

Ladder equation for the three-particle vertex and its approximate solution

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We generalize the three two-particle Bethe-Salpeter equations to ten three-particle ladders. These equations are exact and yield the exact three-particle vertex, if we knew the three-particle vertex irreducible in one of the ten channels. However, as we do not have this three-particle irreducible vertex at hand, we approximate this building block for the ladder by the sum of two-particle irreducible vertices, each connecting two fermionic lines. The comparison to the exact solution shows that this approximation is only good for rather weak interactions and even then only qualitatively—at least for the nonlinear response function analyzed.

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I. INTRODUCTION

Feynman diagrams are at the heart of the theory of strongly correlated electrons. Textbooks [1] study diagrams for one- and two-particle Green's functions, which provide renormalizations (and lifetimes) of the quasiparticles and susceptibilities, respectively. One-particle Green's functions and self-energies also form the basis of dynamical mean field theory (DMFT) [2–5], whereas two-particle Green's functions and vertices build the fundament of diagrammatic extensions of DMFT [6–8].

Electronic correlations on the next level of three-particle Feynman diagrams are hitherto hardly explored. A calculation of selected three-particle contributions shows that these may become relevant for diagrammatic extensions of DMFT [9–11]. Similarly, for the functional renormalization group the next level, hitherto largely neglected, is the three-particle level [12]. This calls for a better understanding and for developing methods to actually calculate three-particle Green's functions and vertices more systematically.

Physics-wise, three-particle Green's functions are relevant for calculating Raman and Hall responses [13] as well as for nonlinear response functions [14–18]. Traditionally, such calculations have been restricted to calculating the three-particle correlator from bubble contributions with quasiparticle renormalizations of the Green's functions but without vertex corrections; or more recently by including a two-particle vertex between the electron-hole pair of one of the bosonic fields/responses [16]. The three-particle Green's function has also recently been used to obtain electronic spectra [19,20].

In related research fields, three-particle physics is also relevant for trions in semiconductors, which are typically

treated as a three-particle Hamiltonian [21,22]. In quantum chromodynamics (QCD), three-particle extensions of the Bethe-Salpeter equations, the so-called Faddeev equations [23], are employed for solving the three-particle problem of, e.g., quarks forming protons or neutrons. Approximations such as the rainbow-ladder truncation [24] have been developed. The Faddeev equations have also been employed in nuclear physics to study the propagation of two holes and a particle interacting with each other through phonons [25]. A notable difference is that in solid-state physics our three particles or holes propagate in a background of many more electrons with which they interact strongly. This requires more involved Feynman diagrams where we can have at a given time many more (or fewer) than three particle or hole excitations. A mapping onto a three-particle Hamiltonian is no longer possible.

In this paper, we derive a three-particle analog of the Bethe-Salpeter equation. Irreducibility on the three-particle level is more involved and leads to additional one-particle reducible diagrams that need to be considered for the nine particle-particle-hole channels but not for the particle-particle-particle channel. Further, we solve this generalized Bethe-Salpeter ladder for an approximate irreducible three-particle vertex that consists only of the two-particle vertices connecting all possible pairs of particle (hole) lines. To fulfill crossing symmetries of the vertex, contributions from multiple channels need to be considered. The thus approximated three-particle vertex is then compared to the exact one for an Anderson impurity model (AIM) at DMFT self-consistency. For this AIM, the vertex is local and can be calculated exactly.

The outline of the paper is as follows: Sec. II sets the stage, defining the AIM and recalling some essentials for the two-particle diagrammatics. Section III defines the three-particle Green's function and vertex, as well as our frequency and spin notation. Section IV is the main part of this paper. Here, we derive the three-particle Bethe-Salpeter-like ladder equations in Sec. IV A and develop an approximation in terms of two particle irreducible vertices in Sec. IV B. Section V presents numerical results for the latter and compares them to

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the exact ones. Finally, Sec. VI summarizes our results and provides a brief outlook.

II. THEORETICAL BACKGROUND

In this section, we define the AIM, the two-particle Green's function and vertex. We further recall the parquet and Bethe-Salpeter ladder equation as well as the crossing symmetry, which is very helpful for later understanding the extensions to three particles.

A. Anderson impurity model

The AIM, introduced in 1961 by P. W. Anderson to describe magnetic impurities in metals [26], has become a popular model in the field of correlated many-electron systems. Arguably, this is because even though its Hamilton operator, which is described below, is rather simple, it already shows effects of strong correlation, more specifically the Kondo effect [27,28]. Another important aspect is that its solution is connected to local correlation functions of more complex lattice Hamilton operators in DMFT [4] and its diagrammatic extensions [8]. For an in-depth review of the physics of the AIM and the Kondo problem, see Refs. [29,30].

The Hamilton operator of the AIM reads

$$\hat{H}_{\text{AIM}} = \epsilon \hat{n} + U \hat{n}_{\uparrow} \hat{n}_{\downarrow} + \sum_{k,\sigma} \epsilon_k \hat{c}_{k\sigma}^{\dagger} \hat{c}_{k\sigma} + \sum_{k,\sigma} (V_k \hat{f}_{\sigma}^{\dagger} \hat{c}_{k\sigma} + \text{H.c.}). \quad (1)$$

The first two terms describe the impurity with one-particle energy ϵ . Electrons with spin $\sigma = \uparrow, \downarrow$ on the impurity are created and annihilated with $\hat{f}_{\sigma}^{\dagger}$ and $\hat{f}_{\sigma}$, respectively. As usual, the density operators are given by $\hat{n} = \hat{n}_{\uparrow} + \hat{n}_{\downarrow}$, with $\hat{n}_{\sigma} = \hat{f}_{\sigma}^{\dagger} \hat{f}_{\sigma}$. If the impurity is doubly occupied, the local Coulomb interaction U comes into play. The third term models a bath of noninteracting electrons with dispersion relation ϵ_k in terms of creation and annihilation operators $\hat{c}_{k\sigma}^{\dagger}$ and $\hat{c}_{k\sigma}$. The last two terms describe hopping (hybridization) from the bath to the impurity (V_k) and vice versa (Hermitian conjugate; V_k^*).

Here, we employ the AIM with a real, k -independent hybridization $V_k \equiv V \in \mathbb{R}$ and with a bath density of states (DOS) given by DMFT self-consistency for the Hubbard model [4] with the same U , hopping $t \equiv 1$ and inverse temperature $\beta = 1/T = 10$ (we set the Boltzmann constant k_B to 1 and use $\hbar \equiv 1$). The motivation behind this choice is that we are eventually interested in diagrammatic extensions of DMFT, which have the local two- or, on the next level, three-particle vertices of such an AIM as a starting point (see Ref. [8]). However, here we do not pursue further calculations of nonlocal correlations of the Hubbard model. For the purpose of this paper, we only calculate one-, two-, and three-particle Green's functions and vertices of an AIM whose bath is determined by DMFT self-consistency.

B. Two-particle Green's function

The two-particle Green's function G_2 is defined as

$$G_{2,1234}(\tau_1, \tau_2, \tau_3, \tau_4) := (-1)^2 \langle T \hat{c}_1(\tau_1) \hat{c}_2^{\dagger}(\tau_2) \hat{c}_3(\tau_3) \hat{c}_4^{\dagger}(\tau_4) \rangle, \quad (2)$$

where T is the Wick imaginary-time ordering operator [1], $\tau_1, \dots, \tau_4 \in [0, \beta]$ are imaginary time variables (for details on

TABLE I. Frequency notations for the ph, pp, and $\overline{\text{ph}}$ channel.

Channel	ν_1	ν_2	ν_3	ν_4
ph	ν	$\nu - \omega$	$\nu' - \omega$	ν'
pp	ν	$\omega - \nu'$	$\omega - \nu$	ν'
$\overline{\text{ph}}$	ν	ν'	$\nu' - \omega$	$\nu - \omega$

the imaginary time Matsubara formalism, see Refs. [1,31]), and where we use compound indices 1–4 for all quantum numbers such as spin, orbitals, and sites or momenta. The Fourier transformation from imaginary time to Matsubara frequencies $\nu_n = (2n + 1)\pi/\beta$, $n \in \mathbb{Z}$ can be rewritten by explicitly including energy conservation as follows:

$$\begin{aligned} G_{2,1234}^{\nu_1 \nu_2 \nu_3 \nu_4} &:= \iiint_0^{\beta} d\tau_1, \tau_2, \tau_3, \tau_4 G_{2,1234}(\tau_1, \tau_2, \tau_3, \tau_4) \\ &\quad \times e^{i(\nu_1 \tau_1 - \nu_2 \tau_2 + \nu_3 \tau_3 - \nu_4 \tau_4)} \\ &= \beta \delta^{\nu_1 - \nu_2 + \nu_3 - \nu_4, 0} \iiint_0^{\beta} d\tau'_1, \tau'_2, \tau'_3 \\ &\quad G_{2,1234}(\tau'_1, \tau'_2, \tau'_3) e^{i(\nu_1 \tau'_1 - \nu_2 \tau'_2 + \nu_3 \tau'_3)} \\ &=: \beta \delta^{\nu_1 - \nu_2 + \nu_3 - \nu_4, 0} G_{2,1234}^{\nu_1 \nu_2 \nu_3}, \end{aligned} \quad (3)$$

where the time-translation invariance was used to obtain the Kronecker δ in Matsubara frequencies. With this, we can infer the dimension (indicated in the following by $[\dots]$) of the two-particle Green's function in imaginary time and Matsubara space:

$$[G(\tau_1, \tau_2, \tau_3, \tau_4)] = [G(\tau_1, \tau_2, \tau_3, \tau_4)] = 1, \quad (4)$$

$$[G^{\nu_1 \nu_2 \nu_3 \nu_4}] = [\tau]^4, \quad (5)$$

$$[G^{\nu_1 \nu_2 \nu_3}] = [\tau]^3. \quad (6)$$

For the two-particle Green's function, we can also define new combinations ω, ν, ν' of the three independent frequencies ν_1, ν_2, ν_3 as defined in Table I and Fig. 1. The Bethe-Salpeter equation then becomes diagonal in ω for the particle-hole (ph), transverse-particle-hole ($\overline{\text{ph}}$), and particle-particle (pp) channel [see Eq. (14) below].

For the sake of completeness, let us also define the one-particle Green's function and its Fourier transform:

$$G_{1,12}(\tau_1, \tau_2) := (-1) \langle T \hat{c}_1(\tau_1) \hat{c}_2^{\dagger}(\tau_2) \rangle, \quad (7)$$

$$\begin{aligned} G_{1,12}^{\nu_1 \nu_2} &:= \int_0^{\beta} d\tau_1, \tau_2 G_{1,12}(\tau_1, \tau_2) e^{i(\nu_1 \tau_1 - \nu_2 \tau_2)} \\ &=: \beta \delta^{\nu_1 - \nu_2, 0} G_{1,12}^{\nu_1}. \end{aligned} \quad (8)$$

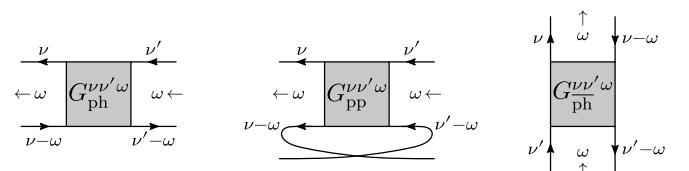


FIG. 1. The same two-particle Green's function in the three frequency notations from Table I (only the connected part is shown).

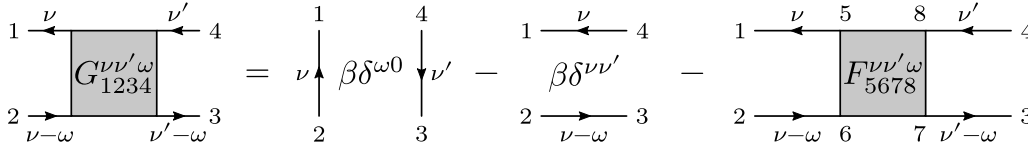


FIG. 2. Decomposition of the two-particle Green's function into two disconnected terms and a connected term, introducing the full two-particle vertex F .

C. Full two-particle vertex

In the following, we use skeleton diagrams that are defined in terms of the full (interacting) one-particle Green's function and thus must not contain one-particle insertions (i.e., no internal parts that can be separated completely from the rest of the diagram by cutting two Green's function lines) [1]. Furthermore, the terms of the two-particle Green's function that actually connect the two in- and outgoing particle lines can be collected into an interaction vertex, which we call the full two-particle vertex F_2 . In the following, we usually drop the particle-ness index (here "2") if it can be inferred from the (number of) arguments. With this, the whole series expansion can be decomposed into vertex contributions and disconnected Green's function lines (cf. Fig. 2):

$$G_{1234}^{vv'\omega} = \beta\delta^{\omega,0} G_{12}^v G_{34}^{v'} - \beta\delta^{vv'} G_{14}^v G_{32}^{v-\omega} - G_{15}^v G_{62}^{v-\omega} F_{5678}^{vv'\omega} G_{37}^{v'} G_{84}^{v'-\omega}. \quad (9)$$

Here, the sign of the vertex is just a convention. Our choice leads to the following weak coupling (first order) terms of F for a local interaction:

$$\begin{aligned} \lim_{U \rightarrow 0^+} F_{\uparrow\uparrow\downarrow\downarrow} &\equiv \lim_{U \rightarrow 0^+} F_{\uparrow\downarrow} = +U, \\ \lim_{U \rightarrow 0^+} F_{\uparrow\downarrow\uparrow\downarrow} &\equiv \lim_{U \rightarrow 0^+} F_{\uparrow\downarrow} = -U. \end{aligned} \quad (10)$$

From Eq. (9), we can also deduce the dimension of the full vertex to be $[F^{vv'\omega}] = [\tau]^{-1}$, consistent with the bare interaction U , which also has the dimension of energy or inverse time.

D. Irreducible two-particle vertices

A further step is to classify the two-particle diagrams in terms of their reducibility. For two-particle interactions, all fermionic two-particle diagrams are inherently one-particle irreducible (1PI); i.e., it is not possible to separate a two-particle diagram by cutting one (single-particle) Green's function line (otherwise the conservation of the number of fermions would be violated). In contrast, three-particle diagrams discussed later will not necessarily be 1PI.

On the two-particle level, of course, we also need to think about two-particle reducibility. This means that we check if diagrams can be separated into two disconnected parts by cutting two Green's function lines. If not, we call the diagram fully two-particle irreducible. If yes, the diagram is two-particle reducible (2PR). We can further refine the classification of reducible diagrams by looking at pairs of external points, which stay connected: a particle-hole pair that runs horizontally in Fig. 1, a particle-hole pair that runs vertically, or a particle-particle pair. These are the three channels (ph, $\overline{\text{ph}}$, and pp) we already mentioned in Sec. II B when

introducing the different frequency notations. While the frequency notations are just different parametrizations for the same object, convenient for evaluating Bethe-Salpeter equations [see Eq. (14)] in the respective channels, the diagrams reducible in one channel are different from the diagrams reducible in another channel. Moreover, it turns out every two-particle diagram can only be reducible in one of the three channels [32–34]. This allows us to uniquely split up the full two-particle vertex F into four terms

$$F_{1234} = \Lambda_{1234} + \Phi_{\text{ph},1234} + \Phi_{\overline{\text{ph}},1234} + \Phi_{\text{pp},1234}, \quad (11)$$

where Λ is the fully irreducible two-particle vertex, and Φ_{ph} , $\Phi_{\overline{\text{ph}}}$, and Φ_{pp} are reducible vertices in ph, $\overline{\text{ph}}$, and pp channels, respectively. Equation (11) is called the parquet equation or parquet decomposition [34].

Let us now briefly talk about the crossing symmetry (i.e., the symmetry under swapping the two in and outgoing legs) of the different terms in Eqs. (9) and (11). This symmetry will become relevant later for three-particle diagrams. Since the full two-particle Green's function is crossing symmetric and the two disconnected terms in Eq. (9), each map to the other one under crossing, the full two-particle vertex is crossing symmetric as well. Things are similar for the components of the parquet decomposition in Eq. (11). When swapping the two in or outgoing legs, the ph channel maps onto the $\overline{\text{ph}}$ channel and vice versa. The fully irreducible vertex Λ never maps to any reducible diagram under exchange of external legs, and Φ_{pp} cannot map to Λ for the same reason. Therefore, these two components are crossing symmetric on their own. Putting everything together, we have the following crossing symmetries:

$$\begin{aligned} F_{1234} &= -F_{3214} = -F_{1432}, \\ \Lambda_{1234} &= -\Lambda_{3214} = -\Lambda_{1432}, \\ \Phi_{\text{ph},1234} &= -\Phi_{\overline{\text{ph}},3214} = -\Phi_{\overline{\text{ph}},1432}, \\ \Phi_{\overline{\text{ph}},1234} &= -\Phi_{\text{ph},3214} = -\Phi_{\text{ph},1432}, \\ \Phi_{\text{pp},1234} &= -\Phi_{\text{pp},3214} = -\Phi_{\text{pp},1432}. \end{aligned} \quad (12)$$

Equation (11) is not the only useful decomposition of the full two-particle vertex F , regarding reducibility. Instead of working with the fully irreducible vertex Λ , we can look at one channel at a time and define vertices Γ that are only two-particle irreducible (2PI) in each of them:

$$\Gamma_r = F - \Phi_r, \quad r \in \{\text{ph}, \overline{\text{ph}}, \text{pp}\}. \quad (13)$$

With this, we are back to a binary property for each channel r (each diagram is part of either Γ_r or Φ_r). From every reducible diagram in Φ_r , we can cut off the left-most irreducible part and again be left with the whole series of diagrams for the

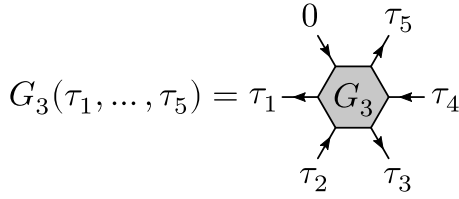


FIG. 3. Diagrammatic representation of the three-particle Green's function in imaginary times.

full vertex F . This leads to the so-called Bethe-Salpeter equations [35]

$$\begin{aligned} F_{1234} &= \Gamma_{\text{ph},1234} + \sum_{5678} \Gamma_{\text{ph},1256} G_{67} G_{85} F_{7834}, \\ F_{1234} &= \Gamma_{\overline{\text{ph}},1234} - \sum_{5678} \Gamma_{\overline{\text{ph}},1654} G_{67} G_{85} F_{7238}, \\ F_{1234} &= \Gamma_{\text{pp},1234} + \frac{1}{2} \sum_{5678} \Gamma_{\text{pp},1836} G_{67} G_{85} F_{7254}, \end{aligned} \quad (14)$$

where the different signs between the ph and $\overline{\text{ph}}$ channels respect the crossing relations in Eq. (12) and the factor 1/2 in the pp channel comes from the indistinguishability of the particles [34] [for a detailed explanation of why the factor of 1/2 is necessary, cf. the discussion after Eq. (44) in Sec. IV B].

III. THREE-PARTICLE GREEN'S FUNCTION

Let us now turn to the three-particle Green's function, visualized in Fig. 3 and defined as

$$\begin{aligned} G_{3,1-6}(\tau_1, \dots, \tau_5) \\ := (-1)^3 \langle T \hat{c}_1(\tau_1) \hat{c}_2^\dagger(\tau_2) \hat{c}_3(\tau_3) \hat{c}_4^\dagger(\tau_4) \hat{c}_5(\tau_5) \hat{c}_6^\dagger(0) \rangle, \end{aligned} \quad (15)$$

with imaginary times τ_i and all other parameters and quantum numbers condensed into compound indices 1...6. Note that we directly used time translation invariance (energy conservation) to get rid of one time argument, analogous to Sec. II B for the two-particle Green's functions.

The Fourier transformation to fermionic Matsubara frequencies $\nu_i = (2n_i + 1)\pi/\beta$, $n_i \in \mathbb{Z}$, is given by

$$\begin{aligned} G_{3,1-6}^{\nu_1 \dots \nu_5} &= \int \dots \int_0^\beta d\tau_1 \dots d\tau_5 G_{3,1-6}(\tau_1, \dots, \tau_5) \\ &\times e^{i(\nu_1 \tau_1 - \nu_2 \tau_2 + \nu_3 \tau_3 - \nu_4 \tau_4 + \nu_5 \tau_5)}, \end{aligned} \quad (16)$$

and the inverse transformation reads.

$$\begin{aligned} G_{3,1-6}(\tau_1, \dots, \tau_5) \\ = \frac{1}{\beta^5} \sum_{\nu_1 \dots \nu_5} G_{3,1-6}^{\nu_1 \dots \nu_5} e^{-i(\nu_1 \tau_1 - \nu_2 \tau_2 + \nu_3 \tau_3 - \nu_4 \tau_4 + \nu_5 \tau_5)}. \end{aligned} \quad (17)$$

With that we can infer the dimension of the three-particle Green's function in imaginary time and Matsubara space:

$$[G_{3,1-6}(\tau_1, \dots, \tau_5)] = 1, \quad (18)$$

$$[G_{3,1-6}^{\nu_1 \dots \nu_5}] = [\tau]^5. \quad (19)$$

From now on, we drop the index 3 if the three-particle-ness can be inferred from the (number of) arguments.

TABLE II. The 15 different two-particle frequency notations of three-particle diagrams [18].

Channel	ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
ph	ν_a	$\nu_a - \omega_a$	ν_b	$\nu_b - \omega_b$	ν_c	$\nu_c - \omega_c$
ph'	ν_a	$\nu_b - \omega'_b$	ν_b	$\nu_c - \omega'_c$	ν_c	$\nu_a - \omega'_a$
ph	ν_a	$\nu_c - \overline{\omega}_c$	ν_b	$\nu_a - \overline{\omega}_a$	ν_c	$\nu_b - \overline{\omega}_b$
ph $_{\overline{a}}$	ν_a	$\nu_b - \omega'_b$	ν_b	$\nu_a - \overline{\omega}_a$	ν_c	$\nu_c - \omega_c$
ph $_{\overline{b}}$	ν_a	$\nu_a - \omega_a$	ν_b	$\nu_c - \omega'_c$	ν_c	$\nu_b - \overline{\omega}_b$
ph $_{\overline{c}}$	ν_a	$\nu_c - \overline{\omega}_c$	ν_b	$\nu_b - \omega_b$	ν_c	$\nu_a - \omega'_a$
pp $_{24-13}$	ν_a	ν_b	$\omega_a - \nu_a$	$\omega_b - \nu_b$	ν_c	$\nu_c - \omega_c$
pp $_{26-13}$	$\omega_b - \nu_b$	ν_a	ν_b	$\nu_c - \omega'_c$	ν_c	$\omega_a - \nu_a$
pp $_{26-15}$	$\omega_c - \nu_c$	$\omega_a - \nu_a$	ν_b	$\nu_b - \omega_b$	ν_c	ν_a
pp $_{46-15}$	ν_a	$\nu_b - \omega'_b$	ν_b	$\omega_c - \nu_c$	$\omega_a - \nu_a$	ν_c
pp $_{46-35}$	ν_a	$\nu_a - \omega_a$	ν_b	ν_c	$\omega_b - \nu_b$	$\omega_c - \nu_c$
pp $_{24-35}$	ν_a	$\omega_b - \nu_b$	$\omega_c - \nu_c$	ν_b	ν_c	$\nu_a - \omega'_a$
pp $_{26-35}$	ν_a	ν_b	$\omega_c - \nu_c$	$\nu_a - \overline{\omega}_a$	ν_c	$\omega_b - \nu_b$
pp $_{46-13}$	$\omega_b - \nu_b$	$\nu_c - \overline{\omega}_c$	ν_b	$\omega_a - \nu_a$	ν_c	ν_a
pp $_{24-15}$	ν_a	$\omega_c - \nu_c$	ν_b	ν_c	$\omega_a - \nu_a$	$\nu_b - \overline{\omega}_b$

A. Frequency notations

In Sec. II B, we saw that there are three channels for the two-particle Green's function, each with its own frequency notation. They are chosen such that the in and outgoing particle-particle or particle-hole pairs have a total energy of ω .

As shown in Ref. [18], generalizing this yields 15 different two-particle frequency notations for three-particle diagrams. They are listed in Table II.

We can generalize this to three-particle frequency notations where we combine either two particle lines and one hole line (pph) or three particle lines (ppp) such that they have a total energy of $\bar{\nu}$. In the pph case, there are $\binom{3}{2} \cdot \binom{3}{1} = 9$ such combinations, while in the ppp case there is only one for a total of ten three-particle frequency notations. All of them are listed in Table III, while a diagrammatic representation is shown for four of them in Fig. 4. The cases with three holes and two holes and one particle can be obtained from ppp and pph by inverting the directions of the lines so we do not consider them here explicitly.

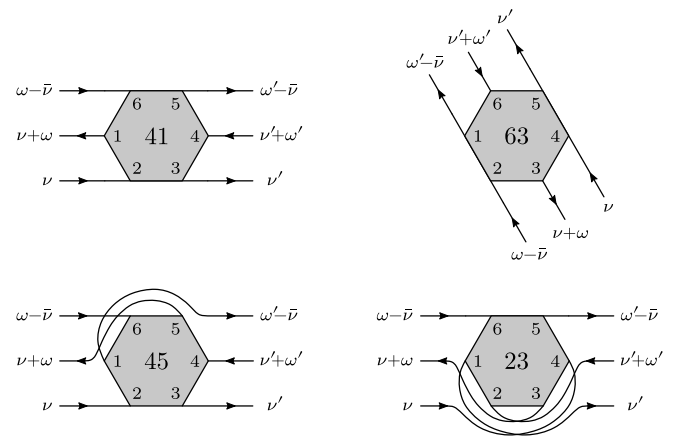


FIG. 4. Diagrammatic representation of four of the ten three-particle frequency notations listed in Table III.

TABLE III. The ten different three-particle frequency notations of three-particle diagrams. In our notation, the channel names in the first column (the two bracketed triplets) denote which particles and holes remain together. These triplets sum to a fermionic transfer frequency $\bar{\nu}$. The second column is a shorthand notation for these channel names; they are simply the middle numbers of the two triplets in the first column. For the pph channels (the first nine rows), they specify the particle running in the opposite direction. Diagrammatic representations for four of them are shown in Fig. 4.

Channel		ν_1	ν_2	ν_3	ν_4	ν_5	ν_6
(345)(612)	41	$\nu + \omega$	ν	ν'	$\nu' + \omega'$	$\omega' - \bar{\nu}$	$\omega - \bar{\nu}$
(123)(456)	25	ν'	$\nu' + \omega'$	$\omega' - \bar{\nu}$	$\omega - \bar{\nu}$	$\nu + \omega$	ν
(561)(234)	63	$\omega' - \bar{\nu}$	$\omega - \bar{\nu}$	$\nu + \omega$	ν	ν'	$\nu' + \omega'$
(341)(652)	45	$\omega' - \bar{\nu}$	ν	ν'	$\nu' + \omega'$	$\nu + \omega$	$\omega - \bar{\nu}$
(361)(452)	65	$\omega' - \bar{\nu}$	ν	ν'	$\omega - \bar{\nu}$	$\nu + \omega$	$\nu' + \omega'$
(365)(412)	61	$\nu + \omega$	ν	ν'	$\omega - \bar{\nu}$	$\omega' - \bar{\nu}$	$\nu' + \omega'$
(325)(614)	21	$\nu + \omega$	$\nu' + \omega'$	ν'	ν	$\omega' - \bar{\nu}$	$\omega - \bar{\nu}$
(125)(634)	23	ν'	$\nu' + \omega'$	$\nu + \omega$	ν	$\omega' - \bar{\nu}$	$\omega - \bar{\nu}$
(145)(632)	43	ν'	ν	$\nu + \omega$	$\nu' + \omega'$	$\omega' - \bar{\nu}$	$\omega - \bar{\nu}$
(315)(642)	ppp	$\omega' - \nu'$	ν	ν'	$\omega - \nu$	$-\omega' - \bar{\nu}$	$-\omega - \bar{\nu}$

With regard to the possible spin components, there are only three independent spin combinations for the six compound indices $1 \dots 6$ of Eq. (15): $\sigma_1 \dots \sigma_6 \in \{\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow, \uparrow\uparrow\uparrow\uparrow\downarrow\downarrow, \uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\}$, which from now on we write as $\uparrow\uparrow\uparrow, \uparrow\uparrow\downarrow, \uparrow\uparrow\downarrow, \uparrow\uparrow\downarrow*$, respectively [18].

Similar to the two-particle Green's function in Sec. II, one can define a full three-particle vertex F_3 , which contains all diagrams that connect all incoming and outgoing lines of G_3 in Fig. 3 [18] (additionally G_3 contains disconnected diagrams).

The decomposition of the three-particle Green's function is, cf. Fig. 5:

$$G_{123456} = -\langle \hat{c}_1^\dagger \hat{c}_2 \hat{c}_3^\dagger \hat{c}_4 \hat{c}_5^\dagger \hat{c}_6 \rangle \quad (20)$$

$$= -\langle \hat{c}_1 \hat{c}_2^\dagger \rangle \langle \hat{c}_3 \hat{c}_4^\dagger \rangle \langle \hat{c}_5 \hat{c}_6^\dagger \rangle - \langle \hat{c}_1 \hat{c}_6^\dagger \rangle \langle \hat{c}_3 \hat{c}_2^\dagger \rangle \langle \hat{c}_5 \hat{c}_4^\dagger \rangle$$

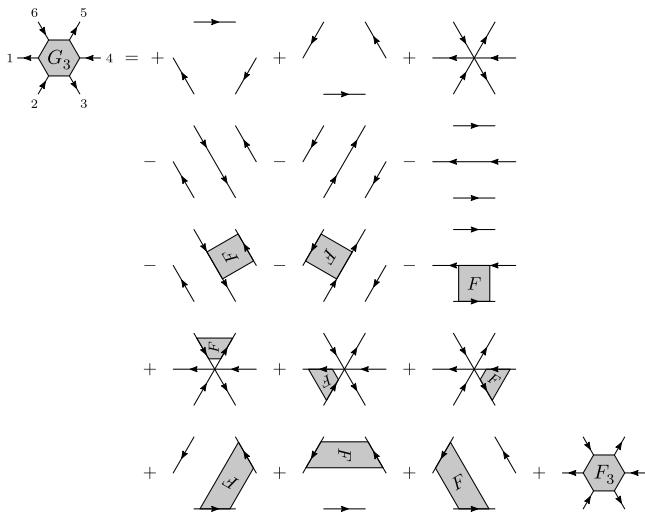


FIG. 5. Diagrammatic representation of Eq. (21), the decomposition of the three-particle Green's function.

$$\begin{aligned}
& -\langle \hat{c}_1 \hat{c}_4^\dagger \rangle \langle \hat{c}_3 \hat{c}_6^\dagger \rangle \langle \hat{c}_5 \hat{c}_2^\dagger \rangle + \langle \hat{c}_1 \hat{c}_2^\dagger \rangle \langle \hat{c}_3 \hat{c}_6^\dagger \rangle \langle \hat{c}_5 \hat{c}_4^\dagger \rangle \\
& + \langle \hat{c}_1 \hat{c}_6^\dagger \rangle \langle \hat{c}_3 \hat{c}_4^\dagger \rangle \langle \hat{c}_5 \hat{c}_2^\dagger \rangle + \langle \hat{c}_1 \hat{c}_4^\dagger \rangle \langle \hat{c}_3 \hat{c}_2^\dagger \rangle \langle \hat{c}_5 \hat{c}_6^\dagger \rangle \\
& - \langle \hat{c}_1 \hat{c}_2^\dagger \rangle \langle \hat{c}_3 \hat{c}_4^\dagger \hat{c}_5 \hat{c}_6^\dagger \rangle - \langle \hat{c}_3 \hat{c}_4^\dagger \rangle \langle \hat{c}_5 \hat{c}_6^\dagger \hat{c}_1 \hat{c}_2^\dagger \rangle \\
& - \langle \hat{c}_5 \hat{c}_6^\dagger \rangle \langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4^\dagger \rangle + \langle \hat{c}_1 \hat{c}_4^\dagger \rangle \langle \hat{c}_3 \hat{c}_2^\dagger \hat{c}_5 \hat{c}_6^\dagger \rangle \\
& + \langle \hat{c}_3 \hat{c}_6^\dagger \rangle \langle \hat{c}_5 \hat{c}_4^\dagger \hat{c}_1 \hat{c}_2^\dagger \rangle + \langle \hat{c}_5 \hat{c}_2^\dagger \rangle \langle \hat{c}_1 \hat{c}_6^\dagger \hat{c}_3 \hat{c}_4^\dagger \rangle \\
& + \langle \hat{c}_1 \hat{c}_6^\dagger \rangle \langle \hat{c}_3 \hat{c}_4^\dagger \hat{c}_5 \hat{c}_2^\dagger \rangle + \langle \hat{c}_3 \hat{c}_2^\dagger \rangle \langle \hat{c}_5 \hat{c}_6^\dagger \hat{c}_1 \hat{c}_4^\dagger \rangle \\
& + \langle \hat{c}_5 \hat{c}_4^\dagger \rangle \langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_6^\dagger \rangle - \langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4^\dagger \hat{c}_5 \hat{c}_6^\dagger \rangle, \quad (21)
\end{aligned}$$

where underlined expectation values denote fully connected diagrams. On the one-particle level this means

$$G_{12} = -\langle \hat{c}_1 \hat{c}_2^\dagger \rangle = -\langle \hat{c}_1 \hat{c}_2^\dagger \rangle, \quad (22)$$

and on the two-particle level we get

$$\begin{aligned}
G_{1234} = \langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4^\dagger \rangle &= \langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4^\dagger \rangle + \langle \hat{c}_1 \hat{c}_2^\dagger \rangle \langle \hat{c}_3 \hat{c}_4^\dagger \rangle \\
&+ (-1)^3 \langle \hat{c}_1 \hat{c}_4^\dagger \rangle \langle \hat{c}_3 \hat{c}_2^\dagger \rangle, \quad (23)
\end{aligned}$$

where comparison with Eq. (9) reveals that the four-point fully connected expectation value is given by

$$\langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4^\dagger \rangle = -G_{15} G_{62} F_{5678} G_{37} G_{84}. \quad (24)$$

Finally, the last term in Sec. III A introduces the full three-particle vertex F_3 . Its sign is chosen as

$$\begin{aligned}
-\langle \hat{c}_1 \hat{c}_2^\dagger \hat{c}_3 \hat{c}_4^\dagger \hat{c}_5 \hat{c}_6^\dagger \rangle &= G_{1'1} G_{2'2} G_{3'3} F_{3,1'2'3'4'5'6'} G_{4'4} G_{5'5} G_{6'6'}. \quad (25)
\end{aligned}$$

B. Nonlinear response functions

As shown in Ref. [18], nonlinear response functions are the connected part (conn) of three-particle correlators. Specifically, the second-order spin response functions $\chi_{\sigma_1 \sigma_2 \sigma_3}^{(2)}$ are defined as

$$\chi_{\sigma_1 \sigma_2 \sigma_3}^{(2)}(\tau_1, \tau_2) = \langle \hat{T} \hat{n}_{\sigma_1}(\tau_1) \hat{n}_{\sigma_2}(\tau_2) \hat{n}_{\sigma_3}(0) \rangle, \quad (26)$$

with the usual definition of the density operators $\hat{n}_\sigma = \hat{c}_\sigma^\dagger \hat{c}_\sigma$, and the underline again denotes fully connected diagrams. Comparing this to Eq. (15) reveals that we can also write it in terms of the connected part (conn) of the three-particle Green's function:

$$\chi_{\sigma_1 \sigma_2 \sigma_3}^{(2)}(\tau_1, \tau_2) = -\text{conn} G_{\sigma_1 \sigma_3 \sigma_2}(\tau_1, \tau_1^+, 0, 0^+, \tau_2, \tau_2^+). \quad (27)$$

Furthermore, the second-order response functions can be decomposed into three different parts [18] (see Fig. 6):

$$\chi^{(2)} = \chi_0^{(2)} + \chi_1^{(2)} + \chi_{\text{vertex}}^{(2)}. \quad (28)$$

Here, $\chi_0^{(2)}$ is the bare or bubble part that contains diagrams with only one-particle Green's functions, $\chi_1^{(2)}$ are the first-order terms, which are three-particle diagrams with a single two-particle vertex F , and $\chi_{\text{vertex}}^{(2)}$ is the contribution from the full three-particle vertex F_3 .

Let us finally also define the Fourier transform,

$$\chi_{\sigma_1 \sigma_2 \sigma_3}^{\omega_1 \omega_2} = \int_0^\beta \int_0^\beta \chi_{\sigma_1 \sigma_2 \sigma_3}(\tau_1, \tau_2) e^{i\omega_1 \tau_1 + i\omega_2 \tau_2} d\tau_1 d\tau_2, \quad (29)$$

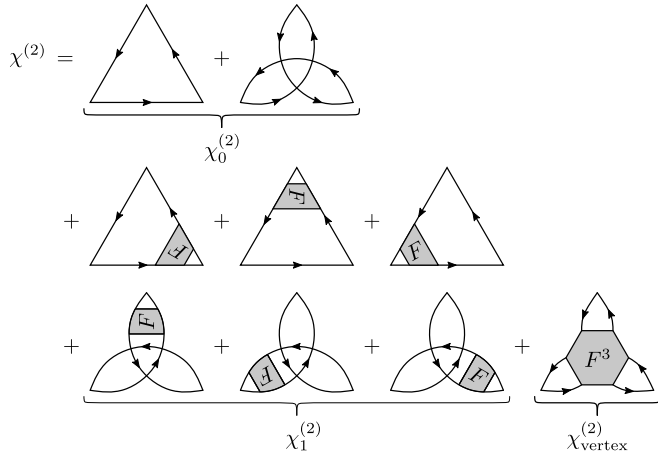


FIG. 6. Diagrammatic representation of the decomposition of the second-order response function $\chi^{(2)}$ into bare or bubble terms χ_0 , first-order terms χ_1 and full vertex terms χ_{vertex} . Time and frequency labels are omitted to avoid clutter.

where ω_1 and ω_2 are bosonic Matsubara frequencies.

IV. THREE-PARTICLE LADDER

The full three-particle vertex is a complex object, which is expensive to compute and even storing it becomes difficult if we do not restrict ourselves to its local part. Fortunately, we can build it completely from simpler two-particle vertices since the only interaction term we consider is a two-particle interaction.

In this section, we first express the three-particle vertex as a geometric ladder series in terms of irreducible two-particle vertices. Our motivation for this are the ladder diagrams generated by the Bethe-Salpeter equations on the two-particle level. However, calculating the fully irreducible vertex in a given three-particle channel is presently not feasible.

We thus approximate the irreducible three-particle vertex by a sum of irreducible two-particle vertices. This makes an actual calculation possible. If we instead constructed the ladder series in terms of the bare interaction U , we would have a three-particle analog of the random phase approximation (RPA). However, expressing the ladder in terms of the two-particle vertex includes many more Feynman diagrams, among others screening effects.

The local two-particle vertex can be calculated by solving an AIM numerically. The difference to QCD calculations with rainbow-ladder truncation [24] is that the QCD calculations are, to the best of our knowledge, restricted to one ladder of three quarks, whereas we calculate the ladder in various pph channels and the ppp channel. Further, we keep the full frequency dependence of the irreducible two-particle vertex that arises from more complicated local Feynman diagrams, rather than just the bare effective interaction used in the rainbow-ladder truncation.

A. Three-particle Bethe-Salpeter-like equations

Let us start by writing down the two-particle Bethe-Salpeter equations that we introduced in Eq. (14) in a very

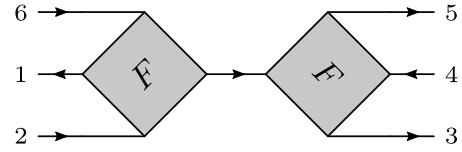


FIG. 7. The only diagram 1PR in the channel that separates (612) from (345). Looking at Table III, this is the same as the three-particle channel 41.

simplified form,

$$F = \Gamma_r + \Gamma_r \cdot F, \quad (30)$$

where F is the full vertex, Γ_r are the vertices irreducible in a single channel r , and $\cdot$ denotes the proper connection of two vertex diagrams with Green's function lines in the correct channel. Generalizing this from the two-particle to the three-particle level seems straightforward. We define a three-particle diagram as three-particle reducible (3PR) if it can be separated into two disconnected three-particle parts by cutting three Green's function lines, and as three-particle irreducible (3PI) otherwise. Note that a less stringent definition of cutting it into any kind of parts is not helpful since then any diagram would be 3PR: It could be simply cut around an outermost two-particle interaction (that we consider here) into two disconnected parts (a four-particle and a two-particle one). In Sec. III, we already identified the ten three-particle channels, so we need to define $\Gamma_{3\text{PI},r}$ as the vertex that is 3PI in one three-particle channel r , use three instead of two Green's functions to connect everything, and we are done.

As it turns out, it is not that easy. The two-particle level has the very nice advantage that all diagrams are inherently 1PI (see Sec. II). This is not true for the three-particle level. With a four-point interaction, we can easily draw a diagram that goes from three lines down to a single one and then back to three again. Such a diagram is shown in Fig. 7. Cutting the single Green's function line in the middle separates the diagram into two connected parts: (612) and (345). This is the same separation that happens when cutting the three Green's function lines of a diagram 3PR in the 41 = (345)(612) channel (see Table III). We can do this for all other pph channels, too.

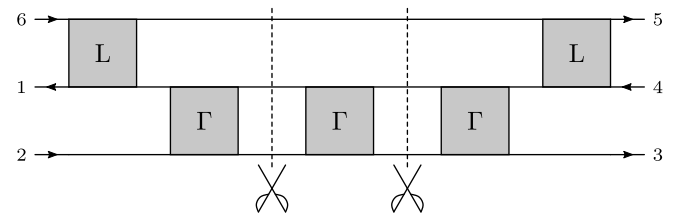


FIG. 8. A simple example diagram that illustrates the ambiguity that arises when cutting 3PR diagrams into 3PI parts. In our notation, it is reducible in the (345)(612) or 41 channel. Note that cutting after the leftmost or before the rightmost vertex is not allowed since then we would end up with disconnected parts that are not three-particle vertices anymore. Also, the upper vertices are upside down because, in our notation, the orientation of the letter Γ is with respect to the incoming and outgoing particles as defined in Fig. 1 for the standard orientation.

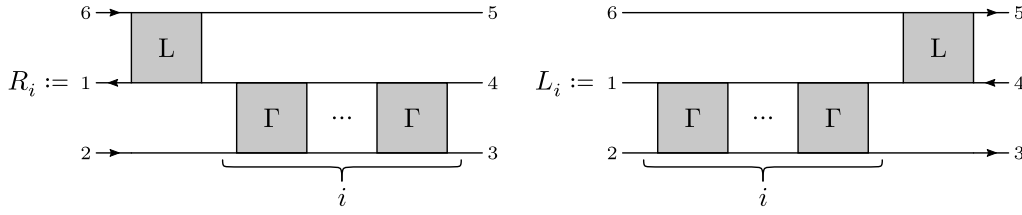


FIG. 9. Definition of R_i and L_i . Again, the upper vertices are upside down because of how we defined them in Fig. 1.

This shows that the channels where we encounter one-particle reducibility are the very same as the nine pph channels for three-particle reducibility [36].

If we were to connect two diagrams that are 1PR in the same channel, we would have built a one-particle insertion. Since we are drawing our diagrams with full Green's functions this would lead to double counting and is therefore not allowed. To avoid this, we do not build a three-particle Bethe-Salpeter-like equation with F_3 and $\Gamma_{3\text{PI},r}$, but subtract diagrams 1PR in r first. We denote the three-particle vertex that is 1PI in channel r with $\Gamma_{1\text{PI},r}$; and the one that is 1PI and 3PI in r with $\Gamma_{(1,3)\text{PI},r}$.

Let us note here that one needs to be careful with the 1PR diagrams when calculating physical properties from these. This often involves connecting some of the legs of the three-particle vertex with Green's functions. Depending on the specific pph channel and connection, the 1PR diagrams may (or may not) generate diagrams that are (are not) already contained as a self-energy inclusion. Then, these must (must not) be discarded. In our case of the second-order response studied below, this is not the case, the 1PR diagrams contribute.

Even with the $\Gamma_{1\text{PI},r}$ and $\Gamma_{(1,3)\text{PI},r}$ thus defined, there is still one remaining problem: Some 3PR diagrams cannot be uniquely cut into 3PI parts. A simple example of this is shown in Fig. 8, where there are two possible ways to cut the diagram and each one results in different 3PI parts. The underlying issue is that 3PI diagrams can be 2PR in related channels. This means that two-particle vertices can be added or cut off from those diagrams without changing their three-particle reducibility. If we use the notation defined in Fig. 9, where R_i has i two-particle vertices on the right and L_i has i vertices on the left, we see that

$$R_i \cdot L_j = R_n \cdot L_m, \quad \forall i + j = n + m. \quad (31)$$

Since both R_i and L_i are elements of $\Gamma_{1\text{PI},r}$ and $\Gamma_{(1,3)\text{PI},r}$, we would again invoke double counting.

One way to prevent this and make cutting off 3PI parts unique is to require that we always cut off the “leftmost” part, i.e., that we fix $m = i + j$ and $n = 0$ in Eq. (31). [37]

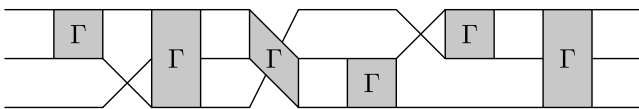


FIG. 10. Example diagram for an approximate three-particle ladder built only from two-particle vertices. Only Green's function lines touching the corners of a vertex are really connected to it. The middle line on the right side, e.g., is not connected to the right-most vertex but runs through “behind” it.

This is equivalent to requiring that the vertices 1PI and 3PI in a channel r must also be 2PI in the three related two-particle channels “on the right.” Denoting this quantity with $\Gamma_{(1,\bar{2},3)\text{PI},r}$, we can finally write down the three-particle equivalent of the Bethe-Salpeter equation:

$$\Gamma_{1\text{PI},r} = \Gamma_{(1,\bar{2},3)\text{PI},r} + \Gamma_{(1,\bar{2},3)\text{PI},r} \cdot \Gamma_{1\text{PI},r}. \quad (32)$$

To recover the full vertex F_3 , we need to add the diagrams 1PR in channel r . As it turns out there is only a single one for each channel. They are all of the same form: two full two-particle vertices F_2 connected by a single Green's function line G . One of them is depicted in Fig. 7. With this, we have

$$F_3 = \Gamma_{1\text{PI},r} + (F_2 G F_2)_r. \quad (33)$$

For a detailed discussion on three-particle (ir)reducibilities, see the Supplemental Material [38].

Let us also note here that our Bethe-Salpeter-like equations are similar to the Faddeev equations employed in other fields of physics. The fundamental difference is that Faddeev [23] considered a three-particle Hamiltonian, whereas we consider three particles and holes that propagate through a solid. Thereby, they strongly interact with many other electrons. Consequently, in between the three incoming and outgoing particles (holes), there can be further particle (hole) pairs generated through the Coulomb interaction. This is hidden here in the more complicated Feynman diagrams of the irreducible vertex $\Gamma_{(1,\bar{2},3)\text{PI},r}$. The opposite effect that we can have, a particle-hole annihilation in between, is more apparent in the equations, and leads to the additional contribution of the 1PR diagram of Fig. 7. This contribution is absent in the ppp channel and the Faddeev equations.

B. Approximate three-particle ladder

In the last section, we saw that the exact three-particle ladders generated by the Bethe-Salpeter-like equations are built from three-particle vertices that are 1PI and 3PI in a certain channel and 2PI in the three related channels “on the right.” The problem is that we have no easy way to compute them. We could construct them order by order from two-particle vertices, but that is tedious and unfeasible. Instead, we propose approximating the exact three-particle ladder with a ladder of two-particle vertices.

The general idea is to find all possible ways to connect a two-particle vertex to three lines on the left and three lines on the right, and then build a ladder from that. Figure 10 shows an example diagram for such a ladder. Formally, we can write

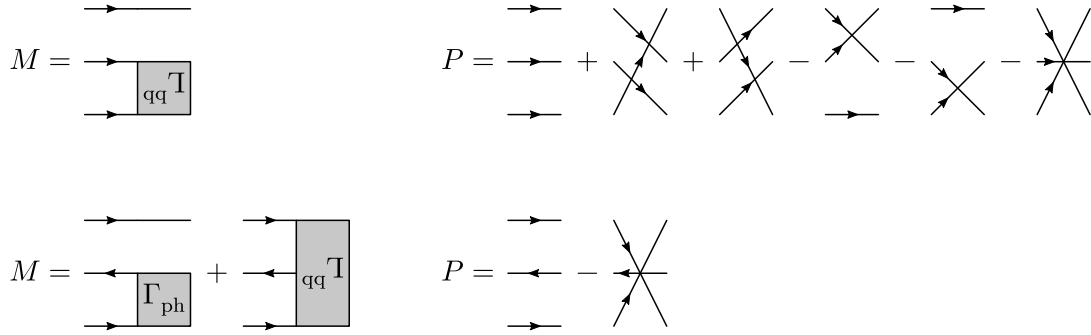


FIG. 11. Diagrammatic representation of M and P for ppp ladders (top) and pph ladders (bottom). The pp vertex is mirrored because the frequencies of the incoming and outgoing lines are opposite to the definition in Fig. 1.

this as

$$\tilde{L} = \sum_{n=1}^{\infty} P(MP)^n, \quad (34)$$

where $\tilde{L}$ is the approximate ladder, P consists of all permutations of the three lines of the ladder, and M contains a two-particle vertex. Since the ladder can have multiple vertices right next to each other, using the full two-particle vertex in M would lead to double counting. To avoid this issue, we use Γ_r , the two-particle vertex irreducible in channel r . Which channel we need depends on which kinds of three-particle ladder we build: either one with three particles (ppp) or one with two particles and a hole (pph). [39] In the ppp case, we only need Γ_{pp} ; in the pph case, we need to add Γ_{ph} as well. The permutation matrix P also differs between the two cases because we are not allowed to swap particles with holes and vice versa. Thus, for a pph ladder, the permutation matrix only consists of 2 instead of $3! = 6$ terms. Figure 11 shows a diagrammatic representation of M and P for both cases.

From now on, we only focus on the pph ladder since it directly matches with our definition of the three-particle Green's function shown in Fig. 3. Because of that it is also easier to compute the vertex corrections to the second-order response functions $\chi_{\text{vertex}}^{(2)}$ from it, which is convenient for our comparison tests. It is, however, straightforward to apply the ideas, concepts, issues, and solutions presented in the rest of this section to the ppp case.

Let us continue by introducing some notation. We label the lines of the ladder with the numbers 1–3 starting from the top. Since in the first term of M shown in Fig. 11 (bottom left), the ph vertex sits between lines 2 and 3 we call it M_{23} . The second term with the pp vertex is then called M_{13} , and we can write

$$M = M_{23} + M_{13}. \quad (35)$$

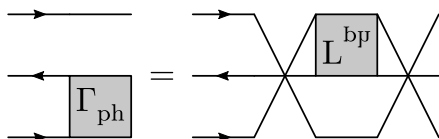


FIG. 12. Diagrammatic representation of Eq. (37), the relation between M_{12} and M_{23} .

In combination with the permutation matrix P the crossing symmetry of M_{13} , inherited from Γ_{pp} , causes the following double-counting issue:

$$PM_{13} = M_{13}P = 2M_{13}. \quad (36)$$

This can easily be corrected with an additional factor of $1/2$.

Equation (36) also shows that M_{13} commutes with P . If this were true for the whole M we could simplify Eq. (34), by pulling all permutation matrices to one side, disentangling the ladder. M_{23} prevents this because swapping the two particle lines folds the ph vertex up, creating a new diagram, which we call M_{12} (it connects the first and second line), that is not in M . However, swapping the particle lines of M_{12} brings us back to M_{23} , so the two diagrams turn into each other under the considered permutation. This means that in order to make M commute with P , all we need to do is to symmetrize its ph part and write it as the sum of both diagrams. Denoting the permutation matrix that exchanges the two particle lines with P_{13} , we can write M_{23} in terms of M_{12}

$$M_{23} = P_{13}M_{12}P_{13}. \quad (37)$$

Figure 12 shows a diagrammatic representation of this. Applying P_{13} to the whole permutation matrix P only gives a sign

$$P_{13}P = PP_{13} = P_{13} - P_{13}P_{13} = P_{13} - \mathbb{I} = -P, \quad (38)$$

where $\mathbb{I}$ is the identity permutation. The diagrams for this equation can be found in Fig. 13. Putting everything together, we can compute the desired symmetrization,

$$PM_{23}P = \frac{1}{2}P(M_{23} + P_{13}M_{12}P_{13})P = \frac{1}{2}P(M_{23} + M_{12})P. \quad (39)$$

For later convenience, we pull out the factors of $1/2$ from Eq. (39) and the double counting issue in Eq. (36) when redefining M :

$$M = M_{12} + M_{23} + M_{13}. \quad (40)$$



FIG. 13. Diagrammatic representation of Eq. (38).

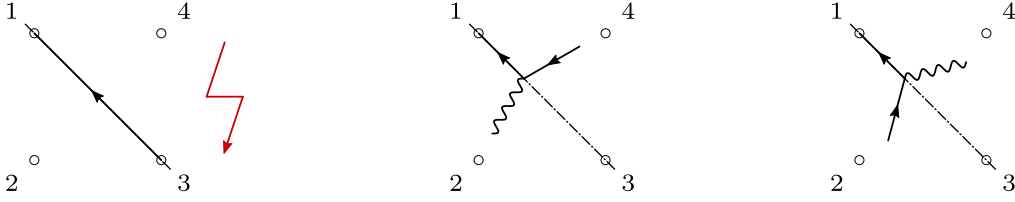


FIG. 14. Visual proof that a diagram with a two-particle interaction cannot be symmetric along a diagonal. The first diagram is not allowed since in our convention, an annihilation operator sits at both coordinates “1” and “3” [see Eq. (2)]. The second and third diagrams illustrate that it is impossible to add an interaction term and keep the diagram symmetric along the diagonal. Therefore, a single diagram cannot be crossing symmetric on its own.

This new M commutes with P

$$\begin{aligned} PM &= M - P_{13}M_{12} - P_{13}M_{23} - P_{13}M_{13} \\ &= M - M_{23}P_{13} - M_{12}P_{13} - M_{13}P_{13} = MP. \end{aligned} \quad (41)$$

With the previously pulled out factor of $1/2$, we get

$$\tilde{L} = \sum_{n=1}^{\infty} P \left(\frac{1}{2} MP \right)^n = \sum_{n=1}^{\infty} M^n P \left(\frac{1}{2} P \right)^n \quad (42)$$

for the approximate ladder. One can easily check that $P/2$ is idempotent, and we can thus further simplify the ladder equation:

$$\tilde{L} = \sum_{n=1}^{\infty} M^n P \left(\frac{1}{2} P \right)^n = \sum_{n=1}^{\infty} M^n P \frac{1}{2} P = \sum_{n=1}^{\infty} M^n P. \quad (43)$$

The ladder is now disentangled, with only a single permutation matrix at one end. This also shows that the ladder is crossing symmetric with respect to the two particle lines: It fulfills crossing symmetries with respect to exchange of incoming particle legs on the left, and of outgoing ones at the right. The full three-particle vertex, however, is crossing symmetric with respect to all particle and hole lines: It has six crossing symmetries (four with respect to exchanging particle or hole legs from left to right). This difference in symmetries is an important issue that we will come back to later.

The simple form of Eq. (43) also reveals that we generate a lot of disconnected terms. They are the ones where we do not mix the different components of M and therefore build a two-particle ladder with a disconnected Green’s function running next to it. There is one such disconnected term for each ladder. Subtracting them leaves us with

$$L = \sum_{n=1}^{\infty} (M^n - M_{12}^n - M_{23}^n - M_{13}^n) P. \quad (44)$$

Now, let us focus on the last double-counting issue. Again, it comes from the irreducible pp vertex in M_{13} , but this time it has nothing to do with the permutation matrix. Γ_{pp} is the sole perpetrator and this issue already appears on the two-particle level. There it mandates the factor of $1/2$ in the Bethe-Salpeter equation of the pp channel [see Eq. (14)].

Let us hence start by looking at the crossing symmetry for a two-particle vertex diagram. With a two-particle interaction term, it is not possible that any given diagram contributing to the vertex is crossing symmetric on its own. The reason is that with our established conventions such a diagram would

have to be symmetric along one of the two diagonals (1–3 or 2–4) and that is impossible as illustrated in Fig. 14. Without any interaction terms, we would have to draw a Green’s function line from 1 to 3, which is not allowed because in our convention an annihilation operator sits at both coordinates [see Eq. (2)]. Adding an interaction term effectively splits the Green’s function line into an interaction line and another Green’s function line. No matter at what angle or on what side we draw that this will never be symmetric along the 1–3 diagonal because they are two different types of lines.

Objects like the two-particle Green’s function, full vertex, or irreducible pp vertex are crossing symmetric because they consist of a sum of terms and this sum contains pairs of diagrams that turn into each other under crossing exchange. The reason for the diagrams to come in pairs and not in larger groups is that crossing is an involution, i.e., applying it twice yields the identity. Probably the simplest example for such a pair of diagrams are the disconnected parts of the two-particle Green’s function G_2 shown in Fig. 2. Swapping $1 \leftrightarrow 3$ or $2 \leftrightarrow 4$ turns the first diagram into the second and vice versa. For a general discussion, let $\gamma_1, \gamma_2 \in \Gamma_{pp}$ be a crossing-related pair of diagrams, i.e.,

$$\begin{aligned} \gamma_1 &= C\gamma_2 = \gamma_2 C, \\ \gamma_2 &= C\gamma_1 = \gamma_1 C, \end{aligned} \quad (45)$$

where C denotes the crossing operation. If two irreducible pp vertices are connected with two particle lines both terms $\gamma_1\gamma_2$ and $\gamma_2\gamma_1$ appear. However, since crossing is its own inverse we can write

$$\gamma_1\gamma_2 = \gamma_1 C C \gamma_2 = \gamma_2\gamma_1. \quad (46)$$

Therefore, we count all diagrams twice and need the factor of $1/2$ in the Bethe-Salpeter equation for the pp channel.

For the three-particle ladder, the case is similar. The main difference is that we can have diagrams from ph vertices in between the pp ones, so we need to consider that in our argument. Let m be a general combination of ph diagrams that can appear in the ladder, i.e., $m \in (M_{12} + M_{23})^n$. Its crossing-related counterpart $\bar{m} = P_{13}mP_{13}$ is the same diagram but with the M_{12} and M_{23} parts swapped [remember Eq. (37)], so it is also generated by the ladder. If we pick an arbitrary pair of crossing-related diagrams $\gamma_1, \gamma_2 \in M_{13}$, the ladder generates both $\gamma_1 m \gamma_2$ and $\gamma_2 \bar{m} \gamma_1$. Using the same trick as before, we can write

$$\gamma_1 m \gamma_2 = \gamma_1 P_{13} P_{13} m P_{13} P_{13} \gamma_2 = \gamma_2 \bar{m} \gamma_1, \quad (47)$$

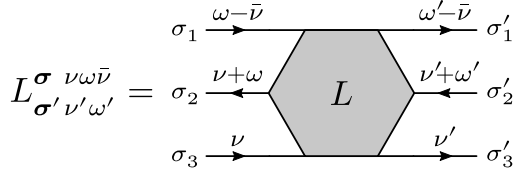


FIG. 15. Frequency and spin notation for the three-particle ladder.

and show that we count all such diagrams twice. Therefore, we must add a factor of $1/2$ in front of Γ_{pp} , as well.

With the last topological issue resolved, we can finally work out the full equations for the three-particle ladder and its components with all prefactors, indices, and arguments. So far we always drew horizontal ladders in the 41 channel, so we choose the matching frequency notation. Both the channel and its frequency notation are defined in Table III. A diagrammatic representation with all spin and frequency indices is shown in Fig. 15. Ladders in different pph channels can easily be obtained by rotation or swapping of external legs. An example of this is illustrated in Fig. 16. Due to implementation details, the frequency notations for the irreducible two-particle vertices are not the ones introduced in Table I and Fig. 1. Instead, all frequencies are shifted by ω as shown in Fig. 17. We also denote frequency and spin indices on the right side of the diagrams as subscripts to save horizontal space.

To connect the two-particle vertices in the ladder, we need Green's functions. We choose to add two on the right of each vertex in the M 's and then three on the very left of the entire ladder. This means that the ladder is not an approximation for a “naked” three-particle vertex but has Green's functions attached to every external point. This is convenient since we need them anyway for computing the vertex contribution to second-order response functions $\chi_{\text{vertex}}^{(2)}$. Putting everything together yields

$$M_{12, \sigma' \nu' \omega'}^{\sigma \nu \omega \bar{\nu}} := \frac{1}{\beta} \delta_{\sigma'_3}^{\sigma_3} \delta_{\nu'}^{\nu} \Gamma_{\text{ph}, \sigma'_2 \sigma'_1}^{\sigma_2 \sigma_1 (\omega - \bar{\nu})(\nu + \bar{\nu})} G^{\omega' - \bar{\nu}} G^{\omega' + \nu}, \quad (48)$$

$$M_{23, \sigma' \nu' \omega'}^{\sigma \nu \omega \bar{\nu}} := \frac{1}{\beta} \delta_{\sigma'_1}^{\sigma_1} \delta_{\omega'}^{\omega} \Gamma_{\text{ph}, \sigma'_2 \sigma'_3}^{\sigma_2 \sigma_3 \nu \omega} G^{\nu'} G^{\omega + \nu'}, \quad (49)$$

$$M_{13, \sigma' \nu' \omega'}^{\sigma \nu \omega \bar{\nu}} := \frac{1}{2\beta} \delta_{\sigma'_2}^{\sigma_2} \delta_{\nu' + \omega'}^{\nu + \omega} \Gamma_{\text{pp}, \sigma'_1 \sigma'_3}^{\sigma'_1 \sigma'_3 \nu (\omega + \nu - \bar{\nu})} G^{\omega' - \bar{\nu}} G^{\nu'}, \quad (50)$$

for the components of M , where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ and similarly for σ' . The factors $1/\beta$ ensure that M is dimensionless, which is necessary because we sum over different powers of them in the ladder. A diagrammatic representation of the M 's is shown in Fig. 18. The permutation matrix is simply given

by a combination of Kronecker deltas

$$P_{\sigma' \nu' \omega'}^{\sigma \nu \omega \bar{\nu}} = \delta_{\sigma'_1}^{\sigma_1} \delta_{\sigma'_2}^{\sigma_2} \delta_{\sigma'_3}^{\sigma_3} \delta_{\omega'}^{\omega} \delta_{\nu'}^{\nu} - \delta_{\sigma'_3}^{\sigma_1} \delta_{\sigma'_2}^{\sigma_2} \delta_{\sigma'_1}^{\sigma_3} \delta_{\nu'}^{\omega - \bar{\nu}} \delta_{\omega' + \nu'}^{\nu + \omega}. \quad (51)$$

Finally, the full equation for the approximate three-particle ladder reads

$$L_{\sigma' \nu' \omega'}^{\sigma \nu \omega \bar{\nu}} = -\beta^2 G^{\omega - \bar{\nu}} G^{\nu + \omega} G^{\nu} \sum_{\sigma_1, \nu_1, \omega_1} \left(\sum_{n=0}^{\infty} (M^n - M_{12}^n - M_{23}^n - M_{13}^n) + 2 \right)_{\sigma_1 \nu_1 \omega_1}^{\sigma \nu \omega \bar{\nu}} P_{\sigma' \nu' \omega'}^{\sigma_1 \nu_1 \omega_1 \bar{\nu}}, \quad (52)$$

where the prefactor of β^2 ensures a dimension of $[\tau]^5$, as it should be for a quantity depending on five Matsubara frequencies. The addition of 2 is necessary because the sum now starts at $n = 0$ to turn it into a proper geometric series. The notation also shows that the equation is diagonal in $\bar{\nu}$ and the terms can be viewed as simple matrices when condensing (σ, ν, ω) into a single compound index. This makes it easy to employ the closed-form formula for the geometric series.

Substituting the 1PI vertex $\Gamma_{1\text{PI}, r}$ in Eq. (33), with the approximate three-particle ladder L , turns out to yield even qualitatively bad results. The reason for that lies in the crossing symmetries. As mentioned before, the approximate ladder only satisfies two of the six crossing symmetries of the full three-particle vertex F_3 . The 1PR diagram $(F_2 G F_2)_r$ in Eq. (33) is in the same channel r as $\Gamma_{1\text{PI}, r}$ or in this case the ladder, and therefore has the same problem. To solve this, we compute the average of the approximate ladder and the 1PR diagram $(F_2 G F_2)_r$ over all nine pph channels defined in Table III. The full three-particle vertex (with legs) in this approximation is thus given by

$$GGGF_3 GGG \approx \frac{1}{9} \sum_r [L_r + GGG(F_2 G F_2)_r GGG], \quad (53)$$

where r runs over the nine pph channels.

Averaging is preferable to summation to avoid overcounting of lower-order diagrams. Considering second-order diagrams of G_3 , every pph ladder generates eight (out of a total of nine of them) and the 1PR diagram added separately is the ninth. This means that a single channel already contains all diagrams up to second order in F_2 and not averaging would lead to overcounting them by a factor of 9. Averaging guarantees that the thus calculated vertex is correct to second order. [40]

Note that we do not need to come up with nine versions of Eq. (52) to compute the ladders in all pph channels. Instead, it is much easier to convert the ladder in the 41 channel to the

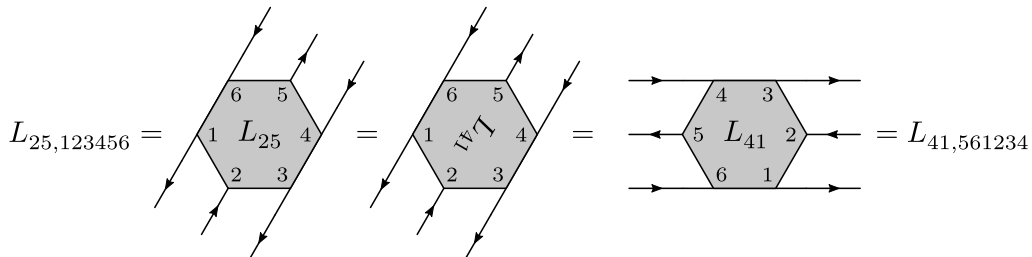


FIG. 16. The pph ladder in the 25 channel, obtained from the one in the 41 channel.

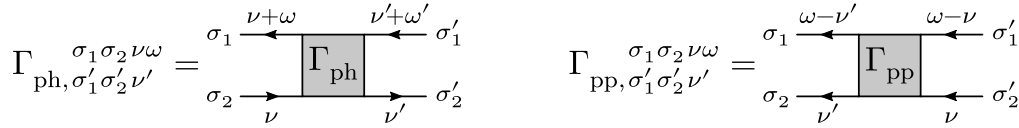


FIG. 17. Frequency and spin notations for the two-particle vertices used in the three-particle ladder.

other ones by rotation or swapping of legs as exemplified in Fig. 16.

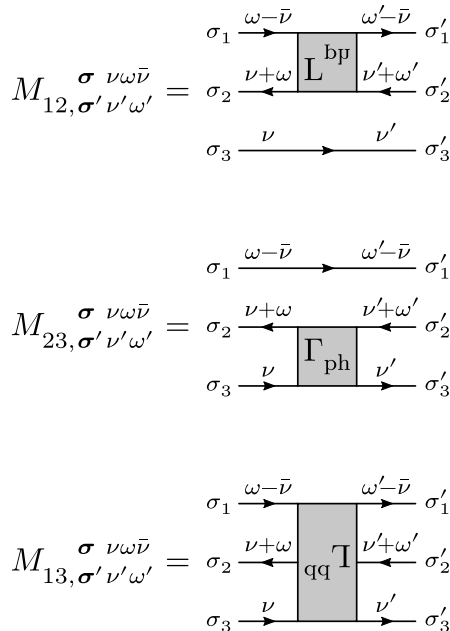
C. Second-order response function

The last step in our computations is using the approximate three-particle vertex and calculating its contribution to the second-order response function $\chi_{\text{vertex}}^{(2)}$, which we here compare to the exact solution. Since our approximation already comes attached with six Green's functions, this is, at least in theory, easily done by summing over the fermionic frequencies:

$$\chi_{\text{vertex}}^{\omega\omega'} = \sum_{\nu\nu'\bar{\nu}} (GGGF_3GGG)_{\nu'\omega'}^{\nu\omega\bar{\nu}}. \quad (54)$$

In numerical calculations, these infinite sums are, of course, limited by the grid size. As it turns out it is important how exactly the sums are implemented because some terms need to cancel. The reason for that is that the imaginary part of $\chi_{\text{vertex},\uparrow\uparrow\uparrow}$ and $\chi_{\text{vertex},\uparrow\uparrow\downarrow}$ must vanish. This can easily be shown when remembering that complex conjugation inverts the order of spins and fermionic frequencies while also negating the latter [41,42]:

$$(F_{123456}^{\nu_1\cdots\nu_6})^* = F_{654321}^{-\nu_6\cdots-\nu_1}. \quad (55)$$

FIG. 18. Diagrammatic representation of Eqs. (48)–(50), the definitions of the three components of M .

If we now use, e.g., the first ph notation from Table II,

$$\begin{aligned} \omega_a &= \nu_1 - \nu_2, \\ \omega_b &= \nu_3 - \nu_4, \\ \omega_c &= \nu_5 - \nu_6, \end{aligned} \quad (56)$$

we see that the bosonic frequencies also change their order but keep their signs after complex conjugation

$$\begin{aligned} \omega_a &\rightarrow -\nu_6 + \nu_5 = \omega_c, \\ \omega_b &\rightarrow -\nu_4 + \nu_3 = \omega_b, \\ \omega_c &\rightarrow -\nu_2 + \nu_1 = \omega_a. \end{aligned} \quad (57)$$

For the second-order response functions, we therefore have

$$(\chi_{\text{vertex},123456}^{\omega_a\omega_b\omega_c})^* = \chi_{\text{vertex},654321}^{\omega_c\omega_b\omega_a}. \quad (58)$$

Using the swapping symmetries introduced in Ref. [18] and Eqs. (G3)–(G5), we see that the $\uparrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$ components of $\chi_{\text{vertex}}^{(2)}$ are indeed purely real:

$$(\chi_{\text{vertex},\uparrow\uparrow\uparrow}^{\omega_a\omega_b\omega_c})^* = \chi_{\text{vertex},\uparrow\uparrow\uparrow}^{\omega_c\omega_b\omega_a} = \chi_{\text{vertex},\uparrow\uparrow\uparrow}^{\omega_a\omega_b\omega_c}, \quad (59)$$

$$(\chi_{\text{vertex},\uparrow\uparrow\downarrow}^{\omega_a\omega_b\omega_c})^* = \chi_{\text{vertex},\downarrow\uparrow\uparrow}^{\omega_c\omega_b\omega_a} = \chi_{\text{vertex},\uparrow\uparrow\downarrow}^{\omega_a\omega_b\omega_c}. \quad (60)$$

The problem for the approximate ladder is that it does not have those swapping symmetries. [43] Fortunately, they are not required if we do the complex conjugation of the ladder properly and choose the right ph notation. To show what we mean by the first part, let us do an explicit complex conjugation for a term that appears in the ladder. A simple example is

$$(\Gamma^{\nu_1\nu_2\nu_3\nu} G^{\nu} \Gamma^{\nu\nu_6\nu_5\nu_4})^* = \Gamma^{\nu-\nu_3-\nu_2-\nu_1} G^{-\nu} \Gamma^{-\nu_4-\nu_5-\nu_6-\nu}. \quad (61)$$

The corresponding Feynman diagrams are found in Fig. 19 and show that the positions of the vertices and frequencies get mirrored along the vertical axis with the frequencies also being negated. This holds in general for all ladder terms as can be seen when computing a few more simple diagrams and then using induction. Since the ladder generates all possible arrangements of two-particle vertices, it also contains all mirrored terms. Therefore, the correct way to complex conjugate a ladder is

$$(L_{123456}^{\nu_1\cdots\nu_6})^* = L_{432165}^{-\nu_4-\nu_3-\nu_2-\nu_1-\nu_6-\nu_5}. \quad (62)$$

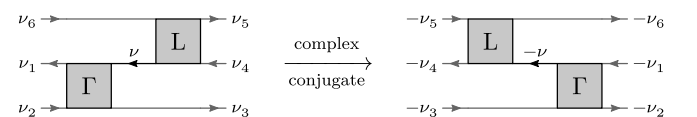


FIG. 19. Diagrammatic representation of Eq. (61). The complex conjugation mirrors the positions of the vertices and frequencies along the vertical axis. The frequencies are also negated.

This does not contradict Eq. (55) since the full three-particle vertex has all crossing and swapping symmetries, and we can write

$$(F_{123456}^{v_1 \dots v_6})^* = F_{654321}^{-v_6 \dots -v_1} = F_{432165}^{-v_4 - v_3 - v_2 - v_1 - v_6 - v_5}. \quad (63)$$

To ensure that the $\uparrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$ components of $\chi_{\text{vertex}}^{(2)}$ are real, we have to find a ph notation where the imaginary parts of the ladder cancel when summing over the fermionic frequencies. This means that the complex conjugate of a frequency component of L must map to the same bosonic frequencies. The $\text{ph}_{\bar{a}}$ notation from Table II achieves exactly that

$$\begin{aligned} \bar{\omega}_a &= v_1 - v_4 \rightarrow -v_4 + v_1 = \bar{\omega}_a, \\ \omega'_b &= v_3 - v_2 \rightarrow -v_2 + v_3 = \omega'_b, \\ \omega_c &= v_5 - v_6 \rightarrow -v_6 + v_5 = \omega_c, \end{aligned} \quad (64)$$

and therefore

$$(L_{123456}^{v_a \bar{\omega}_a v_b \omega'_b v_c})^* = L_{432165}^{-v_a \bar{\omega}_a - v_b \omega'_b - v_c}. \quad (65)$$

In the numerical implementation, we only have to make sure that we sum over a symmetric interval of fermionic frequencies to ensure cancellation.

So far, we only considered the approximate three-particle ladder in the 41 channel. However, in Eq. (53), we average over ladders in all nine pph channels. Fortunately, this does not cause additional issues with the cancellation of imaginary parts: When converting the ladder in the 41 channel to some other channels, we have to swap one or two pairs of legs. Channels 23 and 65 are the ones requiring two pairs. Their Feynman diagrams turn out to be symmetric along the vertical axis, so the same considerations as for the 41 channel hold, and the imaginary parts cancel. The remaining six channels are not symmetric on their own, but they form mirror pairs 25 and 63, 45 and 61, as well as 21 and 43. When summing over those pairs, they cancel each other's imaginary parts for the $\uparrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$ component as well.

Putting everything together, we end up with the following approximation for the vertex contribution to the second-order response function:

$$\begin{aligned} \bar{\chi}_{\text{vertex}}^{\omega'_a \omega'_b} &\approx \sum_{v_a v_b v_c} \frac{1}{9} \sum_r [L_r^{v_a \bar{\omega}_a v_b \omega'_b v_c} \\ &\quad + (GGG(F_2 GF_2)_r GGG)^{v_a \bar{\omega}_a v_b \omega'_b v_c}], \end{aligned} \quad (66)$$

where the ladder L and the 1PR diagram $F_2 GF_2$ are in $\text{ph}_{\bar{a}}$ notation, and r runs over the nine pph channels.

V. NUMERICAL RESULTS

A. Numerical methods employed

All numerical results presented in this section are computed for the AIM of the DMFT solution for a single-band, square lattice Hubbard model with nearest-neighbor hopping $t = 1$, total density $n = 1.1$, inverse temperature $\beta = 10$, and local Coulomb interaction $U \in \{0.5, 1, 2, 3, 4\}$. Here, the DMFT solution is obtained with w2dynamcis [44], a continuous-time quantum Monte Carlo (QMC) solver, which also allows calculating the local two-particle Green's function,

Eq. (2), and then, by employing the parquet and two-particle Bethe-Salpeter equations, Eq. (14), all local two-particle vertices. [45] The hybridization expansion used by w2dynamics is, however, not well suited in the limit of small U since the hybridization becomes relatively large compared to the interaction. This means that while the one-particle Green's function can still be obtained with high enough accuracy and precision, the irreducible vertices are too noisy to be used in the three-particle ladder. Therefore, we employ different methods for computing Γ .

For the smallest interactions, $U \in \{0.5, 1, 2\}$, we use a parquet equations solver [46,47] to compute the irreducible vertices in the parquet approximation $\Lambda \approx U$, which yields noise-free results. For $U \in \{3, 4\}$, we use the same parquet solver, but take the local fully irreducible vertex Λ from the QMC calculation as a starting point because it turns out that the resulting Γ has less noise than the Γ computed directly from the QMC results.

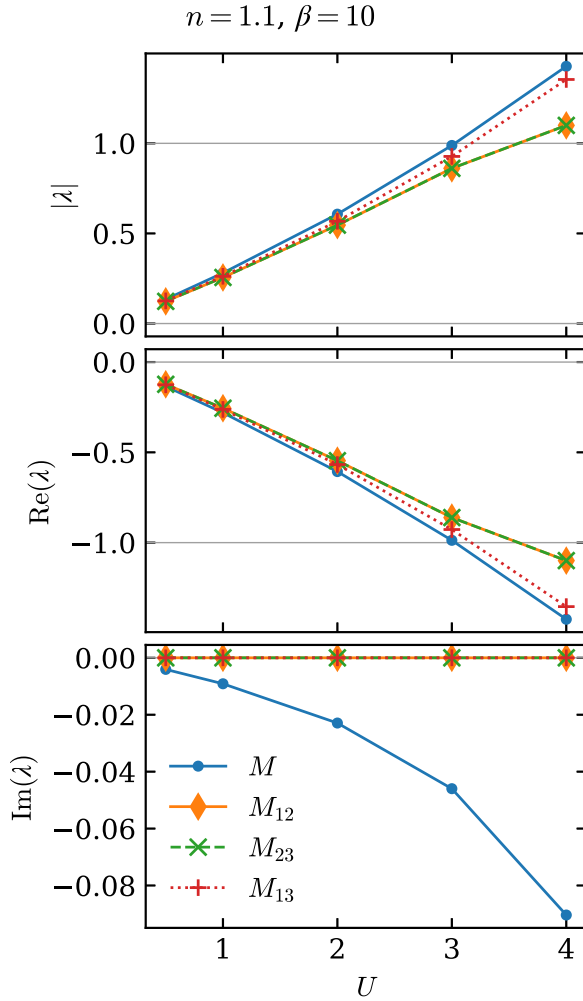
In all cases, we then construct the M 's from two-particle irreducible vertices Γ as in Eqs. (48)–(50). Together with the one-particle Green's function, this is the input for the three-particle BSE, Eq. (30). The ladder solution of the BSE, L , Eq. (52), is then evaluated for the AIM. That is, this way we can compute three-particle local Green's functions and response functions of the AIM with the derived ladder approximation and compare these against numerically calculated exact ones.

To obtain the exact three-particle (second order) response function $\chi^{(2)}$, Eq. (29), exact diagonalization (ED) calculations are performed using the ED code of [48] with six bath sites. The latter are obtained from the DMFT(QMC) solution via pole fitting [49]. In ED, we calculate the eigenfunctions and eigenvalues of this AIM (1) with six bath sites and from it $\chi^{(2)}$ via the Lehmann representation. We have also calculated $\chi^{(2)}$ in QMC, which agrees well with ED, except for a substantial level of statistical noise for larger frequency values (which is why we present here only the ED results). A further alternative, which is, however, beyond the scope of the present paper, would be to use the numerical renormalization group for calculating the local two-particle vertex [50,51].

B. Eigenvalues of M 's

To obtain the ladder solution of the three-particle BSE from Eq. (52), we need to perform the sum of a geometric series. Before we compute any three-particle ladders, we need to make sure that the geometric series in Eq. (52) actually converges. To this end, we compute the eigenvalues of the M 's (i.e., M, M_{12}, M_{23} , and M_{13}) and check if their absolute values are less than 1. More precisely, when looking at Eqs. (48)–(50) (the definitions of the M 's), we condense (v, ω, σ) and (v', ω', σ') into two compound indices. For every $\bar{v}$, we then have a sparse square matrix ($\approx 30\,000 \times 30\,000$) for which the eigenvalues are calculated.

The absolute largest eigenvalues λ over all values of $\bar{v}$ are shown in Fig. 20 for different interaction strengths U . We see that the eigenvalues of M are larger than those of its components, and the difference grows with U . At $U = 3$, the magnitude of the largest eigenvalue of M is just below 1, so the ladder converges only up to about this point. Despite that,

FIG. 20. Largest absolute eigenvalues of M 's plotted over U .

we do not expect the ladder to blow up numerically because we compute the ladder using the closed-form solution for the geometric series, $1/(1-q)$, and the eigenvalues are close to -1 and not $+1$. We also see that M_{12} and M_{23} yield identical results, which is not surprising since they both contain Γ_{ph} and are mirror versions of each other. Furthermore, M_{13} and therefore Γ_{pp} seem to give the dominant contribution to the largest eigenvalue of M and therefore the three-particle ladder as a whole. The last thing to mention is that only M seems to have eigenvalues with an imaginary part. However, when looking at more than just the largest eigenvalue, we find that the components of M , especially M_{13} , have eigenvalues with similar imaginary parts as well (not shown), so this is actually not an exceptional result.

1. $\chi_{\text{vertex}}^{(2)}$: Exact diagonalization versus approximate ladder

Next, we compare the ladder approximation to the ED for three-particle vertex contributions to the second-order response functions. Similarly as in Ref. [18]: First one-, two-, and three-particle correlators are computed with the ED code [48]. Then, the disconnected parts are subtracted to obtain the full second-order response functions $\chi^{(2)}$. Next, the bubble terms $\chi_0^{(2)}$ and first-order terms $\chi_1^{(2)}$ are computed

TABLE IV. Static values ($\omega_1 = \omega_2 = 0$) of $\chi_{\text{vertex}}^{(2)}$ cut off from the color bars of Fig. 21.

U	$\chi_{\text{vertex}, \uparrow\uparrow\uparrow}^{(2)00}$		$\chi_{\text{vertex}, \uparrow\uparrow\downarrow}^{(2)00}$	
	ED	Ladder	ED	Ladder
0.5	5.6×10^{-05}	1.5×10^{-05}	-6.3×10^{-04}	-3.4×10^{-04}
1.0	4.0×10^{-04}	4.8×10^{-05}	-2.3×10^{-03}	-1.1×10^{-03}
2.0	2.4×10^{-03}	-9.1×10^{-04}	-7.1×10^{-03}	-2.2×10^{-03}
3.0	5.5×10^{-03}	-8.9×10^{-03}	-1.2×10^{-02}	9.5×10^{-04}
4.0	7.5×10^{-03}	-1.5×10^{-02}	-1.6×10^{-02}	5.7×10^{-03}

from one- and two-particle quantities (see Fig. 6). Finally, $\chi_0^{(2)}$ and $\chi_1^{(2)}$ are subtracted from the full second-order response function yielding the vertex term $\chi_{\text{vertex}}^{(2)}$. The difference to Ref. [18] is that instead of the “physical” response functions χ_{nnn} , χ_{nzz} , and χ_{xyz} we compute and compare the three spin components $\chi_{\uparrow\uparrow\uparrow}$, $\chi_{\uparrow\uparrow\downarrow}$, and $\chi_{\uparrow\downarrow\downarrow}$. The reason for that is that these spin components are what we can actually compute directly from the approximate ladder. As shown in Ref. [18], the physical response functions are a linear combination of the spin components, and we do not want that linear combination to hide or disguise potential differences between the ED results and the ladder.

As explained at the end of Sec. IV, the contribution to $\chi_{\text{vertex}}^{(2)}$ from the approximate ladder is computed in $\text{ph}_{\bar{a}}$ notation Eq. (64). However, for better consistency and comparability, all results shown in this section use the same frequency notation as in Ref. [18], i.e., the ph notation from Table II. That is, we have to translate back from Eq. (64) to Eq. (56).

Figure 21 compares the ED and ladder results of spin components $\uparrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$ of $\chi_{\text{vertex}}^{(2)\omega_1\omega_2}$ for different values of the on-site Coulomb interaction U . We only plot the real parts since, as expected from the discussion at the end of Sec. IV, the imaginary parts are at least 7 orders of magnitude smaller than the real part. The static values of the second-order response functions, i.e., those at $\omega_1 = \omega_2 = 0$, are much larger (by magnitude) than the other frequency components and would dominate the plot. Therefore, they are cut off from the color bars and instead shown in Table IV.

The first thing we see when looking at Fig. 21 is that the approximate ladder yields qualitatively good results only for small values of the interaction. For the $\uparrow\uparrow\uparrow$ component this is until $U = 1$; for the $\uparrow\uparrow\downarrow$ component, it is until $U = 3$. Even then, however, the results are off by a factor of 2 to 10, so quantitatively the approximate ladder is not good.

Figure 22 compares the real and imaginary parts of the ED and ladder results of spin component $\uparrow\uparrow\downarrow$, $\uparrow\uparrow\downarrow^*$ of $\chi_{\text{vertex}}^{(2)\omega_1\omega_2}$ for different values of the interaction U . Similar to the spin component $\uparrow\uparrow\uparrow$ the approximate ladder only yields qualitatively good results until $U = 1$ —at least for the real parts. The imaginary parts look fine for all values of U . However, looking at the color bars reveals that quantitatively the ladder results for spin component $\uparrow\uparrow\downarrow$, $\uparrow\uparrow\downarrow^*$ are just as bad as those for the others.

The fact that for all spin components, the qualitatively good-looking results are consistently too small is no surprise.

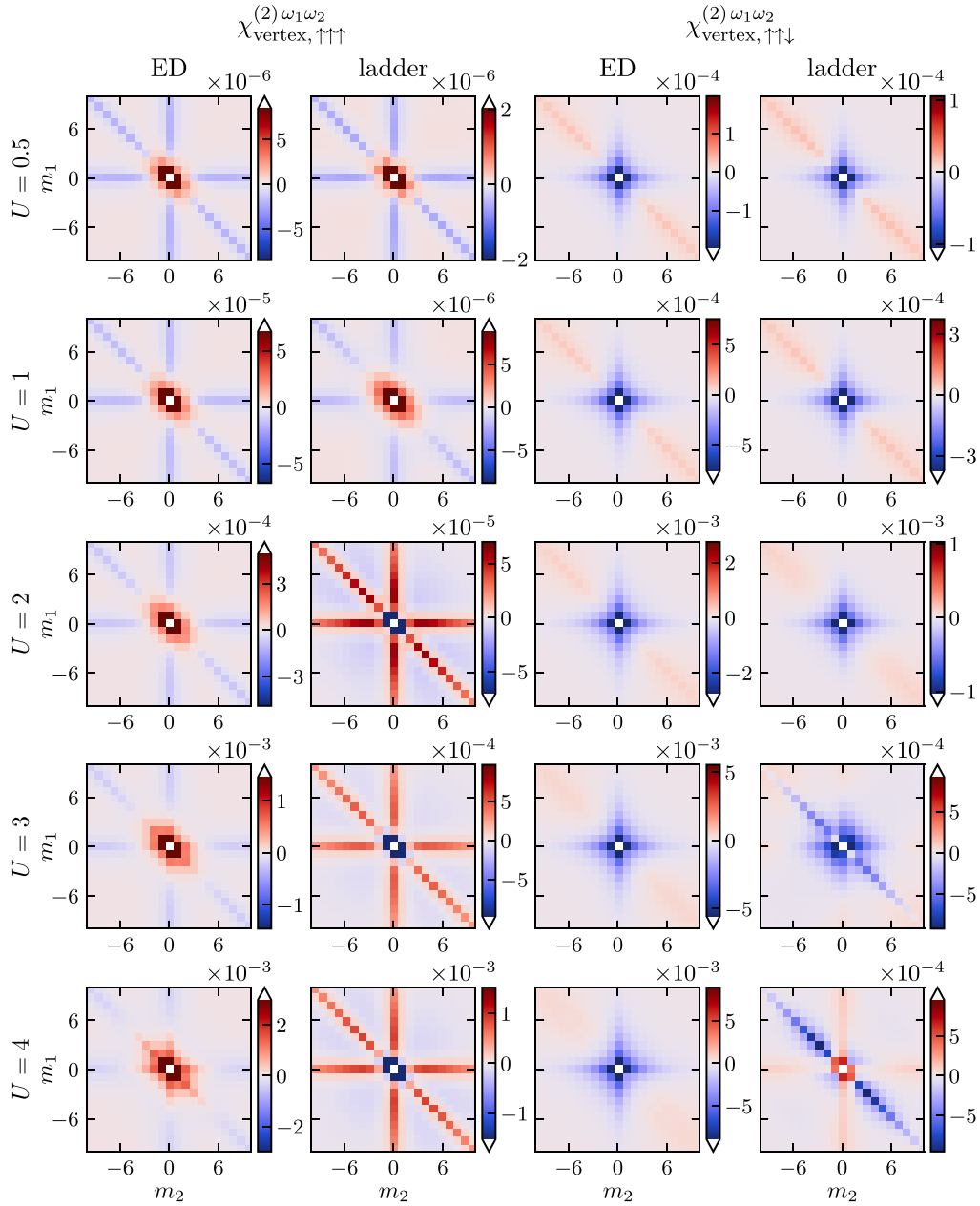


FIG. 21. Comparison of spin component $\uparrow\uparrow\uparrow$ and $\uparrow\uparrow\downarrow$ of $\chi_{\text{vertex}}^{(2)\omega_1\omega_2}$ between ED and the approximate ladder for different values of the interaction U (here and in the following figures inverse temperature is $\beta = 10$). The labels m_i are the indices of the bosonic frequencies $\omega_i = 2\pi m_i/\beta$. The static values ($\omega_1 = \omega_2 = 0$) are much larger than the other frequency components, so they are cut off from the color bars and instead shown in Table IV. Please note, the color scale is different for each subplot.

After all, we average over all nine pph channels instead of summing. Of course, as we have shown at the end of Sec. IV, summing would overcount diagrams with few vertices, but we conjecture that ladder terms of high enough order, i.e., number of vertices, are exclusive to a channel. Averaging therefore cuts down higher-order contributions by a factor of 9.

C. Approximate ladder in different channels

In this section, we take a closer look at the contributions of the different pph channels r to the second-order response

function computed only from the approximate ladder L , i.e.,

$$\chi_{L,r}^{\omega_1\omega_2} = \sum_{v_1 v_2 v_3} L_r^{v_1 \omega_1 v_2 \omega_2 v_3}. \quad (67)$$

We already pointed out at the end of Sec. IV that six of the nine channels form mirror pairs. These pairs have the same real part but opposing imaginary parts, which all cancel eventually. Therefore, only six channels are of interest. Figure 23 compares the spin component $\uparrow\uparrow\uparrow$ of the real parts of $\chi_{L,r}^{\omega_1\omega_2}$ in six such channels at interaction strengths $U = 1$ and $U = 2$. As in Fig. 21, the static frequency components

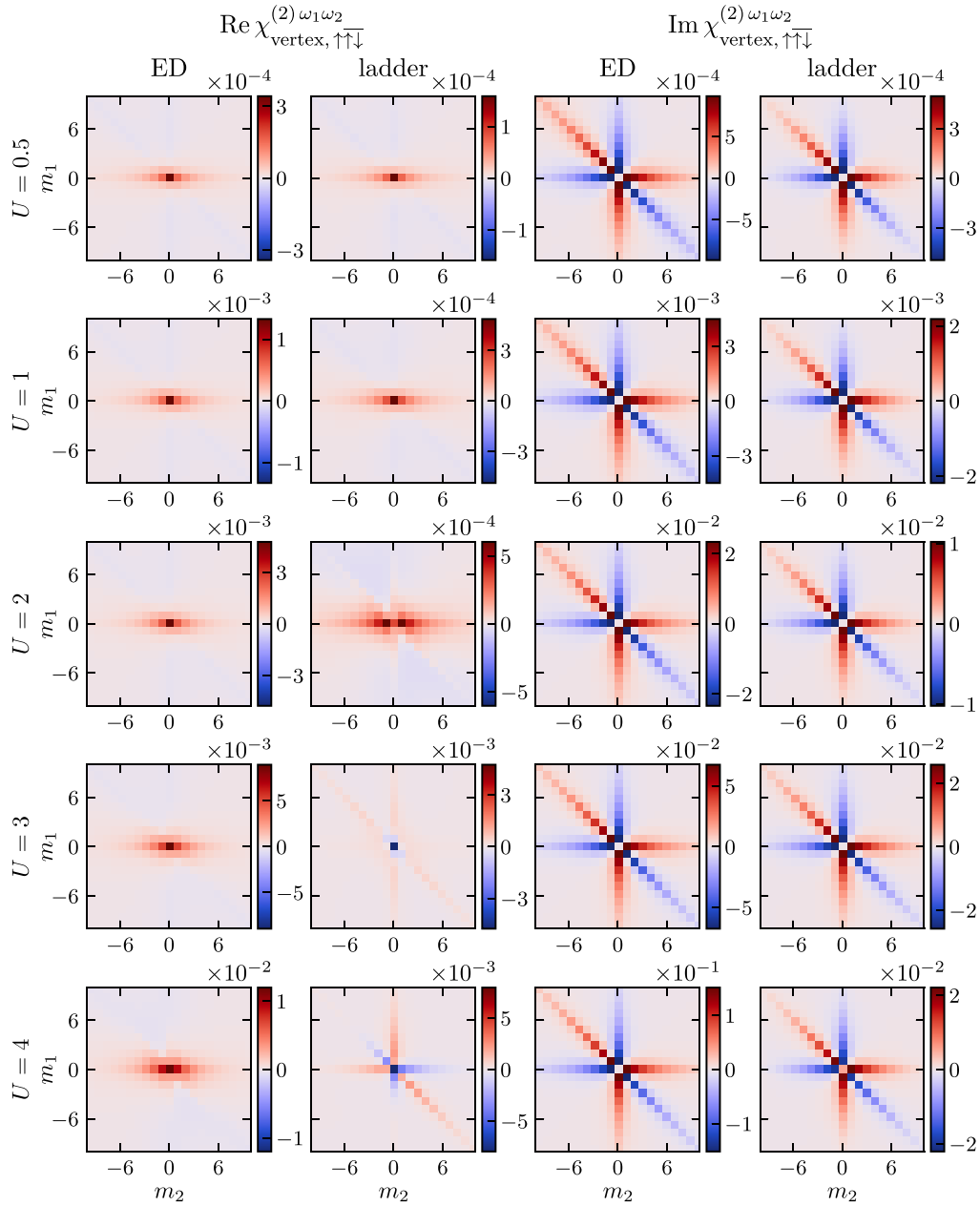


FIG. 22. Comparison of the real and imaginary parts of spin component $\uparrow\downarrow, \uparrow\uparrow\downarrow$ of $\chi_{\text{vertex}}^{(2)\omega_1\omega_2}$ between ED and the approximate ladder for different values of the on-site Coulomb interaction U . The axis labels m_i are the indices of the bosonic frequencies $\omega_i = 2\pi m_i/\beta$. Please note, the color scale is different for every subplot.

($\omega_1 = \omega_2 = 0$) would dominate the plot and are therefore cut off and presented separately in Table V.

When looking at Fig. 23, we see that all results share two features: First, the main contributions are around the center;

second, one of the three lines $\omega_i = 0$, $i \in \{1, 2, 3\}$, is more pronounced than the others. The latter is not surprising, since the Feynman diagrams for a single ladder have a distinguished direction. This also highlights once more why averaging over

TABLE V. Static values ($\omega_1 = \omega_2 = 0$) of $\chi_{L,r,\uparrow\uparrow\uparrow}^{(2)}$ cut off from the color bars of Fig. 23.

U	$\chi_{L,r,\uparrow\uparrow\uparrow}^{00}$					
	$r = 41$	$r = 23$	$r = 65$	$r = 25$	$r = 45$	$r = 21$
1.0	-3.3×10^{-04}	-3.3×10^{-04}	-3.3×10^{-04}	2.6×10^{-04}	2.6×10^{-04}	2.6×10^{-04}
2.0	-4.4×10^{-03}	-4.4×10^{-03}	-4.4×10^{-03}	1.2×10^{-03}	1.2×10^{-03}	1.2×10^{-03}

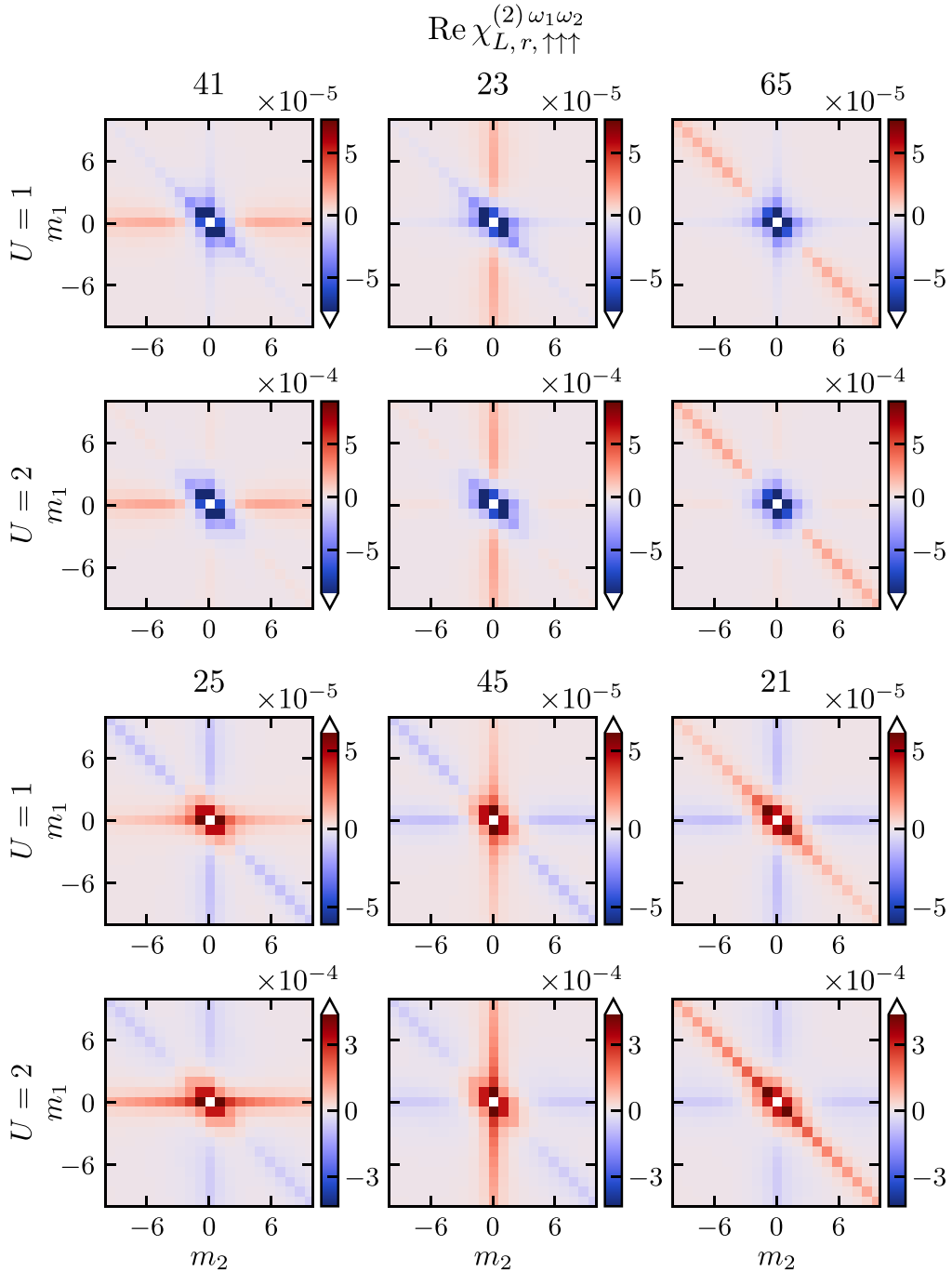


FIG. 23. Comparison of the contributions of the approximate ladder L in six pph channels $r \in \{41, 23, 65, 25, 45, 21\}$ to the $\uparrow\uparrow\uparrow$ component of the second-order response function $\chi_{L,r}^{(2)\omega_1\omega_2}$ for Coulomb interactions $U = \{1, 2\}$. The labels m_i are the indices of the bosonic frequencies $\omega_i = 2\pi m_i/\beta$. As in Fig. 21, the static components ($\omega_1 = \omega_2 = 0$) are cut off and shown in Table V instead. The color scale is the same for all three subplots in each row.

the approximate ladders in all channels is important if we want to get the right structure of the three-particle vertex.

We also see that the contributions from the upper and lower three channels in Fig. 23 have opposite signs. For $U = 1$, they even have a very similar magnitude. However, since for each of the lower three channels there is a second one with the same real part, those contributions outweigh the upper three channels. The final result for $\chi_{\text{vertex},\uparrow\uparrow\uparrow}^{(2)}$ at $U = 1$,

shown in Fig. 21, has therefore positive values around the center.

When comparing the results between $U = 1$ and $U = 2$ in Fig. 23, we notice that while the plots still look qualitatively similar, the balance in magnitude shifts. The static frequency components in Table V show this best. While the values for the first three channels rise by a factor of more than 10, those of the last three channels only rise by a factor of less than 5.

In absolute terms, the channels 41, 23, and 65 now outweigh the other channels by a factor of more than 3. Therefore, the sign of the total result for $\chi_{\text{vertex}, \uparrow\uparrow\uparrow}^{(2)}$ shown in Fig. 21 changes at $U = 2$.

VI. CONCLUSION AND OUTLOOK

We have generalized the Bethe-Salpeter equations from two to three particle ladders. Due to the increased complexity of three-particle diagrams when it comes to the property of reducibility, the resulting equations are much more involved than those on the two-particle level. Also, the fully irreducible building blocks of the exact three-particle ladder are more complicated, and we do not yet have a feasible way of computing them. For this reason, we have derived an approximate ladder, built simply from irreducible two-particle vertices Γ and full Green's functions. Admittedly, even this approximation turned out to be quite complex and involved, but it yields a viable way for approximately computing the full three-particle vertex F_3 . Our three-particle ladder equations bear some similarities to the Faddeev equations [23] for the three-body problem; they are, however, somewhat more involved since we do not keep the particle(hole) number fixed in between the three incoming and the three outgoing particles (holes).

If we knew the 3PI vertex in a given channel exactly, [52] the corresponding ladder equation in that channel is exact and thus yields the exact full three-particle vertex. But, we do not have a feasible way of computing that 3PI vertex yet. An approximation will most likely be necessary. In the spirit of diagrammatic extensions of DMFT [8], it might be easier to find a good approximation or a numerical way to calculate the *local* irreducible vertex than for the full one. Here, we employ an approximation where the 3PI vertex is built up, as mentioned above, from the three irreducible two-particle vertices that each connect two of the particle (hole) lines.

The numerical computations show that the approximated ladder only yields good results for very small values of the local Coulomb interaction U and even then only qualitatively. At least this holds for the investigated parameters and for the nonlinear response function studied. There might be parameter regimes where the approximation is generally better,

or quantities where we do not combine fermionic lines from both ends of the ladder. For example, two-particle ph ladders provide a quite good approximation for the magnetic susceptibility, if expressed in terms of Γ instead of the bare Coulomb interaction. But there, we combine the particle and hole line from one side of the ladder to a bosonic (para)magnon line. Calculating instead the $\overline{\text{ph}}$ ladder and then combining particle and hole lines from opposite sides of the ladder would be a rather bad approximation for the magnetic susceptibility. Similarly, for a three-particle quantity where we do not have to average over ladders in all nine channels because the physics happens predominantly in one “direction” might also give better results for the three-particle ladder. One could also look at a better way to avoid the double-counting issues that arise from summing the nine channels. This would require an additional major effort beyond the scope of the present paper. That is, one would need to identify all diagrams that are included twice or more in different three-particle ladders (including at least all second-order diagrams) and subtract them from the added contributions of the nine channels. At the moment, it is not possible to determine which of these two aspects is more important for the deviations from the exact result: (1) the approximation for the 3PI vertex by a two-particle irreducible vertex Γ and a Green's function or (2) the plain and unadorned averaging of all nine channels.

In the end, computing three-particle vertices is still in its very early stages of development. So while the current results fall short of expectations, they are still useful and a good first step that can be built upon.

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DATA AVAILABILITY

The code for the calculation of the three-particle ladder is available under open source license at [56].

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