.2.5).

The corresponding MF function is defined as

$$K(\mathrm{i}\nu) = \int_0^\beta \mathrm{d}\tau\, e^{\mathrm{i}\nu\tau} \big\langle \mathcal{T} \big(d^\dagger_{\sigma_1} d_{\sigma_2}\big)(\tau) \big(d^\dagger_{\sigma_3} d_{\sigma_4}\big)(0) \big\rangle. \tag{4.3.3}$$

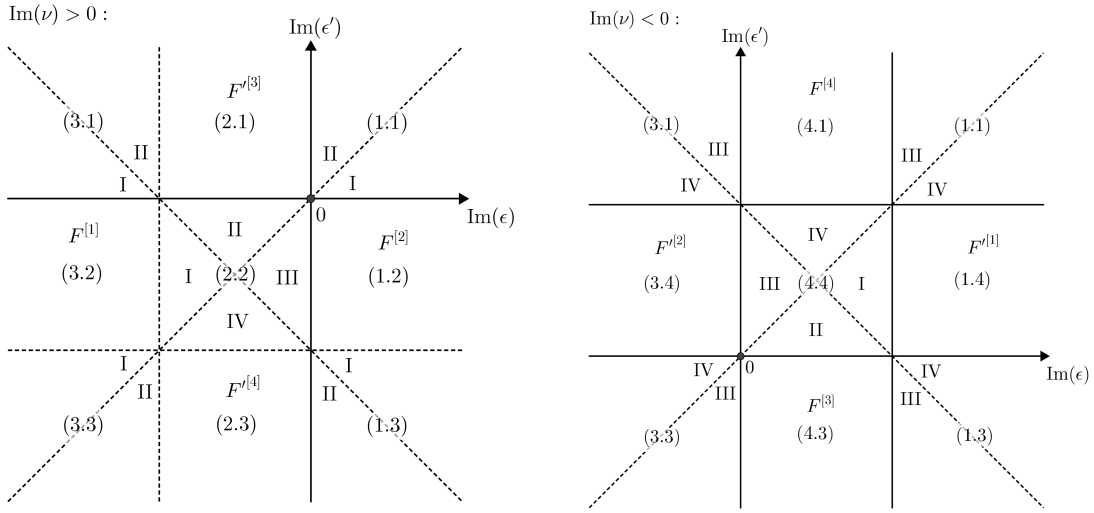

Figure 4.3: Regions of analyticity of vertex functions (adapted from Ref. [13]): The regions are identical to those of the correlators. The frequencies are parametrized in the convention $\boldsymbol{\omega} = (-\epsilon, \epsilon + \nu, -\epsilon' - \nu, \epsilon')$. Following Ref. [13] we denote the rectangular parts by arabic numbers. Roman numbers are used to differentiate between regions which are separated by the diagonals. The notation of the analytically continued vertex functions follows that of the regions, such that e.g. $2\,F^{[1]} = F_{3.2}$.

This 2p correlator can be obtained from the 4p correlator

$$G(\mathrm{i}\boldsymbol{\omega}) = \int_0^\beta \mathrm{d}^3\tau\, e^{\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{\tau}} \left\langle \mathcal{T} d^\dagger_{\sigma_1}(\tau_1) d_{\sigma_2}(\tau_2) d^\dagger_{\sigma_3}(\tau_3) d_{\sigma_4}(0) \right\rangle. \tag{4.3.4}$$

by summing over two fermionic frequencies ϵ and ϵ', as represented in Fig. 4.2. This gives

$$K(\mathrm{i}\nu) = -\frac{1}{\beta^2} \sum_{\epsilon,\epsilon'} \left(G_{(\mathrm{disc.})}(\mathrm{i}\boldsymbol{\omega}) + \left[\prod_{i=1}^{4} G(\mathrm{i}\omega_i) \right] F(\mathrm{i}\boldsymbol{\omega}) \right), \tag{4.3.5}$$

where we have split the 4p correlator into its disconnected and connected part. The frequencies of the 4p correlator are parametrized by

$$\omega_1 = -\epsilon, \quad \omega_2 = \epsilon + \nu, \quad \omega_3 = -\epsilon - \nu, \quad \omega_4 = \epsilon'. \tag{4.3.6}$$

The disconnected part can be treated with the analytic continuation of 2p functions already. We therefore focus on the vertex contribution to $K(\mathrm{i}\nu)$. Eliashberg then made use of the analytic continuation method to replace the sums over the frequencies ϵ and ϵ' by contour integrals which pick up the pole contributions of tanh or coth functions. To make sure that no other pole contributions are picked up, every contour has to stay within

a region on which the correlator is analytic. Since the branch cuts of correlators and, identically, of vertex functions run along the real axis and contour contributions at infinity are zero, it remains to integrate along the real axis. For the poles which lie directly on the branch cuts at $\mathrm{Im}(\omega_{13}) = 0$ and $\mathrm{Im}(\omega_{14}) = 0$ (see the diagonals in Fig. 4.3) one needs to take the Cauchy principal value integral which avoids the points with $\omega_{13} = 0$ and $\omega_{14} = 0$, respectively. The final result is given in Eqs. (9)-(12) of [35] where the vertex contributions are sorted by the analytic continuation of the external legs.

Now we derive the KF formula for the computation of the retarded function K^{21} and compare the contributions to those by Eliashberg. In the KF one not only needs to integrate out the fermionic frequencies ϵ and ϵ', but also has to account for the ordering due to the two branches of the Keldysh contour. In the contour basis the two constituents of the composite operator $(\mathcal{AB})$ also need to be on the same (forward or backward) branch. With c being the contour index, this amounts to

$$(\mathcal{AB})^c = \mathcal{A}^c\mathcal{B}^c, \quad c \in \{-,+\}. \tag{4.3.7}$$

In the Keldysh basis this leads to the correspondence

$$\sqrt{2}(\mathcal{AB})^1 = \mathcal{A}^1\mathcal{B}^2 + \mathcal{A}^2\mathcal{B}^1, \quad \sqrt{2}(\mathcal{AB})^2 = \mathcal{A}^1\mathcal{B}^1 + \mathcal{A}^2\mathcal{B}^2. \tag{4.3.8}$$

For a direct comparison of the resulting vertex contributions with the result of Eliashberg, it serves to group the contributions according to the analytic continuation of the external legs. For this purpose it is convenient to transform the vertex contributions of the retarded function K^{21} into the R/A basis. Inserting Eq. (4.3.2) into Eq. (4.3.8) gives

$$\begin{aligned}\sqrt{2}(\mathcal{AB})^1 &= -(N_a + N_b)\mathcal{A}^A\mathcal{B}^A - \mathcal{A}^A\mathcal{B}^R - \mathcal{A}^R\mathcal{B}^A,\\ \sqrt{2}(\mathcal{AB})^2 &= N_aN_b\mathcal{A}^A\mathcal{B}^A + N_a\mathcal{A}^A\mathcal{B}^R + N_b\mathcal{A}^R\mathcal{B}^A + \mathcal{A}^R\mathcal{B}^R,\end{aligned} \tag{4.3.9}$$

with the statistical factors N_a and N_b defined according to Eq. (2.2.4) where the frequencies ω_a and ω_b belong to the operators $\mathcal{A}$ and $\mathcal{B}$. Hence the operator product in the definition of the retarded function K^{21} gives

$$\begin{aligned}&2(\mathcal{AB})^2(\mathcal{CD})^1\\ &= -N_aN_b(N_c + N_d)\mathcal{A}^A\mathcal{B}^A\mathcal{C}^A\mathcal{D}^A - N_aN_b\mathcal{A}^A\mathcal{B}^A\mathcal{C}^A\mathcal{D}^R - N_aN_b\mathcal{A}^A\mathcal{B}^A\mathcal{C}^R\mathcal{D}^A\\ &\quad - N_a(N_c + N_d)\mathcal{A}^A\mathcal{B}^R\mathcal{C}^A\mathcal{D}^A - N_a\mathcal{A}^A\mathcal{B}^R\mathcal{C}^A\mathcal{D}^R - N_a\mathcal{A}^A\mathcal{B}^R\mathcal{C}^R\mathcal{D}^A\\ &\quad - N_b(N_c + N_d)\mathcal{A}^R\mathcal{B}^A\mathcal{C}^A\mathcal{D}^A - N_b\mathcal{A}^R\mathcal{B}^A\mathcal{C}^A\mathcal{D}^R - N_b\mathcal{A}^R\mathcal{B}^A\mathcal{C}^R\mathcal{D}^A\\ &\quad - (N_c + N_d)\mathcal{A}^R\mathcal{B}^R\mathcal{C}^A\mathcal{D}^A - (N_c + N_d)\mathcal{A}^R\mathcal{B}^R\mathcal{C}^A\mathcal{D}^R - (N_c + N_d)\mathcal{A}^R\mathcal{B}^R\mathcal{C}^R\mathcal{D}^A.\end{aligned} \tag{4.3.10}$$

Plugging creation and annihilation operators into this formula allows us to write the retarded function as

$$K^R(\nu) = -\frac{1}{2}\int_{\mathbb{R}} \frac{\mathrm{d}\epsilon\mathrm{d}\epsilon'}{(2\pi\mathrm{i})^2}\, I(\boldsymbol{\omega})$$

with

$$\begin{aligned}I = &-N_1(N_3 + N_4)G^{ARAA} - N_1G^{ARAR} - N_1G^{ARRA} - N_2(N_3 + N_4)G^{RAAA}\\ &- N_2G^{RAAR} - N_2G^{RARA} - (N_3 + N_4)G^{RRAA} - G^{RRAR} - G^{RRRA}.\end{aligned} \tag{4.3.11}$$

Here we already used that $G^{AAAA} = G^{[]} = 0$ and that

$$\int_{-\infty}^{\infty} \mathrm{d}\epsilon \mathrm{d}\epsilon' N_1 N_2 \left[G^{AAAR} + G^{AARA}\right] = 0. \tag{4.3.12}$$

These integrals yield zero since the statistical factors N_1 and N_2 contain no poles for ϵ'. Also, the functions $G^{AAAR} = -G^{[4]}$ and $G^{AARA} = -G^{[3]}$ are analytic functions on their respective region. Each region extends to $|\mathrm{Im}(\epsilon')| \to \infty$. We can therefore close the contour with a half-circle over the upper or lower complex half-plane of ϵ' and get zero due to the lack of poles.

Be aware that we always worked in the R/A basis according to Eq. (4.2.7) which assumes that all external legs are outgoing, such that e.g.

$$G_{\mathrm{con}}^{RRAA}(\boldsymbol{\omega}) = G^R(\omega_1)G^R(\omega_2)G^A(\omega_3)G^A(\omega_4)F^{RRAA}(\boldsymbol{\omega}). \tag{4.3.13}$$

For our computations it is convenient to work in this basis. However, for a direct comparison of the external legs with Eliashberg's result we have to account for the fact that the first and third leg are incoming. Following the remark after Eq. (4.2.19) we transform

$$G^{R/A}(\omega_i) \to G^{A/R}(-\omega_i), \quad \text{for } i \in \{1, 3\}. \tag{4.3.14}$$

Our above example in Eq. (4.3.13) now has the external legs

$$G^A(-\omega_1)G^R(\omega_2)G^R(-\omega_3)G^A(\omega_4) = G^A(\epsilon)G^R(\epsilon+\nu)G^R(\epsilon'+\nu)G^A(\epsilon').$$

Adopting the notation of external legs from Ref. [13] we define

$$\begin{aligned} g_1(\epsilon,\nu) &= G^R(\epsilon+\nu)G^R(\epsilon), \\ g_2(\epsilon,\nu) &= G^R(\epsilon+\nu)G^A(\epsilon), \\ g_3(\epsilon,\nu) &= G^A(\epsilon+\nu)G^A(\epsilon), \\ g_4(\epsilon,\nu) &= G^A(\epsilon+\nu)G^R(\epsilon). \end{aligned} \tag{4.3.15}$$

For the retarded correlator $K^R(\nu)$ the vertex contributions can be read off from Eq. (4.3.11)

$$K_{\mathrm{vertex}}^R(\nu) = -\frac{1}{2(2\pi\mathrm{i})^2} \int_{-\infty}^{\infty} \mathrm{d}\epsilon \mathrm{d}\epsilon' \sum_{i,j} g_i(\epsilon,\nu)\mathcal{L}_{ij}(\boldsymbol{\omega})g_j(\epsilon',\nu) \tag{4.3.16}$$

with

$$\begin{aligned}
\mathcal{L}_{11} &= -N_1 F^{ARAR} = -N_1(F^{[24]} + N_4\Gamma^{[2]} + N_2\Gamma^{[4]}),\\
\mathcal{L}_{12} &= -N_1(N_3+N_4)F^{ARAA} = N_1(N_3+N_4)F^{[2]},\\
\mathcal{L}_{13} &= -N_1 F^{ARRA} = -N_1(F^{[23]} + N_3F^{[2]} + N_2F^{[3]}),\\
\mathcal{L}_{21} &= -F^{RRAR} = (1+N_1N_2+N_1N_4+N_2N_4)F'^{[3]},\\
\mathcal{L}_{22} &= -(N_3+N_4)F^{RRAA} = -(N_1+N_2)F'^{AARR} = -(N_1+N_2)[F'^{[34]} + N_4F'^{[3]} + N_3F'^{[4]}],\\
\mathcal{L}_{23} &= -F^{RRRA} = (1+N_1N_2+N_1N_3+N_2N_3)F'^{[4]},\\
\mathcal{L}_{31} &= -N_2 F^{RAAR} = -N_2[F^{[14]} + N_4F^{[1]} + N_1F^{[4]}],\\
\mathcal{L}_{32} &= -N_2(N_3+N_4)F^{RAAA} = N_2(N_3+N_4)F^{[1]},\\
\mathcal{L}_{33} &= -N_2 F^{RARA} = -N_2[F^{[13]} + N_3F^{[1]} + N_1F^{[3]}]
\end{aligned} \tag{4.3.17}$$

where for $\mathcal{L}_{21}$, $\mathcal{L}_{22}$ and $\mathcal{L}_{23}$ we used the generalized FDRs to make the connection to Eliashberg's result more obvious.

The relations in Eq. (4.3.17) already show the one-to-one correspondence between Eliashberg's vertex contributions and the KF components. To see that these are indeed identical we have to express the Keldysh vertices in terms of AC functions using Eqs. (B.2.2). For the primed correlators like G'^{34} the AC functions for constructing $G^{[34]}$ are replaced by those with the opposite imaginary frequencies. Thereby we e.g. obtain the vertex contributions

$$\begin{aligned}
\mathcal{L}_{12} &= +\tfrac{1}{2}N_1(N_3+N_4)\,F_{1.2},\\
\mathcal{L}_{21} &= +\tfrac{1}{2}(1+N_1N_2+N_1N_4+N_2N_4)\,F_{2.1},\\
\mathcal{L}_{22} &= -\tfrac{1}{2}(N_1+N_2)[N_4(F^{\mathrm{II}}_{2.2}) + N_{23}(F^{\mathrm{II}}_{2.2} - F^{\mathrm{III}}_{2.2}) + N_{13}(F^{\mathrm{III}}_{2.2} - F^{\mathrm{IV}}_{2.2}) + N_3(F^{\mathrm{IV}}_{2.2})].
\end{aligned}$$

For all the AC functions which do not belong to the central region with the label (2.2) one can then use the argument under Eq. (4.3.12) to cross out the summands which do not contribute poles for both ϵ and ϵ'. By doing so, we obtain

$$\begin{aligned}
\mathcal{L}_{11} &= -\tfrac{1}{2}N_1\big[\cancel{N_2F^{\mathrm{III}}_{1.1}} + N_4\Gamma^{\mathrm{I}}_{1.1} + N_{14}(F^{\mathrm{II}}_{1.1} - F^{\mathrm{I}}_{1.1}) + N_{12}(\cancel{F^{\mathrm{II}}_{1.1}} - \cancel{F^{\mathrm{III}}_{1.1}})\big]\\
\mathcal{L}_{12} &= +\tfrac{1}{2}N_1(N_3+N_4)F_{1.2}\\
\mathcal{L}_{13} &= -\tfrac{1}{2}N_1\big[\cancel{N_2F^{\mathrm{III}}_{1.3}} + N_3F^{\mathrm{I}}_{1.3} + N_{13}(F^{\mathrm{II}}_{1.3} - F^{\mathrm{I}}_{1.3}) + N_{12}(\cancel{F^{\mathrm{II}}_{1.3}} - \cancel{F^{\mathrm{III}}_{1.3}})\big]\\
\mathcal{L}_{21} &= +\tfrac{1}{2}(\cancel{1+N_1N_2} + N_1N_4 + N_2N_4)F_{2.1}\\
\mathcal{L}_{22} &= -\tfrac{1}{2}(N_1+N_2)\big[N_4(F^{\mathrm{II}}_{2.2}) + N_{23}(F^{\mathrm{II}}_{2.2} - F^{\mathrm{III}}_{2.2}) + N_{13}(F^{\mathrm{III}}_{2.2} - F^{\mathrm{IV}}_{2.2}) + N_3(F^{\mathrm{IV}}_{2.2})\big]\\
\mathcal{L}_{23} &= +\tfrac{1}{2}(\cancel{1+N_1N_2} + N_1N_3 + N_2N_3)F_{2.3}\\
\mathcal{L}_{31} &= -\tfrac{1}{2}N_2\big[\cancel{N_1F^{\mathrm{III}}_{3.1}} + N_4\Gamma^{\mathrm{I}}_{3.1} + N_{12}(\cancel{F^{\mathrm{II}}_{3.1}} - \cancel{F^{\mathrm{III}}_{3.1}}) + N_{13}(F^{\mathrm{I}}_{3.1} - F^{\mathrm{II}}_{3.1})\big]\\
\mathcal{L}_{32} &= +\tfrac{1}{2}N_2(N_3+N_4)F_{3.2}\\
\mathcal{L}_{33} &= -\tfrac{1}{2}N_2\big[\cancel{N_1F^{\mathrm{III}}_{3.3}} + N_3\Gamma^{\mathrm{I}}_{3.3} + N_{12}(\cancel{F^{\mathrm{II}}_{3.3}} - \cancel{F^{\mathrm{III}}_{3.3}}) + N_{14}(F^{\mathrm{I}}_{3.3} - F^{\mathrm{II}}_{3.3})\big]
\end{aligned} \tag{4.3.18}$$

Expressing the factors $N_i = \tanh[\beta\omega_i/2]$ and $N_{ij} = \coth[\beta(\omega_i + \omega_j)/2]$ in terms of the frequencies ν, ϵ and ϵ' we find that Eq. (4.3.18) exactly gives Eliashbergs vertex contributions.

Now, knowing the direct correspondence between vertex contributions by Eliashberg and the KF components, one can directly translate formulas from one formalism to the other. For instance, Oguri derived a formula for the linear conductance of quantum point contacts with non-interacting leads in [14]. Working with Eliashberg's method he was able to apply simplifications on the general formula which allowed him to neglect all vertex contributions but the central $\mathcal{L}_{22}$. From Eq. (4.3.17) we read off

$$\mathcal{L}_{22} = -\tfrac{1}{2}(N_3 + N_4)F^{RRAA} = -\tfrac{1}{2}(N_3 + N_4)[F^{[12]} + N_2 F^{[1]} + N_1 F^{[2]}].$$

This agrees with the result which Heyder et al. derived separately in Eq. (23) of Ref. [15] within the framework of the KF. However, instead of the 'standard' approach (computing the susceptibility by integrating out two fermionic frequencies) they made use of an exact flow equation from the functional renormalization group. We have thereby closed a gap between the two formalisms on the two-particle level, showing that the KF is not just conceptually expected to yield the same results as the MF. But also one also obtains a result in the KF by first performing calculations in the MF and then analytically continue to a KF function, here via the relations in Eq. (4.3.17).

At last, a short note on the anomalous contributions which have been neglected so far: While we integrate out ϵ and ϵ' we take care of the divergencies of the factors N_{ij} by using the Cauchy principal value integral in both the MF and the KF which avoids the points with $\omega_{ij} = 0$. This is necessary in the MF to take into account the pole contributions of the regular MF correlator which lie directly on the branch cut. However, in the above AC functions the anomalous contributions are not contained yet. They have to be added separately to make sure that the Matsubara sum and the contour integral take on the same value. From our construction of the KF correlator with AC functions we know that these are exactly the points for which the reconstruction of an PSF anti-commutator fails (see Sec. 3.1.3). This issue is reconciled by adding the anomalous contributions. Since these are proportional to a delta function, e.g. $\delta(\epsilon' - \epsilon)$, the integral or the sum over ϵ' is trivial and the correspondence of the MF and KF calculation is checked analogously to the disconnected part of the susceptibility.

Chapter 5

The Hubbard atom in the Keldysh formalism

In this chapter we compute the one-particle and two-particle correlator of the Hubbard atom within the Keldysh formalism. The Hubbard atom describes a system of spin–$\frac{1}{2}$ fermions (electrons) which consists of a single lattice site. Due to the Pauli exclusion principle only fermions with different quantum numbers can occupy this site simultaneously. Two electrons on the same site interact via the Coulomb repulsion. This very simple model is of high interest since it is one of the few which are accessible via *analytically exact* computations. The Hubbard atom can be obtained from the Hubbard model and the single-impurity Anderson model in the *atomic limit*. It can thus serve as a benchmark for numerical methods. The difficulty of solving these models can be traced back to the competition of the kinetic and interaction terms of the Hamiltonian which impedes analytic calculations [5].

The one-particle and two-particle correlator of the Hubbard atom have already been computed in the Matsubara formalism (MF) [16–20]. The vertex function of the Hubbard atom has been used as a starting point for a perturbative expansion around strong coupling [17, 36]. It has been found that (despite the simplicity of the model) the two–particle irreducible (2PI) vertex functions display a complicated frequency dependence [37]. The divergencies in these 2PI vertices are an object of ongoing research. Such divergencies have been related to the breakdown of the perturbative expansion due to the multivaluedness of the Luttinger-Ward functional [38–41].

The corresponding correlators in the Keldysh formalism can be computed directly via a spectral representation. They can also be computed via our formula for analytic continuation (see App. B) which allows us to "recycle" formulas obtained within the MF. The generalized fluctuation-dissipation relations (FDR) reduce the number of independent components of the Keldysh correlator to $2^\ell - 1$ [12, 33] and can thus be used to facilitate the computations.

In the remaining part of this chapter we first introduce the model and the results in MF in Sec. 5.1. In Sec. 5.2 we introduce an alternative spectral representation for KF correlators in which we then (in Sec. 5.3) compute the results directly. Next, in Sec. 5.4 we

show, using the example of some Keldysh components, that analytic continuation of the MF correlator delivers the same result. We confirm the consistency of the computed results by checking the generalized fluctuation-dissipation relations and the SU(2) symmetry in Sec. C.3. Lastly, in Sec. 5.5 we derive formulas for the vertex function in KF and investigate the asymptotics of the vertex function for high frequencies.

5.1 Review of results on the Hubbard atom

5.1.1 The model

In the following we consider an interacting fermionic spin-$\frac{1}{2}$ system which consists of a single site. The corresponding Hamiltonian reads

$$\mathcal{H} = U\, n_\uparrow n_\downarrow - \mu \cdot (n_\uparrow + n_\downarrow) \tag{5.1.1}$$

with $n_\sigma = d_\sigma^\dagger d_\sigma$ being the number operators for spin $\sigma \in \{\uparrow, \downarrow\}$. These are expressed in terms of fermionic creation and annihilation operators $d_\sigma^\dagger$ and d_σ. The parameter $U > 0$ is the effective strength of the local interaction and μ the chemical potential. We use $u = U/2$ to minimize the factors of $1/2$ in the following sections.

This very simple system can be obtained from the Hubbard model and the Single-Impurity Anderson Model (SIAM) in the atomic limit [5,19,42]. For instance the one-band Hubbard model is a tight-binding approximation of a crystal. It is assumed that electrons can occupy the lattice sites which form a discrete set of points in space. The Hubbard Hamiltonian is

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} d_i^\dagger d_j + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_{i,\sigma} n_{i,\sigma} \tag{5.1.2}$$

with the creation and annihilation operators $d_{i,\sigma}^\dagger$ and $d_{i,\sigma}$ for an electron at site i with spin $\sigma \in \{\uparrow, \downarrow\}$. The number operators $n_{i,\sigma} = d_{i,\sigma}^\dagger d_{i,\sigma}$ are defined correspondingly. In the first term the tunneling with amplitude t is restricted to neighboring lattice sites $\langle i, j \rangle$. We only consider on-site interaction with strength U. The Coulomb interaction is assumed to be screened on longer distances and μ is the chemical potential. An exact solution for the correlation functions of the Hubbard model can be computed in two limits. In the free theory ($U = 0$) Wick's theorem allows to write any correlator in terms of one-particle correlators and the Hamiltonian is diagonal in momentum space. In the atomic limit ($t = 0$) the Hamiltonian is diagonal in position space, such that the individual sites decouple and it remains to compute the correlations on a single site. The corresponding Hamiltonian is given in Eq. (5.1.1).

The SIAM hosts a single interacting impurity which is coupled to a non-interacting bath. Its Hamiltonian reads

$$\mathcal{H} = \sum_{\ell,\sigma} \varepsilon_\ell\, c_{\ell,\sigma}^\dagger c_{\ell,\sigma} + \sum_{\ell,\sigma} V_\ell\, (d_\sigma^\dagger c_{\ell,\sigma} + c_{\ell,\sigma}^\dagger d_\sigma) + U\, n_\uparrow n_\downarrow - \mu\, (n_\uparrow + n_\downarrow). \tag{5.1.3}$$

Electrons are created, $d_\sigma^\dagger$, and annihilated, d_σ, at the impurity where they interact with strength u. On the impurity the chemical potential is μ. The bath electrons occupy the energy levels ε_ℓ and are created and annihilated with the operators $c_{\ell,\sigma}^\dagger$ and $c_{\ell,\sigma}$. The second term introduces a coupling between the impurity and the bath with hybridization strengths V_ℓ. Similar to the Hubbard model both the free theory ($u = 0$) and the atomic limit ($V_\ell = 0$) can be solved analytically. In the latter case the impurity site decouples from the bath such that it remains to compute the local correlations given by the Hamiltonian in Eq. (5.1.1).

There are only a few energy eigenstates for the Hubbard atom. In the system according to Eq. (5.1.1) it can only be either unoccupied, $|\emptyset\rangle$, singly occupied, $|\uparrow\rangle$ or $|\downarrow\rangle$, or doubly occupied $|\downarrow\uparrow\rangle$ such that the eigenenergies are given by

$$\mathcal{H}\big(\,|\emptyset\rangle\,,|\downarrow\rangle\,,|\uparrow\rangle\,,|\downarrow\uparrow\rangle\,\big) = \big(0\,|\emptyset\rangle\,,-\mu\,|\uparrow\rangle\,,-\mu\,|\downarrow\rangle\,,(U-2\mu)\,|\downarrow\uparrow\rangle\,\big). \tag{5.1.4}$$

Using the above basis any state can be expressed as a vector $\boldsymbol{v} = v_1\,|\emptyset\rangle + v_2\,|\downarrow\rangle + v_3\,|\uparrow\rangle + v_4\,|\downarrow\uparrow\rangle$. We can also compute the matrix elements of the fermionic creation and annihilation operators. These are given in the occupation number basis [11]

$$\begin{aligned} d_j^\dagger\,|n_1,n_2,...,n_j,...\rangle &= (-1)^{\sum_{i<j} n_i}\cdot(1-n_j)\cdot|n_1,n_2,...,n_j+1,...\rangle\,,\\ d_j\,|n_1,n_2,...,n_j,...\rangle &= (-1)^{\sum_{i<j} n_i}\cdot n_j\cdot|n_1,n_2,...,n_j-1,...\rangle\,, \end{aligned} \tag{5.1.5}$$

where the fermionic sign factor $(-1)^{\sum_{i<j} n_i}$ is defined for a fixed order of the states, given by $|n_1,n_2,...,n_j,...\rangle$. In the following we choose the order $|n_\downarrow,n_\uparrow\rangle$ for which we can represent the operators with the matrices

$$d_\uparrow = \begin{pmatrix} 0&0&1&0\\ 0&0&0&-1\\ 0&0&0&0\\ 0&0&0&0 \end{pmatrix}, \quad d_\downarrow = \begin{pmatrix} 0&1&0&0\\ 0&0&0&0\\ 0&0&0&1\\ 0&0&0&0 \end{pmatrix}, \quad d_\uparrow^\dagger = d_\uparrow^T, \quad d_\downarrow^\dagger = d_\downarrow^T. \tag{5.1.6}$$

These operators fulfill the fermionic anti-commutation relations and allow us to compute correlators directly via a spectral representation in the MF given in Refs. [13, 16, 21] and as we derive for the KF in Sec. 5.1.4. Note that the matrix elements of these operators are real. Since the Hamiltonian is a real function of the creation and annihilation operators, all partial spectral functions are real in frequency space [see Eq. (2.1.9)]. Hence, the primed KF correlators equal the complex conjugated ones, $G' = G^*$ [see Eq. (2.1.28)].

5.1.2 Correlators and symmetries of the Hubbard atom

In the following sections we consider the one- and two-particle correlator of the Hubbard atom. The general n-particle correlator in MF is defined as

$$\mathcal{G}_{\sigma_1,...,\sigma_{2n}}(\boldsymbol{\tau}) = (-1)^{\ell-1}\left\langle \mathcal{T}\left[d_{\sigma_1}(\tau_1)d_{\sigma_2}^\dagger(\tau_2)...d_{\sigma_{2n-1}}(\tau_{2n-1})d_{\sigma_{2n}}^\dagger(\tau_\ell)\right]\right\rangle \tag{5.1.7}$$

and correspondingly in the KF

$$\mathcal{G}^{k_1\dots k_{2n}}_{\sigma_1,\dots,\sigma_{2n}}(\boldsymbol{t}) = (-1)^{\ell-1}\left\langle \mathcal{T}_c\left[d^{k_1}_{\sigma_1}(t_1)d^{\dagger\,k_2}_{\sigma_2}(t_2)\dots d^{k_{2n-1}}_{\sigma_{2n-1}}(t_{2n-1})d^{\dagger\,k_{2n}}_{\sigma_{2n}}(t_\ell)\right]\right\rangle, \tag{5.1.8}$$

where $\mathcal{T}$ and $\mathcal{T}_c$ denotes the imaginary time ordering and contour ordering, respectively. The operators $d^\dagger_{\sigma_i}$ and d_{σ_i} create and annihilate a fermion with spin $\sigma_i \in \{\uparrow,\downarrow\}$. The time-evolution of the operators in imaginary and real time is given in the Heisenberg picture

$$\mathcal{O}(\tau) = e^{\mathcal{H}\tau}\mathcal{O}e^{-\mathcal{H}\tau}, \qquad\qquad \mathcal{O}(t) = e^{\mathrm{i}\mathcal{H}t}\mathcal{O}e^{-\mathrm{i}\mathcal{H}t}, \tag{5.1.9}$$

with the time-independent full Hamiltonian $\mathcal{H}$.

Following Refs. [19, 33] we summarize the general properties of the correlators. For the sake of notational convenience the symmetry properties of the Hubbard atom and its consequences on the correlators are presented for MF correlators only [19]. However, they are not specific to the formalism. For KF correlators one obtains very analogous relations, following the same lines of arguments. The Hubbard atom has several symmetries which can be exploited to simplify the computation of correlators. It displays time-translational invariance, time-reversal symmetry and SU(2) spin symmetry. A symmetry relation due to the SU(2) spin symmetry is used in Sec. C.3.2 to check the consistency of the result on the KF correlator. Furthermore we assume equilibrium at finite temperature $T = 1/\beta$. For $\mu = U/2$ we additionally have particle-hole symmetry and a further $SU(2)$ symmetry.

Within the MF the assumption of an *equilibrium* system at finite temperature is built into the formalism. The Boltzmann factor $e^{-\beta\mathcal{H}}$ corresponds to a time-evolution $e^{-\mathrm{i}t\mathcal{H}}$ along the imaginary time axis. After a Wick rotation $t \to -\mathrm{i}\tau$ the MF correlator Eq. (5.1.7) is (anti-)periodic in each time-argument. Due to the (anti-)periodicity of the MF correlator its Fourier transform is given by an integration of all time variables τ_i over an interval of length β. In the KF the equilibrium condition leads to the generalized FDRs allowing one to reduce the number of independent KF correlators [12, 33]. *Time-translational invariance* yields a further simplification of the calculation. Since correlators only depend on relative time differences, one can translate all times by an arbitrary amount, e.g. setting one of the times to zero. In the frequency domain this leads to the global factor of $\beta\delta_{\omega_{1\dots\ell},0}$ or $2\pi\delta(\omega_{1\dots\ell})$ which ensures total energy conservation as expected for a time-translationally invariant system. The *exchange symmetry* (or *crossing symmetry*) is expressed in the time-ordering by the sign factors $\boldsymbol{\zeta}^p$ [see Eq. (2.1.7)]. One can thereby relate correlators which merely differ in the permutation of their operators. For instance, by exchanging two fermionic creation operators one finds that $G^{k_1k_2k_3k_4}_{\sigma_1\sigma_2\sigma_3\sigma_4}(\omega_1,\omega_2,\omega_3,\omega_4) = -G^{k_1k_4k_3k_2}_{\sigma_1\sigma_4\sigma_3\sigma_2}(\omega_1,\omega_4,\omega_3,\omega_2)$.

In general, a given unitary operator $\mathcal{U}$ is associated with a *symmetry* if it commutes with the Hamiltonian

$$[\mathcal{U},\mathcal{H}] = 0, \qquad \Leftrightarrow \qquad \mathcal{U}\mathcal{H}\mathcal{U}^{-1} = \mathcal{H}. \tag{5.1.10}$$

In this case, one can transform the creation and annihilation operators

$$d'^{(\dagger)}_\sigma = \mathcal{U}^{-1}d^{(\dagger)}_\sigma\,\mathcal{U}, \qquad \text{with} \quad d'^{(\dagger)}_\sigma(\tau) = e^{\tau\mathcal{H}}d'^{(\dagger)}_\sigma e^{-\tau\mathcal{H}}, \tag{5.1.11}$$

where the time-evolution is defined with the untransformed Hamiltonian. One obtains the transformed n-particle correlator

$$G'_{\sigma_1\ldots\sigma_{2n}}(\boldsymbol{\tau}) = (-1)^{2n-1}\left\langle \mathcal{T}[d'_{\sigma_1}(\tau_1)d'^{\dagger}_{\sigma_2}(\tau_2)\ldots d'^{\dagger}_{\sigma_{2n}}(\tau_{2n})]\right\rangle, \tag{5.1.12}$$

Plugging the transformation in Eq. (5.1.11) and using the symmetry according to Eq. (5.1.10) one finds

$$\begin{aligned} G'_{\sigma_1\ldots\sigma_{2n}}(\boldsymbol{\tau}) &= (-1)^{2n-1}\big\langle \mathcal{T}[e^{\tau_1\mathcal{H}}\mathcal{U}^{-1}d_{\sigma_1}\underbrace{\mathcal{U}e^{-\tau_1\mathcal{H}}e^{\tau_2\mathcal{H}}\mathcal{U}^{-1}}_{e^{-\tau_1\mathcal{H}}e^{\tau_2\mathcal{H}}}d^{\dagger}_{\sigma_2}\mathcal{U}e^{-\tau_2\mathcal{H}}\ldots d'^{\dagger}_{\sigma_{2n}}(\tau_{2n})]\big\rangle \\ &= (-1)^{2n-1}\big\langle \mathcal{T}[e^{\tau_1\mathcal{H}}d_{\sigma_1}e^{-\tau_1\mathcal{H}}e^{\tau_2\mathcal{H}}d^{\dagger}_{\sigma_2}e^{-\tau_2\mathcal{H}}\ldots d^{\dagger}_{\sigma_{2n}}(\tau_{2n})]\big\rangle \\ &= G_{\sigma_1\ldots\sigma_{2n}}(\boldsymbol{\tau}). \end{aligned} \tag{5.1.13}$$

Thus, given a symmetry $\mathcal{U}$ the correlator G' with the symmetry-transformed operators $d'^{(\dagger)}_{\sigma_i}$ is equal to the untransformed correlator G. This can be used to derive identities for the correlators.

Let us now consider the spin symmetry. The spin operators are defined as

$$\mathcal{S}^a = d^{\dagger}_{\sigma'}\sigma^a_{\sigma'\sigma}d_{\sigma}, \qquad \text{for } a \in \{x, y, z\}, \tag{5.1.14}$$

with σ_i being the corresponding Pauli matrix. They commute with the Hamiltonian of the Hubbard atom

$$[\mathcal{S}_i, \mathcal{H}] = 0 \tag{5.1.15}$$

and are thus the generators of symmetry transformations

$$\mathcal{U}_i(\varphi) = e^{\mathrm{i}\varphi\mathcal{S}_i}. \tag{5.1.16}$$

From the commutation relation Eq. (5.1.15) follows that both matrices can be diagonalized simultaneously. In a suitable basis, the eigenvalues of $\mathcal{S}_i$ are hence conserved quantities during time evolution. For spins one usually uses the operator $\mathcal{S}_z$ and the total spin $\boldsymbol{\mathcal{S}}^2$ as a maximal set of operators which can be simultaneously diagonalized with the Hamiltonian. In this basis the total spin and the z-component are conserved quantities. For the one-particle correlator $G_{\sigma\sigma'}$ this means that it is non-vanishing only for $\sigma = \sigma'$. Similarly, most spin configurations for the two-particle correlator vanish.

Explicitly computing the symmetry transformation $\mathcal{U}_y(\varphi)$ one finds for $\varphi = \pi/2$ that the transformed creation (annihilation) operators give [19]

$$d'^{(\dagger)}_{\uparrow} = \frac{1}{\sqrt{2}}(d^{(\dagger)}_{\uparrow} + d^{(\dagger)}_{\downarrow}), \qquad d'^{(\dagger)}_{\downarrow} = \frac{1}{\sqrt{2}}(d^{(\dagger)}_{\downarrow} - d^{(\dagger)}_{\uparrow}). \tag{5.1.17}$$

Plugging these transformed operators in Eq. (5.1.12) and by use of the fermionic exchange symmetry of the operators, Rohringer concluded in Ref. [19] that

$$G_{\uparrow\uparrow\uparrow\uparrow}(\omega_1, \omega_2, \omega_3, \omega_4) = G_{\uparrow\uparrow\downarrow\downarrow}(\omega_1, \omega_2, \omega_3, \omega_4) - G_{\uparrow\uparrow\downarrow\downarrow}(\omega_1, \omega_4, \omega_3, \omega_2). \tag{5.1.18}$$

He concluded that $G_{\uparrow\uparrow\downarrow\downarrow}$ is the only two-particle correlator which has to be computed. All other spin configurations can be deduced by use of symmetry relations. We use this equation as a consistency check for the computed correlators.

So, henceforth we define the four-point functions

$$\mathcal{G}_{\sigma\sigma'}(\tau_1,\tau_2,\tau_3,\tau_4) = (-1)^3\langle\mathcal{T}\left[d_\sigma(\tau_1)d^\dagger_\sigma(\tau_2)d_{\sigma'}(\tau_3)d^\dagger_{\sigma'}(\tau_4)\right]\rangle \tag{5.1.19}$$

with $\tau_i \in [0,\beta]$, $\sigma,\sigma' \in \{\uparrow,\downarrow\}$. Given this definition, the symmetry relation in Eq. (5.1.18) reads

$$G_{\uparrow\uparrow}(\omega_1,\omega_2,\omega_3,\omega_4) = G_{\uparrow\downarrow}(\omega_1,\omega_2,\omega_3,\omega_4) - G_{\uparrow\downarrow}(\omega_1,\omega_4,\omega_3,\omega_2). \tag{5.1.20}$$

The corresponding symmetry relation in the KF is obtained by additionally attaching a Keldysh index to every operator, giving

$$G^{k_1k_2k_3k_4}_{\uparrow\uparrow}(\omega_1,\omega_2,\omega_3,\omega_4) = G^{k_1k_2k_3k_4}_{\uparrow\downarrow}(\omega_1,\omega_2,\omega_3,\omega_4) - G^{k_1k_4k_3k_2}_{\uparrow\downarrow}(\omega_1,\omega_4,\omega_3,\omega_2). \tag{5.1.21}$$

5.1.3 Results in the Matsubara formalism at half-filling

In this section we summarize results on the one- and two-particle correlators for the Hubbard atom at half-filling ($\mu = u$) at inverse temperature $\beta = 1/T$ in the imaginary-time formalism (MF) [16–20]. To avoid factors of $1/2$ in the subsequent formulas we introduced the constant $u = U/2$ such that the energy eigenstates $(|\emptyset\rangle, |\downarrow\rangle, |\uparrow\rangle, |\downarrow\uparrow\rangle)$ have the eigenenergies $(0,-u,-u,0)$.

For the one-particle correlators it is conventional to express them only in terms of the time and frequency argument of the first operator $\omega = \omega_1 = -\omega_2$. Thus, the one-particle correlator of the Hubbard atom at half-filling gives in frequency space

$$G(\mathrm{i}\omega) = -\int_0^\beta \mathrm{d}\tau\, \langle\mathcal{T}\left[d_\sigma(\tau)d^\dagger_\sigma(0)\right]\rangle e^{\mathrm{i}\omega\tau} = \frac{\mathrm{i}\omega}{(\mathrm{i}\omega)^2 - u^2}, \tag{5.1.22}$$

which is identical for any spin $\sigma \in \{\uparrow,\downarrow\}$. Hence we drop the spin indices for $G(\mathrm{i}\omega)$. Due to SU(2)-symmetry the one-particle correlator is diagonal in spin space, i.e. correlators of unequal spin like $\langle\mathcal{T}[d_\uparrow(\tau)d^\dagger_\downarrow(0)]\rangle$ vanish.

As mentioned at the end of the last section, it suffices to compute the 4p correlator $G_{\uparrow\downarrow}$ to account for all other spin configurations. The two-particle correlator can be separated in two contributions $G_{\uparrow\downarrow} = G_{\uparrow\downarrow,\mathrm{dis}} + G_{\uparrow\downarrow,\mathrm{con}}$ (see Fig. 5.1). The *disconnected part* $G_{\uparrow\downarrow,\mathrm{dis}}$ is the product of one-particle correlators, i.e. in this case

$$G_{\uparrow\downarrow,\mathrm{dis}}(\mathrm{i}\omega_1,\mathrm{i}\omega_2,\mathrm{i}\omega_3,\mathrm{i}\omega_4) = -\beta\delta_{\omega_{12},0}G(\mathrm{i}\omega_1)G(\mathrm{i}\omega_3)$$

and corresponds to the independent propagation of two particles without scattering. The *connected part* of the two-particle correlator $G_{\uparrow\downarrow,\mathrm{con}}$ gives in frequency space

$$G_{\uparrow\downarrow,\mathrm{con}} = \widetilde{G}_{\uparrow\downarrow,\mathrm{con}} + \widehat{G}^{(\omega_{12})}_{\uparrow\downarrow,\mathrm{con}} + \widehat{G}^{(\omega_{13})}_{\uparrow\downarrow,\mathrm{con}} + \widehat{G}^{(\omega_{14})}_{\uparrow\downarrow,\mathrm{con}}, \tag{5.1.23a}$$

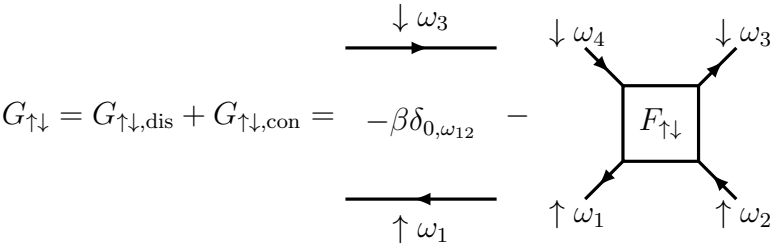

Figure 5.1: Diagrammatic representation of the correlator $G_{\uparrow\downarrow}$ which consists of a disconnected part $G_{\uparrow\downarrow,\mathrm{dis}}$ and a connected part $G_{\uparrow\downarrow,\mathrm{con}}$. The latter consists of a vertex $F_{\uparrow\downarrow}$ and four external legs (one-particle correlators) G.

with the regular part

$$\widetilde{G}_{\uparrow\downarrow,\mathrm{con}}(\mathrm{i}\boldsymbol{\omega}) = \frac{2u\prod_{i=1}^{4}(\mathrm{i}\omega_i) + u^3\sum_{i=1}^{4}(\mathrm{i}\omega_i)^2 - 6u^5}{\prod_{i=1}^{4}[(\mathrm{i}\omega_i)^2 - u^2]}, \tag{5.1.23b}$$

and the anomalous parts containing Kronecker symbols

$$\widehat{G}^{(\omega_{12})}_{\uparrow\downarrow,\mathrm{con}}(\mathrm{i}\boldsymbol{\omega}) = \frac{\beta u^2}{\prod_{i=1}^{4}[\mathrm{i}\omega_i - u]}\delta_{0,\omega_{12}}\mathrm{th}, \tag{5.1.23c}$$

$$\widehat{G}^{(\omega_{13})}_{\uparrow\downarrow,\mathrm{con}}(\mathrm{i}\boldsymbol{\omega}) = \frac{\beta u^2}{\prod_{i=1}^{4}[\mathrm{i}\omega_i - u]}\delta_{0,\omega_{13}}(\mathrm{th}-1), \tag{5.1.23d}$$

$$\widehat{G}^{(\omega_{14})}_{\uparrow\downarrow,\mathrm{con}}(\mathrm{i}\boldsymbol{\omega}) = \frac{\beta u^2}{\prod_{i=1}^{4}[\mathrm{i}\omega_i - u]}\delta_{0,\omega_{14}}(\mathrm{th}+1), \tag{5.1.23e}$$

where we used the abbreviation $\mathrm{th} = \tanh(\beta u/2)$.

Furthermore, the interaction vertex $F_{\uparrow\downarrow}$ is obtained from the connected part $G_{\uparrow\downarrow,\mathrm{con}}$ by factoring out the propagators $G(\mathrm{i}\omega_i)$ (*external legs* in a diagrammatic language) of the incoming and outgoing particles, yielding

$$F_{\uparrow\downarrow}(\mathrm{i}\omega_1,\mathrm{i}\omega_2,\mathrm{i}\omega_3,\mathrm{i}\omega_4) = \frac{G_{\uparrow\downarrow,\mathrm{con}}(\mathrm{i}\omega_1,\mathrm{i}\omega_2,\mathrm{i}\omega_3,\mathrm{i}\omega_4)}{G(\mathrm{i}\omega_1)G(-\mathrm{i}\omega_2)G(\mathrm{i}\omega_3)G(-\mathrm{i}\omega_4)} = \widetilde{F}_{\uparrow\downarrow} + \widehat{F}^{(\omega_{12})}_{\uparrow\downarrow} + \widehat{F}^{(\omega_{13})}_{\uparrow\downarrow} + \widehat{F}^{(\omega_{14})}_{\uparrow\downarrow}, \tag{5.1.24a}$$

with the regular part

$$\widetilde{F}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}) = 2u + \frac{u^3 \sum_{i=1}^{4} (\mathrm{i}\omega_i)^2 - 6u^5}{\prod_{i=1}^{4} (\mathrm{i}\omega_i)}, \tag{5.1.24b}$$

and the anomalous parts containing Kronecker symbols

$$\widehat{F}^{(\omega_{12})}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}) = \beta u^2 \frac{\prod_{i=1}^{4} [\mathrm{i}\omega_i + u]}{\prod_{i=1}^{4} (\mathrm{i}\omega_i)} \delta_{0,\omega_{12}} \mathrm{th}, \tag{5.1.24c}$$

$$\widehat{F}^{(\omega_{13})}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}) = \beta u^2 \frac{\prod_{i=1}^{4} [\mathrm{i}\omega_i + u]}{\prod_{i=1}^{4} (\mathrm{i}\omega_i)} \delta_{0,\omega_{13}} (\mathrm{th} - 1), \tag{5.1.24d}$$

$$\widehat{F}^{(\omega_{14})}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}) = \beta u^2 \frac{\prod_{i=1}^{4} [\mathrm{i}\omega_i + u]}{\prod_{i=1}^{4} (\mathrm{i}\omega_i)} \delta_{0,\omega_{14}} (\mathrm{th} + 1). \tag{5.1.24e}$$

5.1.4 Susceptibilities

One of the main motivations for computing two-particle correlators is their close relationship to susceptibilities. They are physical observables measurable by experiment. For Hubbard-like interactions it has been shown [19, 20] that the susceptibilities are related to certain asymptotic functions of the vertex (see Sec. 5.5). Here we describe the standard approach to the computation of a susceptibility. A susceptibility is for example obtained from the MF function[1]

$$K(\tau) = \langle \mathcal{T}[n_\uparrow(\tau) n_\downarrow] \rangle - \langle n_\uparrow \rangle \langle n_\downarrow \rangle,$$

which can be computed from the 2p and 4p correlator via the limit

$$K(\tau) = \lim_{\substack{\tau_2 \to \tau^- \\ \tau_3 \to 0^-}} \langle \mathcal{T}[d_\uparrow(\tau_1) d^\dagger_\uparrow(\tau) d_\downarrow(\tau_3) d^\dagger_\downarrow] \rangle - \langle \mathcal{T}[d_\uparrow(\tau_1) d^\dagger_\uparrow(\tau)] \rangle \langle \mathcal{T}[d_\downarrow(\tau_3) d^\dagger_\downarrow] \rangle.$$

In frequency space this limit can be taken by parametrizing the frequencies in a suitable manner and then summing over the two fermionic frequencies. By use of frequency conservation we can express the 4-point correlator in terms of three independent frequencies

$$G_{\uparrow\downarrow}(\mathrm{i}\nu, \mathrm{i}\nu', \mathrm{i}\omega) = \int_0^\beta \mathrm{d}\tau_1 \mathrm{d}\tau_2 \mathrm{d}\tau_3 \, G_{\uparrow\downarrow}(\tau_1, \tau_2, \tau_3, 0) e^{\mathrm{i}\nu(\tau_2 - \tau_1) + \mathrm{i}\omega(\tau_2 - \tau_3) - \mathrm{i}\nu'\tau_3},$$

[1] The corresponding real-time response functions is obtained in frequency space via the well-known analytic analytic continuation for retarded 2p functions $K^R(\omega) = K(\mathrm{i}\omega)|_{\mathrm{i}\omega \to \omega + \mathrm{i}0^+}$ [10].

such that the above susceptibility is obtained by summing over the fermionic Matsubara frequencies ν and ν'

$$K(\mathrm{i}\omega) = -\sum_{\nu,\nu'}[G_{\uparrow\downarrow}(\mathrm{i}\nu,\mathrm{i}\nu',\mathrm{i}\omega) - \beta\delta_{0,\omega}G(\mathrm{i}\nu)G(\mathrm{i}\nu')]e^{-\mathrm{i}(\nu+\nu')0^+}.$$

Different "pairings" of the four operators in $G_{\sigma_1\sigma_2\sigma_3\sigma_4}$ correspond to different generalized susceptibilities [19, 20]. Using the definition of the three channels in Ref. [43] they give

$$\begin{aligned}
\chi_{a,\sigma\sigma'}(\mathrm{i}\nu_a,\mathrm{i}\nu'_a,\mathrm{i}\omega_a) &= -G_{\sigma\sigma'}(\mathrm{i}\nu_a,\mathrm{i}\nu'_a,\mathrm{i}\omega_a) + \zeta\beta\delta_{\omega_a,0}\delta_{\sigma\sigma'}G(\mathrm{i}\nu_a)G(\mathrm{i}\nu'_a),\\
\chi_{t,\sigma\sigma'}(\mathrm{i}\nu_t,\mathrm{i}\nu'_t,\mathrm{i}\omega_t) &= -G_{\sigma\sigma'}(\mathrm{i}\nu_t,\mathrm{i}\nu'_t,\mathrm{i}\omega_t) + \beta\delta_{\omega_t,0}G(\mathrm{i}\nu_t)G(\mathrm{i}\nu'_t),\\
\chi_{p,\sigma\sigma'}(\mathrm{i}\nu_p,\mathrm{i}\nu'_p,\mathrm{i}\omega_p) &= -G_{\sigma\sigma'}(\mathrm{i}\nu_p,\mathrm{i}\nu'_p,\mathrm{i}\omega_p),
\end{aligned} \tag{5.1.25}$$

for which we defined suitable frequency parametrizations by

$$\begin{aligned}
&\omega_1 = \nu_a, && \omega_1 = \nu_t, && \omega_1 = \nu_p,\\
&\omega_2 = -\nu'_a, && \omega_2 = -\nu_t - \omega_t, && \omega_2 = \nu'_p + \omega_p,\\
&\omega_3 = \nu'_a + \omega_a, && \omega_3 = \nu'_t + -\omega_t, && \omega_3 = -\nu_p - \omega_p,\\
&\omega_4 = -\nu_a - \omega_a, && \omega_4 = -\nu'_t, && \omega_4 = -\nu'_p.
\end{aligned} \tag{5.1.26}$$

Hence, the physical susceptibilities are obtained by summing over the corresponding fermionic frequencies, i.e.

$$\chi_{r,\sigma\sigma'}(\mathrm{i}\omega_r) = \sum_{\nu_r,\nu'_r}\chi_{r,\sigma\sigma'}(\mathrm{i}\nu_r,\mathrm{i}\nu'_r,\mathrm{i}\omega_r). \tag{5.1.27}$$

These susceptibilities can be computed directly for the Hubbard atom and give for example

$$\chi_{a,\uparrow\downarrow}(\mathrm{i}\omega_a) = -\frac{\beta}{4}\delta_{\omega_a,0}(\mathrm{th}+1), \tag{5.1.28a}$$

$$\chi_{t,\uparrow\downarrow}(\mathrm{i}\omega_t) = -\frac{\beta}{4}\delta_{\omega_t,0}\mathrm{th}, \tag{5.1.28b}$$

$$\chi_{p,\uparrow\downarrow}(\mathrm{i}\omega_p) = -\frac{\beta}{4}\delta_{\omega_p,0}(\mathrm{th}-1). \tag{5.1.28c}$$

They are constants in the time domain. The factor of β is merely an artifact of the Fourier transformation for which one integrates over an interval of length β. In the KF only the Keldysh component is nonzero and e.g. gives for the a-channel $\chi^K_{a,\uparrow\downarrow} = -\pi\mathrm{i}\delta(\omega_a)(\mathrm{th}+1)$. These results will be recovered in Sec. 5.5 by computing the vertex asymptotics according to Wentzell et al. [20].

5.2 Another spectral representation for the KF

In this section we derive a spectral representation for Keldysh correlators which deviates from the one used in chapter 2. It is however widely used in the literature [22–24, 26]. Even

though the final results are independent of the representation, the following one provided simpler intermediate results. It shifts a part of the complexity to the partial spectral functions, while the convolution kernels are exclusively time-ordered ones.

The idea behind this spectral representation is to attach the contour index not to the kernel but to the operators. Hence, every operator carries a *contour index* $\mathcal{O}^{i,c_i}(t_i)$ with $c_i \in \{-,+\}$. Note that $\mathcal{O}^{i,c_i}(t_i)$ and $\mathcal{O}^{i}(t_i^{c_i})$ are in fact equivalent. In a spectral representation the first notation is prefered when allocating the contour and Keldysh indices to the PSF, the latter notation when allocating them to the kernel.

Both contour index and time determine the ordering of operators on the *Keldysh contour*. The Keldysh contour consists of a time-ordered branch (associated with index $c_i = -$) followed by an anti-time-ordered branch ($c_i = +$), such that the *contour ordering operator* $\mathcal{T}_c$ sorts all operators with contour index $+$ to the left of those with index $-$. The operators on the time-ordered branch ($c_i = -$) are ordered such that operators $\mathcal{O}^{i,-}(t_i)$ with a smaller time appear on the right of those with a bigger time. Operators on the anti-time-ordered branch ($c_i = +$) are ordered conversely. Thereby we obtain the Keldysh ℓ-point correlator in the contour basis

$$\mathcal{G}^{c_1\dots c_\ell}(t_1,\dots,t_\ell) = (-\mathrm{i})^{\ell-1}\langle\mathcal{T}_c\big[\mathcal{O}^{1,c_1}(t_1)\dots\mathcal{O}^{\ell,c_\ell}(t_\ell)\big]\rangle. \tag{5.2.1}$$

In the following we choose to work in the *Keldysh basis* in which the correlators are given by linear combinations of correlators in the contour basis. The Keldysh indices $k_i \in \{1,2\}$ determine the exact linear combination via the transformation matrix D with the entries A ℓ-point correlator in the Keldysh basis is then given by

$$\mathcal{G}^{k_1\dots k_\ell} = \sum_{c_1,\dots,c_\ell\in\{-,+\}} \left(\prod_{i=1}^{\ell} D^{k_i,c_i}\right)\mathcal{G}^{c_1\dots c_\ell}, \qquad \text{with } D^{k_i\pm} = \frac{(\mp 1)^{k_i}}{\sqrt{2}}. \tag{5.2.2}$$

Alternatively, one can define the operator $\mathcal{O}^{i,k_i}$ with Keldysh index $k_i \in \{1,2\}$ as

$$\mathcal{O}^{i,k_i} = \frac{1}{\sqrt{2}}(\mathcal{O}^{i,-} + (-1)^k\mathcal{O}^{i,+}) \tag{5.2.3}$$

such that the correlator becomes

$$\mathcal{G}^{k_1\dots k_\ell}(t_1,\dots,t_\ell) = (-\mathrm{i})^{\ell-1}\langle\mathcal{T}_c[\mathcal{O}^{1,k_1}(t_1)\dots\mathcal{O}^{\ell,k_\ell}(t_\ell)]\rangle. \tag{5.2.4}$$

The Keldysh basis has the advantage that it exploits the linear dependence of correlators in the contour basis. Thereby a correlator for which all Keldysh indices are $k_i = 1$ is known to give zero, i.e. $G^{1\dots1} = 0$. This fact is closely linked to a *theorem of causality* [22, 32] by which the correlator vanishes if the operator with biggest time argument carries the Keldysh index 1. The situation is demonstrated in Fig. 5.2 where the correlators are independent of the contour index c_1. For $k_1 = 1$ the Keldysh rotation according to D subtracts the correlators with $c_1 = -$ and with $c_1 = +$ to give zero.

Another advantage of the Keldysh basis is that it has a close relation to the results in Matsubara formalism. As shown in chapters 2 and 3 one can express the correlators in Keldysh formalism in terms of analytic continuations of the correlator in Matsubara formalism.

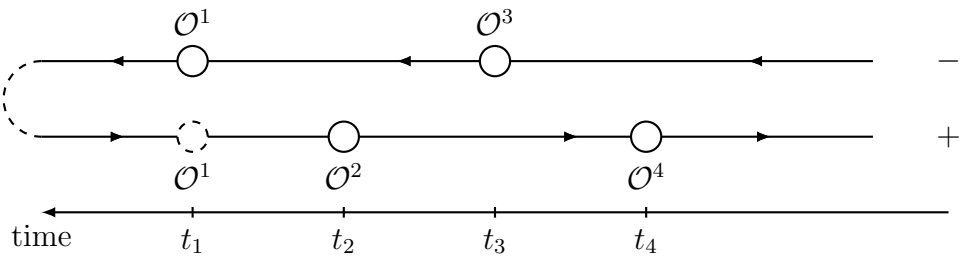

Figure 5.2: Demonstration of the ordering on the Keldysh contour: The effect of the ordering operator on the depicted situation $\mathcal{T}_c[\mathcal{O}^{1,c_1}(t_1)\mathcal{O}^{2,+}(t_2)\mathcal{O}^{3,-}(t_3)\mathcal{O}^{4,+}(t_4)] = \mathcal{O}^{4,+}(t_4)\mathcal{O}^{2,+}(t_2)\mathcal{O}^{1,c_1}(t_1)\mathcal{O}^{3,-}(t_3)$ is independent of the contour index $c_1 \in \{-,+\}$ of the operator $\mathcal{O}^1$ with the biggest time.

Spectral representation of KF correlators

For a systematic computation of Keldysh correlators we want to make use of a spectral representation which explicitly takes into account the ordering structure of the Keldysh contour. For brevity we write the arguments of an ℓ-point correlator with tuples, e.g. $\boldsymbol{k} = (k_1, ..., k_\ell)$. In the spectral representation the correlator is expressed as a sum over all permutations $p = (\overline{1}, ..., \overline{\ell})$ of the indices $(1, ..., \ell)$. A tuple which has been permuted according to permutation p gives e.g. $\boldsymbol{t}_p = (t_{\overline{1}}, ..., t_{\overline{\ell}})$.

A simple spectral representation can be given for the time-ordered correlator (with contour indices $\boldsymbol{c} = (-, ..., -)$). It can be written as

$$\mathcal{G}^{-\cdots-}(\boldsymbol{t}) = \sum_p \mathcal{S}_p(\boldsymbol{t}_p)\, \mathcal{K}^{\mathcal{T}}(\boldsymbol{t}_p) \tag{5.2.5}$$

where the kernel

$$\mathcal{K}^{\mathcal{T}}(\boldsymbol{t}_p) = \prod_{i=1}^{\ell-1} [-\mathrm{i}\, \theta(t_{\overline{i}} - t_{\overline{i+1}})] \tag{5.2.6}$$

is a product of step functions θ which explicitly implements time-ordering. It picks out the correctly ordered *partial spectral function* for given times $\boldsymbol{t}_p$. The partial spectral function (PSF) for the permutation $p = (\overline{1}, ..., \overline{\ell})$ of the operators is defined as

$$\mathcal{S}_p(\boldsymbol{t}_p) = \boldsymbol{\zeta}^p \langle \mathcal{O}^{\overline{1}}(t_{\overline{1}}) ... \mathcal{O}^{\overline{\ell}}(t_{\overline{\ell}}) \rangle. \tag{5.2.7}$$

We have included the sign factor $\boldsymbol{\zeta}^p$ into the definition of the partial spectral function to simplify our notation. It accounts for the bosonic or fermionic exchange symmetry of the operators $\mathcal{O}^i$ and is $+1$ or -1 if the permutation p contains an even or uneven number of transpositions of fermionic operators. By including the sign factor in the partial spectral function S_p we avoid notational clutter when we take linear combinations of them by (anti-)commutators

$$\mathcal{S}_{[A;B]_\pm} = \mathcal{S}_{AB} \pm \mathcal{S}_{BA} \tag{5.2.8}$$

where the tuples A and B have been combined to a permutation p once in the order AB and once in the order BA.

We will argue that the Keldysh correlator is given by

$$\mathcal{G}^{\boldsymbol{k}}(\boldsymbol{t}) = 2^{1-\ell/2} \sum_p \mathcal{S}_p^{\boldsymbol{k}_p}(\boldsymbol{t}_p)\, \mathcal{K}^{\mathcal{T}}(\boldsymbol{t}_p) \tag{5.2.9}$$

where the partial spectral function (with Keldysh indices $\boldsymbol{k}_p$) for permutation $p = (\overline{1}, ..., \overline{\ell})$ is defined as

$$\mathcal{S}_p^{\boldsymbol{k}_p}(\boldsymbol{t}_p) = \begin{cases} 0, & \text{for } k_{\overline{1}} = 1, \\ \mathcal{S}_{[...[[\overline{1};\overline{2}]_{(-1)^{k_{\overline{2}}}};\overline{3}]_{(-1)^{k_{\overline{3}}}};...;\overline{\ell}]_{(-1)^{k_{\overline{\ell}}}}}, & \text{for } k_{\overline{1}} = 2. \end{cases} \tag{5.2.10}$$

For purely bosonic (fermionic) operators we can write this more explicitly as

$$\mathcal{S}_p^{\boldsymbol{k}_p}(\boldsymbol{t}_p) = \begin{cases} 0, & \text{for } k_{\overline{1}} = 1, \\ \boldsymbol{\zeta}^P \langle [...[[\mathcal{O}^{\overline{1}}(t_{\overline{1}}), \mathcal{O}^{\overline{2}}(t_{\overline{2}})]_{\zeta(-1)^{k_{\overline{2}}}}, \mathcal{O}^{\overline{3}}(t_{\overline{3}})]_{\zeta^2(-1)^{k_{\overline{3}}}}, ..., \mathcal{O}^{\overline{\ell}}(t_{\overline{\ell}})]_{\zeta^{\ell-1}(-1)^{k_{\overline{\ell}}}} \rangle, & \text{for } k_{\overline{1}} = 2. \end{cases} \tag{5.2.11}$$

with $\zeta = +1$ ($\zeta = -1$) where the (anti-)commutators of operators are defined in the usual way as $[\mathcal{O}^1, \mathcal{O}^2]_\pm = \mathcal{O}^1\mathcal{O}^2 \pm \mathcal{O}^2\mathcal{O}^1$. Note that by including the sign factor $\boldsymbol{\zeta}^p$ into the definition of $\mathcal{S}$ we are able to express Eq. (5.2.9) without specifying for the bosonic and fermionic exchange symmetry. Especially mixed systems with both bosonic and fermionic operators would otherwise lead to a clutter of sign factors. The sign factor $\boldsymbol{\zeta}^p$ is, of course, only defined with respect to a standard ordering which is given by the definition of the correlator in Eq. (5.2.4).

To derive the spectral representation in Eq. (5.2.9) we use the kernels $\mathcal{K}^{\mathcal{T}}$ only to obtain a partition of $\mathbb{R}^\ell$. In each of these partitions the ordering of the times $\boldsymbol{t}$ is fixed. Now consider one fixed time-ordering by picking a $p = (\overline{1}, ..., \overline{\ell})$ such that $t_{\overline{i}} > t_{\overline{i+1}}$.

By definition of the correlator in the Keldysh basis according to Eqs. (5.2.3) and (5.2.4) we have to consider all possible contour indices $\boldsymbol{c}$ and add them with the correct sign factor. Each configuration of $\boldsymbol{c}$ corresponds to a certain ordering. To depict the situation we can align the operators along the time axis as in Fig. 5.2 and consider for each operator the possibilities $c_i = -$ and $c_i = +$. The operator $\mathcal{O}^{\overline{\ell}}$ with the smallest time argument appears either on the right of all the others (for $c_\ell = -$) or on the left of the others (for $c_{\overline{\ell}} = +$). The latter partial spectral function $\mathcal{S}_p$ needs to be added with the sign factor $(-1)^{k_\ell}$. Such a linear combination can be written with the (anti-)commutator notation introduced in Eq. (5.2.8). In general, the operator $\mathcal{O}^{\overline{j}}$ appears on the right of those $\mathcal{O}^{\overline{i}}$ with $i < j$ for $c_{\overline{j}} = -$ and on the left of them for $c_{\overline{j}} = +$. For the biggest time operator $\mathcal{O}^{\overline{1}}$ one reproduces the theorem of causality.

The spectral representation in Eq. (5.2.9) can also be used in frequency space. The partial spectral functions $\mathcal{S}_p$ and the kernels $\mathcal{K}^{\mathcal{T}}$ can be Fourier transformed individually. By the convolution theorem the multiplicative structure turns into a ℓ-fold convolution of

the partial spectral function and the kernel, giving

$$\mathcal{G}^{\boldsymbol{k}}(\boldsymbol{\omega}) = 2^{1-\ell/2}\sum_p \big(\mathcal{S}_p^{\boldsymbol{k}_p} * \mathcal{K}^{\mathcal{T}}\big)(\boldsymbol{\omega}_p) = 2^{1-\ell/2}\sum_p \int_{\mathbb{R}^\ell} \frac{\mathrm{d}^\ell \omega'_p}{(2\pi)^\ell}\, \mathcal{S}_p^{\boldsymbol{k}_p}(\boldsymbol{\omega}'_p)\, \mathcal{K}^{\mathcal{T}}(\boldsymbol{\omega}_p - \boldsymbol{\omega}'_p), \tag{5.2.12}$$

where the kernel in frequency space is

$$\mathcal{K}^{\mathcal{T}}(\boldsymbol{\omega}_p) = 2\pi\delta(\omega_{1\ldots\ell})\prod_{i=1}^{\ell-1}(\omega^+_{\bar{1}\ldots\bar{i}})^{-1}. \tag{5.2.13}$$

Here we again abbreviate the sum of frequencies with $\omega_I = \sum_{i\in I}\omega_i$. The superscript of such a sum of frequencies indicates whether the infinitesimal imaginary part of the sum is positive or negative, i.e. $\omega_I^\pm = \omega_I \pm \mathrm{i}0^+$. The significance of the sign of the imaginary part becomes obvious when one considers the inverse Fourier transformation of a step function in Eq. (2.3.5) which is sensitive to this sign. It is thus important to recover the correct kernel $\mathcal{K}^{\mathcal{T}}$ on the time-domain.

5.3 Explicit computation of the correlators

We use the spectral representation from the previous section to compute the connected part of the KF correlator $G_{\uparrow\downarrow,\mathrm{con}}$ of the fermionic Hubbard atom at half-filling. The full 4-point correlator is defined as

$$\mathcal{G}^{k_1k_2k_3k_4}_{\uparrow\downarrow}(t_1,t_2,t_3,t_4) = (-\mathrm{i})^3\langle\mathcal{T}_c\big[d^{k_1}_\uparrow(\tau_1)d^{\dagger,k_2}_\uparrow(\tau_2)d^{k_3}_\downarrow(\tau_3)d^{\dagger,k_4}_\downarrow(\tau_4)\big]\rangle. \tag{5.3.1}$$

In App. C.1 we present explicit computations of selected the KF components. Defining the function

$$\Phi_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = \frac{1}{2}\frac{2u\prod_{i=1}^4 z_i + u^3\sum_{i=1}^4 (z_i)^2 - 6u^5}{\prod_{i=1}^4[(z_i)^2-u^2]}. \tag{5.3.2}$$

we obtain for the connected part of the correlator $G_{\uparrow\downarrow,\mathrm{con}}$:

$$G^{1111}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = 0, \tag{5.3.3a}$$
$$G^{2111}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-), \tag{5.3.3b}$$
$$G^{1211}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-), \tag{5.3.3c}$$
$$G^{1121}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-), \tag{5.3.3d}$$
$$G^{1112}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+). \tag{5.3.3e}$$
$$G^{1122}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{2\pi\mathrm{i}u^2[\delta(\omega_{14})-\delta(\omega_{13})]}{[(\omega_1^-)^2-u^2][(\omega_2^-)^2-u^2]}$$

$$+ u^2\mathrm{th} \times \left[\frac{1}{[(\omega_3^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \left(\frac{1}{\omega_{24}^-} + \frac{1}{\omega_{14}^-} \right) - \text{ c.c. } \right], \tag{5.3.3f}$$

$$G^{1212}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{2\pi \mathrm{i} u^2 \delta(\omega_{14})}{[(\omega_1^-)^2 - u^2][(\omega_3^-)^2 - u^2]}$$
$$+ u^2\mathrm{th} \times \left[\frac{1}{[(\omega_2^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \left(\frac{1}{\omega_{34}^-} + \frac{1}{\omega_{14}^-} \right) - \text{ c.c. } \right], \tag{5.3.3g}$$

$$G^{1221}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{-2\pi \mathrm{i} u^2 \delta(\omega_{13})}{[(\omega_1^-)^2 - u^2][(\omega_4^-)^2 - u^2]}$$
$$+ u^2\mathrm{th} \times \left[\frac{1}{[(\omega_2^+)^2 - u^2][(\omega_3^-)^2 - u^2]} \left(\frac{1}{\omega_{34}^-} + \frac{1}{\omega_{13}^-} \right) - \text{ c.c. } \right], \tag{5.3.3h}$$

$$G^{2112}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{-2\pi \mathrm{i} u^2 \delta(\omega_{13})}{[(\omega_2^-)^2 - u^2][(\omega_3^-)^2 - u^2]}$$
$$+ u^2\mathrm{th} \times \left[\frac{1}{[(\omega_1^+)^2 - u^2][(\omega_4^-)^2 - u^2]} \left(\frac{1}{\omega_{34}^-} + \frac{1}{\omega_{24}^-} \right) - \text{ c.c. } \right], \tag{5.3.3i}$$

$$G^{2121}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{2\pi \mathrm{i} u^2 \delta(\omega_{14})}{[(\omega_2^-)^2 - u^2][(\omega_4^-)^2 - u^2]}$$
$$+ u^2\mathrm{th} \times \left[\frac{1}{[(\omega_1^+)^2 - u^2][(\omega_3^-)^2 - u^2]} \left(\frac{1}{\omega_{34}^-} + \frac{1}{\omega_{23}^-} \right) - \text{ c.c. } \right], \tag{5.3.3j}$$

$$G^{2211}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{2\pi \mathrm{i} u^2 [\delta(\omega_{14}) - \delta(\omega_{13})]}{[(\omega_3^-)^2 - u^2][(\omega_4^-)^2 - u^2]}$$
$$+ u^2\mathrm{th} \times \left[\frac{1}{[(\omega_1^+)^2 - u^2][(\omega_2^-)^2 - u^2]} \left(\frac{1}{\omega_{24}^-} + \frac{1}{\omega_{23}^-} \right) - \text{ c.c. } \right], \tag{5.3.3k}$$

$$G^{1222}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-, \omega_2^+, \omega_3^+, \omega_4^+)$$
$$+ 2\pi^2 u\,\mathrm{th} \times [\delta(\omega_2 - u) + \delta(\omega_2 + u)][\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{\left(\omega_1^-\right)^2 - u^2}, \tag{5.3.3l}$$

$$G^{2122}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+, \omega_2^-, \omega_3^+, \omega_4^+)$$
$$+ 2\pi^2 u\,\mathrm{th} \times [\delta(\omega_1 - u) + \delta(\omega_1 + u)][\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{\left(\omega_2^-\right)^2 - u^2}, \tag{5.3.3m}$$

$$G^{2212}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+, \omega_2^+, \omega_3^-, \omega_4^+)$$
$$+ 2\pi^2 u\,\mathrm{th} \times [\delta(\omega_4 - u) + \delta(\omega_4 + u)][\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{\left(\omega_3^-\right)^2 - u^2}, \tag{5.3.3n}$$

$$G^{2221}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+, \omega_2^+, \omega_3^+, \omega_4^-)$$
$$+ 2\pi^2 u\,\mathrm{th} \times [\delta(\omega_3 - u) + \delta(\omega_3 + u)][\delta(\omega_{14}) - \delta(\omega_{13})] \frac{1}{\left(\omega_4^-\right)^2 - u^2}, \tag{5.3.3o}$$

$$G^{2222}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \frac{\mathrm{th}}{u} \Big[\omega_1^+ \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+, \omega_2^-, \omega_3^-, \omega_4^-) + \omega_2^+ \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-, \omega_2^+, \omega_3^-, \omega_4^-)$$

$$+\omega_3^+\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)+\omega_4^+\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\Big]$$
$$-\mathrm{i}4\pi^3\mathrm{th}^2\times\delta(\omega_{12})[\delta(u+\omega_1)-\delta(u-\omega_1)][\delta(u+\omega_3)-\delta(u-\omega_3)], \quad (5.3.3\mathrm{p})$$

where c.c. is the complex conjugate and we abbreviated $\mathrm{th}=\tanh(\beta u/2)$. In App. C.3 we check the consistency of the results. There we verify that the components fulfill the FDRs and the spin symmetry relation in Eq. (5.1.21). The disconnected part of the correlators can be computed separately with the one-particle correlators $G^{k_1k_2}$ and $G^{k_3k_4}$.

5.4 Derivation of the correlator $G_{\uparrow\downarrow}$ via analytic continuation

An alternative way to compute the correlator in Keldysh formalism is by analytic continuation of the Matsubara correlator. The corresponding formulas are derived in chapter 2. To do so we first analyze the correlator in Matsubara formalism given in Eq. (5.1.23). It consists of a *regular part* $\widetilde{G}_{\uparrow\downarrow,\mathrm{con}}$ which is analytic in its frequency arguments and several anomalous parts $\widehat{G}^{(\omega_I)}_{\uparrow\downarrow,\mathrm{con}}\propto\delta_{\omega_I,0}$.

The analytic continuation of the regular part to complex frequencies $z_i=\omega_i+\mathrm{i}\gamma$ is given by the function

$$\Phi_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4)=\frac{1}{2}\frac{2u\prod_{i=1}^4 z_i+u^3\sum_{i=1}^4(z_i)^2-6u^5}{\prod_{i=1}^4[(z_i)^2-u^2]}. \quad (5.4.1)$$

Here we have already included the global prefactor of 1/2 due to the Keldysh rotation. Note that, as we discussed in 2.3.1, the analytic continuation of a 4p correlator $\overline{\Phi}$ generally has branchcuts at

$$\mathrm{Im}(z_i)=0,\quad i\in\{1,..,4\},\qquad\text{and}\qquad\mathrm{Im}(z_{ij})=0,\quad i,j\in\{1,..,4\}\text{ with }i\neq j.$$

However, for $\Phi_{\uparrow\downarrow,\mathrm{con}}$ in Eq. (5.4.1) there are no branchcuts of the type $\mathrm{Im}(\omega_{ij})=0$. Since the function $\Phi_{\uparrow\downarrow,\mathrm{con}}$ is analytic at these branchcuts also the corresponding discontinuities of $\Phi_{\uparrow\downarrow,\mathrm{con}}$ are zero. Therefore $\Phi_{\uparrow\downarrow,\mathrm{con}}$ is sufficiently characterized by specifying $z_i\in\{\omega_i^\pm\}$ for the four single complex frequencies, e.g. $\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)=G^{[1]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega})$ is an analytic continuation equivalent to a retarded correlator.

For the anomalous parts $\widehat{G}^{(\omega_I)}_{\uparrow\downarrow,\mathrm{con}}\propto\delta_{\omega_I,0}$ in Eq. (5.1.23) we follow the prescription in Sec. 3.1.3: we replace the Kronecker symbol by a Dirac delta function $\beta\delta_{\omega_I,0}\to 2^{1-\ell/2}4\pi\mathrm{i}\delta(\omega_I)$, thereby already including the factor due to the Keldysh rotation, and define the following functions as the analytic continuations of the anomalous parts

$$\widehat{\Phi}_{\uparrow\downarrow,\mathrm{dis}}(z_1,z_2,z_3,z_4)=-\frac{z_1z_3}{\prod_{i=1}^4[z_i-u]}2\pi\mathrm{i}\delta(\omega_{12}), \quad (5.4.2\mathrm{a})$$

$$\widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = \frac{u^2}{\prod_{i=1}^{4}[z_i-u]} 2\pi\mathrm{i}\delta(\omega_{12})\tanh(\beta u/2), \tag{5.4.2b}$$

$$\widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = \frac{u^2}{\prod_{i=1}^{4}[z_i-u]} 2\pi\mathrm{i}\delta(\omega_{13})[\tanh(\beta u/2)-1], \tag{5.4.2c}$$

$$\widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = \frac{u^2}{\prod_{i=1}^{4}[z_i-u]} 2\pi\mathrm{i}\delta(\omega_{14})[\tanh(\beta u/2)+1]. \tag{5.4.2d}$$

Note that the complex frequencies $\boldsymbol{z}$ are subject to the constraint of conservation of total real frequency such that the imaginary parts have to be consistent, e.g. $\omega_1^{\pm} = -\omega_{234}^{\mp}$ must hold. This is most easily ensured by demanding that also the imaginary frequencies add up to zero, i.e. $z_{1234} = 0$. For the analytic continuations of the anomalous parts we have the additional Dirac delta function, such that we get e.g. $z_{12} = 0 = z_{34}$ for $\widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}$.

The correlators with up to two 2-indices can be easily obtained by analytic continuation following the formula in App. B. In the following we already make use of the fact that the AC functions for $\Phi_{\uparrow\downarrow,\mathrm{con}}$ are sufficiently specified by choosing $z_i \in \{\omega_i^+, \omega_i^-\}$ for the four single frequencies. Using the statistical factor $N_i = \tanh(\beta\omega_i/2)$ the connected part of the correlators are expressed in terms of the functions, defined in Eq. (5.4.1) and Eqs. (5.4.2),

$$G^{[]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = 0, \tag{5.4.3a}$$

$$G^{[4]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+), \tag{5.4.3b}$$

$$G^{[3]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-), \tag{5.4.3c}$$

$$G^{[2]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-), \tag{5.4.3d}$$

$$G^{[1]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-), \tag{5.4.3e}$$

$$\begin{aligned} G^{[34]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = {} & +N_3\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\big] \\ & + N_4\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)\big] \\ & + \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+), \end{aligned} \tag{5.4.3f}$$

$$\begin{aligned} G^{[24]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = {} & +N_2\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\big] \\ & + N_4\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\big] \\ & + \widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+) + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+), \end{aligned} \tag{5.4.3g}$$

$$\begin{aligned} G^{[23]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = {} & +N_2\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)\big] \\ & + N_3\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\big] \\ & + \widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) + \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-), \end{aligned} \tag{5.4.3h}$$

$$\begin{aligned} G^{[14]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = {} & +N_1\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\big] \\ & + N_3\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)\big] \end{aligned}$$

$$+\widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^+)+\widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^+), \tag{5.4.3i}$$

$$\begin{aligned} G^{[13]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = &+N_1\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^+,\omega_4^-)-\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)\big]\\ &+N_3\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^+,\omega_4^-)-\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)\big]\\ &+\widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^+,\omega_4^-)+\widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^+,\omega_4^-), \end{aligned} \tag{5.4.3j}$$

$$\begin{aligned} G^{[12]}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = &+N_1\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-)-\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\big]\\ &+N_2\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-)-\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)\big]\\ &+\widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-)+\widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-), \end{aligned} \tag{5.4.3k}$$

In App. C.2 we demonstrate that these components agree with those obtained by a direct computation. The remaining KF components can most easily be computed by use of the generalized FDR in [12]. In Sec. C.3.1 we exemplify such a computation with some KF components.

5.5 The vertex function

In Sec. 4.2 we already discussed vertex functions in general. We argued that they have the very same analytic structure as the corresponding correlators and can be computed with the same linear combinations of AC functions. We confirm this in App. C.4 with a direct computation for the components with up to two 1's in the Keldysh indices.

In the next step we consider the asymptotic behavior of the vertex. For this purpose it is convenient to express the vertex in terms of the corresponding AC functions. Thereby the asymptotics of a KF component of the vertex depends on the asymptotics of the AC functions and the statistical factors needed for its construction. As we argued in Sec. 5.5 one obtains the KF vertex with the very same formulas as for KF correlators. The analytic continuation of the regular and anomalous contributions in Eq. (5.1.24) reads

$$\widetilde{\Phi}^{(F)}_{\uparrow\downarrow}(\boldsymbol{z}) = u + \frac{u^3\sum_{i=1}^{4} z_i^2 - 6u^5}{2\prod_{i=1}^{4} z_i}, \tag{5.5.1a}$$

$$\widehat{\Phi}^{(F,12)}_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = u^2\frac{\prod_{i=1}^{4}[z_i+u]}{\prod_{i=1}^{4} z_i} 2\pi\mathrm{i}\delta(\omega_{12})\tanh(\beta u/2), \tag{5.5.1b}$$

$$\widehat{\Phi}^{(F,13)}_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = u^2\frac{\prod_{i=1}^{4}[z_i+u]}{\prod_{i=1}^{4} z_i} 2\pi\mathrm{i}\delta(\omega_{13})[\tanh(\beta u/2)-1], \tag{5.5.1c}$$

$$\widehat{\Phi}^{(F,14)}_{\uparrow\downarrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = u^2 \frac{\prod_{i=1}^{4}[z_i+u]}{\prod_{i=1}^{4} z_i} 2\pi\mathrm{i}\delta(\omega_{14})[\tanh(\beta u/2)+1]. \tag{5.5.1d}$$

Using these functions one can express the vertex function conveniently using the same linear combinations as for correlators. These are exactly the same linear combinations as for correlators [see Eqs. (5.4.3)], the only difference being that for vertex functions the roles of the Keldysh indices 1 and 2 interchange, such that e.g. a retarded vertex is given by

$$F^{[1]}_{\uparrow\downarrow} = F^{1222}_{\uparrow\downarrow} = \widetilde{\Phi}^{(F)}_{\uparrow\downarrow}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-).$$

For the statistical factors in Eq. (5.4.3) the low-temperature and high-frequency limit is given by

$$|\tanh(\beta\omega_i)| \overset{\beta\to\infty}{\longrightarrow} 1, \quad |\tanh(\beta\omega_i)| \overset{\omega_i\to\pm\infty}{\longrightarrow} 1. \tag{5.5.2}$$

Hence, the asymptotic behavior of the vertex is mostly determined by the AC functions in Eq. (5.5.1). While the regular part $\widetilde{\Phi}^{(F)}_{\uparrow\downarrow}$ is temperature-independent, the anomalous parts depend on the expression $\tanh(\beta u/2) \overset{\beta\to\infty}{\longrightarrow} 1$, leading to a vanishing $\widehat{\Phi}^{(F,13)}_{\uparrow\downarrow,\mathrm{con}}$. Note that the anomalous parts of the MF carry a factor of $\beta\delta_\omega$ which has to be replaced by a $2\pi\mathrm{i}\delta(\omega)$ as part of the analytic continuation to the KF correlator. So, unlike in the MF [19], there is no divergence of the vertex at zero temperature. As we mentioned after Eq. (5.1.28), the factors of β accompanying a Kronecker symbol are merely artifacts of the integration interval in the MF.

In the following we consider the asymptotic behavior of the Hubbard atom, following the discussion of Wentzell et al. in Ref. [20]. There the authors analyzed the asymptotics of vertex functions diagrammatically and presented the asymptotic functions of the Hubbard atom in MF. The bottom line of our discussion is that their results can be directly adopted to the KF via our formula for analytic continuation. Wentzell et al. used a decomposition of the full Matsubara vertex $F_{\uparrow\downarrow}$ in four functions

$$F_{\uparrow\downarrow} = \mathcal{F}_{\mathrm{odd}} + \mathcal{F}_a + \mathcal{F}_t + \mathcal{F}_p \tag{5.5.3}$$

which is identical to our decomposition in regular and anomalous parts according to Eq. (5.1.24)

$$\mathcal{F}_{\mathrm{odd}}(\mathrm{i}\boldsymbol{\omega}) = \widetilde{F}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}), \quad \mathcal{F}_a(\mathrm{i}\boldsymbol{\omega}) = \widehat{F}^{(\omega_{14})}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}), \quad \mathcal{F}_t(\mathrm{i}\boldsymbol{\omega}) = \widehat{F}^{(\omega_{12})}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}), \quad \mathcal{F}_p(\mathrm{i}\boldsymbol{\omega}) = \widehat{F}^{(\omega_{13})}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}). \tag{5.5.4}$$

The asymptotic behavior of these four functions can be analyzed separately. The Matsubara functions $\mathcal{F}$ and the corresponding AC functions in Eqs. (5.5.1) have very similar asymptotic behavior. For the Keldysh correlators the AC functions are multiplied with prefactors of $\tanh(x) \overset{x\to\pm\infty}{\longrightarrow} \pm 1$ which do not significantly change the asymptotic behavior of the functions.

For a quick example we present an asymptotic Keldysh function in the a-channel by adopting the results from Ref. [20]. Firstly, we realize that we indeed obtain the *bare* vertex of the onsite-interaction in case all frequencies ω_i are sent to infinity, giving

$$\lim_{\substack{|\omega_i|\to\infty \\ \forall i\in\{1,..,4\}}} \widetilde{\Phi}^{(F)}_{\uparrow\downarrow} = u, \qquad \Rightarrow \quad F^{k_1k_2k_3k_4}_{0,\uparrow\downarrow} = \begin{cases} u, & \text{if } k_1+k_2+k_3+k_4 \text{ is odd,} \\ 0, & \text{else.} \end{cases} \tag{5.5.5}$$

These constant contributions can be subtracted when investigating the asymptotic behavior. Using the a-channel frequency variables defined in Eq. (5.1.26) Wentzell et al. find that the MF vertex has the asymptotic function

$$\begin{aligned} \mathcal{K}_{1,a}(\mathrm{i}\omega_a) &= \lim_{|\nu_a|,|\nu'_a|\to\infty} F_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}) - F_{0,\uparrow\downarrow} \\ &= \lim_{|\nu_a|,|\nu'_a|\to\infty} \mathcal{F}_a(\mathrm{i}\nu_a, \mathrm{i}\nu'_a, \mathrm{i}\omega_a) = \beta u^2 \delta(\omega_a)(\mathrm{th}+1). \end{aligned} \tag{5.5.6}$$

The asymptotic behavior of the corresponding AC function is

$$\mathcal{K}_{1,a}(\omega_a) = \lim_{|\nu_a|,|\nu'_a|\to\infty} \widehat{\Phi}^{(F,\,14)}_{\uparrow\downarrow,\mathrm{con}}(\nu_a,\nu'_a,\omega_a) = 2\pi\mathrm{i}u^2\delta(\omega_a)(\mathrm{th}+1). \tag{5.5.7}$$

Since all other AC functions decay in this limit and since $\mathcal{K}_{1,a}$ belongs to the anomalous contribution $\widehat{F}^{(\omega_{14})}_{\uparrow\downarrow}$ we find the asymptotics of the Keldysh vertex by inserting $\mathcal{K}_{1,a}$ in place of $\widehat{F}^{(\omega_{14})}_{\uparrow\downarrow}$ into the formula for analytic continuation, yielding

$$\lim_{|\nu_a|,|\nu'_a|\to\infty} F^{\boldsymbol{k}}_{\uparrow\downarrow}(\mathrm{i}\boldsymbol{\omega}) - F^{\boldsymbol{k}}_{0,\uparrow\downarrow} = \begin{cases} \mathcal{K}_{1,a}(\omega_a), & \text{for } \boldsymbol{k}\in\{2211,2121,1212,1122\}, \\ 0, & \text{else.} \end{cases} \tag{5.5.8}$$

For a proper motivation and interpretation of the asymptotic functions, one can make use of diagrammatic relations. We summarize the properties of vertex functions which are necessary for an interpretation of the asymptotic functions. For a complete and self-contained discussion we however refer to the literature [18–20]. The asymptotic behavior of the vertex function is related to the two-particle reducibility of the diagrams. A diagram is called one-particle reducible if it consists of two parts which are connected by exactly one propagator line. Cutting this line would make the diagram a disconnected one. This characteristic is important because the self-energy consists of the one-particle irreducible (1PI) two-point diagrams. Via the Dyson equation one obtains the full propagator by resummation of the 1PI diagrams which the self-energy is comprised of. By considering only diagrams with full propagators one finds that every diagrammatic contribution to the vertex has to be 1PI since the external legs of the diagrams are amputated. We henceforth only consider diagrams with full propagators which are also called *skeleton diagrams*.

The two-particle (ir)reducibility is a property which divides the set of vertex diagrams in four disjoint classes. A diagram is two-particle reducible if it consists of two parts which are connected by exactly one pair of full propagator lines, dubbed a *bubble*. It transfers a bosonic frequency $\omega_{12} = \omega_t, \omega_{13} = \omega_p$ or $\omega_{14} = \omega_a$, depending on the orientation of

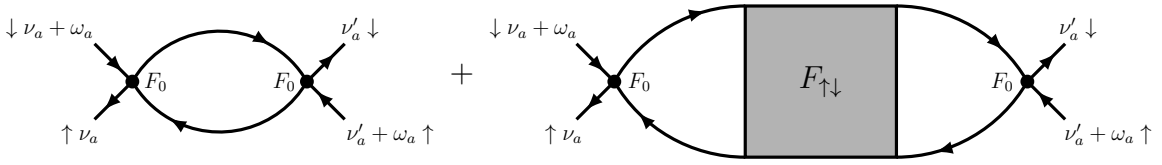

Figure 5.3: Diagrammatic contributions to the asymptotic function $\mathcal{K}_{a,\uparrow\downarrow}$. Two pairs of external legs enter the diagrams via the same bare vertex F_0.

the bubble. One hence distinguishes two-particle reducibility in three different channels, the anti-parallel (a), transverse-antiparallel (t) and the parallel (p) channel [43]. (See Eq. (5.1.26) for the appropriate frequency parametrizations in the three channels.) Again, there are diagrams which are two-particle irreducible (2PI) in any channel. The full vertex is given by the parquet equation

$$F = R + \gamma_a + \gamma_t + \gamma_p \tag{5.5.9}$$

with the 2PI diagrams R and the two-particle reducible diagrams γ_r in channel $r \in \{a, t, p\}$. It has been shown that the 2PI diagrams R decay in all directions to the bare Hubbard interaction F_0 [18]. We can therefore neglect these for the investigation of the asymptotic behavior.

Now consider the diagram in Fig. 5.3. The bare vertex is frequency-independent and merely ensures conservation of frequencies in MF. Since the two external legs on the left enter via the same bare vertex the diagram depends on the bosonic frequency ω_a but not on the fermionic frequency ν_a. The same holds for the other two external legs. Hence this diagram is even independent of the other fermionic frequency ν'_a. The diagram is obviously two-particle reducible in the a-channel. For different options of attaching two (out of four) external legs to a bare vertex, one distinguishes three channels. For every channel $r \in \{a, t, p\}$ we hence define in the resp. frequency parametrization

$$\mathcal{K}_{1,r}(\omega_r) = \lim_{|\nu_r|,|\nu'_r|\to\infty} \gamma_r(\nu_r, \nu'_r, \omega_r), \tag{5.5.10}$$

$$\mathcal{K}_{2,r}(\nu_r, \omega_r) = \lim_{|\nu'_r|\to\infty} \gamma_r(\nu_r, \nu'_r, \omega_r) - \mathcal{K}_{1,r}(\omega_r), \tag{5.5.11}$$

$$\overline{\mathcal{K}}_{2,r}(\nu'_r, \omega_r) = \lim_{|\nu_r|\to\infty} \gamma_r(\nu_r, \nu'_r, \omega_r) - \mathcal{K}_{1,r}(\omega_r). \tag{5.5.12}$$

The $\mathcal{K}_{1,r}$-function is the collection of bubble diagrams with vertex corrections in the r-channel, as shown for the a-channel in Fig. 5.3. The $\mathcal{K}_{2,r}$- and the $\overline{\mathcal{K}}_{2,r}$-function correspond to the collection of diagrams with exactly two external lines entering via the same bare vertex. The other two external lines enter via different vertices, resulting in a dependence on the two frequencies ω_r and $\nu_r^{(\prime)}$.

In the MF it has been shown that $\mathcal{K}_{1,r}$ functions are proportional to the susceptibilities χ_r in the resp. channels

$$\mathcal{K}_{1,r}(\mathrm{i}\omega_r) = -U^2 \chi_r(\mathrm{i}\omega_r). \tag{5.5.13}$$

By comparison with Eq. (5.1.28a) we find that $\mathcal{K}_{1,a}$ is indeed proportional to the susceptibility χ_a. The very same diagrams contribute to the susceptibility and the $K_{1,r}$ function. In the KF the bare vertex additionally ensures that all attached legs are on the same (forward or backward) time-branch. Hence, the Keldysh structure of the bare vertex F_0 gives our previous example in Eq. (5.5.8) its structure in Keldysh space. The asymptotics is unchanged upon exchanging the Keldysh indices of the two external legs which enter into the same bare vertex. By use of the asymptotic functions and its symmetries one can simplify the parametrization of the vertex in the KF. A more detailed and general analysis of the asymptotic functions in the MF and the KF can be found in Refs. [20, 44].

Chapter 6

Conclusion

In this thesis we investigated the analytic continuation of Matsubara multi-point correlators to the Keldysh formalism (KF). Knowing the Matsubara correlator as a function of its imaginary frequency arguments, the goal was to obtain the corresponding correlator in the (real-frequency) Keldysh formalism. To answer the question in general, without any further assumptions[1], we used a spectral representation derived in Ref. [21]. It expresses the correlator in terms of *formalism-independent* partial spectral functions (PSFs) and *formalism-specific* kernels. Using this analytically exact starting point we have shown that it is indeed possible to fully recover KF correlators from a MF function. Even though most of our results hold for ℓ-point (ℓp) correlators with any ℓ, our focus was on the particularly relevant cases of $\ell \leq 4$. For the latter we derived explicit formulas (AC formulas) summarized in App. B.

We approached the problem in the following way: We first analyzed the consequences of the equilibrium condition on KF correlators which gives rise to the statistical factors in our formulas. After a review of the analytic structure of MF functions we used their analytic continuations (AC functions) to construct discontinuities which are fit for the application of the equilibrium condition. We showed that the KF components $G^{[\eta_1\eta_2]}$ can be expanded into a sum of functions. Using the equilibrium condition, the latter can be identified with discontinuities multiplied with an statistical factor. This expansion could be reused, such that analogous steps yielded expressions for the KF components $G^{[\eta_1\eta_2\eta_3]}$ and $G^{[\eta_1\eta_2\eta_3\eta_4]}$.

During our analysis we took special care of so-called anomalous parts of the MF correlator, proportional to a factor of $\beta\delta_{\omega,0}$. We have found that these have to be treated separately. For instance, they do not contribute to the construction of the retarded correlators via analytic continuation. However, they are required for fully recovering other components of the KF correlator. While an "analytic continuation" of the Kronecker symbol is not unique in the first place, we were able to make sense of these anomalous contributions.

In the subsequent sections we applied the formulas in different contexts. Exploiting the relations between KF correlators and AC functions, we presented in Sec. 4.1 a deriva-

[1] Time-translational symmetry and equilibrium are formalism-inherent assumptions of the Matsubara formalism (MF).

tion of the generalized fluctuation-dissipation relations (FDRs) for 3p and 4p correlators. These establish relations between KF components and *primed* KF components. While our derivation did not require any further assumption, we reproduce the results in Refs. [12,33] under certain conditions for which primed correlators equal the complex conjugated ones, i.e. $G' = G^*$. In Sec. 4.2 we argued by use of the R/A basis that for vertex functions analogous formulas hold. The R/A basis is particularly convenient to work with. Propagators are diagonal in this basis, facilitating diagrammatic computations. While the FDRs are rather lengthy in the Keldysh basis, they have a very concise and general form in the R/A basis. In combination with the FDRs every KF component is represented by very few AC functions.

In Sec. 4.3 we compared the computation of response functions in MF and KF. These are 2p functions which are typically obtained from 4p correlators by integrating out two frequencies. Using the relations between MF and KF functions we find for every vertex contribution from Eliashberg's method the corresponding KF function. The latter is proportional to a KF component in the R/A basis. Thereby the arguments by Eliashberg and Oguri, based on the analytic continuations of MF correlators, can be directly transfered to the KF. They found that only a single vertex contribution has to be considered for the linear response of the model under their consideration.

In chapter 5 we directly computed the 4p KF correlator of the Hubbard atom, an exactly solvable interacting model which can be used as benchmark for the Hubbard model or Anderson impurity model. The results were summarized in Eqs. (5.4.3) and (C.3.3) for the two relevant spin configurations. By application of the results of the previous chapters we were able to reproduce the results via the AC formulas and via the FDRs. The AC formulas enabled us to adopt the results on the high-frequency asymptotics for the vertex of the Hubbard atom , computed by Wentzell et al. [20] in the MF.

In summary, our main result comprises the formulas (3.1.11) and (3.2.9) for the construction of the ℓp KF components $G^{[\eta_1 \cdots \eta_\alpha]}$ for $\alpha < 4$ and arbitrary ℓ.[2] We have shown how to obtain the necessary building blocks from discontinuities [cf. 2.3.9]. For 3p and 4p functions we summarized the AC formulas in App. B. Using a spectral respresentation our results are exact and hold for any equilibrium system with time translation symmetry. In particular, our result does not rely on any approximation. It also covers the anomalous contributions of the MF correlator which arise if the spectrum has degeneracies (see e.g. the Hubbard atom). Our formulas can be used for correlators of bosonic, fermionic or mixed operators. Their exchange symmetry is fully respected via the the statistical factors.

We found that the complexity of the construction of KF correlators mostly increases with the number of 2's in the Keldysh indices. While the retarded components $G^{[\eta]}$ directly correspond to an AC function, we found that the components $G^{[\eta_1 \eta_2]}$ can be obtained via a reasonably complicated formula. The length of the formulas increased quickly for the components $G^{[\eta_1 \cdots \eta_\alpha]}$ with $\alpha \geq$. However, it may be possible to focus on a subset of the Keldysh components. As Eliashberg, Oguri and Heyder et al. have shown, certain

[2] In fact, our formula for the analytic continuation of the component G^{2222} can easily be generalized to arbitrary ℓ by use of the kernel expansion as explained at the end of Sec. 3.2.1.

observables require just the knowledge of a few [13–15]. For computation of 3p and 4p functions via analytic continuation we recommend the procedure in App. B in which only the components $G^{[\eta_1\eta_2]}$ are computed via analytic continuation. The remaining components can be obtained more conveniently by use of the FDRs.

We note that similar formulas where also found by other authors: Guerin [45] computed diagrams in the lowest order of the bare vertex and, with a careful analysis of the diagrammatic rules in the R/A basis, derived formulas for the analytic continuation of KF vertices with two R's and an arbitrary number of A's. Taylor [46] used a spectral representation and transformed the KF correlator into the R/A basis, yielding frequency dependent coefficients in the permutation expansion of the correlator into PSFs and kernels. He then made an ansatz by taking a linear combination of AC functions. By comparison of the coefficients he deduced a formula for the analytic continuation of 4p correlators. However, both authors do not cover the treatment of anomalous contributions. As demonstrated by the example of the Hubbard atom, the latter cannot be neglected. For bosonic operators an anomalous contribution arises even for 2p functions which has to be considered for the diagonalization of the propagator. While these works either pertain to a perturbative approximation or to the 4p case, our approach still seems to be the most general one.

Appendix A

Identities for kernels

A.1 Discontinuities of AC functions

In Sec. 2.3.2 we have discussed the discontinuities of analytically continued MF correlators at the branch cuts. In this appendix we derive a general formula for discontinuities. Let I and I^c be two non-empty complementary subsets of $L = \{1,...\ell\}$. To quantify these discontinuities we consider two regions which are separated by the branch cut $\mathcal{B}_I$ where $\gamma_I = 0$. The corresponding AC functions are $C^{\boldsymbol{\gamma}^{[I,+]}}(\boldsymbol{\omega})$ and $C^{\boldsymbol{\gamma}^{[I,-]}}(\boldsymbol{\omega})$, with $\boldsymbol{\gamma}^{[I,\pm]}$ representing the two regions such that in the domain of all $\boldsymbol{\gamma}$s the sums $\gamma_I^{[I,\pm]} \gtrless 0$ are positive or negative on the respective side of the branch cut (or equivalently $\gamma_{I^c}^{\mp} \gtrless 0$, due to $\gamma_I = -\gamma_{I^c}$). The following fact is of great importance for the computation of discontinuities: Since $\boldsymbol{\gamma}^{[I,+]}$ and $\boldsymbol{\gamma}^{[I,-]}$ are only separated by the branch cut $\gamma_I = 0$, all other sums $\gamma_J^{[I,\pm]}$ with $J \neq I$ ($J \subsetneq L$) are equivalent, i.e. $\mathrm{sgn}(\gamma_{J\neq I}^{[I,+]}) = \mathrm{sgn}(\gamma_{J\neq I}^{[I,-]})$.

The discontinuity has been defined as [cf. Eq. (2.3.7)]

$$\Delta C_I^{\boldsymbol{\gamma}}(\boldsymbol{\omega}) = C^{\boldsymbol{\gamma}^{[I,+]}}(\boldsymbol{\omega}) - C^{\boldsymbol{\gamma}^{[I,-]}}(\boldsymbol{\omega}). \tag{A.1.1}$$

Using the permutation expansion of the AC function $C^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega})$ according to Eq. (2.3.3), the discontinuity can be computed by subtracting the corresponding two kernels for every permutation, $\Delta\widetilde{K}^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega}_p) = \widetilde{K}(\boldsymbol{z}_p^{[I,+]}) - \widetilde{K}(\boldsymbol{z}_p^{[I,-]})$, where $\boldsymbol{z}_p^{[I,\pm]} = \boldsymbol{\omega}_p + \mathrm{i}\boldsymbol{\gamma}^{[I,\pm]}$ denote the form of the complex frequencies infinitesimally close to and on either side of the branch cut.

For any permutation p which is neither of the type $\overline{I}\,\overline{I}^c$ nor $\overline{I}^c\overline{I}$, the difference of the kernels gives $\Delta\widetilde{K}^{\boldsymbol{\gamma}^{[I,\pm]}} = 0$.[1] The reason is that according to Eq. (2.1.10) the regular kernel $\widetilde{K}(\boldsymbol{z}_p)$ consists of the factors $z_{\overline{1}...\overline{i}}$, being sums of the first i components of the permuted tuple $\boldsymbol{z}_p = (z_{\overline{1}},...z_{\overline{\ell}})$. The regular kernels $\widetilde{K}(\boldsymbol{z}_p^{[I,+]})$ and $\widetilde{K}(\boldsymbol{z}_p^{[I,-]})$ are identical since they contain neither the factor $z_I^{[I,\pm]}$ nor $z_{I^c}^{[I,\pm]}$ (since neither $p = \overline{I}\,\overline{I}^c$ nor $p = \overline{I}^c\overline{I}$). Hence, the only non-vanishing contributions in the permutation expansion are those for

[1] Remember that by our notation $\overline{I}$ is an index tuple built from the elements of I. And $\overline{I}\,\overline{I}^c$ is a tuple containing the entries of $\overline{I}$ followed by those of $\overline{I}^c$.

the permutations of the type $\overline{I}\,\overline{I}^c$ and $\overline{I}^c\overline{I}$. Consider as an example for $\ell = 3$ the branch cut $\mathcal{B}_{13} = \mathcal{B}_2$ along $\gamma_{13} = \gamma_2 = 0$. On either side of the branch cut we have the sums $z_{13}^{[I,\pm]} = \omega_{13} \pm \mathrm{i}0^+$, all other frequency sums are equivalent on both sides. Hence $\widetilde{K}(\boldsymbol{z}_{132}^{[I,\pm]}) = 1/[z_1(\omega_{13} \pm \mathrm{i}0^+)]$ is different on both sides while $\widetilde{K}(\boldsymbol{z}_{123}^{[I,\pm]}) = 1/[z_1 z_{12}]$ yields the same result on both sides of $\mathcal{B}_{13}$.

For a permutation of the type $p = \overline{I}\,\overline{I}^c$ we obtain for the kernel of the discontinuity

$$\Delta\widetilde{K}_I^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega}_{\overline{I}\,\overline{I}^c}) = \widetilde{K}(\boldsymbol{z}_{\overline{I}\,\overline{I}^c}^{[I,+]}) - \widetilde{K}(\boldsymbol{z}_{\overline{I}\,\overline{I}^c}^{[I,-]}) \tag{A.1.2a}$$

$$= \prod_{i=1}^{|I|-1} (z_{\overline{1}\ldots\overline{i}})^{-1} [(z_I^{[I,+]})^{-1} - (z_I^{[I,-]})^{-1}] \prod_{i=|I|+1}^{\ell-1} (z_{\overline{1}\ldots\overline{i}})^{-1} \tag{A.1.2b}$$

$$= \prod_{i=1}^{|I|-1} (z_{\overline{1}\ldots\overline{i}})^{-1} \hat{\delta}(\omega_I) \prod_{i=|I|+1}^{\ell-1} (z_{\overline{|I|+1}\ldots\overline{i}})^{-1} \tag{A.1.2c}$$

$$= \hat{\delta}(\omega_I) \widetilde{K}(\boldsymbol{z}_{\overline{I}}) \widetilde{K}(\boldsymbol{z}_{\overline{I}^c}). \tag{A.1.2d}$$

The second line is obtained since all factors $z_{\overline{1}\ldots\overline{i}}^{[I,+]} = z_{\overline{1}\ldots\overline{i}}^{[I,-]}$ are equivalent except for $z_I^{[I,\pm]} = \omega_I \pm \mathrm{i}\,0^+$. Hence we only have to treat the latter separately and drop the superscript for the other factors. For the third line we need

$$\lim_{\gamma_I \to 0} \left(\frac{1}{z_I^{[I,+]}} - \frac{1}{z_I^{[I,-]}} \right) = \lim_{\gamma \searrow 0} \left(\frac{1}{\omega_I + \mathrm{i}\gamma} - \frac{1}{\omega_I - \mathrm{i}\gamma} \right) = -2\pi\mathrm{i}\delta(\omega_I) = \hat{\delta}(\omega_I). \tag{A.1.3}$$

In the factors with $i > |I|$, we exploit $\hat{\delta}(\omega_I)$ to set $\omega_{\overline{1}\cdots\overline{|I|}} = 0$, and also set $\gamma_{\overline{1}\cdots\overline{|I|}} = \gamma_I = 0$, since these factors are equal on either side of the branch cut. Together, these two simplifications imply $z_{\overline{1}\ldots\overline{i}} = z_{\overline{|I|+1}\ldots\overline{i}}$ for $i > |I|$. In the last line, the tuple of complex frequencies $\boldsymbol{z}_{\overline{I}\,\overline{I}^c}$ has been separated into subtuples as $(\boldsymbol{z}_{\overline{I}}, \boldsymbol{z}_{\overline{I}^c})$.

A similar computation as for Eq. (A.1.2d) gives for a permutation of the type $p = \overline{I}^c\overline{I}$

$$\Delta\widetilde{K}_I^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega}_{\overline{I}^c\overline{I}}) = \widetilde{K}(\boldsymbol{z}_{\overline{I}^c\overline{I}}^{[I,+]}) - \widetilde{K}(\boldsymbol{z}_{\overline{I}^c\overline{I}}^{[I,-]}) = -\hat{\delta}(\omega_I) \widetilde{K}(\boldsymbol{z}_{\overline{I}}) \widetilde{K}(\boldsymbol{z}_{\overline{I}^c}). \tag{A.1.4}$$

This result differs from the one in Eq. (A.1.2d) only by a minus sign. So, in total we can summarize

$$\begin{aligned} \Delta\widetilde{K}_I^{\boldsymbol{\gamma}^{[I,\pm]}}(\boldsymbol{\omega}_p) &= \widetilde{K}(\boldsymbol{z}_p^{[I,+]}) - \widetilde{K}(\boldsymbol{z}_p^{[I,-]}) \\ &= \begin{Bmatrix} +\hat{\delta}(\omega_I), \\ -\hat{\delta}(\omega_I), \\ 0, \end{Bmatrix} \widetilde{K}(\boldsymbol{z}_{\overline{I}}) \widetilde{K}(\boldsymbol{z}_{\overline{I}^c}) \begin{Bmatrix} \text{for } p = \overline{I}\,\overline{I}^c, \\ \text{for } p = \overline{I}^c\overline{I}, \\ \text{else.} \end{Bmatrix} \end{aligned} \tag{A.1.5}$$

On the right-hand side the kernels give equivalent results for $\boldsymbol{z}_{\overline{I}^{(c)}}^{[I,+]}$ and $\boldsymbol{z}_{\overline{I}^{(c)}}^{[I,-]}$. By taking the limit $\gamma_I^{[I,\pm]} \to 0$ this kernel is now a function of $\ell - 2$ independent complex variables $\boldsymbol{\gamma}$ satisfying $\gamma_I = 0$ and $\gamma_{I^c} = 0$.

A.2 Proof for the expansion of $K^{[\mu\nu]}$

Here we prove Eq. (3.1.2), which expands the kernel $K^{[\mu\nu]} = K^{[\mu]} - K^{[\nu]}$ in a manner allowing KF correlators to be related to AC functions. Using the notation according to Eq. (2.1.24) this difference is proportional to $\prod_{i=\mu}^{\nu-1}(\omega^{+}_{\bar{1}\dots\bar{i}})^{-1} - \prod_{i=\mu}^{\nu-1}(\omega^{-}_{\bar{1}\dots\bar{i}})^{-1}$. The latter can be expressed as a sum $\sum_{y=\mu}^{\nu-1}$, with each summand proportional to $(\omega^{+}_{\bar{1}\dots\bar{y}})^{-1} - (\omega^{-}_{\bar{1}\dots\bar{y}})^{-1} = \hat{\delta}(\omega_{\bar{1}\dots\bar{y}})$.

For a compact exposition, we introduce the shorthand:

$$K^{\pm}_{\mu\nu}(\boldsymbol{\omega}_p) = \prod_{i=\mu}^{\nu-1} \frac{1}{\omega^{\pm}_{\bar{1}\dots\bar{i}}}\,, \quad (\mu < \nu), \qquad K^{\pm}_{\mu\mu} = 1\,. \tag{A.2.1}$$

Then, the following identities hold for any argument $\boldsymbol{\omega}_p$:

$$K^{\pm}_{\mu y} K^{\pm}_{y\nu} = K^{\pm}_{\mu\nu}\,, \qquad K^{[\eta]} = K^{-}_{1\eta} K^{+}_{\eta\ell}\,. \tag{A.2.2}$$

Using these, we can express $K^{[\mu\nu]}(\boldsymbol{\omega}_p)$ as follows:

$$\begin{aligned} K^{[\mu\nu]} = K^{[\mu]} - K^{[\nu]} &= K^{-}_{1\mu}\Big[K^{+}_{\mu\nu} - K^{-}_{\mu\nu}\Big] K^{+}_{\nu\ell} \\ &= \sum_{y=\mu}^{\nu-1} K^{-}_{1\mu}\Big[K^{+}_{\mu\,y+1} K^{-}_{y+1\,\nu} - K^{+}_{\mu y} K^{-}_{y\nu}\Big] K^{+}_{\nu\ell} \\ &= \sum_{y=\mu}^{\nu-1} K^{-}_{1\mu} K^{+}_{\mu y} \underbrace{\left[\frac{1}{\omega^{+}_{\bar{1}\dots\bar{y}}} - \frac{1}{\omega^{-}_{\bar{1}\dots\bar{y}}}\right]}_{\hat{\delta}(\omega_{\bar{1}\dots\bar{y}})} K^{-}_{y+1\nu} K^{+}_{\nu\ell}\,. \end{aligned}$$

In the second line, the terms with $y = \nu - 1$ or μ represent the first line, the remaining terms cancel pairwise. In the last line, where $\hat{\delta}$ enforces $\omega_{\bar{1}\dots\bar{y}} = 0$, we may substitute $\omega^{\pm}_{\bar{1}\dots\bar{i}} = \omega^{\pm}_{\overline{y+1}\dots\bar{i}}$ for $i > y$ in the arguments of $K^{-}_{y+1\nu} K^{+}_{\nu\ell}$. This leads to a form equivalent to Eq. (3.1.2),

$$K^{[\mu\nu]}(\boldsymbol{\omega}_{(\bar{1}\dots\bar{\ell})}) = \sum_{y=\mu}^{\nu-1} K^{[\mu]}(\boldsymbol{\omega}_{(\bar{1}\dots\bar{y})})\hat{\delta}(\omega_{\bar{1}\dots\bar{y}}) K^{[\nu-y]}(\boldsymbol{\omega}_{(\overline{y+1}\dots\bar{\ell})}) \tag{A.2.3}$$

$$= \sum_{y=\mu}^{\nu-1} \widetilde{K}(\boldsymbol{\omega}^{[\overline{\mu}]}_{(\bar{1}\dots\bar{y})})\hat{\delta}(\omega_{\bar{1}\dots\bar{y}})\widetilde{K}(\boldsymbol{\omega}^{[\overline{\nu}]}_{(\overline{y+1}\dots\bar{\ell})}) \tag{A.2.4}$$

$$= \sum_{y=\mu}^{\nu-1} K_{(\bar{1}\dots\bar{y})^{[\overline{\mu}]}(\overline{y+1}\dots\bar{\ell})^{[\overline{\nu}]}}(\boldsymbol{\omega}_{(\bar{1}\dots\bar{\ell})}). \tag{A.2.5}$$

In the second to last line we used the definition of the retarded kernel in Eq. (2.1.29). And in the last line we inserted the definition of the retarded product kernel Eq. (2.1.30).

Appendix B

Explicit formulas for analytic continuation

In the following we summarize the results for the most relevant cases of 3-point and 4-point functions. The following functions hold both for correlators G and for vertex functions Γ. For brevity we only write the version for correlators. The version for vertex functions is obtained by replacing the symbol G by Γ and by exchanging all 1's for 2's and vice versa.

We defined the analytic continuation $\Phi(\boldsymbol{z})$ which is obtained from the regular part of the correlator in MF by the simple replacement

$$\begin{aligned} \mathrm{i}\omega_i &\longrightarrow z_i = \omega_i + \mathrm{i}\gamma_i \\ \widetilde{G}(\mathrm{i}\boldsymbol{\omega}) &\longrightarrow \Phi(\boldsymbol{z}) = 2^{1-\ell/2} \times \overline{G}(\mathrm{i}\boldsymbol{\omega}))\big|_{\mathrm{i}\boldsymbol{\omega}\to\boldsymbol{z}} \,. \end{aligned} \tag{B.0.1}$$

Here we have already included the global factor $2^{1-\ell/2}$ originating from the Keldysh rotation. A retarded correlator is obtained by analytic continuation to the complex frequency $\boldsymbol{\omega}^{[\eta]}$ according to Eq. (2.1.23), i.e.

$$G^{[\eta]} = \overline{\Phi}(\boldsymbol{\omega}^{[\eta]}). \tag{B.0.2}$$

The corresponding advanced correlators $G'^{[\eta]}$ are then obtained by conjugating all complex frequencies.

B.1 Three-point functions

For three-point functions the situation is still relatively simple. All analytic continuations of the (regular) MF correlator correspond directly to retarded or advanced KF correlators, $G^{[\eta]}$ and $G'^{[\eta]}$ (see Fig. 2.2). Any other KF correlator can be computed from the generalized fluctuation-dissipation relations (FDR). One just has to take special care of divergencies of the factors N_i which indicate that we additionally need to include an analytic continuation of an anomalous MF correlator.

Let us assume that the first operator, $\mathcal{O}^1$, is bosonic and the last two, $\mathcal{O}^2$ and $\mathcal{O}^3$, are fermionic. Then $N_1 = \coth(\beta\omega_1/2)$ can diverge for $\omega_1 = 0$. According to Sec. 3.1.3 the corresponding anomalous MF correlator $\widehat{G}_1 \propto \beta\delta_{\omega_1,0}$ can be analytically continued independently for the frequencies $\{\mathrm{i}\omega_1\}$ and for $\{\mathrm{i}\omega_2, \mathrm{i}\omega_3\}$. However, for a single frequency the regular kernel is one, $\widetilde{K}(\mathrm{i}\omega_1) = 1$, which makes the analytic continuation of $\mathrm{i}\omega_1$ superfluous. For the frequencies $\{\mathrm{i}\omega_2, \mathrm{i}\omega_3\}$ the analytic structure is identical to that of 2p functions. Hence, it suffices to specify for a single frequency e.g. $z_2 = \omega_2^+$ or $z_2 = \omega_2^-$. We obtain an analytic continuation of the anomalous part according to Sec. 3.1.3 by

$$\begin{aligned} \beta\delta_{\omega_1,0} &\longrightarrow 2^{3/2}\pi\mathrm{i}\delta(\omega_1), \\ \widehat{G}_1(\mathrm{i}\boldsymbol{\omega}) &\longrightarrow \widehat{\Phi}_1(\boldsymbol{z}). \end{aligned} \tag{B.1.1}$$

The exact Keldysh correlators can be computed from these functions via the following formulas:

$$G^{122} = N_2(G'^{[1]} - G^{[2]}) + N_3(G'^{[1]} - G^{[3]}), \tag{B.1.2a}$$

$$G^{212} = N_1(G'^{[2]} - G^{[3]}) + N_3(G'^{[2]} - G^{[1]}) + \widehat{\Phi}_1(\omega_2^-), \tag{B.1.2b}$$

$$G^{221} = N_1(G'^{[3]} - G^{[2]}) + N_2(G'^{[3]} - G^{[1]}) + \widehat{\Phi}_1(\omega_2^+), \tag{B.1.2c}$$

$$\begin{aligned} G^{222} = {} & (1 + N_2N_3)G'^{[1]} + (1 + N_1N_3)G'^{[2]} + (1 + N_1N_2)G'^{[3]} \\ & + N_2N_3G^{[1]} + N_1N_3G^{[2]} + N_1N_2G^{[3]} - N_3\big[\widehat{\Phi}_1(\omega_2^+) - \widehat{\Phi}_1(\omega_2^-)\big], \end{aligned} \tag{B.1.2d}$$

These are basically the same formulas as in Ref. [12]. Additionally we have included the functions $\widehat{\Phi}$ which cannot be obtained from the retarded or advanced correlators. The very same formulas hold for vertex functions as discussed in Sec. 4.2.

B.2 Four-point functions

Here we focus on the most relevant case in which all four operators are fermionic. This assumption restricts the possible anomalous terms in the MF correlator according to Sec. 2.1.2.

There are four retarded correlators $G^{[\eta]}$ $(1 \leq \eta \leq 4)$ which are easily obtained by analytic continuation according to Eq. (2.1.23). The correlators $G^{[\eta_1\eta_2]}$ are still rather easily obtained via analytic continuation. However, for $G^{\eta_1\cdots\eta_\alpha}$ with $\alpha = 3, 4$ it is advisable to reuse those components with $\alpha \leq 2$ via the FDR. Since the FDR only relate 8 correlators to the rest we have to at least compute 3 correlators of the type $G^{[\eta_1\eta_2]}$.

Note that in the following we express the Keldysh components in terms of the AC functions which correspond to the individual regions in Fig. 2.3. They labeling with arabic and roman numbers is thus identical for the region and the AC function. However, the representation by these AC functions is not unique. As explained after Eq. (2.3.12) we for example have the identity $0 = C^I_{2.2} - C^I_{2.2} + C^{III}_{2.2} - C^{IV}_{2.2}$.

We define the analytically continued anomalous parts of the MF correlator $\widehat{G}_I(\mathrm{i}\boldsymbol{\omega}) \propto \delta_{\omega_I,0}$ according to Sec. 3.1.3 by

$$\begin{aligned} \beta\delta_{\omega_I,0} &\longrightarrow 2\pi\mathrm{i}\delta(\omega_I), \\ \widehat{G}_I(\mathrm{i}\boldsymbol{\omega}) &\longrightarrow \widehat{\Phi}_I(\boldsymbol{z}) \end{aligned} \tag{B.2.1}$$

for $I \in \{12, 13, 14\}$. For instance, the analytic continuation of the frequencies in $\widehat{\Phi}_{12}$ is performed independently on the sets $\{z_1, z_2\}$ and on $\{z_3, z_4\}$. The analytic structure of each of these corresponds to a two-point function, in which frequency conservation ensures $\omega_1^{\pm} = -\omega_2^{\mp}$ and $\omega_3^{\pm} = -\omega_4^{\mp}$. It is hence sufficient to declare the analytic continuation by the imaginary parts of single frequencies, e.g. $\widehat{\Phi}_{12}(\omega_1^+, \omega_2^-, \omega_3^+, \omega_4^-)$. Corresponding statements hold also for $\widehat{\Phi}_{13}$ and $\widehat{\Phi}_{14}$.

$$\begin{aligned} G^{[34]} &= N_3\big(C^{\mathrm{IV}}_{4.4} - C_{4.1}\big) + N_4\big(C^{\mathrm{II}}_{4.4} - C_{4.3}\big) + N_{13}\big(C^{\mathrm{II}}_{4.4} - C^{\mathrm{I}}_{4.4}\big) + N_{14}\big(C^{\mathrm{IV}}_{4.4} - C^{\mathrm{I}}_{4.4}\big) \\ &\quad + \widehat{\Phi}_{13}(\omega_1^-, \omega_2^-, \omega_3^+, \omega_4^+) + \widehat{\Phi}_{14}(\omega_1^-, \omega_2^-, \omega_3^+, \omega_4^+), && \text{(B.2.2a)} \\ G^{[24]} &= N_2\big(C^{\mathrm{III}}_{1.1} - C_{4.1}\big) + N_4\big(C^{\mathrm{I}}_{1.1} - C_{1.2}\big) + N_{12}\big(C^{\mathrm{II}}_{1.1} - C^{\mathrm{III}}_{1.1}\big) + N_{14}\big(C^{\mathrm{II}}_{1.1} - C^{\mathrm{I}}_{1.1}\big) \\ &\quad + \widehat{\Phi}_{12}(\omega_1^-, \omega_2^+, \omega_3^-, \omega_4^+) + \widehat{\Phi}_{14}(\omega_1^-, \omega_2^+, \omega_3^-, \omega_4^+), && \text{(B.2.2b)} \\ G^{[23]} &= N_2\big(C^{\mathrm{III}}_{1.3} - C_{4.3}\big) + N_3\big(C^{\mathrm{I}}_{1.3} - C_{1.2}\big) + N_{12}\big(C^{\mathrm{II}}_{1.3} - C^{\mathrm{III}}_{1.3}\big) + N_{13}\big(C^{\mathrm{II}}_{1.3} - C^{\mathrm{I}}_{1.3}\big) \\ &\quad + \widehat{\Phi}_{12}(\omega_1^-, \omega_2^+, \omega_3^+, \omega_4^-) + \widehat{\Phi}_{13}(\omega_1^-, \omega_2^+, \omega_3^+, \omega_4^-), && \text{(B.2.2c)} \\ G^{[14]} &= N_1\big(C^{\mathrm{III}}_{3.1} - C_{4.1}\big) + N_4\big(C^{\mathrm{I}}_{3.1} - C_{3.2}\big) + N_{12}\big(C^{\mathrm{II}}_{3.1} - C^{\mathrm{III}}_{3.1}\big) + N_{13}\big(C^{\mathrm{I}}_{3.1} - C^{\mathrm{II}}_{3.1}\big) \\ &\quad + \widehat{\Phi}_{12}(\omega_1^+, \omega_2^-, \omega_3^-, \omega_4^+) + \widehat{\Phi}_{13}(\omega_1^+, \omega_2^-, \omega_3^-, \omega_4^+), && \text{(B.2.2d)} \\ G^{[13]} &= N_1\big(C^{\mathrm{III}}_{3.3} - C_{4.3}\big) + N_3\big(C^{\mathrm{I}}_{3.3} - C_{3.2}\big) + N_{12}\big(C^{\mathrm{II}}_{3.3} - C^{\mathrm{III}}_{3.3}\big) + N_{14}\big(C^{\mathrm{I}}_{3.3} - C^{\mathrm{II}}_{3.3}\big) \\ &\quad + \widehat{\Phi}_{12}(\omega_1^+, \omega_2^-, \omega_3^+, \omega_4^-) + \widehat{\Phi}_{14}(\omega_1^+, \omega_2^-, \omega_3^+, \omega_4^-), && \text{(B.2.2e)} \\ G^{[12]} &= N_1\big(C^{\mathrm{III}}_{2.2} - C_{1.2}\big) + N_2\big(C^{\mathrm{I}}_{2.2} - C_{3.2}\big) + N_{13}\big(C^{\mathrm{I}}_{2.2} - C^{\mathrm{II}}_{2.2}\big) + N_{14}\big(C^{\mathrm{II}}_{2.2} - C^{\mathrm{III}}_{2.2}\big) \\ &\quad + \widehat{\Phi}_{13}(\omega_1^+, \omega_2^+, \omega_3^-, \omega_4^-) + \widehat{\Phi}_{14}(\omega_1^+, \omega_2^+, \omega_3^-, \omega_4^-), && \text{(B.2.2f)} \end{aligned}$$

The AC functions in round brackets are discontinuities, e.g. in the first line $\big(C^{\mathrm{IV}}_{4.4} - C_{4.1}\big)$ is a discontinuity at the branchcut $\mathrm{Im}(z_3) = 0$ [see Sec. 2.3.2].

The above correlators are related by the FDRs given in Eqs. (53) in Ref. [12]. Since we are considering a fermionic system we have to redefine the statistical factors $N_i = \tanh(\beta\omega_i/2)$ according to Eq. (2.2.4). This gives

$$\begin{aligned} G^{[12]} &= -N_1 G^{[2]} - N_2 G^{[1]} + N^{(12)}_{(34)}[N_3 G'^{[4]} + N_4 G'^{[3]} + G'^{[34]}], && \text{(B.2.3a)} \\ G^{[13]} &= -N_1 G^{[3]} - N_3 G^{[1]} + N^{(13)}_{(24)}[N_2 G'^{[4]} + N_4 G'^{[2]} + G'^{[24]}], && \text{(B.2.3b)} \\ G^{[14]} &= -N_1 G^{[4]} - N_4 G^{[1]} + N^{(14)}_{(23)}[N_2 G'^{[3]} + N_3 G'^{[2]} + G'^{[23]}], && \text{(B.2.3c)} \end{aligned}$$

with $N^{(ij)}_{(kl)} = \frac{N_i + N_j}{N_k + N_l}$.

With the above components the remaining ones can be computed via the FDRs, giving

$$\begin{aligned} G^{[123]} &= (1+N_1N_3+N_1N_2+N_2N_3)G'^{[4]} - N_2N_3G^{[1]} - N_1N_3G^{[2]} - N_1N_2G^{[3]} \\ &\quad - N_3G^{[12]} - N_2G^{[13]} - N_1G^{[23]}, \end{aligned} \tag{B.2.4a}$$

$$\begin{aligned} G^{[124]} &= (1+N_1N_4+N_1N_2+N_2N_4)G'^{[3]} - N_2N_4G^{[1]} - N_1N_4G^{[2]} - N_1N_2G^{[4]} \\ &\quad - N_4G^{[12]} - N_2G^{[14]} - N_1G^{[24]}, \end{aligned} \tag{B.2.4b}$$

$$\begin{aligned} G^{[134]} &= (1+N_1N_4+N_1N_3+N_3N_4)G'^{[2]} - N_3N_4G^{[1]} - N_1N_4G^{[3]} - N_1N_3G^{[4]} \\ &\quad - N_4G^{[13]} - N_3G^{[14]} - N_1G^{[34]}, \end{aligned} \tag{B.2.4c}$$

$$\begin{aligned} G^{[234]} &= (1+N_2N_4+N_2N_3+N_3N_4)G'^{[1]} - N_3N_4G^{[2]} - N_2N_4G^{[3]} - N_2N_3G^{[4]}, \\ &\quad - N_4G^{[23]} - N_3G^{[24]} - N_2G^{[34]}, \end{aligned} \tag{B.2.4d}$$

$$\begin{aligned} G^{[1234]} &= 2N_2N_3N_4G^{[1]} + (N_2N_3N_4+N_2+N_3+N_4)G'^{[1]} \\ &\quad + 2N_1N_3N_4G^{[2]} + (N_1N_3N_4+N_1+N_3+N_4)G'^{[2]} \\ &\quad + 2N_1N_2N_4G^{[3]} + (N_1N_2N_4+N_1+N_2+N_4)G'^{[3]} \\ &\quad + 2N_2N_3N_4G^{[4]} + (N_1N_2N_3+N_1+N_2+N_3)G'^{[4]} \\ &\quad + N_3N_4G^{[12]} + N_2N_4G^{[13]} + N_2N_3G^{[14]} \\ &\quad + N_1N_4G^{[23]} + N_1N_3G^{[24]} + N_1N_2G^{[34]}. \end{aligned} \tag{B.2.4e}$$

Note that a primed correlator is equivalent to a complex conjugated one (such that $G' = G^*$) for certain correlators as mentioned after Eq. (2.1.28).

Appendix C

Explicit calculations on the Hubbard atom

C.1 Explicit calculation of the four-point correlator

In the following we explicitly compute components of the (connected part of the) 4p correlator $G_{\uparrow\downarrow,\mathrm{con}}$ for the Hubbard atom at half-filling. The final results are summarized in Eq. (5.3.3).

For the computation of the correlators in frequency space we draw attention to the subtlety of the infinitesimal imaginary parts of the complex frequencies $\omega_i^{\pm}$ in the KF. (In the MF there is no such problem.) Previously we have elucidated the importance of these infinitesimal parts already. However, when we encounter a sum like $\omega_1^+ + \omega_2^-$, it is ambiguous whether this sum has a positive or negative imaginary part. This ambiguity can be avoided when one only allows to sum complex frequencies with the same imaginary parts. While we simplify expressions it is advisable to *exclusively* work with frequency sums ω_I^+ carrying positive imaginary parts (or exclusively with frequency sums ω_I^- carrying negative imaginary parts, $I \subsetneq \{1,..,\ell\}$). In this case one can perform simplifications in the same way as with purely real frequencies. For instance, one can simplify the following sum by

$$\frac{1}{\omega_{23}^-}\left[\frac{1}{\omega_2^-}+\frac{1}{\omega_3^-}\right] = \frac{\omega_2^- + \omega_3^-}{\omega_{23}^-\omega_2^-\omega_3^-} = \frac{1}{\omega_2^-\omega_3^-}. \tag{C.1.1}$$

Above relation can also be verified in the time domain where it translates to

$$-\theta(t_1-t_3)\theta(t_3-t_2) - \theta(t_1-t_2)\theta(t_2-t_3) = -\theta(t_1-t_3)\theta(t_1-t_2).$$

Due to the conservation of the total frequency one can express the sum over frequencies in terms of the complementary ones, e.g. for 4p functions $\omega_1^- = -\omega_{234}^+$.

C.1.1 The two-point correlator $G^{k_1k_2}$

As an introductory example, we first compute the two-point (2p) function. Both the direct computation and the analytic continuation from the MF correlator are easily done. For

any $\sigma \in \{\uparrow, \downarrow\}$ the 2p correlator is defined as

$$\mathcal{G}^{k_1 k_2}(t,0) = -\mathrm{i}\langle \mathcal{T}_c[d_\sigma^{k_1}(t) d_\sigma^{\dagger,k_2}(0)]\rangle \tag{C.1.2}$$

and obtain the PSFs for the permutations $p \in \{(12),(21)\}$

$$\begin{aligned} \mathcal{S}_{(12)}(t,0) &= +\langle d_\sigma^{k_1}(t) d_\sigma^{\dagger,k_2}(0)\rangle = +\frac{e^{\mathrm{i}ut} + e^{\beta u} e^{-\mathrm{i}ut}}{2(1+e^{\beta u})}, \\ \mathcal{S}_{(21)}(0,t) &= -\langle d_\sigma^{\dagger,k_2}(0) d_\sigma^{k_1}(t)\rangle = -\frac{e^{\beta u} e^{\mathrm{i}ut} + e^{-\mathrm{i}ut}}{2(1+e^{\beta u})}. \end{aligned} \tag{C.1.3}$$

Plugging these into the spectral representation Eq. (5.2.9) gives the correlators

$$\begin{aligned} &\mathcal{G}^{11}(t_1,t_2) = 0, \\ &\mathcal{G}^{12}(t_1,t_2) = \mathcal{S}_{[2;1]_-}(t_2,t_1) \times K^{\mathcal{T}}(t_2,t_1) = -\frac{1}{2} e^{-\mathrm{i}t_{12}u}(e^{2\mathrm{i}t_1 u} + e^{2\mathrm{i}t_2 u}) \mathcal{K}^{\mathcal{T}}(t_2,t_1), \\ &\mathcal{G}^{21}(t_1,t_2) = \mathcal{S}_{[1;2]_-}(t_1,t_2) \times K^{\mathcal{T}}(t_1,t_2) = \frac{1}{2} e^{-\mathrm{i}t_{12}u}(e^{2\mathrm{i}t_1 u} + e^{2\mathrm{i}t_2 u}) \mathcal{K}^{\mathcal{T}}(t_1,t_2), \\ &\mathcal{G}^{22}(t_1,t_2) = \mathcal{S}_{[1;2]_+}(t_1,t_2) \times (-\mathrm{i}) = -\mathrm{i}\frac{\mathrm{th}}{2} e^{-\mathrm{i}t_{12}u}(-e^{2\mathrm{i}t_1 u} + e^{2\mathrm{i}t_2 u}). \end{aligned} \tag{C.1.4}$$

Here we used the abbreviation $t_I = \sum_{i\in I} t_i$ for sums. Expressing 2-point functions only in terms of the frequency argument of the first operator $\omega = \omega_1 = -\omega_2$ we obtain

$$\begin{aligned} G(\omega) &= \begin{pmatrix} 0 & G^A(\omega) \\ G^R(\omega) & G^K(\omega) \end{pmatrix} = \begin{pmatrix} G^{11}(\omega) & G^{12}(\omega) \\ G^{21}(\omega) & G^{22}(\omega) \end{pmatrix} \\ &= \begin{pmatrix} 0 & \frac{\omega^-}{(\omega^-)^2 - u^2} \\ \frac{\omega^+}{(\omega^+)^2 - u^2} & -\pi\mathrm{i}\mathrm{th} \times \big[\delta(\omega - u) - \delta(\omega + u)\big] \end{pmatrix} \end{aligned} \tag{C.1.5}$$

where we used the abbreviation $\omega^\pm = \omega \pm \mathrm{i}\gamma$ with infinitesimal $\gamma > 0$. One can easily check that $G^R = G^{21}$ is obtained from the MF correlator in Eq. (5.1.22) via the analytic continuation $\mathrm{i}\omega \to \omega + \mathrm{i}\gamma$ and $G^A = G^{12}$ is obtained by $\mathrm{i}\omega \to \omega - \mathrm{i}\gamma$. Furthermore the fluctuation-dissipation theorem

$$G^K = G^{22} = \tanh(\beta\omega/2)\big[G^{21} - G^{12}\big] \tag{C.1.6}$$

is fulfilled.

C.1.2 The retarded correlators $G^{2111}_{\uparrow\downarrow}$, $G^{1211}_{\uparrow\downarrow}$, $G^{1121}_{\uparrow\downarrow}$ and $G^{1112}_{\uparrow\downarrow}$

The correlators with only one 2 in the Keldysh indices (2-index) are also called *retarded correlators*. We first compute the retarded correlators directly by use of the spectral representation in Eq. (5.2.9) and e.g. get

$$G^{2111}_{\uparrow\downarrow}(\boldsymbol{t}) = \frac{e^{-\mathrm{i}t_{1234}u}}{4} \sum_{P,\overline{1}=1} (e^{2\mathrm{i}t_1 u} - e^{2\mathrm{i}t_{\overline{2}} u})(e^{2\mathrm{i}t_{\overline{3}} u} + e^{2\mathrm{i}t_{\overline{4}} u}) \times K^{\mathcal{T}}(t_1, t_{\overline{2}}, t_{\overline{3}}, t_{\overline{4}}), \tag{C.1.7}$$

where we restricted permutations $P = (\overline{1}, \overline{2}, \overline{3}, \overline{4})$ to those with $\overline{1} = 1$. In frequency space this gives, after use of simplifications of the type in Eq. (C.1.1),

$$\begin{aligned} G^{2111}_{\uparrow\downarrow}(\boldsymbol{\omega}) &= \frac{1}{4}\left[\frac{1}{\omega_1^+ + u} - \frac{1}{\omega_1^+ - u}\right] \\ &\quad \times \left[\frac{1}{\omega_2^- + u}\left(\frac{1}{\omega_3^- - u} + \frac{1}{\omega_4^- - u}\right) + \frac{1}{\omega_3^- + u}\left(\frac{1}{\omega_2^- - u} + \frac{1}{\omega_4^- - u}\right)\right. \\ &\quad \left. + \frac{1}{\omega_4^- + u}\left(\frac{1}{\omega_3^- - u} + \frac{1}{\omega_2^- - u}\right)\right] \\ &= \frac{1}{2}\frac{2u \cdot \omega_1^+\omega_2^-\omega_3^-\omega_4^- + u^3 \cdot [(\omega_1^+)^2 + (\omega_2^-)^2 + (\omega_3^-)^2 + (\omega_4^-)^2] - 6u^5}{[(\omega_1^+)^2 - u^2][(\omega_2^-)^2 - u^2][(\omega_3^-)^2 - u^2][(\omega_4^-)^2 - u^2]}. \end{aligned} \tag{C.1.8}$$

In the last step we used $\omega^-_{234} = -\omega_1^+$. It has been shown that each of these retarded correlators can be directly obtained from the Matsubara correlator by a certain choice of analytic continuation [10, 23, 30]. We find that this can indeed be related to the Matsubara correlator. Therefore we isolate the *regular part* of the Matsubara correlator $\widetilde{G}_{\uparrow\downarrow,\mathrm{con}}$ in Eq. (5.1.23b) which is the part without Kronecker symbols and define the analytically continued function of complex frequencies z_i

$$\Phi_{\uparrow\downarrow,\mathrm{con}}(z_1, z_2, z_3, z_4) = \frac{1}{2}\frac{2u\prod_{i=1}^{4} z_i + u^3\sum_{i=1}^{4}(z_i)^2 - 6u^5}{\prod_{i=1}^{4}[(z_i)^2 - u^2]}. \tag{C.1.9}$$

Then the above retarded correlator can be expressed as

$$G^{2111}_{\uparrow\downarrow}(\boldsymbol{\omega}) = \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+, \omega_2^-, \omega_3^-, \omega_4^-). \tag{C.1.10}$$

A complete derivation of the Keldysh correlator via analytic continuation from the Matsubara correlator will be delivered in Sec. 5.4.

C.1.3 Other Keldysh correlators

In the following we compute the connected parts $G^{1212}_{\uparrow\downarrow,\mathrm{con}}$, $G^{2221}_{\uparrow\downarrow,\mathrm{con}}$ and $G^{2222}_{\uparrow\downarrow,\mathrm{con}}$. For correlators with more than one 2-index we might have a non-vanishing disconnected part. It can be computed separately with our previous result in Eq. (C.1.5) and subtracted to obtain the connected part of the correlators.

For instance the disconnected part of the correlator $G^{1212}_{\uparrow\downarrow}$ is

$$G^{1212}_{\uparrow\downarrow,\mathrm{dis}}(\boldsymbol{\omega}) = -2\pi\mathrm{i}\delta(\omega_{12})G^{12}(\omega_1, \omega_2)G^{12}(\omega_3, \omega_4) = -\left(\frac{1}{\omega^-_{12}} + \frac{1}{\omega^-_{34}}\right)\frac{\omega_2^-\omega_4^-}{[(\omega_2^-)^2 - u^2][(\omega_4^-)^2 - u^2]} \tag{C.1.11}$$

Using the spectral representation in Eq. (5.2.9) the full correlator is

$$\begin{aligned}
G^{1212}_{\uparrow\downarrow}(\boldsymbol{t}) = \frac{\mathrm{th}\times}{4} e^{-\mathrm{i}t_{1234}u}\Big[&(e^{2\mathrm{i}ut_1}-e^{2\mathrm{i}ut_2})(e^{2\mathrm{i}ut_3}-e^{2\mathrm{i}ut_4})[\mathcal{K}^{\mathcal{T}}(t_1,t_2,t_4,t_3)+\mathcal{K}^{\mathcal{T}}(t_3,t_4,t_2,t_1)]\\
&-(e^{2\mathrm{i}ut_1}-e^{2\mathrm{i}ut_4})(e^{2\mathrm{i}ut_2}-e^{2\mathrm{i}ut_3})[\mathcal{K}^{\mathcal{T}}(t_1,t_4,t_2,t_3)+\mathcal{K}^{\mathcal{T}}(t_3,t_2,t_4,t_1)]\Big]\\
+\frac{e^{-\mathrm{i}t_{1234}u}}{4}\Big[&(e^{2\mathrm{i}ut_1}+e^{2\mathrm{i}ut_2})(e^{2\mathrm{i}ut_3}+e^{2\mathrm{i}ut_4})[\mathcal{K}^{\mathcal{T}}(t_1,t_2,t_3,t_4)+\mathcal{K}^{\mathcal{T}}(t_3,t_4,t_1,t_2)]\\
&+(e^{2\mathrm{i}ut_1}+e^{2\mathrm{i}ut_3})(e^{2\mathrm{i}ut_2}+e^{2\mathrm{i}ut_4})[\mathcal{K}^{\mathcal{T}}(t_1,t_3,t_2,t_4)+\mathcal{K}^{\mathcal{T}}(t_3,t_1,t_2,t_4)\\
&\qquad+\mathcal{K}^{\mathcal{T}}(t_1,t_3,t_4,t_2)+\mathcal{K}^{\mathcal{T}}(t_3,t_1,t_4,t_2)]\\
&+(e^{2\mathrm{i}ut_1}-e^{2\mathrm{i}ut_4})(e^{2\mathrm{i}ut_2}-e^{2\mathrm{i}ut_3})[\mathcal{K}^{\mathcal{T}}(t_1,t_4,t_3,t_2)+\mathcal{K}^{\mathcal{T}}(t_3,t_2,t_1,t_4)]\Big]
\end{aligned} \tag{C.1.12}$$

where we abbreviated $\mathrm{th} = \tanh(\beta u/2)$. After subtracting the disconnected part $G^{1212}_{\uparrow\downarrow,\mathrm{dis}}$ and after simplifications the connected part gives in frequency space

$$\begin{aligned}
G^{1212}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) &= u^2\mathrm{th}\times\Bigg[\frac{1}{[u^2-(\omega_2^+)^2][u^2-(\omega_4^-)^2]}\left(\frac{1}{\omega_{34}^-}+\frac{1}{\omega_{14}^-}\right)\\
&\qquad-\frac{1}{[u^2-(\omega_2^-)^2][u^2-(\omega_4^+)^2]}\left(\frac{1}{\omega_{34}^+}+\frac{1}{\omega_{14}^+}\right)\Bigg]\\
&\quad+\frac{2\pi\mathrm{i}u^2\delta(\omega_{14})}{[u^2-(\omega_1^-)^2][u^2-(\omega_3^-)^2]}\\
&= u^2\mathrm{th}\times\left[\frac{1}{[u^2-(\omega_2^+)^2][u^2-(\omega_4^-)^2]}\left(\frac{1}{\omega_{34}^-}+\frac{1}{\omega_{14}^-}\right)+\mathrm{c.c.}\right]\\
&\quad+\frac{2\pi\mathrm{i}u^2\delta(\omega_{14})}{[u^2-(\omega_1^-)^2][u^2-(\omega_3^-)^2]}.
\end{aligned} \tag{C.1.13}$$

where c.c. stands for the complex conjugate. The other correlators with two Keldysh indices $k_i = 2$ (and $k_i = 1$ else) give similar results.

For the correlators with three Keldysh indices $k_i = 2$ (and $k_i = 1$ else) we have a disconnected part like

$$\begin{aligned}
G^{2221}_{\uparrow\downarrow,\mathrm{dis}}(\boldsymbol{\omega}) &= -2\pi\mathrm{i}\delta(\omega_{12})G^{22}(\omega_1,\omega_2)G^{21}(\omega_3,\omega_4)\\
&= -2\pi^2\mathrm{th}\times\delta(\omega_{12})[\delta(\omega_1-u)-\delta(\omega_1+u)]\frac{-\omega_4^-}{(\omega_4^-)^2-u^2}
\end{aligned} \tag{C.1.14}$$

The corresponding full correlator is

$$\begin{aligned}
&G^{2221}_{\uparrow\downarrow}(\boldsymbol{t}) \\
&= \frac{e^{-\mathrm{i}t_{1234}u}}{4}\sum_{P,\overline{4}=4}(e^{2\mathrm{i}t_{\overline{1}}u}+e^{2\mathrm{i}t_{\overline{2}}u})(e^{2\mathrm{i}t_{\overline{3}}u}-e^{2\mathrm{i}t_4u})\times K^{\mathcal{T}}(t_{\overline{1}},t_{\overline{2}},t_{\overline{3}},t_4) \\
&\quad + \mathrm{th}\times\frac{e^{-\mathrm{i}t_{1234}u}}{4} \\
&\quad\times\Big\{(e^{2\mathrm{i}t_1u}-e^{2\mathrm{i}t_2u})(e^{2\mathrm{i}t_3u}+e^{2\mathrm{i}t_4u})[\mathcal{K}^{\mathcal{T}}(t_1,t_2,t_4,t_3)+\mathcal{K}^{\mathcal{T}}(t_2,t_1,t_4,t_3) \\
&\qquad\qquad -\mathcal{K}^{\mathcal{T}}(t_3,t_4,t_1,t_2)-\mathcal{K}^{\mathcal{T}}(t_3,t_4,t_2,t_1)] \\
&\qquad +(e^{2\mathrm{i}t_1u}-e^{2\mathrm{i}t_4u})(e^{2\mathrm{i}t_2u}+e^{2\mathrm{i}t_3u})[\mathcal{K}^{\mathcal{T}}(t_1,t_4,t_2,t_3)+\mathcal{K}^{\mathcal{T}}(t_1,t_4,t_3,t_2) \\
&\qquad\qquad -\mathcal{K}^{\mathcal{T}}(t_2,t_3,t_4,t_1)-\mathcal{K}^{\mathcal{T}}(t_3,t_2,t_4,t_1)] \\
&\qquad +(e^{2\mathrm{i}t_2u}-e^{2\mathrm{i}t_4u})(e^{2\mathrm{i}t_1u}+e^{2\mathrm{i}t_3u})[\mathcal{K}^{\mathcal{T}}(t_1,t_3,t_4,t_2)+\mathcal{K}^{\mathcal{T}}(t_3,t_1,t_4,t_2) \\
&\qquad\qquad -\mathcal{K}^{\mathcal{T}}(t_2,t_4,t_1,t_3)-\mathcal{K}^{\mathcal{T}}(t_2,t_4,t_3,t_1)]\Big\},
\end{aligned} \tag{C.1.15}$$

where, in the second line, we restricted the permutations $p=(\overline{1},\overline{2},\overline{3},\overline{4})$ to those with $\overline{4}=4$. The second line yields very analogous expressions in frequency space as for G^{2111} in Eq. (C.1.8). It produces the *advanced correlator* $\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^+,\omega_4^-)=[G^{1112}_{\uparrow\downarrow}(\omega)]^*$. After subtracting the disconnected part we obtain for the connected part

$$\begin{aligned}
G^{2221}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) &= \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^+,\omega_4^-) \\
&\quad + 2\pi^2 u\,\mathrm{th}\times[\delta(\omega_3-u)+\delta(\omega_3+u)][\delta(\omega_{13})-\delta(\omega_{14})]\frac{1}{u^2-\left(\omega_4^-\right)^2}.
\end{aligned} \tag{C.1.16}$$

The correlators $G^{2212}_{\uparrow\downarrow,\mathrm{con}}$, $G^{2122}_{\uparrow\downarrow,\mathrm{con}}$ and $G^{1222}_{\uparrow\downarrow,\mathrm{con}}$ are computed analogously.

Now the remaining correlator is, using the spectral representation in Eq. (5.2.9),

$$G^{2222}_{\uparrow\downarrow}(\boldsymbol{t}) = -\mathrm{th}\times\frac{e^{-\mathrm{i}t_{1234}u}}{4}\sum_p(e^{2\mathrm{i}t_{\overline{1}}u}+e^{2\mathrm{i}t_{\overline{2}}u})(e^{2\mathrm{i}t_{\overline{3}}u}+e^{2\mathrm{i}t_{\overline{4}}u})\times K^{\mathcal{T}}(t_{\overline{1}},t_{\overline{2}},t_{\overline{3}},t_{\overline{4}}) \tag{C.1.17}$$

By comparison of its Fourier transform with the retarded correlator in Eq. (C.1.7) we find that this can be written in terms of the function $\Phi_{\uparrow\downarrow,\mathrm{con}}$ again. For instance, for the permutations $p=(\overline{1},\overline{2},\overline{3},\overline{4})$ with $\overline{1}=1$ we can reuse Eq. (C.1.8) and only have to replace the factor

$$\left[\frac{1}{\omega_1^+ + u}-\frac{1}{\omega_1^+ - u}\right] = \frac{2u}{u^2-(\omega_1^-)^2}$$

by the factor

$$-\mathrm{th}\times\left[\frac{1}{\omega_1^+ + u}+\frac{1}{\omega_1^+ - u}\right] = \mathrm{th}\times\frac{2\omega_1^-}{u^2-(\omega_1^-)^2}$$

This gives for the full correlator

$$G^{2222}_{\uparrow\downarrow} = \frac{\mathrm{th}}{u}\Big[\omega_1^+\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-) + \omega_2^+\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-) + \omega_3^+\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-) + \omega_4^+\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\Big]. \tag{C.1.18}$$

C.2 Comparison of direct computation and analytic continuation

Next we demonstrate that the results of the analytic continuation agree with those from direct computation. Since the fulfillment of the FDR is checked separately in App. C.3.1 it suffices to confirm agreement of the results for correlators with two 2-indices. For these components the analytic continuation proceeds analogously. Here we use the example of $G^{1122}_{\uparrow\downarrow,\mathrm{con}}$. To do so we have to get explicit formulas for the discontinuities. Above formulas in Eqs. (5.4.3f)-(5.4.3k) contain the factors N_i. To compare these with the direct computation we have to evaluate the frequency in $N_i = \tanh(\beta\omega_i/2)$ at certain energies $\pm u$. We hence expect the discontinuities to contain suitable Dirac delta functions.

These delta functions are easily obtained after rewriting $\Phi_{\uparrow\downarrow,\mathrm{con}}$ e.g. as

$$\Phi_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{z}) = \frac{1}{4}\left[\frac{1}{z_4+u}-\frac{1}{z_4-u}\right]\left[\frac{1}{z_1+u}\left(\frac{1}{z_2-u}+\frac{1}{z_3-u}\right)+\frac{1}{z_2+u}\left(\frac{1}{z_1-u}+\frac{1}{z_3-u}\right)\right. \tag{C.2.1}$$

$$\left.+\frac{1}{z_3+u}\left(\frac{1}{z_1-u}+\frac{1}{z_2-u}\right)\right]. \tag{C.2.2}$$

When subtracting two AC functions which differ by the frequency $\omega_3^\pm$ we can consider every summand of the type $[(z_4+u)(z_1+u)(z_2-u)]^{-1}$ individually. Then, a discontinuity can be read off from Eq. (C.2.1) to be

$$\begin{aligned}
&N_3[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)]\\
&= \frac{N_3}{4}\left[\frac{1}{\omega_4^+ + u} - \frac{1}{\omega_4^+ - u}\right]\\
&\quad\times\left[-2\pi\mathrm{i}\delta(\omega_3-u)\left(\frac{1}{\omega_1^-+u}+\frac{1}{\omega_2^-+u}\right) - 2\pi\mathrm{i}\delta(\omega_3+u)\left(\frac{1}{\omega_1^--u}+\frac{1}{\omega_2^--u}\right)\right]
\end{aligned}$$

and using the delta functions we obtain

$$= \pi\mathrm{i}\,\mathrm{th}\frac{u}{(\omega_4^+)^2-u^2}\Big[\delta(\omega_3-u)-\delta(\omega_3+u)\Big]\left(\frac{1}{\omega_{13}^-}+\frac{1}{\omega_{23}^-}\right). \tag{C.2.3}$$

Other discontinuities are computed analogously and in total we obtain

$$G^{1122}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) = N_3\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\big]$$

$$
\begin{aligned}
&+ N_4\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)\big] \\
&+ \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) \\
&= \mathrm{th}\frac{-2\pi\mathrm{i}}{4}\frac{-2u}{(\omega_4^+)^2-u^2}\left[\delta(\omega_3-u)-\delta(\omega_3+u)\right]\left(\frac{1}{\omega_{13}^-}+\frac{1}{\omega_{23}^-}\right) \\
&+ \mathrm{th}\frac{-2\pi\mathrm{i}}{4}\frac{-2u}{(\omega_3^+)^2-u^2}\left[\delta(\omega_4-u)-\delta(\omega_4+u)\right]\left(\frac{1}{\omega_{14}^-}+\frac{1}{\omega_{24}^-}\right) \\
&+ \frac{2\pi\mathrm{i}u^2}{[(\omega_3^+)^2-u^2][(\omega_4^+)^2-u^2]}\left[\delta(\omega_{13})[\mathrm{th}-1]+\delta(\omega_{14})[\mathrm{th}+1]\right],
\end{aligned}
$$

and sorting the expressions by the factor $\mathrm{th} = \tanh(\beta u/2)$ we get

$$
\begin{aligned}
&= \frac{2\pi\mathrm{i}u^2[\delta(\omega_{14})-\delta(\omega_{13})]}{[(\omega_3^+)^2-u^2][(\omega_4^+)^2-u^2]} \\
&+ \mathrm{th}\frac{2\pi\mathrm{i}}{4}\Bigg[\frac{-2u}{(\omega_4^+)^2-u^2}\left[\delta(\omega_3+u)-\delta(\omega_3-u)\right]\left(\frac{1}{\omega_{13}^-}+\frac{1}{\omega_{23}^-}\right) \\
&\qquad + \frac{-2u}{(\omega_3^+)^2-u^2}\left[\delta(\omega_4+u)-\delta(\omega_4-u)\right]\left(\frac{1}{\omega_{14}^-}+\frac{1}{\omega_{24}^-}\right) \\
&\qquad + \frac{4u^2}{[(\omega_3^+)^2-u^2][(\omega_4^+)^2-u^2]}\left[\delta(\omega_{13})+\delta(\omega_{14})\right]\Bigg],
\end{aligned}
$$

by writing out the delta functions e.g. as $2\pi\mathrm{i}[\delta(\omega_3+u)-\delta(\omega_3-u)] = \frac{-2u}{(\omega_3^-)^2-u^2} - \frac{-2u}{(\omega_3^+)^2-u^2}$ we can cancel many terms and recover

$$
= \frac{2\pi\mathrm{i}u^2[\delta(\omega_{14})-\delta(\omega_{13})]}{[(\omega_3^+)^2-u^2][(\omega_4^+)^2-u^2]} + \frac{\mathrm{th}}{4}\left[\frac{-2u}{(\omega_3^+)^2-u^2}\frac{-2u}{(\omega_4^-)^2-u^2}\left(\frac{1}{\omega_{24}^-}+\frac{1}{\omega_{14}^-}\right) - \text{ c.c. }\right]
$$

which is exactly the result from direct computation Eq. (5.3.3f).

C.3 Consistency checks

C.3.1 Generalized fluctuation dissipation relations

In this appendix we verify that our result for the KF correlator in Eq. (5.3.3) fulfills the generalized Fluctuation-Dissipation Relations (FDRs) and have been derived in Ref. [12,32] and in 4.1. They are summarized in Eqs. (B.2.3) and (B.2.4) for the fermionic operators. As we mentioned at the end of Sec. 5.1 the primed correlator equals the complex conjugated one ($G' = G^*$) since the Hamiltonian is a real function of the creation and annihilation operators.

We only consider the connected part of the correlator since the disconnected part also fulfills them. The FDR for $G^{2211}_{\uparrow\downarrow,\mathrm{con}}$ and $G^{1122}_{\uparrow\downarrow,\mathrm{con}}$ can be easily verified by use of the formulas obtained from analytic continuation in Eqs. (5.4.3f) and (5.4.3k). The formulas obtained from direct computation are not well suited for an analytical check of the FDR. In the correlators G^{1122} and G^{2211} the statistical factors N_i have been evaluated at certain frequencies which empedes a direct comparison with frequency-dependent factors N_i.

The right-hand side of Eq. (B.2.3a) gives for $G^{2211}_{\uparrow\downarrow,\mathrm{con}}$

$$- N_2 G^{2111}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) - N_1 G^{1211}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) + \frac{N_1+N_2}{N_3+N_4}\Big(N_4 G^{1121}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) + N_3 G^{1112}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) + G^{1122}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega})\Big)^*$$

and plugging in the relations in Eqs. (5.4.3) we find

$$\begin{aligned}
&= -N_2\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-) - N_1\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\\
&\quad + \frac{N_1+N_2}{N_3+N_4}\Big(N_4\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-) + N_3\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\\
&\qquad + N_4\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)\big] + \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+)\\
&\qquad + N_3\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)\big] + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+)\Big)^*\\
&= -N_2\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-) - N_1\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\\
&\quad + \frac{N_1+N_2}{N_3+N_4}\Big((N_3+N_4)\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+)\\
&\qquad\qquad + \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+)\Big)^*\\
&= -N_2\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-) - N_1\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\\
&\quad + (N_1+N_2)\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-)\\
&\quad - \frac{N_1+N_2}{N_3+N_4}\Big(\widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-)\Big),
\end{aligned}$$

using $\widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}} \propto \delta(\omega_{14})$ and $\frac{N_1+N_2}{N_3+N_4}\delta(\omega_{14}) = -\delta(\omega_{14})$ and similar relations for $\widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}$ we find

$$\begin{aligned}
&= +N_2\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)\big]\\
&\quad + N_1\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)\big]
\end{aligned}$$

$$
\begin{aligned}
&+ \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) \\
&\overset{Eq.\ (5.3.3k)}{=} G^{2211}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}).
\end{aligned}
$$

We also check the FDR for $G^{1222}_{\uparrow\downarrow,\mathrm{con}}$ for which the right-hand side of Eq. (B.2.4d) gives

$$
\begin{aligned}
&(1+N_2N_3+N_2N_4+N_3N_4)[G^{2111}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega})]^* - N_3N_4G^{1211}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) - N_2N_4G^{1121}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) \\
&\quad - N_2N_3G^{1112}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) - N_4G^{1221}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) - N_3G^{1212}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}) - N_2G^{1122}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega})
\end{aligned}
$$

plugging in the relations in Eqs. (5.4.3) we find

$$
\begin{aligned}
&= \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^+) + N_3N_4[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) \\
&\qquad\qquad - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+) + \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)] \\
&\quad + N_2N_4[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) \\
&\qquad\qquad - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) + \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^-)] \\
&\quad + N_2N_3[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^+) - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+) \\
&\qquad\qquad - \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+) + \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^-,\omega_4^+)] \\
&\quad + N_3[\widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) - \widehat{\Phi}^{(12)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+)] \\
&\quad + N_2[\widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^-) - \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+)] \\
&\quad + N_2[\widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^+) - \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^-,\omega_3^+,\omega_4^+)].
\end{aligned}
$$

The discontinuities in square brackets can be computed similarly to the one in Eq. (C.2.3). They give delta functions which allow to evaluate the factors N_i to $\pm\mathrm{th} = \pm\tanh(\beta u/2)$.

$$
\begin{aligned}
&= \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^+) + N_3N_4 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_4-u)+\delta(\omega_4+u)]\delta(\omega_{34}) \\
&\quad + N_2N_4 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_2-u)+\delta(\omega_2+u)]\delta(\omega_{24}) \\
&\quad + N_2N_3 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_2-u)+\delta(\omega_2+u)]\delta(\omega_{23}) \\
&\quad - N_3\mathrm{th}\, 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_4-u)-\delta(\omega_4+u)]\delta(\omega_{34}) \\
&\quad - N_2(\mathrm{th}-1)\, 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_2-u)-\delta(\omega_2+u)]\delta(\omega_{24}) \\
&\quad - N_2(\mathrm{th}+1)\, 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_2-u)-\delta(\omega_2+u)]\delta(\omega_{23}) \\
&= \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^+,\omega_4^+) + \mathrm{th}\, 2\pi^2 \frac{u}{(\omega_1^-)^2-u^2}[\delta(\omega_2-u)+\delta(\omega_2+u)][\delta(\omega_{24})-\delta(\omega_{23})] \\
&\overset{Eq.\ (5.3.3l)}{=} G^{1222}_{\uparrow\downarrow,\mathrm{con}}(\boldsymbol{\omega}).
\end{aligned}
$$

We see that for the above components our result fully agrees with the FDRs.

C.3.2 SU(2) spin symmetry

Due to the SU(2) spin symmetry of the Hubbard model we only need to compute the 4p correlator $G_{\uparrow\downarrow}$. It has been shown in Ref. [19] that every other spin configuration can be obtained by use of the fermionic exchange symmetry and the SU(2) symmetry. In the following we demonstrate that the corresponding relation in the KF [see Eq. (5.1.21)] is fulfilled for our result for the Hubbard atom.

In Ref. [19] the correlator $G_{\uparrow\uparrow}$ has been computed in the Matsubara formalism in which its disconnected part gives

$$G_{\uparrow\uparrow,\mathrm{dis}}(\mathrm{i}\omega_1,\mathrm{i}\omega_2,\mathrm{i}\omega_3,\mathrm{i}\omega_4) = -\beta\delta_{\omega_{12},0}G(\mathrm{i}\omega_1,\mathrm{i}\omega_2)G(\mathrm{i}\omega_3,\mathrm{i}\omega_4) + \beta\delta_{\omega_{14}}G(\mathrm{i}\omega_1,\mathrm{i}\omega_4)G(\mathrm{i}\omega_3,\mathrm{i}\omega_2) \tag{C.3.1}$$

and the connected part is

$$G_{\uparrow\uparrow,\mathrm{con}}(\mathrm{i}\omega_1,\mathrm{i}\omega_2,\mathrm{i}\omega_3,\mathrm{i}\omega_4) = \frac{u^2\beta[\delta_{\omega_{14},0}-\delta_{\omega_{12},0}]}{\prod_{i=1}^{4}[\mathrm{i}\omega_i - u]}. \tag{C.3.2}$$

Since the disconnected part fulfills Eq. (5.1.21) separately, we can focus on the connected part of the correlator. By direct computation of the correlators, as discussed for $G_{\uparrow\downarrow}$, we obtain

$$G^{1111}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = G^{1112}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = G^{1121}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = G^{1211}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = G^{2111}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 0, \tag{C.3.3a}$$

$$G^{1122}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi\mathrm{i}u^2\frac{\delta(\omega_{14})}{[(\omega_2^-)^2-u^2][(\omega_4^+)^2-u^2]}, \tag{C.3.3b}$$

$$G^{1212}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi\mathrm{i}u^2\frac{\delta(\omega_{14})-\delta(\omega_{12})}{[(\omega_2^+)^2-u^2][(\omega_4^+)^2-u^2]}, \tag{C.3.3c}$$

$$G^{1221}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi\mathrm{i}u^2\frac{-\delta(\omega_{12})}{[(\omega_2^+)^2-u^2][(\omega_4^-)^2-u^2]}, \tag{C.3.3d}$$

$$G^{2112}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi\mathrm{i}u^2\frac{-\delta(\omega_{12})}{[(\omega_2^-)^2-u^2][(\omega_4^+)^2-u^2]}, \tag{C.3.3e}$$

$$G^{2121}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi\mathrm{i}u^2\frac{\delta(\omega_{14})-\delta(\omega_{12})}{[(\omega_2^-)^2-u^2][(\omega_4^-)^2-u^2]}, \tag{C.3.3f}$$

$$G^{2211}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi\mathrm{i}u^2\frac{\delta(\omega_{14})}{[(\omega_2^+)^2-u^2][(\omega_4^-)^2-u^2]}, \tag{C.3.3g}$$

$$G^{1222}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi^2 u\,\mathrm{th}\,\frac{1}{(\omega_1^-)^2-u^2}[\delta(\omega_3-u)+\delta(\omega_3+u)][\delta(\omega_{14})-\delta(\omega_{12})], \tag{C.3.3h}$$

$$G^{2122}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi^2 u\,\mathrm{th}\,\frac{1}{(\omega_2^-)^2-u^2}[\delta(\omega_4-u)+\delta(\omega_4+u)][\delta(\omega_{14})-\delta(\omega_{12})], \tag{C.3.3i}$$

$$G^{2212}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi^2 u\,\mathrm{th}\,\frac{1}{(\omega_3^-)^2-u^2}[\delta(\omega_1-u)+\delta(\omega_1+u)][\delta(\omega_{14})-\delta(\omega_{12})], \tag{C.3.3j}$$

$$G^{2221}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = 2\pi^2 u\,\mathrm{th}\,\frac{1}{(\omega_4^-)^2-u^2}[\delta(\omega_2-u)+\delta(\omega_2+u)][\delta(\omega_{14})-\delta(\omega_{12})], \tag{C.3.3k}$$

$$G^{2222}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega}) = -\mathrm{i}4\pi^3\mathrm{th}^2\times[\delta(\omega_{12})-\delta(\omega_{14}][\delta(u+\omega_1)-\delta(u-\omega_1)][\delta(u+\omega_3)-\delta(u-\omega_3)]. \tag{C.3.3l}$$

A convenient way to reproduce these results is by use of the formulas for analytic continuation and the FDR. We have the analytically continued functions

$$\Phi_{\uparrow\uparrow}(z_1,z_2,z_3,z_4) = 0, \tag{C.3.4}$$

$$\widehat{\Phi}^{(12)}_{\uparrow\uparrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = -\frac{u^2 2\pi\mathrm{i}\delta(\omega_{12})}{\prod_{i=1}^{4}[z_i-u]}, \tag{C.3.5}$$

$$\widehat{\Phi}^{(14)}_{\uparrow\uparrow,\mathrm{con}}(z_1,z_2,z_3,z_4) = +\frac{u^2 2\pi\mathrm{i}\delta(\omega_{14})}{\prod_{i=1}^{4}[z_i-u]}. \tag{C.3.6}$$

The correspondence between these functions and the correlators is directly visible for those with two Keldysh indices $k_i = 2$. And the remaining correlators are conveniently checked with the FDRS.

One can now check whether Eq. (5.1.21) is fulfilled. This is easily done for the retarded correlators since $\Phi_{\uparrow\downarrow,\mathrm{con}}$ is symmetric under exchange of frequency arguments. To give an explicit example we consider the correlator $G^{1122}_{\uparrow\uparrow,\mathrm{con}}(\boldsymbol{\omega})$ for which we have to subtract

$$\begin{aligned} G^{1122}_{\uparrow\downarrow,\mathrm{con}}(\omega_1,\omega_2,\omega_3,\omega_4) = {} & \frac{2\pi\mathrm{i}u^2[\delta(\omega_{14})-\delta(\omega_{13})]}{[(\omega_1^-)^2-u^2][(\omega_2^-)^2-u^2]} \\ & + u^2\mathrm{th}\times\left[\frac{1}{[(\omega_3^+)^2-u^2][(\omega_4^-)^2-u^2]}\left(\frac{1}{\omega_{24}^-}+\frac{1}{\omega_{14}^-}\right) - \text{ c.c.}\right], \end{aligned} \tag{C.3.7}$$

and

$$\begin{aligned} G^{1221}_{\uparrow\downarrow,\mathrm{con}}(\omega_1,\omega_4,\omega_3,\omega_2) = {} & \frac{-2\pi\mathrm{i}u^2\delta(\omega_{13})}{[(\omega_1^-)^2-u^2][(\omega_2^-)^2-u^2]} \\ & + u^2\mathrm{th}\times\left[\frac{1}{[(\omega_3^+)^2-u^2][(\omega_4^-)^2-u^2]}\left(\frac{1}{\omega_{24}^-}+\frac{1}{\omega_{14}^-}\right) - \text{ c.c.}\right]. \end{aligned} \tag{C.3.8}$$

So we obtain the result

$$G^{1122}_{\uparrow\downarrow,\mathrm{con}}(\omega_1,\omega_2,\omega_3,\omega_4) - G^{1221}_{\uparrow\downarrow,\mathrm{con}}(\omega_1,\omega_4,\omega_3,\omega_2) = 2\pi\mathrm{i}u^2\frac{\delta(\omega_{14})}{[(\omega_2^-)^2-u^2][(\omega_4^+)^2-u^2]} \tag{C.3.9}$$

$$= G^{1122}_{\uparrow\uparrow,\mathrm{con}}(\omega_1,\omega_2,\omega_3,\omega_4), \tag{C.3.10}$$

which fulfills the relation in Eq. (5.1.21) due to SU(2) spin symmetry.

C.4 The vertex function

Given the one- and the two-particle correlator we can extract an interaction vertex. It can be obtained from the connected part of the Keldysh correlator $G_{\uparrow\downarrow,\mathrm{con}}$ by factoring out the four one-particle propagators (in diagrammatic terms this is called "amputation" of external legs). In Sec. 4.2 we already discussed vertex functions in general. We argued that they have the very same analytic structure as the corresponding correlators and can be computed with the same linear combinations of AC functions. However, in this appendix we use a more direct approach to confirm the results of Sec. 4.2 .

The amputation of the external legs reads

$$F^{\boldsymbol{k}}(\boldsymbol{\omega}) = \sum_{\{\boldsymbol{k}'\}} [G^{-1}(\omega_1)]^{k_1 k_1'} [G^{-1}(\omega_3)]^{k_3 k_3'} G_{\mathrm{con}}^{k_1' k_2' k_3' k_4'}(\boldsymbol{\omega}) [G^{-1}(-\omega_2)]^{k_2' k_2} [G^{-1}(-\omega_4)]^{k_4' k_4}. \tag{C.4.1}$$

For a fermionic one-particle correlator the fluctuation-dissipation theorem $G^K(\omega_i) = N_i\big(G^R(\omega_i) - G^A(\omega_i)\big)$ is exactly fulfilled. The inverse is in general

$$G^{-1}(\omega_i) = \begin{pmatrix} [G^{-1}(\omega_i)]^K & [G^{-1}(\omega_i)]^R \\ [G^{-1}(\omega_i)]^A & 0 \end{pmatrix} = \begin{pmatrix} N_i\big([G^R(\omega_i)]^{-1} - [G^A(\omega_i)]^{-1}\big) & [G^R(\omega_i)]^{-1} \\ [G^A(\omega_i)]^{-1} & 0 \end{pmatrix}. \tag{C.4.2}$$

For comparison we also directly invert the one-particle correlator in Eq. (C.1.5), giving

$$G^{-1}(\omega) = \begin{pmatrix} \tanh(\beta u/2)\frac{4\mathrm{i}u\omega\gamma}{\omega^2+\gamma^2} & \frac{(\omega+\mathrm{i}\gamma)^2-u^2}{\omega+\mathrm{i}\gamma} \\ \frac{(\omega-\mathrm{i}\gamma)^2-u^2}{\omega-\mathrm{i}\gamma} & 0 \end{pmatrix}, \tag{C.4.3}$$

where we use the parametrization of the complex frequency $\omega^{\pm} = \omega \pm \mathrm{i}\gamma$ with $\gamma > 0$. By use of Eq. (C.4.1) we can now directly compute the vertex function $F_{\uparrow\downarrow}^{\boldsymbol{k}}(\boldsymbol{\omega})$ from the four-point correlator $G_{\uparrow\downarrow,\mathrm{con}}^{\boldsymbol{k}}(\boldsymbol{\omega})$. Note however that, analytically, one must not take the limit $\gamma_i \to 0$ or use a delta distribution yet since this is only sensible for the final expression, e.g. we incautiously cannot take the limit

$$\lim_{\gamma \searrow 0} [G^{-1}(\omega)]^K \propto \lim_{\gamma \searrow 0} \frac{\mathrm{i}\gamma\omega}{\omega^2+\gamma^2} = 2\pi\mathrm{i}\delta(\omega)\omega = 0.$$

These infinitesimal regularizations cannot be neglected. In this simple example even the one-particle correlator would not be recovered, otherwise. Vertex functions are used to construct more complicated diagrams for which they are multiplied with propagators and other vertex functions. In particular the vertex function F has to recover the connected part of the correlator G_{con} when multiplied with the one-particle correlators.

Since $[G^{-1}(\omega)]^{k_1 k_2}$ is not diagonal in Keldysh space the sum over $\boldsymbol{k}'$ in Eq. (C.4.1) can give several contributions. Due to $[G^{-1}]^{22} = 0$ and $G^{1111} = 0$ the number of contributions increases with the number of Keldysh indices $k_i = 1$ in $F^{\boldsymbol{k}}$. One finds that $F^{2222} = 0$

always holds. Similarly, for a *retarded* vertex function (with a single Keldysh index $k_i = 1$ and $k_i = 2$ else) the only non-vanishing contribution is e.g.

$$F^{1222}(\boldsymbol{\omega}) = [G^R(\omega_1)]^{-1}[G^A(\omega_3)]^{-1}G^{2111}_{\mathrm{con}}(\boldsymbol{\omega})[G^R(-\omega_2)]^{-1}[G^R(-\omega_4)]^{-1}. \tag{C.4.4}$$

Since the retarded correlator $G^{2111}_{\uparrow\downarrow}(\boldsymbol{\omega})$ is the analytic continuation $\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)$ we see that the analytic continuation of the propagators (the external legs)

$$G^R(\omega) = G(\mathrm{i}\omega)|_{\mathrm{i}\omega\to\omega+\mathrm{i}0^+}\,, \quad G^A(\omega) = G(\mathrm{i}\omega)|_{\mathrm{i}\omega\to\omega-\mathrm{i}0^+}\,, \tag{C.4.5}$$

is consistent with that of the correlators. Hence we can define the analytic continuation of the regular part of the vertex function in Eq. (5.1.24b) as

$$\widetilde{\Phi}^{(F)}_{\uparrow\downarrow}(\boldsymbol{z}) = u + \frac{u^3\sum_{i=1}^{4} z_i^2 - 6u^5}{2\prod_{i=1}^{4} z_i}, \tag{C.4.6}$$

such that the above vertex functions can be written as $F^{1222}_{\uparrow\downarrow}(\boldsymbol{\omega}) = \widetilde{\Phi}^{(F)}_{\uparrow\downarrow}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)$. Those vertex functions with two Keldysh indices $k_i = 1$ (and $k_i = 2$ else) give three contributions, e.g.

$$\begin{aligned} F^{1122}(\boldsymbol{\omega}) &= [G^R(\omega_1)]^{-1}[G^A(\omega_3)]^{-1}G^{2211}_{\mathrm{con}}(\boldsymbol{\omega})[G^A(-\omega_2)]^{-1}[G^R(-\omega_4)]^{-1} \\ &+ [G^{-1}(\omega_1)]^K[G^A(\omega_3)]^{-1}G^{1211}_{\mathrm{con}}(\boldsymbol{\omega})[G^A(-\omega_2)]^{-1}[G^R(-\omega_4)]^{-1} \\ &+ [G^{-1}(\omega_1)]^R[G^A(\omega_3)]^{-1}G^{1211}_{\mathrm{con}}(\boldsymbol{\omega})[G^{-1}(-\omega_2)]^K[G^R(-\omega_4)]^{-1}. \end{aligned} \tag{C.4.7}$$

We can write these in terms of AC functions by plugging in the right-hand side of Eq. (5.4.3k) for $G^{2211}_{\uparrow\downarrow,\mathrm{con}}$ and by use of $[G^{-1}(\omega_i)]^K = N_i\big([G^R(\omega_i)]^{-1} - [G^A(\omega_i)]^{-1}\big)$ we find that

$$\begin{aligned} &F^{1122}_{\uparrow\downarrow}(\boldsymbol{\omega}) \\ &= \Big[N_1\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) - \cancel{\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)}\big] + \widehat{\Phi}^{(13)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) \\ &\quad + N_2\big[\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-) - \cancel{\Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)}\big] + \widehat{\Phi}^{(14)}_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^+,\omega_3^-,\omega_4^-)\Big] \\ &\qquad \times \big[G^R(\omega_1)G^A(\omega_3)G^A(-\omega_2)G^R(-\omega_4)\big]^{-1} \\ &\quad + \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^-,\omega_2^+,\omega_3^-,\omega_4^-)N_1\Big[\cancel{[G^R(\omega_1)]^{-1}} - [G^A(\omega_1)]^{-1}\Big][G^A(\omega_3)G^A(-\omega_2)G^R(-\omega_4)]^{-1} \\ &\quad + \Phi_{\uparrow\downarrow,\mathrm{con}}(\omega_1^+,\omega_2^-,\omega_3^-,\omega_4^-)[G^R(\omega_1)G^A(\omega_3)G^R(-\omega_4)]^{-1}N_2\Big[\cancel{[G^A(-\omega_2)]^{-1}} - [G^R(-\omega_2)]^{-1}\Big]. \end{aligned} \tag{C.4.8}$$

The canceled contributions are those for which the analytic continuation of the 4-point correlator is inconsistent with the analytic continuation of the external legs. We see that indeed only the consistent contributions remain and they can be expressed in terms of AC functions again. For the vertex functions with more than two 1's in the Keldysh indices the FDRs can be used to guarantee this property.

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Erklärung

Hiermit erkläre ich, die vorliegende Arbeit selbstständig verfasst zu haben und keine anderen als die in der Arbeit angegebenen Quellen und Hilfsmittel benutzt zu haben.

München, den 02. November 2020

Anxiang Ge