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Nonequilibrium Green functions

Selfenergy approximation techniques

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Abstract

The framework of nonequilibrium Green functions (NEGFs) is developed to accurately describe interacting quantum systems evolving in the presence of strongly exciting ultra-fast fields. At its core stands the selfconsistent determination of the selfenergy, a functional of the single-particle Green function, which incorporates all relevant many-body physics and, via diagrammatic techniques, guarantees the conservation of the constants of motion. Over the last decades, NEGFs have been successfully applied to a broad range of domains ranging from homogeneous systems such as non-ideal quantum gases and plasmas over condensed matter to highly inhomogeneous systems such as atoms and molecules photo-ionized by laser-fields or colliding nuclear matter. Only recently, the first accurate simulation of the expansion dynamics of clouds of ultra-cold fermionic atoms in a two-dimensional optical lattice could be achieved using NEGFs.

The single-particle Green function is the solution of a coupled set of kinetic equations. Its intrinsic dependence on two independent time-arguments, ranging over the complete past of the system, not only enables the determination of all single-particle observables but also provides access to important two-particle observables and spectral information. With this coupling to the history, though, comes the practical necessity to apply physically motivated approximation techniques to the structure of the selfenergy and the Green functions, to achieve numerical tractability.

This thesis is devoted to provide a thorough overview of the possible approximation techniques including perturbative and non-perturbative approaches. Starting from the exact coupled set of equations of motion for the Green functions, the expressions for all selfenergy approximations are derived in the most general basis representation, i.e., for interaction tensor elements w_{ijkl} . From this, the corresponding expressions in a diagonal basis, where the interaction can be described as a matrix w_{ij} , and for the special case of the Hubbard model, where the interaction is just given as a scalar U , are deduced.

In the second part of this thesis, the quality of the selfenergy approximations to describe time-dependent as well as ground-state properties of interacting systems is tested. The approximations are applied to fermionic Hubbard nano-clusters to generate the interacting ground-state and its spectral function as well as to study the highly inhomogeneous excitation dynamics following a sudden quench in the on-site potential. A special focus lies on the effect of the interaction strength and the filling factor on the performance of the approximations. Finally, a strategy is presented to mitigate the effects of the so-called correlation-induced damping (CID), occurring in selfconsistent calculations, by applying the generalized Kadanoff–Baym ansatz (GKBA). Combined with a suitable selfenergy approximation, the GKBA yields results in excellent agreement with the exact solution also for excitations, where CID had previously rendered NEGF-based results unusable.

Kurzfassung

Das¹ Rahmenkonzept der Nichtgleichgewichts-Greenfunktionen (NGGFn) wurde zur akkuraten Beschreibung der Zeitentwicklung wechselwirkender Quantensysteme in stark anregenden ultra-schnellen Feldern entwickelt. Im Zentrum steht die selbstkonsistente Bestimmung der Selbstenergie, einem Funktional der Einteilchen-Greenfunktion, welche die gesamte relevante Vielteilchen-Physik beschreibt und durch die diagrammatische Technik eine Erhaltung von Invarianten der Bewegung sicherstellt. In den letzten Jahrzehnten sind NGGFn in vielen Domänen, angefangen von homogenen Systemen wie nicht-idealen Quantengasen und -plasmen über kondensierte Materie hin zur Photoionisation von hochgradig inhomogenen Systeme wie Atomen und Molekülen erfolgreich eingesetzt worden. Erst kürzlich gelang mit NGGFn die erste akkurate Simulation der Expansions-Dynamik von ultrakalten fermionischen Atomwolken in einem zweidimensionalen optischen Gitter.

Die Einteilchen-Greenfunktion ist als Lösung eines Satzes von kinetischen Gleichungen gegeben. Ihre intrinsische Abhängigkeit von zwei unabhängigen Zeitargumenten, welche sich über die gesamte Vergangenheit des Systems erstrecken, ermöglicht nicht nur die Bestimmung jeglicher Einteilchen-Observablen sondern erlaubt auch Zugriff auf wichtige Zweiteilchen-Größen sowie spektrale Informationen. Mit dieser Kopplung an die Vergangenheit geht jedoch die Notwendigkeit einher, physikalisch motivierte Näherungen an die Struktur der Greenfunktionen und der Selbstenergie zu machen, um eine sinnvolle numerische Lösbarkeit zu erreichen. Die Thesis will einen gründlichen Überblick über die möglichen perturbativen als auch nicht-perturbativen Approximations-Strategien geben. Ausgehend von dem exakten Satz von gekoppelten Bewegungsgleichungen für die Greenfunktionen werden die Ausdrücke für die Selbstenergie-Näherungen in der allgemeinsten Basis hergeleitet, d.h. für Wechselwirkungs-Tensorelemente w_{ijkl} . Davon werden die entsprechenden Terme in diagonalen Basis, wo die Wechselwirkung durch eine Matrix w_{ij} gegeben ist, und

¹This is a translation of the preceding abstract.

für den Spezialfall der Hubbard-Basis mit skalarer Wechselwirkung U abgeleitet. Im zweiten Teil dieser Thesis wird die Qualität der Beschreibung zeitabhängiger und Grundzustands-Eigenschaften durch die Selbstenergie-Näherungen in wechselwirkenden Systemen untersucht. Dazu werden die Approximationen auf fermionische Hubbard Nano-Verbünde zur Präparation des wechselwirkenden Grundzustands und dessen Spektralfunktion angewendet. Ebenso wird die hochgradig inhomogene Anregungsdynamik nach einem plötzlichen Quench des Gitterplatz-Potentials studiert. Ein besonderes Augenmerk liegt dabei auf dem Effekt der Wechselwirkungsstärke und des Füllfaktors auf die Qualität der Näherungen. Abschließend wird mit dem generalisierten Kadanoff–Baym Ansatz (GKBA) eine Strategie präsentiert, welche die Auswirkungen der sogenannten Korrelations-induzierten Dämpfung (KID), welche bei selbstkonsistenten Rechnungen auftritt, verringert. In Kombination mit einer geeigneten Selbstenergie-Näherung kann mit dem GKBA eine hervorragende Übereinstimmung mit der exakten Lösung auch für solche Anregungen erreicht werden, für die NGGF-basierte Rechnungen zuvor keine verwertbaren Ergebnisse geliefert haben.

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1 Introduction

Unlike systems in equilibrium with their surrounding, where a few global variables—such as temperature, pressure or volume—suffice to completely describe their state, the state of a system in nonequilibrium is strongly influenced by transient phenomena such as external fields. The resulting inhomogeneities in the structure of the system can be measured as a strong time-dependence of its observables. Despite the notion of equilibrium being commonly associated with many processes in nature, it is the state of nonequilibrium that is the most prevalent and natural state on many length and time scales, building a basis for the development of life constantly dissipating heat and entropy into the environment to remain at a highly excited state. Furthermore, nonequilibrium processes become more and more important in technical applications since the ubiquitous miniaturization reduces the relevant system sizes to the order of only a few hundred particles, rendering equilibrium descriptions insufficient, since they cannot describe the strong coupling of the system with its environment and the notion of, e.g., temperature, becomes meaningless.

1.1 Approaches to nonequilibrium physics

As the need for adequate descriptions of ever smaller systems has been increasing over the last 50 years, the field of nonequilibrium physics of (strongly) interacting many-body systems has gained a corresponding amount of attention, both experimentally and theoretically. The fields of application reach from condensed-matter physics [1–6] over laser–matter interaction [7–9], high energy nuclear physics [10] and exotic applications such as leptogenesis [11] to expansion experiments of ultra-cold atoms in optical traps [12–17]. Correspondingly, several frameworks have been developed to theoretically address correlated systems, i.e., systems which cannot be described as simple compositions of independent or weakly interacting particles. The first main group is comprised of exact methods, i.e., approaches which solve the (apart

from relativistic effects) exact time-dependent Schrödinger equation (TDSE) for the time-dependent wavefunction $|\Psi(t)\rangle$, which is an element of a suitable Hilbert space \mathcal{H} ,

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle,$$

with the Hamilton operator $\hat{H}(t)$, which includes all relevant energy contributions. Apart from the direct solution of the Schrödinger equation [18]—which is limited to the treatment of only a few particles, since it is hampered by an exponential scaling of the numerical demand with the particle number—there exist several methods which provide an approximate solution of the TDSE. Examples are the generalized active space configuration interaction methods [19–21], which aims at the restriction to physically relevant states of \mathcal{H} , continuous time quantum Monte Carlo, which improves the sampling of these states but is limited to short time scales, and time-dependent density-matrix renormalization group based approaches [14, 22–25], which allow for an efficient treatment of short-ranged correlations but are limited to (effectively) one-dimensional systems. As an alternative approach, there exists a different class of approximations, which, instead of focusing on the time-dependent many-particle wavefunction $|\Psi(t)\rangle$ containing the full N -particle information, try to find a good approximation for the single-particle density-matrix, by the sole knowledge of which many important observables of the system can be computed. Among others, methods belonging to this class are time-dependent density functional theory [26–29], which uses the principle of correspondence between the electronic density and the many-body wavefunction by an (in practice only approximately known) density functional, time-dependent reduced density-matrix based approaches (TDRDM), which approximately solve the equations of motion for the single-particle density matrix by uncoupling them from the equations of motion for reduced density matrices for higher particle numbers. Closely related to TDRDM is the nonequilibrium Green functions (NEGF) approach, applied in this thesis, which augments the single-particle density matrices by a second time-coordinate which carries spectral information, yielding the single-particle Green function,

$$G(z_1, z_2),$$

where the time arguments denoted with the letter “ z ” are situated on a complex time plane \mathcal{C} . Again corresponding to TDRDM, the NEGF approach aims at solving the equations of motion for the single-particle Green function by means of decoupling it from the equations of motion of Green functions for higher particle numbers by introduction of the so-called single-particle selfenergy. The equations of motion—the (Keldysh–)Kadanoff–Baym equations—which are of integro-differential structure, read

$$\begin{aligned} & \sum_l \left[i\hbar \frac{d}{dz_1} \delta_{il} - h_{il}(z_1) \right] G_{lj}(z_1, z_2) \\ &= \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} + \sum_l \int_{\mathcal{C}} dz_3 \Sigma_{il}(z_1, z_3) G_{lj}(z_3, z_2), \\ & \sum_l G_{il}(z_1, z_2) \left[-i\hbar \frac{\overleftarrow{d}}{dz_2} \delta_{lj} - h_{lj}(z_2) \right] \\ &= \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} + \sum_l \int_{\mathcal{C}} dz_3 G_{il}(z_1, z_3) \Sigma_{lj}(z_3, z_2), \end{aligned}$$

where the terms $h_{ij}(z_1)$ correspond to the single-particle part of the Hamiltonian and $\Sigma_{ij}(z_1, z_2)$ denotes the selfenergy. For a more detailed introduction, see Section 2.4.

1.2 Nonequilibrium Green functions

Compared to TDRDM, the NEGF approach has several advantages. First, the spectral information encoded in the Green function can be used to gain information about the possible energy levels for particle removal and addition energies of the systems containing one fewer/more particle. Second, the structure of the equations for the selfenergy allows for much more straight-forward and natural approximations, which are obscured in the density-matrix based approaches [30]. The technique of nonequilibrium Green functions has been invented more than 50 years ago by *L.V. Keldysh*, *G. Baym*, and *L.P. Kadanoff* [31, 32] as a systematic *ab-initio* approach to time-dependent processes in interacting quantum-systems. Since their inception, Green functions have been successfully applied in many domains of physics [10,

33–44].

Over the years, several important classes of selfenergy approximations—the selfenergy being the main ingredient in the equations of motion for the Green function—have been developed, most prominently the *GW* approximation by *L. Hedin* applied in many contexts [45–49] and the particle–particle *T*-matrix approximation [50–52] as well as the second-order Born approximation [7, 37, 40, 53]. Though all these approximations have their range of applicability, in recent years, especially since the description of inhomogeneous systems is increasingly feasible, it has become obvious that there exist system configurations and modes of excitations where none of the common approximations yields acceptable results [51, 54–56]. This has led several researchers to explore methods which go beyond the standard approximations [47, 57, 58]. This thesis follows this path further by extending the perturbative approximations to third-order in the interaction going beyond the most common second-order (Born) approximation. Further, the possibilities of the combination of the particle–particle as well as the particle–hole *T*-matrix and *GW* to the fluctuating exchange approximation is explored both theoretically and numerically. At the same time, this thesis aims at deducing all approximations in the most general basis representation starting from the common basis of the five coupled Hedin equations extending the previous work done in a diagonal basis set for the particle–particle *T*-matrix and the *GW*-approximation by *R. v. Leeuwen* [52] and *N. Schlünzen* on the particle–particle *T*-matrix in general basis representation [59].

1.3 Outline

The structure of this work is as follows.

Chapter 2 develops the theoretical framework of nonequilibrium Green functions starting from the exact description of indistinguishable particles with the language of the Second Quantization by the definition of canonical creation and annihilation operators acting on the so-called Fock space. Once, a suitable one-particle basis of the Fock space is chosen, which is detailed in Section 2.2, all single-particle and many-particle operators, including the Hamiltonian, can be described in terms of matrix and tensor elements, i.e., multiply indexed quantities. The special case of the Hubbard basis, which also underlies the numerical results, presented in Chapter 3, is detailed in Section 2.3. Ensuing, the equations of motion for the single-particle Green

function and the single-particle selfenergy—a functional of the Green function, which incorporates all many-body effects—are developed. They involve two time-arguments which are defined on a complex contour accompanied by a special calculus which is detailed Section 2.4 and 2.5. In Section 2.6, a set of five coupled equations for the Green function, the selfenergy and three additional dynamical quantities, the polarization, the screened interaction and the so-called (screened or bare) vertex function are introduced, the closed solution of which yields the exact Green function. This set of equations goes back to *Lars Hedin* who developed the well-known *GW* approximation starting from it.

Section 2.7, which is the main part of Chapter 2, deals with strategies for the approximate determination of the selfenergy, which render the process suitable for numerical calculations. Here, the two classes of perturbative and non-perturbative approximations are presented on equal footing and in the most general basis description. The perturbative approaches, described in Section 2.7.1 cover the expansion of all relevant quantities in terms of the order of the interaction starting from first order up to third order. The non-perturbative methods rely on a resummation of certain classes of the infinite series constituting the selfenergy. Here, in Section 2.7.2, the particle–particle and particle–hole *T*-matrix as well as the *GW* and the fluctuating exchange approximation are derived.

Ensuing, in Section 2.8, the generalized Kadanoff–Baym ansatz, an approximation to the time-structure of the equations of motion for the Green function, is described, which improves the numerical performance and at the same time cures artifacts of self-consistent calculations, such as correlation induced damping, which is analyzed in Section 3.3. Concluding Chapter 2, the generation of the interacting ground-state via the method of adiabatic switch-on of the interaction, is detailed.

In Chapter 3, the presented selfenergy approximation techniques are tested for small fermionic Hubbard clusters, where exact reference calculations are available. After introductory notes on the time-propagation algorithm in Section 3.1, the performance of the different approximations for the energy and spectral properties of the interacting ground-state is analyzed in Section 3.2. In the ensuing Section 3.3, the description of the time-dependent response of the systems to a sudden and strong potential quench is compared. A special focus lies on the occurrence of the approximation artifact of correlation-induced damping and how it can be circumvented by the use of the generalized Kadanoff–Baym ansatz in combination with a suitable

selfenergy approximation. Finally, in Chapter 4, conclusions are drawn and the overall performance of the different selfenergy approximations is evaluated.

2 Green function theory and approximation strategies

This chapter gives an overview about the theoretical foundation of the NEGF method and focuses on the interconnection between and classification of common approximate schemes. It provides, probably for the first time, a comprehensive overview of the relevant equations in a fully general basis representation¹. From this, the common cases of a diagonal basis like the spatial basis and the Hubbard basis for fermions and bosons are deduced. Alongside the development of the theory, the numerical scaling of the different approximation techniques will be detailed to enable a suitable choice with respect to the achievable simulation duration and basis size. In Section 2.1, the representation of states of indistinguishable quantum particles such as electrons in the so-called *Fock space* is discussed. The underlying notion of the *Second Quantization* allows for a suitable description of the dynamics for these particles in terms of canonical operators which perform the creation and annihilation in a chosen basis comprised of single-particle orbitals. Section 2.2 explores several possible sets of basis functions and their numerical suitability for different classes of systems. As a special case, the description of bosons and fermions in the basis set of the Hubbard model [60] is described. For general time-dependent problems, it is suitable to work on a complex time-contour, which is covered in Section 2.4. A central quantity on the time-contour, the single-particle Green function, which gives access to all single-particle observables, the single-particle spectrum and some two-particle quantities, is defined in Section 2.5. The equations of motion for the Green functions are a set of integro-differential equations, which are mutually coupled, constituting a hierarchy between Green functions of different particle number, the *Martin–Schwinger hierarchy* (MSH). A suitable reformulation of the MSH has been given in [61], where a set of five contour

¹For the particle–particle T -matrix approximation, a thorough derivation for a general basis set is presented in [59].

quantities is introduced, which also obey coupled equations of motion, the solutions of which yield the same Green function as the solution of the MSH. The representations of these equations in a general basis set are given in Section 2.6. Since the exact solution of either set of equations is numerically impossible for most realistic systems, approximation techniques have to be employed. The approaches presented in this work are based on the common building block of the so-called *selfenergy* the purpose of which is to capture all relevant many-body effects. How it can be approximately determined using both perturbative and non-perturbative methods is detailed in the main part of this part in Section 2.7. In the ensuing Section 2.8, an approximation to the time-structure of the equations of motion for the Green function, the Generalized Kadanoff–Baym Ansatz [62], is described. In the concluding Section 2.9, strategies for the generation of the correlated initial state are presented.

2.1 Dynamics of indistinguishable quantum particles in Second Quantization

The physical properties of all quantum particles are determined by their nature as excitations of an underlying field. These fields are quantized, i.e., they can only accommodate an integral number of elementary excitations, which are identified with the quantum particles. If only a single particle is excited, its state can be described by a wavefunction $|\Psi\rangle$ defined on a single-particle Hilbert space \mathcal{H} over the field of complex numbers \mathbb{C} , which is assumed to be of finite dimension². For excitations of more than one particle, the indistinguishability of quantum particles has to be taken into account properly. Experimentally, it has been found that quantum particles either carry *bosonic* or *fermionic* statistics, i.e., obey either the Fermi–Dirac [63, 64] or the Bose–Einstein [65] distribution. The group of fermions, which all have half-integer spin, contains the quarks and leptons, such as the electron, whereas phonons, W - and Z gauge-particles, gluons and the recently experimentally verified Higgs particle are bosons. Particles composed of elementary fermions or bosons can be of either bosonic (mesons, pions, kaons) or fermionic (baryons [11], nucleons) type, depending on the number of fermions. In the theoretical description, the spin

²In practice, this does not constitute a restriction, since the Hilbert space is either already of finite dimension or has to be approximated as such anyway to make a numerical treatment possible.

statistics amounts to the many-body wavefunction being totally symmetric for bosons or totally antisymmetric for fermions with respect to interchange of two particles. How these statistics can conveniently be built into the description of the many-body system, is detailed in the following section.

2.1.1 Canonical operators

To be able to treat states of varying particle number on an equal footing, it is convenient to define the so-called Fock space $\mathcal{F}_\sigma^{\mathcal{H}}$ induced by the single-particle Hilbert space \mathcal{H} as the (completion of the) direct sum of (anti-)symmetrized n -fold tensor products of \mathcal{H} ,

$$\mathcal{F}_\sigma^{\mathcal{H}} = \overline{\bigoplus_{n=0}^{\infty} S_\sigma \mathcal{H}^{\otimes n}} = \overline{\mathbb{C} \oplus \mathcal{H} \oplus S_\sigma(\mathcal{H} \otimes \mathcal{H}) \oplus \dots} \quad , \quad (2.1)$$

with

$$\mathcal{H}^{\otimes n} = \overbrace{\mathcal{H} \otimes \mathcal{H} \otimes \dots \otimes \mathcal{H}}^{n \text{ times}} \quad \text{for all } n \in \mathbb{N}_0. \quad (2.2)$$

The operator S_σ symmetrizes or anti-symmetrizes tensors for bosonic ($\sigma = -$) or fermionic ($\sigma = +$) particles. To define its action, it is suitable to fix a single-particle orbital basis of \mathcal{H} ,

$$\mathcal{B}^{\text{sp}} = \{|b_i\rangle, i \in I\}, \quad (2.3)$$

for an index set I of cardinality $\dim_{\mathcal{H}}$. With this, for every $n \in \mathbb{N}_0$ and basis elements $|b_1\rangle, \dots, |b_n\rangle \in \mathcal{B}^{\text{sp}}$, the action of S_σ on the standard tensor product is given by

$$\begin{aligned} S_- \left(|b_1\rangle \otimes \dots \otimes |b_n\rangle \right) \\ = \frac{1}{\sqrt{n!}} \sum_{s \in \text{Sym}_n} |b_{s(1)}\rangle \otimes \dots \otimes |b_{s(n)}\rangle =: |b_1\rangle \circ \dots \circ |b_n\rangle \end{aligned} \quad (2.4)$$

and

$$\begin{aligned}
 S_+ \left(|b_1\rangle \otimes \dots \otimes |b_n\rangle \right) & \quad (2.5) \\
 = \frac{1}{\sqrt{n!}} \sum_{s \in \text{Sym}_n} \text{sign}(s) |b_{s(1)}\rangle \otimes \dots \otimes |b_{s(n)}\rangle & =: |b_1\rangle \wedge \dots \wedge |b_n\rangle,
 \end{aligned}$$

for bosons and fermions, respectively. Note that it is sufficient to define the (anti-)symmetrization operator only for basis elements, since it is linear. For example, a general fermionic anti-symmetrized state $|\Psi_2^+\rangle$ on the 2-fold tensor product $\mathcal{H} \otimes \mathcal{H}$ is of the form

$$|\Psi_2^+\rangle = \sum_{i < j \in I} c_{ij} |b_i\rangle \wedge |b_j\rangle \quad \text{for } |b_i\rangle, |b_j\rangle \in \mathcal{B}^{\text{sp}}, \quad (2.6)$$

for $c_{ij} \in \mathbb{C}$. Here, the antisymmetric tensor product $|b_i\rangle \wedge |b_j\rangle$ is given in terms of the standard tensor product as

$$|b_i\rangle \wedge |b_j\rangle = \frac{1}{2} \left(|b_i\rangle \otimes |b_j\rangle - |b_j\rangle \otimes |b_i\rangle \right). \quad (2.7)$$

Note that $|b_i\rangle \wedge |b_i\rangle = 0$, which reflects that, due to the Pauli exclusion principle, no two fermions can occupy the same state. With this, a general state in the Fock space $\mathcal{F}_\sigma^{\mathcal{H}}$, a *Fock state* $|\Psi^\sigma\rangle$, which is a superposition of states with a different number of particles, can be written as

$$|\Psi^\sigma\rangle = c_0 |0\rangle \oplus \sum_{i \in I} c_i |b_i\rangle \oplus \sum_{i < j \in I} c_{ij} |b_i\rangle \otimes_\sigma |b_j\rangle \oplus \dots, \quad (2.8)$$

for $c_0, c_i, c_{ij} \in \mathbb{C}$, where the short-hand notation

$$\otimes_\sigma = \begin{cases} \circ & \text{for bosons,} \\ \wedge & \text{for fermions,} \end{cases} \quad (2.9)$$

has been introduced. The first state, $|0\rangle$, is the vacuum state, which is the state of zero physical particles and of the lowest possible energy E^{vac} —in the context of

this thesis, $E^{\text{vac}} = 0$ is assumed³. With the concept of Fock states that are suitable to describe systems with a varying particle number, it is most natural to define operators that create $(\hat{c}^\dagger[|b_i\rangle] =: \hat{c}_i^\dagger)$ or remove $(\hat{c}[|b_i\rangle] =: \hat{c}_i)$ a particle in a given single-particle orbital $|b_i\rangle$. To characterize their action, it is sufficient to define the action on all (anti-)symmetrized n -particle subspaces of $\mathcal{F}_\sigma^{\mathcal{H}}$ defined in a similar fashion to Eq. (2.2),

$$\mathcal{H}^{\otimes_\sigma n} = \overbrace{\mathcal{H} \otimes_\sigma \mathcal{H} \otimes_\sigma \dots \otimes_\sigma \mathcal{H}}^{\text{n times}}, \quad (2.10)$$

as

$$\begin{aligned} & \hat{c}_i^\dagger \left(\overbrace{|b_1\rangle \otimes_\sigma \dots \otimes_\sigma |b_n\rangle}^{\in \mathcal{H}^{\otimes_\sigma n}} \right) \\ &= \overbrace{|b_i\rangle \otimes_\sigma |b_1\rangle \otimes_\sigma \dots \otimes_\sigma |b_n\rangle}^{\in \mathcal{H}^{\otimes_{n+1}}} \end{aligned} \quad (2.11)$$

and

$$\begin{aligned} & \hat{c}_i \left(\overbrace{|b_1\rangle \otimes_\sigma \dots \otimes_\sigma |b_n\rangle}^{\in \mathcal{H}^{\otimes_\sigma n}} \right) \\ &= \sum_{k \in I} \overbrace{(-\sigma)^k \langle b_i | b_k \rangle |b_1\rangle \otimes_\sigma \dots \otimes_\sigma \cancel{|b_k\rangle} \otimes_\sigma \dots \otimes_\sigma |b_n\rangle}^{\in \mathcal{H}^{\otimes_{n-1}}}. \end{aligned} \quad (2.12)$$

With these equations, the (anti-)commutator between the creation operators and annihilation operators as well as between one creation and one annihilation operator for fermions (bosons) is easily worked out,

$$\left[\hat{c}_i^\dagger, \hat{c}_j^\dagger \right]_\pm = 0, \quad \left[\hat{c}_i, \hat{c}_j \right]_\pm = 0, \quad \left[\hat{c}_i, \hat{c}_j^\dagger \right]_\pm = \langle i | j \rangle \mathbf{1}. \quad (2.13)$$

³In quantum chromodynamics and quantum electrodynamics, the lowest energy state may not have zero energy and allow for quantum fluctuations [66].

The creation and annihilation operators form a basis for all operators acting on the $\mathcal{F}_\sigma^{\mathcal{H}}$. For instance, general single-particle and two-particle operators $\hat{O}^{(1)}$, $\hat{O}^{(2)}$ are given as linear superpositions⁴

$$\hat{O}^{(1)} = \sum_{mn} o_{mn}^{(1)} \hat{c}_m^\dagger \hat{c}_n, \quad (2.14)$$

$$\hat{O}^{(2)} = \sum_{mnpq} o_{mnpq}^{(2)} \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q. \quad (2.15)$$

As a special case, the Hamiltonian, which carries the specific geometries of the studied systems as well as any external (time-dependent) potentials and forces driving the dynamics transforms to

$$\hat{H}(t) = \underbrace{\sum_{mn} h_{mn} \hat{c}_m^\dagger \hat{c}_n}_{\hat{H}^0} + \frac{1}{2} \underbrace{\sum_{mnpq} w_{mnpq} \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q}_{\hat{W}} + \underbrace{\sum_{mn} f_{mn}(t) \hat{c}_m^\dagger \hat{c}_n}_{\hat{F}(t)}, \quad (2.16)$$

containing the single-particle part \hat{H}^0 , the interaction \hat{W} and the time-dependent single-particle excitation part $\hat{F}(t)$. Since all quantities discussed in this section are formulated in terms of the single-particle basis \mathcal{B}^{sp} , its suitable choice is vital for the numerical implementation to achieve the best possible performance. A strategy for the selection of a set of basis functions is detailed in the next section.

2.2 Choice of the one-particle basis

Selecting a single-particle basis constitutes the first step in the process of the theoretical modeling of a system. With the basis, elements $|\Psi\rangle$ of the single-particle Hilbert space \mathcal{H} can be expanded as

$$|\Psi\rangle = \sum_{i \in I} b_i |b_i\rangle, \quad (2.17)$$

where I is an index set of cardinality $\dim_{\mathcal{H}}$. For Hilbert spaces of infinite dimension, I has to be substituted by a finite set I' to make a numerical treatment possible, which renders Eq. (2.17) only approximate valid. For the formulation of the Hamiltonian

⁴From now on, if not stated otherwise, all sums run over the complete basis set.

according to Eq. (2.16), the matrix elements h_{km} , w_{klmn} , $f_{km}(t)$ have to be specified. Once they are given in the natural basis of the studied system, they can be transformed into another single-particle basis $\mathcal{C}^{\text{SP}} = \{|c_j\rangle, j \in J\}$ by

$$h_{km}^{\mathcal{C}} = \sum_{r=1}^{\dim_{\mathcal{H}}} \sum_{s=1}^{\dim_{\mathcal{H}}} b_{rk}^* h_{rs}^{\mathcal{B}} b_{sm}, \quad (2.18)$$

with the expansion of the new basis functions $|c_i\rangle$ in terms of the old $|b_i\rangle$ as

$$\langle c_i | = \sum_{r=1}^{\dim_{\mathcal{H}}} b_{ri}^* \langle b_r |, \quad (2.19)$$

$$|c_i\rangle = \sum_{s=1}^{\dim_{\mathcal{H}}} |b_s\rangle b_{si}, \quad (2.20)$$

for the transformation matrix elements

$$b_{si} = \langle b_s | c_i \rangle, \quad b_{ri}^* = \langle b_r | c_i \rangle^*. \quad (2.21)$$

With these transformations, the basis can be chosen to suit the numerical needs. To this end, two criteria can be formulated which characterize how numerically tractable a set of basis functions is. First, it should consist of as few basis functions as possible to achieve the accuracy demanded, i.e., it describes single-particle orbitals that are as close as possible to the true orbitals occupied by the particles. To work out the other criterion, one notices that, according to Eq. (2.16), the interaction—a central quantity in any exact treatment as well as the approximations discussed in Section 2.7—is represented by a fourth order tensor w_{klmn} in a general basis. This structure is numerically prohibitive since it involves at least a scaling of $\mathcal{O}(N_b^4)$, where N_b is the dimension of the basis set. Fortunately, the interaction tensor can be brought into a diagonal representation, where it is characterized by a second-order tensor, i.e., is of the structure

$$w_{klmn} = \delta_{kn} \delta_{lm} w_{kl}. \quad (2.22)$$

In practice, this diagonalization can be achieved by choosing a quadrature rule for the integrals involved in the computation of the interaction matrix elements and construction of a (finite-element) discrete variable representation upon it [21, 67, 68]. For details, the reader is referred to [20], where various aspects of different choices of quadratures and their implementation are discussed. Accordingly, the second criterion is that the basis functions are chosen such that the interaction matrix elements are (approximately) diagonal in the sense of Eq. (2.22). Unfortunately, both criteria are mostly orthogonal and the user has to chose between them. While physically motivated basis sets achieve a good representation with only a small number of basis functions, they entail a dense fourth-order tensorial structure of the interaction matrix elements. In contrast, discrete variable representation basis sets provide them in diagonal form, but the basis functions are “general purpose” and the worse representation of physical states requires their number to be comparably large. As a rule of thumb, it can be stated that for small systems, which require only few basis functions, physical basis sets are preferable while for large systems, for instance in the description of photo emission experiments [19, 21, 69], a grid-based approach is mostly favorable. In both cases, a close look at the structure of the equations at hand provides a more thorough base for the decision. As an example, looking ahead to Eqs. (2.167) and (2.169) vs. Eqs. (2.141) and (2.150), the index structure of the selfenergy—the central quantity in Green function based calculations—for example, in a particular approximation, looks like (omitting time arguments and scalar factors)

$$\Sigma_{ij}^{(2),\text{diagonal}} = \sum_{np} G_{in} w_{ip} G_{np} G_{pj} w_{nj} \quad (2.23)$$

$$\pm \sum_{pr} G_{ij} w_{ip} G_{rp} G_{pr} w_{rj},$$

$$\Sigma_{ij}^{(2)} = \sum_{mnpqrs} G_{mn} w_{ipqm} G_{sp} G_{qr} (w_{nrjs} \pm w_{rnjs}), \quad (2.24)$$

in a diagonal basis vs. general basis representation. At first glance, the diagonal case of Eq. (2.23) suggests a scaling of $\mathcal{O}(N_b^4)$ stemming from the two external indices i, j and the summation over the two internal indices while in the case of full interaction, according to Eq. (2.24), the summation over six internal indices

(m, n, p, q, r, s) prompts a scaling of $\mathcal{O}(N_b^8)$, which would strongly favor the former over the latter. A quick reordering, though, lets one rewrite Eqs. (2.23) and (2.24) as

$$\Sigma_{ij}^{(2),\text{diagonal}} = \sum_n G_{in} w_{nj} \sum_p w_{ip} G_{np} G_{pj} \quad (2.25)$$

$$\pm G_{ij} \sum_p w_{ip} \sum_r G_{pr} G_{rp} w_{rj},$$

$$\Sigma_{ij}^{(2)} = \sum_{mpq} w_{ipqm} \sum_s G_{sp} \sum_r G_{qr} \sum_n G_{mn} (w_{nrjs} \pm w_{rnjs}). \quad (2.26)$$

This elucidates that, for diagonal interaction, $\Sigma_{ij}^{(2),\text{diagonal}}$ indeed scales as $\mathcal{O}(N_b^4) + \mathcal{O}(N_b^3) = \mathcal{O}(N_b^4)$, whereas, $\Sigma_{ij}^{(2)}$ scales as $\mathcal{O}(N_b^5) + \mathcal{O}(N_b^5) + \mathcal{O}(N_b^5) + \mathcal{O}(N_b^5) = \mathcal{O}(N_b^5)$, in contrast⁵. Thus, the preferable basis choice depends strongly on the respective basis sizes needed.

2.3 The Hubbard model

Since it plays an important role underlying the applications in Chapter 3, the special case of the Hubbard basis and the associated Hubbard model is shortly discussed here. The Hubbard model has been introduced by *John Hubbard*, a British physicist, in 1963 [60] to describe the physics—especially the transition between conducting and insulating behavior—of electrons in narrow energy-bands of solid state systems such as transition metal oxides. At the heart of the Hubbard model is the observation that, in narrow *d*- and *f*-bands, the electrons are mostly located at the nuclei—where they interact—and only rarely move between different positions on the lattice. Therefore, Hubbard proposed to describe these systems in terms of “sites” between which the electrons “hop” with a given amplitude J . At each site, which, in the model, contains one orbital for spin-up and one orbital for spin-down orientation, the electrons experience a repulsion by electrons in the other orbital of strength U . Accordingly, the Hubbard model can be described by the generic Hamiltonian, cf. Eq. (2.16), with

⁵As one notices, the ordering of the terms in Eqs. (2.25) and (2.26) is not unique but there exists no ordering which results in a better scaling.

matrix elements (written in the spin-orbitals $|i\alpha\rangle$),

$$h_{i\alpha j\beta} = -J\delta_{\langle ij\rangle}\delta_{\alpha\beta} - \mu\delta_{ij}\delta_{\alpha\beta}\hat{c}_{i\alpha}^\dagger\hat{c}_{i\alpha}, \quad (2.27)$$

$$w_{i\alpha j\beta k\gamma l\delta} = U\delta_{il}\delta_{\alpha\delta}\delta_{jk}\delta_{\beta\gamma}\delta_{ij}, \quad (2.28)$$

$$f_{i\alpha j\beta}(t) = \delta_{ij}\delta_{\alpha\beta}f_{i\alpha}(t), \quad (2.29)$$

where $\delta_{\langle ij\rangle} = 1$, exactly if the sites i, j are nearest neighbors. The term

$$-\mu\delta_{ij}\delta_{\alpha\beta}\hat{c}_{i\alpha}^\dagger\hat{c}_{i\alpha} \quad (2.30)$$

describes the chemical energy induced by a chemical potential μ . The time-dependent excitation matrices $f_{i\alpha j\beta}(t)$ for all processes considered in this work are both, on-site (δ_{ij}) and spin-conserving ($\delta_{\alpha\beta}$). Inserting Eqs. (2.27), (2.28) and (2.29) into the general form of Eq. (2.16), one arrives at

$$\begin{aligned} \hat{H}(t) &= -J \sum_{men\zeta} \delta_{\langle mn\rangle} \delta_{\epsilon\zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{n\zeta} + \frac{U}{2} \sum_{men\zeta p\eta q\theta} \delta_{mq} \delta_{\epsilon\theta} \delta_{np} \delta_{\zeta\eta} \delta_{mn} \hat{c}_{m\epsilon}^\dagger \hat{c}_{n\zeta}^\dagger \hat{c}_{p\eta} \hat{c}_{q\theta} \\ &\quad + \sum_{men\zeta} \delta_{mn} \delta_{\epsilon\zeta} f_{men\zeta}(t) \hat{c}_{m\epsilon}^\dagger \hat{c}_{n\zeta} - \mu \sum_{m\epsilon} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\epsilon} \\ &= -J \sum_{\langle m,n\rangle} \sum_{\epsilon} \hat{c}_{m\epsilon}^\dagger \hat{c}_{n\epsilon} + \frac{U}{2} \sum_m \sum_{\epsilon\zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\zeta}^\dagger \hat{c}_{m\zeta} \hat{c}_{m\epsilon} \\ &\quad + \sum_{m\epsilon} f_{m\epsilon}(t) \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\epsilon} - \mu \sum_{m\epsilon} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\epsilon}. \end{aligned} \quad (2.31)$$

With the canonical (anti-)commutator relations, cf. Eq. (2.13), for bosons, the interaction term can be rewritten as

$$\begin{aligned}
 \hat{W}_{\text{bosons}}^{\text{Hubbard}} &= \frac{U}{2} \sum_m \sum_{\epsilon\zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\zeta}^\dagger \hat{c}_{m\zeta} \hat{c}_{m\epsilon} = \frac{U}{2} \sum_m \sum_{\epsilon\zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\zeta}^\dagger \hat{c}_{m\epsilon} \hat{c}_{m\zeta} \\
 &= \frac{U}{2} \sum_m \sum_{\epsilon\zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\epsilon} \hat{c}_{m\zeta}^\dagger \hat{c}_{m\zeta} - \frac{U}{2} \sum_m \sum_{\epsilon} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\epsilon} \\
 &=: \frac{U}{2} \sum_m \sum_{\epsilon\zeta} \hat{n}_{m\epsilon} \hat{n}_{m\zeta} - \frac{U}{2} \sum_m \sum_{\epsilon} \hat{n}_{m\epsilon} \\
 &= \frac{U}{2} \sum_m \sum_{\epsilon \neq \zeta} \hat{n}_{m\epsilon} \hat{n}_{m\zeta} + \frac{U}{2} \sum_m \sum_{\epsilon} \hat{n}_{m\epsilon} (\hat{n}_{m\epsilon} - 1). \tag{2.32}
 \end{aligned}$$

The special case of spin-0 bosons results in the Bose–Hubbard interaction,

$$\hat{W}_{\text{bosons},0}^{\text{Hubbard}} = \frac{U}{2} \sum_m \hat{n}_m (\hat{n}_m - 1), \tag{2.33}$$

and the corresponding Bose–Hubbard Hamiltonian (without time-dependent excitation),

$$\hat{H}_{\text{spin-0}}^{\text{Bose-Hubbard}} = -J \sum_{\langle m,n \rangle} \hat{c}_m^\dagger \hat{c}_n + \frac{U}{2} \sum_m \hat{n}_m (\hat{n}_m - 1) - \mu \sum_m \hat{n}_m. \tag{2.34}$$

For fermions, due to the Pauli exclusion principle, Eq. (2.28) can be rewritten as

$$w_{i\alpha j\beta k\gamma l\delta} = U \delta_{il} \delta_{\alpha\delta} \delta_{jk} \delta_{\beta\gamma} \delta_{ij} \bar{\delta}_{\alpha\beta}, \tag{2.35}$$

with $\bar{\delta}_{\alpha\beta} = 1 - \delta_{\alpha\beta}$. Consequently, the interaction part \hat{W} of the Hamiltonian becomes

$$\begin{aligned}
 \hat{W}_{\text{fermions}}^{\text{Hubbard}} &= \frac{U}{2} \sum_m \sum_{\epsilon \neq \zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\zeta}^\dagger \hat{c}_{m\zeta} \hat{c}_{m\epsilon} = -\frac{U}{2} \sum_m \sum_{\epsilon \neq \zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\zeta}^\dagger \hat{c}_{m\epsilon} \hat{c}_{m\zeta} \\
 &= \frac{U}{2} \sum_m \sum_{\epsilon \neq \zeta} \hat{c}_{m\epsilon}^\dagger \hat{c}_{m\epsilon} \hat{c}_{m\zeta}^\dagger \hat{c}_{m\zeta} = \frac{U}{2} \sum_m \sum_{\epsilon \neq \zeta} \hat{n}_{m\epsilon} \hat{n}_{m\zeta}. \tag{2.36}
 \end{aligned}$$

For the special case of spin- $\frac{1}{2}$ fermions, this expression simplifies to

$$\hat{W}_{\text{fermions},1/2}^{\text{Hubbard}} = \frac{U}{2} \sum_m (\hat{n}_{m\uparrow} \hat{n}_{m\downarrow} + \hat{n}_{m\downarrow} \hat{n}_{m\uparrow}) = U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow} \quad (2.37)$$

and the (Fermi-)Hubbard Hamiltonian (again without time-dependent excitation) is given by

$$\begin{aligned} \hat{H}_{\text{spin-1/2}}^{\text{Fermi-Hubbard}} & \quad (2.38) \\ & = -J \sum_{\langle m,n \rangle} \sum_{\epsilon \in \{\uparrow, \downarrow\}} \hat{c}_{m\epsilon}^\dagger \hat{c}_{n\epsilon} + U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow} - \mu \sum_m (\hat{n}_{m\uparrow} + \hat{n}_{m\downarrow}). \end{aligned}$$

One notices that the Hubbard interaction $w_{i\alpha j\beta k\gamma l\delta}$ is highly diagonal, which is very advantageous to the numerical treatment, a property which has contributed greatly to its recurring popularity in computational physics in the last decade [17, 29, 70–74]. Accordingly, for the example of the second-order selfenergy, which will be treated in full detail in Section 2.7, the expression in the Hubbard basis reads, cf. Eq. (2.214),

$$\begin{aligned} \Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{(2),2,0,\text{Hubbard,fermions},1/2}(z_1, z_2) & \quad (2.39) \\ & = \pm (\text{i}\hbar)^2 G_{i\downarrow(\uparrow)j\downarrow(\uparrow)}(z_1, z_2) U(z_1) G_{i\uparrow(\downarrow)j\uparrow(\downarrow)}(z_1, z_2) G_{j\uparrow(\downarrow)i\uparrow(\downarrow)}(z_2, z_1) U(z_2). \end{aligned}$$

This expression only scales as $\mathcal{O}(N_b^2)$, since it involves no matrix multiplications, compared to the case of a general basis with $\mathcal{O}(N_b^5)$ and of $\mathcal{O}(N_b^4)$ in a diagonal basis.

2.4 Time-dependence of observables and the time-contour

The purpose of the formalism of the Second Quantization, introduced in the last section, is to provide a suitable framework for the description of time-dependent processes in quantum systems. Here, one is mostly interested in the expectation values of operators of the form of Eqs. (2.14) and (2.15) at any given time t . With the time-dependent many-particle wavefunction, $|\Psi(t)\rangle$, solution of the time-dependent

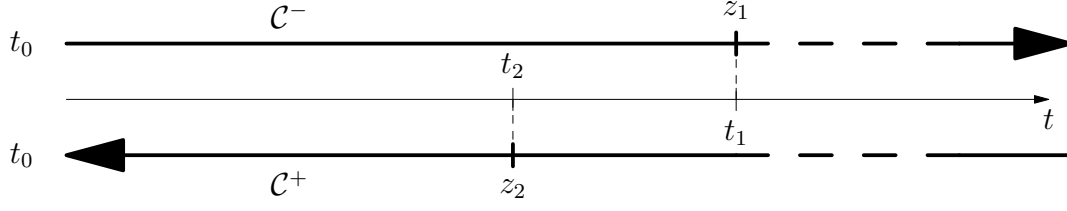


Figure 2.1: Schwinger–Keldysh contour \mathcal{C} . The forward-branch \mathcal{C}^- extends from the initial time t_0 to the current time t , bends and leads back to t_0 along the backward \mathcal{C}^+ -branch. Note that the projections of the contour times $z_1 < z_2$ on the real axis obey the inverse relationship $t_1 > t_2$.

Schrödinger equation, the expectation value can be computed as

$$\begin{aligned} O(t) &= \langle \Psi(t) | \hat{O}(t) | \Psi(t) \rangle \\ &= \left\langle \Psi_0 \left| \hat{\mathcal{T}}_a \left\{ \exp \left(\frac{1}{i\hbar} \int_t^{t_0} d\bar{t} \hat{H}(\bar{t}) \right) \right\} \hat{O}(t) \hat{\mathcal{T}}_c \left\{ \exp \left(-\frac{1}{i\hbar} \int_t^{t_0} d\bar{t} \hat{H}(\bar{t}) \right) \right\} \right| \Psi_0 \right\rangle, \end{aligned} \quad (2.40)$$

where the operators $\hat{\mathcal{T}}_c$ ($\hat{\mathcal{T}}_a$) are the (anti)-chronological time-ordering superoperators, which rearrange the operators acted on such that the latest (earliest) times are moved to the left-hand side as a consequence of causality. A more concise formulation can be achieved by introducing an oriented contour \mathcal{C} which starts from t_0 extends to the turning point t and then reaches back to t_0 ,

$$\mathcal{C} = \underbrace{(t_0, t)}_{\mathcal{C}^-} \oplus \underbrace{(t, t_0)}_{\mathcal{C}^+}, \quad (2.41)$$

with a forward branch \mathcal{C}^- and a backward branch \mathcal{C}^+ , depicted in Fig. 2.1. Henceforth, a general time on the contour \mathcal{C} will be denoted as z and z_{\pm} to refer to a time lying on one of the branches. Accordingly, operators \hat{O} can be extended to the contour having possibly different values on both branches,

$$\hat{O}(z) = \begin{cases} \hat{O}_-(z) & \text{if } z \in \mathcal{C}^- \\ \hat{O}_+(z) & \text{if } z \in \mathcal{C}^+ \end{cases}. \quad (2.42)$$

With this definition, one can define a contour time-ordering superoperator $\hat{\mathcal{T}}_{\mathcal{C}}$ which moves operators at earlier contour times to the left of operators at later contour times. As a consequence, its action agrees with that of $\hat{\mathcal{T}}_{\mathcal{C}}$ for all times $z_- \in \mathcal{C}^-$ and with that of $\hat{\mathcal{T}}_{\mathcal{a}}$ for all times $z_+ \in \mathcal{C}^+$. The integral transforms in a natural way to the contour by defining

$$\int_{z_1}^{z_2} d\bar{z} \hat{O}(\bar{z}) := \begin{cases} \int_{t_1}^{t_2} d\bar{t} \hat{O}_-(\bar{t}) & \text{if } z_1, z_2 \in \mathcal{C}^- \\ \int_{t_1}^t d\bar{t} \hat{O}_-(\bar{t}) + \int_t^{t_2} d\bar{t} \hat{O}_+(\bar{t}) & \text{if } z_1 \in \mathcal{C}^-, z_2 \in \mathcal{C}^+, \\ \int_{t_1}^{t_2} d\bar{t} \hat{O}_+(\bar{t}) & \text{if } z_1, z_2 \in \mathcal{C}^+ \end{cases}$$

assuming z_1 is later than z_2 . Using the contour integral, one can reformulate Eq. (2.40) for operators which have the same value on both branches, i.e., $\hat{O}_- = \hat{O}_+ =: \hat{O}_{\pm}$, as

$$\begin{aligned} O(t) & \quad (2.43) \\ &= \left\langle \Psi_0 \left| \hat{\mathcal{T}}_{\mathcal{C}} \left\{ \exp\left(\frac{1}{i\hbar} \int_{\mathcal{C}^+} d\bar{z} \hat{H}(\bar{z})\right) \hat{O}_{\pm}(t) \exp\left(\frac{1}{i\hbar} \int_{\mathcal{C}^-} d\bar{z} \hat{H}(\bar{z})\right) \right\} \right| \Psi_0 \right\rangle, \end{aligned}$$

which, taking into account the action $\hat{\mathcal{T}}_{\mathcal{C}}$, can be further simplified to

$$O(t) = \left\langle \Psi_0 \left| \hat{\mathcal{T}}_{\mathcal{C}} \left\{ \exp\left(\frac{1}{i\hbar} \int_{\mathcal{C}} d\bar{z} \hat{H}(\bar{z})\right) \hat{O}_{\pm}(t) \right\} \right| \Psi_0 \right\rangle. \quad (2.44)$$

On both branches, the contour Hamiltonian $\hat{H}(\bar{z})$ is set equal to its definition in Eq. (2.16) for the corresponding real-time argument. An undesirable feature of the introduced contour is that it seemingly depends on the value of t . This can be remedied by extending the contour to $t \rightarrow \infty$, which leaves all expressions, in particular Eq. (2.44), invariant, since the additional two integral parts cancel. The corresponding contour is depicted in Fig. 2.2. Finally, one notices that Eq. (2.44) is also true for all contour times z ,

$$O(z) = \left\langle \Psi_0 \left| \hat{\mathcal{T}}_{\mathcal{C}} \left\{ \exp\left(\frac{1}{i\hbar} \int_{\mathcal{C}} d\bar{z} \hat{H}(\bar{z})\right) \hat{O}(z) \right\} \right| \Psi_0 \right\rangle. \quad (2.45)$$

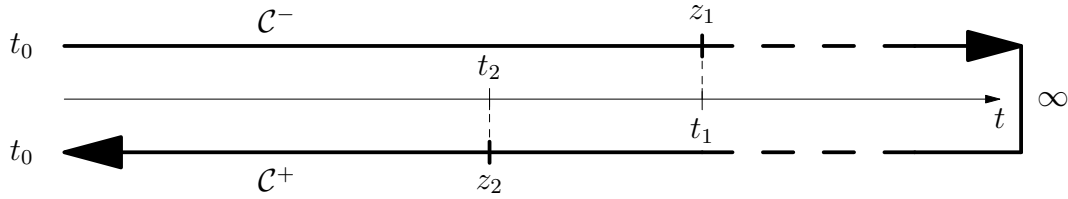


Figure 2.2: Schwinger–Keldysh contour \mathcal{C} extended to ∞ . The forward-branch \mathcal{C}^- spans from the initial time t_0 to ∞ , bends and leads back to t_0 along the backward \mathcal{C}^+ -branch.

2.5 Green functions

To compute time-dependent operator expectation values, there are two immediate choices at hand, following Eq. (2.40), either solving the first or the second line. The first option requires the solution of the equation of motion for the time-dependent wavefunction $|\Psi(t)\rangle$, which is the Schrödinger equation. This is the road taken by wavefunction-based methods like full configuration interaction [8, 75], multiconfigurational time-dependent Hartree–Fock [20, 76, 77], generalized active space configuration interaction [19, 78], exact diagonalization [17], coupled cluster methods [79] and density matrix renormalization group based approaches [22, 24, 80–83].

The other way is to follow the second line and to work with the (known) initial wavefunction $|\Psi_0\rangle$ (as will be shown in Section 2.9, actually, the knowledge of the ideal, i.e., non-interacting, initial state is sufficient) and develop an equation of motion for the term

$$\hat{\mathcal{T}}_{\mathcal{C}} \left\{ \exp \left(\frac{1}{i\hbar} \int_{\mathcal{C}} d\bar{z} \hat{H}(\bar{z}) \right) \hat{O}(z) \right\}, \quad (2.46)$$

according to Eqs. (2.44) and (2.45), respectively. Approaches relying on this method are, among others, time-dependent Hartree–Fock [84], reduced density matrix theory [30, 85], density functional theory [28, 29, 86, 87], dynamical mean-field theory (DMFT) [45, 46, 88, 89] and the method of Green functions [7, 37, 41, 44, 51, 58,

59, 70, 72–74, 90–94], which this thesis is based upon. In principle, both approaches are equivalent and yield the same results. The main difference is the set of available approximation techniques and, foremost, the numerical scaling behavior with respect to the maximal simulation time, particle number, basis size and interaction strength. The wavefunction-based methods, in general, can cope with huge basis sets with a number of basis functions, depending on the system at hand, ranging from thousands to millions and interaction strengths from weak to strong coupling. Additionally, they offer a linear scaling of the numerical effort with the simulation time. The trade-off is the exponential scaling of the numerical effort with the particle number rendering the simulation of systems with more than a few particles impossible [19, 78]. In contrast, the second group of methods, which relies on the equation of motion for the creation and annihilation operators, are not limited by the particle number. The scaling with the basis size is worse compared to the other group but still polynomial and the scaling with the total simulation time is at least quadratic for methods going beyond Hartree–Fock (which has a linear scaling). Apart from DMFT, which is also good for very strong interactions but can simulate only short time-spans, all methods of the second group, including Green functions, are mostly suited for small interaction strengths. In the following, the theory behind the Green functions method will be summarized. For a more in-detail derivation, see, e.g., [52, 68]. In the following section, the definition of the Green functions, their equations of motion and the determination of time-dependent observables from them will be discussed.

2.5.1 Definition and equations of motion

The direct computation of the time-dependent values of operators according to Eq. (2.45) involves the evaluation of the time-ordered exponential, which is impractical apart from very small basis sizes due to the dimensionality of the Hamiltonian. One strategy to bypass the direct evaluation of the exponential is to introduce the contour Heisenberg picture, which will be described in the following. Similar as for standard time, one can define the time-evolution operator $\hat{U}(z_1, z_2)$ on the contour,

$$\hat{U}(z_1, z_2) = \begin{cases} \hat{\mathcal{T}}_C \left\{ \exp \left(\frac{1}{i\hbar} \int_C d\bar{z} \hat{H}(\bar{z}) \right) \right\} & \text{if } z_1 \text{ later than } z_2, \\ \hat{\mathcal{T}}_C^a \left\{ \exp \left(\frac{1}{i\hbar} \int_C d\bar{z} \hat{H}(\bar{z}) \right) \right\} & \text{if } z_1 \text{ earlier than } z_2, \end{cases} \quad (2.47)$$

where, in the second line, the anti-chronological time-ordering operator $\hat{\mathcal{T}}_C^a$ has been introduced, which places operators with later contour times to the right. The contour time-evolution operator has the usual properties, i.e, fulfills

$$i\hbar \frac{d}{dz_1} \hat{U}(z_1, z_0) = \hat{H}(z_1) \hat{U}(z_1, z_0), \quad (2.48)$$

$$i\hbar \frac{d}{dz_1} \hat{U}(z_0, z_1) = -\hat{U}(z_0, z_1) \hat{H}(z_1). \quad (2.49)$$

With this, Eq. (2.45) can be cast into the form

$$O(z_1) = \langle \Psi_0 | \hat{U}(z_{0+}, z_{0-}) \hat{U}(z_{0-}, z_1) \hat{O}(z_1) \hat{U}(z_1, z_{0-}) | \Psi_0 \rangle, \quad (2.50)$$

where z_{0-} and z_{0+} represent the start (end) of the contour. Eq. (2.50) suggests to introduce the contour Heisenberg picture

$$\hat{O}_H(z_1) := \hat{U}(z_{0-}, z_1) \hat{O}(z_1) \hat{U}(z_1, z_{0-}), \quad (2.51)$$

with the equation of motion

$$i\hbar \frac{d}{dz_1} \hat{O}_H(z_1) = [\hat{O}_H(z_1), \hat{H}_H(z_1)]_- + \partial_{z_1} \hat{O}_H(z_1). \quad (2.52)$$

Using the commutator relations, cf. Eq. (2.13), the contour equations of motion for the canonical creation and annihilation operators for systems described by the Hamiltonian in Eq. (2.16) are readily found,

$$i\hbar \frac{d}{dz_1} \hat{c}_i(z_1) = \sum_n (h_{in}(z_1) + f_{in}(z_1)) \hat{c}_n(z_1) \quad (2.53)$$

$$+ \sum_{npq} w_{inpq}(z_1) \hat{c}_n^\dagger(z_1) \hat{c}_p(z_1) \hat{c}_q(z_1),$$

$$-i\hbar \frac{d}{dz_1} \hat{c}_i^\dagger(z_1) = \sum_m \hat{c}_m^\dagger(z_1) (h_{mi}(z_1) + f_{mi}(z_1)) \quad (2.54)$$

$$+ \sum_{mnp} \hat{c}_m^\dagger(z_1) \hat{c}_n^\dagger(z_1) \hat{c}_p(z_1) w_{mnp}(z_1),$$

where

$$\hat{c}(z_1) := \hat{c}_H(z_1), \quad \hat{c}^\dagger(z_1) := \hat{c}_H^\dagger(z_1). \quad (2.55)$$

These equations can be used to derive equations for operator correlators, such as already encountered in Eq. (2.45). For N operators, they are of the form

$$\hat{k}(z_1 \dots z_N) = \hat{\mathcal{T}}_C \left\{ \hat{O}_1(z_1) \dots \hat{O}_N(z_N) \right\}. \quad (2.56)$$

Remembering that any operator is a linear combination of the canonical operators, a special role is played by the correlators of these operators. From Eqs. (2.14) and (2.15), it is evident that especially those with the same number of creation and annihilation operators are of interest, since they give direct access to observables. Thus it is useful to define the correlator of N annihilation and creation operators, i.e., describing N particles, as

$$\begin{aligned} \hat{G}_{i_1 \dots i_N j_1 \dots j_N}^{(N)}(z_1 \dots z_N, z'_1 \dots z'_N) \\ := \frac{1}{(i\hbar)^N} \hat{\mathcal{T}}_C \left\{ \hat{c}_{i_1}(z_1) \dots \hat{c}_{i_N}(z_N) \hat{c}_{j_1}^\dagger(z'_1) \dots \hat{c}_{j_N}^\dagger(z'_N) \right\}, \end{aligned} \quad (2.57)$$

with $2N$ contour arguments. Using some contour calculus, not repeated here (for details see [52, 59]), and the contour Heisenberg equations, one can derive their equations of motion, which couple the N -particle correlator to the $(N-1)$ and $(N+1)$ particle correlator,

$$\begin{aligned} \sum_l \left[i\hbar \frac{d}{dz_k} \delta_{i_k l} - h_{i_k l}(z_k) \right] \hat{G}_{i_1 \dots l \dots i_N j_1 \dots j_N}^{(N)}(z_1 \dots z_N, z'_1 \dots z'_N) \\ = \pm i\hbar \sum_{lmn} \int_C d\bar{z} w_{i_k l m n}(z_k, \bar{z}) \hat{G}_{i_1 \dots m \dots i_N n j_1 \dots j_N m}^{(N+1)}(z_1 \dots z_N, \bar{z}, z'_1 \dots z'_N, \bar{z}) \\ + \sum_p (\pm)^{k+p} \delta_{i_k j_p} \delta_C(z_k, z'_p) \\ \hat{G}_{i_1 \dots \cancel{j_k} \dots i_N j_1 \dots \cancel{j_p} \dots j_N}^{(N-1)}(z_1 \dots \cancel{z_k} \dots z_N, z'_1 \dots \cancel{z'_p} \dots z'_N), \end{aligned} \quad (2.58)$$

$$\begin{aligned}
 & \sum_l \hat{G}_{i_1 \dots i_N j_1 \dots j_N}^{(N)}(z_1 \dots z_N, z'_1 \dots z'_N) \left[-i\hbar \frac{\overleftarrow{d}}{dz'_k} \delta_{lj_k} - h_{lj_k}(z'_k) \right] \quad (2.59) \\
 &= \pm i\hbar \sum_{lmn} \int_{\mathcal{C}} d\bar{z} \hat{G}_{i_1 \dots i_N n j_1 \dots j_N m}^{(N+1)}(z_1 \dots z_N, \bar{z}, z'_1 \dots z'_N, \bar{z}) w_{lmj_k n}(\bar{z}, z'_k) \\
 &+ \sum_p (\pm)^{k+p} \delta_{i_p j_k} \delta_{\mathcal{C}}(z_p, z'_k) \\
 &\hat{G}_{i_1 \dots \cancel{i_p} \dots i_N j_1 \dots \cancel{j_k} \dots j_N}^{(N-1)}(z_1 \dots \cancel{z_p} \dots z_N, z'_1 \dots \cancel{z'_k} \dots z'_N).
 \end{aligned}$$

The expectation value of the operator $\hat{G}^{(N)}$ in the initial state Ψ_0 yields the N -particle Green function $G^{(N)}$,

$$G^{(N)} = \left\langle \Psi_0 \left| \hat{G}^{(N)} \right| \Psi_0 \right\rangle. \quad (2.60)$$

The equations of motion for the Green functions are directly generated from the equations for the underlying operators by taking the expectation value, which corresponds to replacing all correlator operators in Eqs. (2.58) and (2.59) by the respective Green functions,

$$\hat{G}^{(N)} \longrightarrow G^{(N)}. \quad (2.61)$$

These mutually coupled equations form a hierarchy, the *Martin–Schwinger hierarchy* [95]. The solution of the full hierarchy gives access to all observables of the studied system and, by virtue of the connections to the $(N-1)$ -particle and $(N+1)$ -particle spaces, also spectral information is available. Thus, as a subset, the solution of the hierarchy incorporates the solution of the N -particle Schrödinger equation. Unfortunately and as expected, the effort for the full solution of the hierarchy also scales exponentially with the particle number. For the one-particle Green function $G^{(1)}$, which will be simply called the Green function G in the following, the equations

of motion, the *Keldysh–Kadanoff–Baym equations* (KBE), read

$$\begin{aligned} & \sum_l \left[i\hbar \frac{d}{dz_1} \delta_{il} - h_{il}(z_1) \right] G_{lj}(z_1, z_2) \\ &= \delta_c(z_1, z_2) \delta_{ij} \pm i\hbar \sum_{lmn} w_{ilmn}(z_1) G_{mnjl}^{(2)}(z_1, z_1, z_2, z_{1+}), \end{aligned} \quad (2.62)$$

$$\begin{aligned} & \sum_l G_{il}(z_1, z_2) \left[-i\hbar \frac{\overleftarrow{d}}{dz_2} \delta_{lj} - h_{lj}(z_2) \right] \\ &= \delta_c(z_1, z_2) \delta_{ij} \pm i\hbar \sum_{lmn} G_{inlm}^{(2)}(z_1, z_{2-}, z_2, z_2) w_{lmnj}(z_2). \end{aligned} \quad (2.63)$$

Note that the short-hand notation $z_{\pm} := z \pm \epsilon$ has been introduced here to facilitate the correct ordering of the operators under $\hat{\mathcal{T}}_c$. One notices that even the determination of the one-particle Green functions requires the solution of all other hierarchy equations as well, due to the coupling to the two-particle Green function (which, in turn couples to the three-particle Green function, and so on). If the knowledge of the single-particle Green function is sufficient for the physical problem at hand, it is suitable to introduce the so-called single-particle *selfenergy* Σ , which allows to (formally) decouple the time-evolution of the Green function from those of the ($N > 1$)-particle Green functions. It is implicitly defined as

$$\pm i\hbar \sum_{lmn} w_{ilmn}(z_1) G_{mnjl}^{(2)}(z_1, z_1, z_2, z_{1+}) \quad (2.64)$$

$$=: \sum_l \int_{z_3} \Sigma_{il}(z_1, z_3) G_{lj}(z_3, z_2),$$

$$\pm i\hbar \sum_{lmn} G_{inlm}^{(2)}(z_1, z_{2-}, z_2, z_2) w_{lmnj}(z_2) \quad (2.65)$$

$$=: \sum_l \int_{z_3} G_{il}(z_1, z_3) \Sigma_{lj}(z_3, z_2).$$

With this, Eqs. (2.62) and (2.63) transform into

$$\begin{aligned} & \sum_l \left[i\hbar \frac{d}{dz_1} \delta_{il} - h_{il}(z_1) \right] G_{lj}(z_1, z_2) \\ &= \delta_C(z_1, z_2) \delta_{ij} + \sum_l \int_{z_3} \Sigma_{il}(z_1, z_3) G_{lj}(z_3, z_2), \end{aligned} \quad (2.66)$$

$$\begin{aligned} & \sum_l G_{il}(z_1, z_2) \left[-i\hbar \frac{\overleftarrow{d}}{dz_2} \delta_{lj} - h_{lj}(z_2) \right] \\ &= \delta_C(z_1, z_2) \delta_{ij} + \sum_l \int_{z_3} G_{il}(z_1, z_3) \Sigma_{lj}(z_3, z_2). \end{aligned} \quad (2.67)$$

These equations contain the two main quantities in Green functions theory, both depending on two contour times z_1, z_2 : the (single-particle) selfenergy $\Sigma(z_1, z_2)$ (which is a functional of G) and the (single-particle) Green function $G(z_1, z_2)$ itself. Before turning to the self-consistent determination of $\Sigma[G]$ in Section 2.6, and several approximation strategies thereof in Section 2.7, a mapping technique for single-particle contour quantities onto real-time quantities is detailed in Section 2.5.2.

2.5.2 Langreth–Wilkins rules

For the actual computation of expressions containing integrals and products of contour quantities, a mapping to ordinary real-time quantities has to be used. A suitable technique has been provided by *Langreth* and *Wilkins* [96]. Since, in this work, only single-particle correlators like the (single-particle) Green function and selfenergy are of concern, the following technique will only deal with terms of the form, cf. Eq. (2.56),

$$k(z_1, z_2) = \langle \Psi_0 | \hat{\mathcal{T}}_C \{ \hat{O}_1(z_1) \hat{O}_2(z_2) \} | \Psi_0 \rangle, \quad (2.68)$$

with the restriction that the operators have to obey

$$\hat{O}_- = \hat{O}_+, \quad (2.69)$$

i.e., have the same values for contour arguments on the upper and lower branch. The appearance of the contour ordering operator $\hat{\mathcal{T}}_{\mathcal{C}}$ in Eq. (2.68) suggest to split k into

$$\begin{aligned} k(z_1, z_2) & \quad (2.70) \\ & = \delta_{\mathcal{C}}(z_1, z_2)k^{\delta}(z_1) + \Theta_{\mathcal{C}}(z_1, z_2)k^{>}(z_1, z_2) + \Theta_{\mathcal{C}}(z_2, z_1)k^{<}(z_1, z_2), \end{aligned}$$

with

$$k^{>}(z_1, z_2) = \langle \Psi_0 | \hat{O}_1(z_1) \hat{O}_2(z_2) | \Psi_0 \rangle, \quad (2.71)$$

$$k^{<}(z_1, z_2) = \pm \langle \Psi_0 | \hat{O}_2(z_2) \hat{O}_1(z_1) | \Psi_0 \rangle, \quad (2.72)$$

where the \pm stands for bosonic/fermionic operators. Both functions, less and greater, obey

$$k^{\geq}(z_{1+}, z_2) = k^{\geq}(z_{1-}, z_2), \quad (2.73)$$

$$k^{\geq}(z_1, z_{2+}) = k^{\geq}(z_1, z_{2-}).$$

Therefore, only two linearly independent quantities remain and it is thus natural to define the so-called real-time less and greater Keldysh components

$$k^{>}(t_1, t_2) := k(t_{1+}, t_{2-}) = k^{>}(t_{1+}, t_{2-}), \quad (2.74)$$

$$k^{<}(t_1, t_2) := k(t_{1-}, t_{2+}) = k^{<}(t_{1-}, t_{2+}) \quad (2.75)$$

and the δ -component

$$\begin{aligned} k^{\delta}(t_1) & := k(t_{1-}, t_{1-}) = k(t_{1+}, t_{1+}) \\ & = k^{\delta}(t_{1+}, t_{1+}) = k^{\delta}(t_{1-}, t_{1-}), \end{aligned} \quad (2.76)$$

where $t_{1/2\pm}$ are the projections on the backward/forward branch of the contour. The relations are depicted in Fig. 2.3. For convenience, two more (redundant) components,

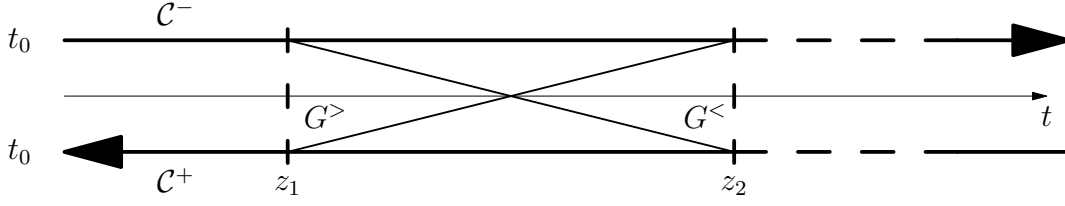


Figure 2.3: Subordinated Green functions on \mathcal{C} with the forward branch \mathcal{C}^- and the backward branch \mathcal{C}^+ . The positions of the two time arguments of $G(z_1, z_2)$ for the \gtrless -components, which can lie on both parts of the contour, are depicted.

the retarded and advanced component, can be defined as

$$k^{\text{R}}(t_1, t_2) = \delta(t_1, t_2)k^\delta(t_1) + \Theta(t_1, t_2)[k^>(t_1, t_2) - k^<(t_1, t_2)], \quad (2.77)$$

$$k^{\text{A}}(t_1, t_2) = \delta(t_1, t_2)k^\delta(t_1) + \Theta(t_2, t_1)[k^<(t_1, t_2) - k^>(t_1, t_2)]. \quad (2.78)$$

With these components, the real-time expressions for two common concatenations of Keldysh functions, i.e., functions satisfying Eqs. (2.70) and (2.73), the convolution and the product, can be worked out. For the convolution

$$c(z_1, z_2) = \int_{\mathcal{C}} dz_3 a(z_1, z_3)b(z_3, z_2), \quad (2.79)$$

one has

$$\begin{aligned} c^{\gtrless}(t_1, t_2) &= \int_{t_0}^{t_1} dt_3 a^{\text{R}}(t_1, t_3)b^{\gtrless}(t_3, t_2) \\ &+ \int_{t_0}^{t_2} dt_3 a^{\gtrless}(t_1, t_3)b^{\text{A}}(t_3, t_2) \end{aligned} \quad (2.80)$$

and

$$c^{\text{R}}(t_1, t_2) = \int_{t_2}^{t_1} dt_3 a^{\text{R}}(t_1, t_3)b^{\text{R}}(t_3, t_2), \quad (2.81)$$

$$c^{\text{A}}(t_1, t_2) = \int_{t_1}^{t_2} dt_3 a^{\text{A}}(t_1, t_3)b^{\text{A}}(t_3, t_2). \quad (2.82)$$

For the product of type

$$c(z_1, z_2) = a(z_1, z_2)b(z_2, z_1), \quad (2.83)$$

with $a^\delta = 0 = b^\delta$, one arrives at

$$c^{\geq}(t_1, t_2) = a^{\geq}(t_1, t_2)b^{\leq}(t_2, t_1) \quad (2.84)$$

and

$$\begin{aligned} c^{\text{R/A}}(t_1, t_2) &= a^{\text{R/A}}(t_1, t_2)b^{<}(t_2, t_1) + a^{<}(t_1, t_2)b^{\text{A/R}}(t_2, t_1) \\ &= a^{\text{R/A}}(t_1, t_2)b^{>}(t_2, t_1) + a^{>}(t_1, t_2)b^{\text{A/R}}(t_2, t_1), \end{aligned} \quad (2.85)$$

while for the product of type

$$c(z_1, z_2) = a(z_1, z_2)b(z_1, z_2), \quad (2.86)$$

with $a^\delta = 0 = b^\delta$, one has

$$c^{\geq}(t_1, t_2) = a^{\geq}(t_1, t_2)b^{\geq}(t_1, t_2) \quad (2.87)$$

and

$$\begin{aligned} c^{\text{R/A}}(t_1, t_2) &= a^{\text{R/A}}(t_1, t_2)b^{<}(t_1, t_2) + a^{>}(t_1, t_2)b^{\text{R/A}}(t_1, t_2) \\ &= a^{\text{R/A}}(t_1, t_2)b^{>}(t_1, t_2) + a^{<}(t_1, t_2)b^{\text{R/A}}(t_1, t_2). \end{aligned} \quad (2.88)$$

With these definitions, the KBE in component representation read

$$\begin{aligned}
 & \sum_l \left[i\hbar \frac{d}{dt_1} \delta_{il} - h_{il}(t_1) \right] G_{lj}^{\geq}(t_1, t_2) \\
 &= \sum_l \int_{t_0}^{t_1} dt_3 \Sigma_{il}^R(t_1, t_3) G_{lj}^{\geq}(\bar{t}, t') + \int_{t_0}^{t_2} dt_3 \Sigma_{il}^{\geq}(t_1, t_3) G_{lj}^A(\bar{t}, t') \\
 &= \sum_l \int_{t_0}^{t_1} dt_3 \left(\Sigma_{il}^>(t_1, t_3) - \Sigma_{il}^<(t_1, t_3) \right) G_{lj}^{\geq}(\bar{t}, t') \\
 & \quad + \sum_l \int_{t_0}^{t_2} dt_3 \Sigma_{il}^{\geq}(t_1, t_3) \left(G_{lj}^<(\bar{t}, t') - G_{lj}^>(\bar{t}, t') \right)
 \end{aligned} \tag{2.89}$$

and

$$\begin{aligned}
 & \sum_l G_{il}^{\geq}(t_1, t_2) \left[-i\hbar \frac{\overleftarrow{d}}{dt_2} \delta_{lj} - h_{lj}(t_2) \right] \\
 &= \sum_l \int_{t_0}^{t_1} dt_3 G_{il}^R(t_1, t_3) \Sigma_{lj}^{\geq}(t_3, t_2) + \int_{t_0}^{t_2} dt_3 G_{il}^{\geq}(t_1, t_3) \Sigma_{lj}^A(t_3, t_2) \\
 &= \sum_l \int_{t_0}^{t_1} dt_3 \left(G_{il}^>(t_1, t_3) - G_{il}^<(t_1, t_3) \right) \Sigma_{lj}^{\geq}(t_3, t_2) \\
 & \quad + \sum_l \int_{t_0}^{t_2} dt_3 G_{il}^{\geq}(t_1, t_3) \left(\Sigma_{lj}^<(t_3, t_2) - \Sigma_{lj}^>(t_3, t_2) \right).
 \end{aligned} \tag{2.90}$$

Note the missing δ_c in the \geq -components of Eqs. (2.89) and (2.90) compared to Eqs. (2.66) and (2.67), which, as it is a time-diagonal function, only enters the retarded and advanced components.

2.6 Hedin's equations

In this brief section, a coupled set of equations of motions for five dynamical quantities, two of which are the Green function and the selfenergy, is summarized. It has been first presented by *Lars Hedin* in 1965 [61] in association with the *GW* method, which

will be discussed in more detail in Section 2.7. If solved exactly, the set of Hedin's equations yields the same G as the solution of the Martin–Schwinger hierarchy⁶ and provides multiple starting points for approximate solution schemes. To determine the solution for $G(z_1, z_2)$, its equations of motion, the KBE, cf. Eqs. (2.66) and (2.67), have to be solved. This can be either done directly in their differential form, or in the integral form, which reads

$$G_{ij}(z_1, z_2) = G_{ij}^{(0)}(z_1, z_2) + \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2), \quad (2.91)$$

with the reference Green function $G^{(0)}$. It is the solution of the ideal pair of equations

$$\sum_l \left[i\hbar \frac{d}{dz_1} \delta_{il} - h_{il}(z_1) \right] G_{lj}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij}, \quad (2.92)$$

$$\sum_l G_{il}(z_1, z_2) \left[-i\hbar \overleftarrow{\frac{d}{dz_2}} \delta_{lj} - h_{lj}(z_2) \right] = \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij}. \quad (2.93)$$

Note that $G^{(0)}$ does not refer to zero particles, but to the property that is of zeroth order with respect to the interaction w . Equation 2.91 is referred to as the *Dyson* equation (for the one-particle Green function). Comparing the KBE, cf. Eqs. (2.66) and (2.67), to the Dyson equation, cf. Eq. (2.91), the question may arise if the solution of one or the other is numerically more favorable. Realizing that the determination of $G^{(0)}$ via Eqs. (2.92) and (2.93) is of $\mathcal{O}(N_b^2)$ and $\mathcal{O}(N_t^2)$, while the solution of the full G via Eq. (2.91) involves two separable time integrations and matrix multiplications, it is of $\mathcal{O}(N_b^3)$ and $\mathcal{O}(N_t^3)$, which is the same scaling as the solution of the KBE, although the prefactors are higher for the Dyson equation. In the following chapter, though, it will be shown that in an expansion of G/Σ with respect to the order of the interaction, only the Dyson equation provides a strict order-per-order expansion scheme. Both, the Dyson equation and the KBE, depend on the knowledge of the

⁶Although, to the knowledge of the author, no strict proof exists that shows the equivalence of the solutions for G of Hedin's equation versus that from the Martin–Schwinger, both approaches agree for all practical relevant approximations.

selfenergy Σ . It fulfills

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{xc}}(z_1, z_2), \quad (2.94)$$

with the (static) time-diagonal Hartree part Σ^{H} ,

$$\Sigma_{ij}^{\text{H}}(z_1, z_2) = \pm i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}(z_1, z_{1+}), \quad (2.95)$$

and the exchange/correlation part Σ^{xc} . To determine Σ^{xc} , there exist two commonly used equivalent exact approaches, either regarding it as a functional of the bare interaction w or of an interaction W which is screened by the particles of the system. Both techniques rely on a so-called vertex function named Λ and Γ , respectively, which involves the derivatives of either Σ or Σ^{xc} with respect to G to determine the vertex function and with it Σ^{xc} . With the coupled equations for Σ^{xc} and the vertex function, both approaches yield a means to generate all selfenergy terms by iteration. With the bare interaction, one has

$$\begin{aligned} \Sigma_{ij}^{\text{xc}}(z_1, z_2) & \\ &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \Lambda_{nqpj}(z_3, z_2, z_1). \end{aligned} \quad (2.96)$$

The bare vertex Λ is self-consistently given as the solution of

$$\begin{aligned} \Lambda_{ijkl}(z_1, z_2, z_3) &= \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl} \\ &+ \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\ &\int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Lambda_{pj kq}(z_6, z_7, z_3). \end{aligned} \quad (2.97)$$

Using the screened interaction W as a basis for the expansion, the exchange/correlation selfenergy reads, cf. Eq. (2.96),

$$\Sigma_{ij}^{\text{xc}}(z_1, z_2) = i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}(z_1, z_3) \quad (2.98)$$

$$\int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}(z_4, z_2, z_3),$$

where W obeys

$$W_{ijkl}(z_1, z_2) = W_{ijkl}^{\text{bare}}(z_1, z_2) + W_{ijkl}^{\text{screened}}(z_1, z_2), \quad (2.99)$$

with

$$W_{ijkl}^{\text{bare}}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2) w_{ijkl}(z_1) \quad (2.100)$$

and

$$W_{ijkl}^{\text{screened}}(z_1, z_2) \quad (2.101)$$

$$= \sum_{mnl} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} P_{nqpm}(z_1, z_3) W_{pjkl}(z_3, z_2).$$

The occurring polarization function P is given by

$$P_{ijkl}(z_1, z_2) = \pm i\hbar \int_{\mathcal{C}} dz_3 \sum_m G_{im}(z_1, z_3) \quad (2.102)$$

$$\int_{\mathcal{C}} dz_4 \sum_n G_{nl}(z_4, z_1) \Gamma_{mjkn}(z_3, z_4, z_2).$$

The screened vertex function Γ —which Σ^{xc} and P depend on—is governed by

$$\begin{aligned} \Gamma_{ijkl}(z_1, z_2, z_3) &= \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl} \\ &+ \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{\text{xc}}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\ &\int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pj kq}(z_6, z_7, z_3). \end{aligned} \quad (2.103)$$

2.7 The selfenergy

To study time-dependent observables of the system of interest, one has to know the less and greater components of the two-time Green function $G^{\lessgtr}(t_1, t_2)$. These components can be generated from the solution of the contour Dyson equation, which is the first equation of Hedin's equations, cf. Eq. (2.91). Its main ingredient is the selfenergy Σ . It is of great importance both from a physical point of view—since it incorporates all different classes of inter-particle effects and processes—as well as from the computational view—since a large portion of the numerical resources is consumed for its determination. Σ is the solution of the second Hedin equation, Eq. (2.94), which, in turn, is dependent on the third to fifth Hedin equation, Eqs. (2.99), (2.102) and (2.103), and, in turn, also on the Dyson equation via the Green function entering it. Since the selfenergy, by iteration of Hedin's equations, consists of an infinite number of terms, a strategy has to be used to reach a good approximation with only a small finite subset. The two most common approaches are detailed in the following, applying either a perturbative approach with respect to the interaction strength, i.e., with respect to the powers of w , or the use of a resummation. The resummation involves (infinitely many) diagrams in all orders of the interaction strength belonging to certain classes, namely the particle–particle (pp), the particle–hole (ph) T -matrix approximation, the GW approximation, or a combination of all or some of these. The immediately following Section 2.7.1 deals with the expansion in orders of the interaction strength up to the third order. In Section 2.7.2, the resummation approaches, which mainly have been applied for the calculations in Section 3, are detailed.

2.7.1 Perturbative expansion of the selfenergy

This section deals with the expansion of the selfenergy with respect to the number of interactions w involved. This means that the n -th order approximation considers only the terms with no more than n interactions. This procedure has two sources of reasoning behind it. First, for small interaction strength S , higher order processes with several interactions usually have small amplitudes proportional to higher powers of S . Second, even for larger S , higher order terms also contain several Green functions corresponding to the correlated creation and annihilation of several particles. The strength of these correlations is not directly coupled to the interaction strength and therefore, a lower order approximation may give good results even for stronger interactions. Regarding the treatment of the Green functions occurring in the expansion of the selfenergy, two different approaches are common. In the self-consistent treatment, one starts from the non-interacting Green function $G^{(0)}$ and one computes the selfenergy according to Eq. (2.94) in the chosen approximation. Then, the Dyson equation is evaluated taking $G = G^{(0)}$ on the right-hand side. With the resulting G , the selfenergy is reevaluated. This procedure is continued until convergence is reached. In contrast, the free approach—like for the other quantities in Hedin’s equations—also expands G with respect to the number of occurrences of the interaction. That way, it is ensured that the n -th order approximation contains no terms of higher order, which is violated in the self-consistent approach through the iteration procedure. Nonetheless, these terms are valid terms of order higher than n , so it cannot be answered beforehand which method is superior. In the following sections, the terms for both approaches of the orders up to third order will be deduced from Hedin’s equation in general, diagonal and Hubbard basis alongside the expressions for the relevant Keldysh components.

2.7.1.1 First-order terms

To determine the first-order contributions to Σ , one starts from the second Hedin equation, Eq. (2.94). The first term, the Hartree term Σ^{H} , is of first-order, since it contains one w . It was already given in Eq. (2.95) and is repeated here for consistency,

$$\Sigma_{ij}^{\text{H}}(z_1, z_2) = \pm i\hbar\delta_C(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}(z_1, z_{1+}). \quad (2.104)$$

Since this expression contains a contour delta function $\delta_{\mathcal{C}}$, the only non-vanishing Keldysh component is

$$\begin{aligned}
 \Sigma_{ij}^{\text{H},\delta}(t_1) &= \Sigma_{ij}^{\text{H}}(z_1, z_1) \\
 &= \pm i\hbar \sum_{mn} w_{mijn}(z_1) G_{nm}(z_1, z_{1+}) \\
 &= \pm i\hbar \sum_{mn} w_{mijn}(t_1) G_{nm}^<(t_1, t_1).
 \end{aligned} \tag{2.105}$$

The second first-order term belongs to Σ^{xc} , cf. Eq. (2.94), generated by the first-order term $W^{(1)}$ of Eq. (2.99),

$$W_{ijkl}^{(1)}(z_1, z_2) = W_{ijkl}^{\text{bare}}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2) w_{ijkl}(z_1) \tag{2.106}$$

and the zeroth order vertex $\Gamma^{(0)}$, cf. Eq. (2.103),

$$\Gamma_{ijkl}^{(0)}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl}. \tag{2.107}$$

It is the so-called *Fock term* Σ^{F} which is of time-diagonal structure like the Hartree term and is given by

$$\begin{aligned}
 \Sigma_{ij}^{\text{F}}(z_1, z_2) &= \Sigma_{ij}^{\text{xc}}(W^{(1)} \equiv W^{\text{bare}}, \Gamma^{(0)}) \\
 &= i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{injm}(z_1) G_{mn}(z_1, z_{1+}).
 \end{aligned} \tag{2.108}$$

The δ -component is given by

$$\Sigma_{ij}^{\text{F},\delta}(t_1) = \Sigma_{ij}^{\text{F}}(z_1, z_1) = \sum_{mn} w_{injm}(t_1) G_{mn}^<(t_1, t_1). \tag{2.109}$$

Since there is no further term stemming from $W^{(0)}$ and $\Gamma^{(1)}$, since $W^{(0)} \equiv 0$, the first-order selfenergy $\Sigma^{(1)}$ is given by

$$\Sigma^{(1)} = \Sigma^{\text{H}} + \Sigma^{\text{F}}, \tag{2.110}$$

which both are time-diagonal. For the non-selfconsistent treatment, the Green functions appearing in Σ^{H} and Σ^{F} are taken as free Green functions, i.e., $G \rightarrow G^{(0)}$.

There are no additional terms containing higher-order Green functions in the first order.

2.7.1.1.1 Diagonal basis In a basis with diagonal interaction $w_{ijkl} = \delta_{il}\delta_{jk}w_{ij}$, the first-order terms read

$$\Sigma_{ij}^{\text{H,diagonal}}(z_1, z_2) = \pm i\hbar\delta_{\mathcal{C}}(z_1, z_2)\delta_{ij}\sum_m w_{mi}(z_1)G_{mm}(z_1, z_{1+}), \quad (2.111)$$

$$\Sigma_{ij}^{\text{F,diagonal}}(z_1, z_2) = i\hbar\delta_{\mathcal{C}}(z_1, z_2)w_{ij}(z_1)G_{ij}(z_1, z_{1+}), \quad (2.112)$$

with δ -components

$$\Sigma_{ij}^{\text{H,diagonal},\delta}(t_1) = \pm i\hbar\delta_{ij}\sum_m w_{mi}(t_1)G_{mm}^<(t_1, t_1), \quad (2.113)$$

$$\Sigma_{ij}^{\text{F,diagonal},\delta}(t_1) = i\hbar w_{ij}(t_1)G_{ij}^<(t_1, t_1). \quad (2.114)$$

The structure of the selfenergy contributions can be suitably visualized by using Feynman diagrams [97]. In this diagrammatic representation, Green functions are depicted as solid lines with an arrow pointing from the second argument to the first argument (since the particle described by it is created at the second argument and annihilated at the first argument). The interaction is represented by a wiggly line which has two connections. Employing the Feynman diagram technique, the first-order contributions to the selfenergy are depicted in Fig. 2.4.

2.7.1.1.2 Hubbard basis For the Hubbard basis, introduced in Section 2.3, the first-order selfenergy terms can be directly worked out for bosons and fermions, cf. Eqs. (2.28) and (2.35), yielding

$$\Sigma_{i\alpha j\alpha}^{\text{H,bosons}}(z_1, z_2) = i\hbar\delta_{\mathcal{C}}(z_1, z_2)\delta_{ij}\sum_{\epsilon} U(z_1)G_{i\epsilon i\epsilon}(z_1, z_{1+}), \quad (2.115)$$

$$\Sigma_{i\alpha j\alpha}^{\text{F,bosons}}(z_1, z_2) = i\hbar\delta_{\mathcal{C}}(z_1, z_2)\delta_{ij}U(z_1)G_{i\alpha i\alpha}(z_1, z_{1+}), \quad (2.116)$$

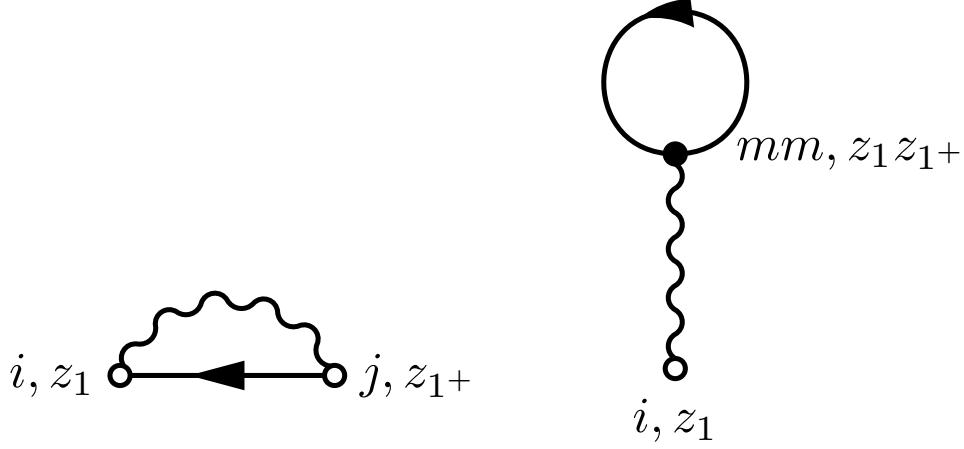


Figure 2.4: First-order diagrams in diagonal basis. **Left:** Fock diagram, $\Sigma^{\text{F,diagonal}}$. **Right:** Hartree diagram, $\Sigma^{\text{H,diagonal}}$. Both diagrams are time-diagonal.

with δ -components

$$\Sigma_{i\alpha j\alpha}^{\text{H,bosons},\delta}(t_1) = i\hbar\delta_{ij} \sum_{\epsilon} U(t_1) G_{i\epsilon i\epsilon}^<(t_1, t_1), \quad (2.117)$$

$$\Sigma_{i\alpha j\alpha}^{\text{F,bosons},\delta}(t_1) = i\hbar\delta_{ij} U(t_1) G_{i\alpha i\alpha}^<(t_1, t_1), \quad (2.118)$$

for bosons and

$$\Sigma_{i\alpha j\alpha}^{\text{H,fermions}}(z_1, z_2) = -i\hbar\delta_c(z_1, z_2) \delta_{ij} \sum_{\epsilon \neq \alpha} U(z_1) G_{i\epsilon i\epsilon}(z_1, z_{1+}), \quad (2.119)$$

$$\Sigma_{i\alpha j\alpha}^{\text{F,fermions}}(z_1, z_2) \equiv 0, \quad (2.120)$$

with δ -components

$$\Sigma_{i\alpha j\alpha}^{\text{H,fermions},\delta}(t_1) = -i\hbar\delta_{ij} \sum_{\epsilon \neq \alpha} U(t_1) G_{i\epsilon i\epsilon}^<(t_1, t_1), \quad (2.121)$$

$$\Sigma_{i\alpha j\alpha}^{\text{F,fermions},\delta}(t_1) \equiv 0, \quad (2.122)$$

for fermions. For spin-0 bosons/spin-1/2 fermions, the terms attain the form

$$\Sigma_{ij}^{\text{H,bosons},0}(z_1) = i\hbar\delta_c(z_1, z_2)\delta_{ij}U(z_1)G_{ii}(z_1, z_{1+}), \quad (2.123)$$

$$\Sigma_{ij}^{\text{F,bosons},0}(z_1) = i\hbar\delta_c(z_1, z_2)\delta_{ij}U(z_1)G_{ii}(z_1, z_{1+}) \quad (2.124)$$

and

$$\Sigma_{i\uparrow j\uparrow}^{\text{H,fermions},1/2}(z_1) = -i\hbar\delta_c(z_1, z_2)\delta_{ij}U(z_1)G_{i\downarrow i\downarrow}(z_1, z_{1+}), \quad (2.125)$$

$$\Sigma_{i\downarrow j\downarrow}^{\text{H,fermions},1/2}(z_1) = -i\hbar\delta_c(z_1, z_2)\delta_{ij}U(z_1)G_{i\uparrow i\uparrow}(z_1, z_{1+}), \quad (2.126)$$

$$\Sigma_{i\alpha j\alpha}^{\text{F,fermions},1/2}(z_1) \equiv 0, \quad (2.127)$$

with δ -components

$$\Sigma_{ij}^{\text{H,bosons},0,\delta}(t_1) = i\hbar\delta_{ij}U(t_1)G_{ii}^<(t_1, t_1), \quad (2.128)$$

$$\Sigma_{ij}^{\text{F,bosons},0,\delta}(t_1) = i\hbar\delta_{ij}U(t_1)G_{ii}^<(t_1, t_1) \quad (2.129)$$

and

$$\Sigma_{i\uparrow j\uparrow}^{\text{H,fermions},1/2,\delta}(t_1) = -i\hbar\delta_{ij}U(t_1)G_{i\downarrow i\downarrow}^<(t_1, t_1), \quad (2.130)$$

$$\Sigma_{i\downarrow j\downarrow}^{\text{H,fermions},1/2,\delta}(t_1) = -i\hbar\delta_{ij}U(t_1)G_{i\uparrow i\uparrow}^<(t_1, t_1), \quad (2.131)$$

$$\Sigma_{i\alpha j\alpha}^{\text{F,fermions},1/2,\delta}(t_1) \equiv 0. \quad (2.132)$$

The corresponding diagrams for spin-0 bosons/spin-1/2 fermions are shown in Figs. 2.5 and 2.6.

2.7.1.2 Second order terms

Returning to Eqs. (2.94) and (2.98), the selfconsistent second-order contribution is given by

$$\Sigma^{(2)} = \Sigma^{\text{xc},(2)}. \quad (2.133)$$

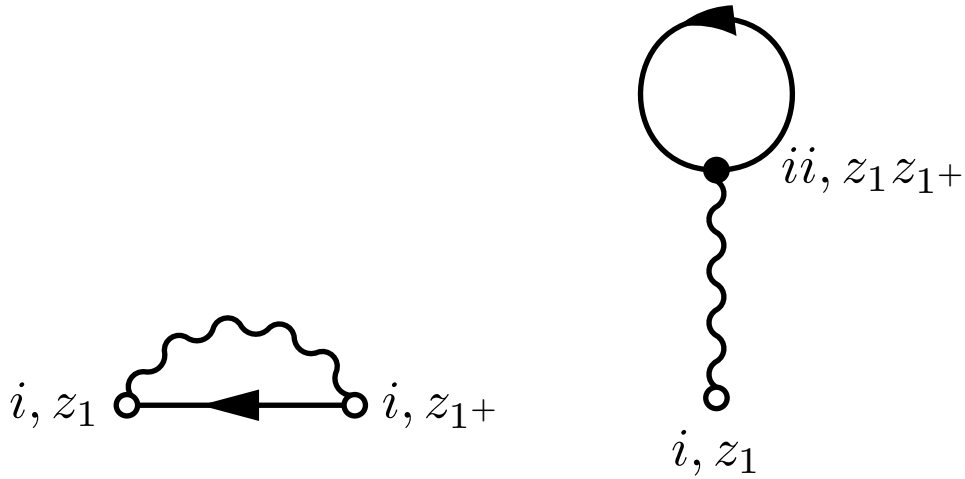


Figure 2.5: First-order diagrams in Hubbard basis for spin-0 bosons. **Left:** Fock diagram, $\Sigma^{\text{F,bosons},0}$. **Right:** Hartree diagram, $\Sigma^{\text{H,bosons},0}$. Note that both diagrams coincide for the Hubbard basis.

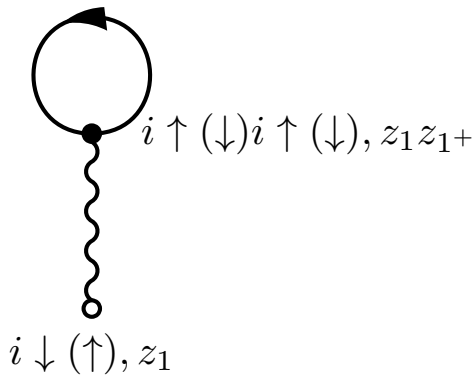


Figure 2.6: First-order (Hartree) diagram in Hubbard basis for spin-1/2 fermions, $\Sigma^{\text{H,fermions},1/2}$.

The second-order terms of $\Sigma^{\text{xc},(2)}$ can only be of either one of the structures

$$\Sigma^{(2),2,0} = \Sigma^{\text{xc},(2)}\left(W^{(2)}, \Gamma^{(0)}\right), \quad (2.134)$$

$$\Sigma^{(2),1,1} = \Sigma^{\text{xc},(2)}\left(W^{(1)}, \Gamma^{(1)}\right).$$

The first structure involves $W^{(2)}$, which structurally is given by, cf. Eq. (2.99),

$$W^{(2)} = W^{\text{screened}}\left(P^{(0)}, W^{(1)}\right). \quad (2.135)$$

The structure of the zeroth order term of the polarization is

$$P^{(0)} = P\left(\Gamma^{(0)}\right). \quad (2.136)$$

Thus, it is given by

$$P_{ijkl}^{(0)}(z_1, z_2) = \pm i\hbar \int_{\mathcal{C}} dz_3 \sum_m G_{im}(z_1, z_3) \quad (2.137)$$

$$\begin{aligned} & \int_{\mathcal{C}} dz_4 \sum_n G_{nl}(z_4, z_1) \delta_{\mathcal{C}}(z_3, z_{4+}) \delta_{\mathcal{C}}(z_2, z_4) \delta_{mk} \delta_{jn} \\ & = \pm i\hbar G_{ik}(z_1, z_2) G_{jl}(z_2, z_1). \end{aligned}$$

Inserting this result into Eq. (2.135), one arrives at

$$W_{ijkl}^{(2)}(z_1, z_2) = \sum_{mn} w_{imnl}(z_1) \quad (2.138)$$

$$\int_{\mathcal{C}} dz_3 \sum_{pq} \left(\pm i\hbar G_{np}(z_1, z_3) G_{qm}(z_3, z_1) \right) \delta_{\mathcal{C}}(z_3, z_2) w_{pj kq}(z_3)$$

and, employing Eq. (2.101), finally, one has

$$W_{ijkl}^{(2)}(z_1, z_2) \quad (2.139)$$

$$= \pm i\hbar \sum_{mn} w_{imnl}(z_1) \sum_{pq} G_{np}(z_1, z_2) G_{qm}(z_2, z_1) w_{pj kq}(z_2).$$

With this, $\Sigma^{(2),2,0}$ can be calculated as, cf. Eq. (2.98),

$$\begin{aligned} \Sigma_{ij}^{(2),2,0}(z_1, z_2) & \quad (2.140) \\ &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} \left(\pm i\hbar \sum_{rs} w_{irsm}(z_1) \sum_{tu} G_{st}(z_1, z_3) G_{ur}(z_3, z_1) w_{tpqu}(z_3) \right) \\ & \quad \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \delta_{\mathcal{C}}(z_4, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{np} \delta_{qj}. \end{aligned}$$

Evaluating the terms, one arrives at

$$\begin{aligned} \Sigma_{ij}^{(2),2,0}(z_1, z_2) & \quad (2.141) \\ &= \pm (i\hbar)^2 \sum_{mn} G_{mn}(z_1, z_2) \sum_{st} G_{st}(z_1, z_2) \\ & \quad \sum_r w_{irsm}(z_1) \sum_u w_{tnju}(z_2) G_{ur}(z_2, z_1). \end{aligned}$$

The other second-order selfenergy term, $\Sigma_{ij}^{(2),1,1}$, requires the first-order term of the vertex Γ , the structure of which is

$$\Gamma^{(1)} = \Gamma(\delta\Sigma^{\text{xc},(1)}/\delta G, \Gamma^{(0)}). \quad (2.142)$$

This term involves the functional derivative of $\Sigma^{\text{xc},(1)}$ with respect to G . One has

$$\frac{\delta\Sigma_{ij}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{rs}(z_5, z_6)} = \frac{\delta\Sigma_{ij}^{\text{xc},(1),\text{F}}(z_1, z_2)}{\delta G_{rs}(z_5, z_6)}. \quad (2.143)$$

Employing Eq. (2.108), one finds

$$\begin{aligned} \frac{\delta\Sigma_{ij}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{rs}(z_5, z_6)} &= i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{injm}(z_1) \frac{\delta G_{mn}(z_1, z_{1+})}{\delta G_{rs}(z_5, z_6)} \\ &= i\hbar \delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_1, z_5) \delta_{\mathcal{C}}(z_1, z_6) w_{isjr}(z_1), \end{aligned} \quad (2.144)$$

where

$$\frac{\delta G_{ij}(z_1, z_2)}{\delta G_{mn}(z_5, z_6)} = \delta_{\mathcal{C}}(z_1, z_5) \delta_{\mathcal{C}}(z_2, z_6) \delta_{im} \delta_{jn} \quad (2.145)$$

has been applied. With this,

$$\begin{aligned} \Gamma_{ijkl}^{(1)}(z_1, z_2, z_3) & \quad (2.146) \\ &= \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\ & \quad \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pj kq}^{(0)}(z_6, z_7, z_3). \end{aligned}$$

Using Eq. (2.144), one has

$$\begin{aligned} \Gamma_{ijkl}^{(1)}(z_1, z_2, z_3) & \quad (2.147) \\ &= i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{inlm}(z_1) \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_1, z_6) \\ & \quad \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_1) \Gamma_{pj kq}^{(0)}(z_6, z_7, z_3). \end{aligned}$$

With Eq. (2.107), finally,

$$\begin{aligned} \Gamma_{ijkl}^{(1)}(z_1, z_2, z_3) & \quad (2.148) \\ &= i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{inlm}(z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_1) \end{aligned}$$

ensues. Inserting this result yields

$$\begin{aligned} \Sigma_{ij}^{(2),1,1}(z_1, z_2) & \quad (2.149) \\ &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(1)}(z_4, z_2, z_3). \end{aligned}$$

Employing Eqs. (2.106) and (2.148), one arrives at

$$\begin{aligned}
 \Sigma_{ij}^{(2),1,1}(z_1, z_2) & \quad (2.150) \\
 &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(1)}(z_4, z_2, z_1) \\
 &= (i\hbar)^2 \sum_{mpq} w_{ipqm}(z_1) \sum_n G_{mn}(z_1, z_2) \sum_{rs} w_{nsjr}(z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2).
 \end{aligned}$$

The corresponding components to the selfconsistent second-order selfenergy contributions $\Sigma_{ij}^{(2),2,0}$ and $\Sigma_{ij}^{(2),1,1}$ read

$$\begin{aligned}
 \Sigma_{ij}^{(2),2,0,\geq}(t_1, t_2) &= \pm (i\hbar)^2 \sum_{mn} G_{mn}^{\geq}(t_1, t_2) \sum_{st} G_{st}^{\geq}(t_1, t_2) \quad (2.151) \\
 &\quad \sum_r w_{irsm}(t_1) \sum_u w_{tnju}(t_2) G_{ur}^{\leq}(t_2, t_1)
 \end{aligned}$$

and

$$\begin{aligned}
 \Sigma_{ij}^{(2),1,1,\geq}(t_1, t_2) &= (i\hbar)^2 \sum_{mpq} w_{ipqm}(t_1) \sum_n G_{mn}^{\geq}(t_1, t_2) \quad (2.152) \\
 &\quad \sum_{rs} w_{nsjr}(t_2) G_{rp}^{\leq}(t_2, t_1) G_{qs}^{\geq}(t_1, t_2).
 \end{aligned}$$

For the non-selfconsistent treatment, the possible second-order classes are

$$\Sigma^{(2),(2),2,0,0} = \Sigma^{\text{xc},(2)}(W^{(2)}, G^{(0)}, \Gamma^{(0)}) \equiv \Sigma^{(2),2,0}(G \rightarrow G^{(0)}), \quad (2.153)$$

$$\Sigma^{(2),(2),1,0,1} = \Sigma^{\text{xc},(2)}(W^{(1)}, G^{(0)}, \Gamma^{(1)}) \equiv \Sigma^{(2),1,1}(G \rightarrow G^{(0)}) \quad (2.154)$$

and

$$\Sigma^{(2),\{\text{H},0\},1} = \Sigma^{\text{H},0}(G^{(1)}), \quad (2.155)$$

$$\Sigma^{(2),\{\text{F},0\},1} = \Sigma^{\text{F},0}(G^{(1)}). \quad (2.156)$$

The first two classes are just the same as in the selfconsistent approximation, cf. Eqs. (2.141) and (2.150), with the replacement $G \rightarrow G^{(0)}$. Likewise, their

components follow directly from Eqs. (2.151) and (2.153). For the third and fourth class, one needs the contributions to $G^{(1)}$, which are

$$\begin{aligned}
 G_{ij}^{(1),\{H,0\},0}(z_1, z_2) & \quad (2.157) \\
 &= \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}^{H,0}(z_3, z_4) G_{nj}^{(0)}(z_4, z_2) \\
 &= \pm i\hbar \int_{\mathcal{C}} dz_3 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \sum_{pq} w_{pmnq}(z_3) G_{qp}^{(0)}(z_3, z_{3+}) G_{nj}^{(0)}(z_3, z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 G_{ij}^{(1),\{F,0\},0}(z_1, z_2) & \quad (2.158) \\
 &= \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}^{F,0}(z_3, z_4) G_{nj}^{(0)}(z_4, z_2) \\
 &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \sum_{pq} w_{mqnp}(z_3) G_{pq}^{(0)}(z_3, z_{3+}) G_{nj}^{(0)}(z_3, z_2).
 \end{aligned}$$

With these results, the additional non-selfconsistent contributions are

$$\begin{aligned}
 \Sigma_{ij}^{(2),\{H,0\},\{1,\{H,0\},0\}}(z_1, z_2) &= \pm i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}^{(1),\{H,0\},0}(z_1, z_{1+}) \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{mijn}(z_1) & (2.159) \\
 & \int_{\mathcal{C}} dz_3 \sum_{pq} G_{np}^{(0)}(z_1, z_3) \sum_{rs} w_{rpqs}(z_3) G_{sr}^{(0)}(z_3, z_{3+}) G_{qm}^{(0)}(z_3, z_{1+})
 \end{aligned}$$

as well as

$$\begin{aligned}\Sigma_{ij}^{(2),\{H,0\},\{1,\{F,0\},0\}}(z_1, z_2) &= \pm i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}^{(1),\{F,0\},0}(z_1, z_{1+}) \\ &= \pm (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{mijn}(z_1)\end{aligned}\quad (2.160)$$

$$\int_{\mathcal{C}} dz_3 \sum_{pq} G_{np}^{(0)}(z_1, z_3) \sum_{rs} w_{psqr}(z_3) G_{rs}^{(0)}(z_3, z_{3+}) G_{qm}^{(0)}(z_3, z_{1+})$$

and

$$\begin{aligned}\Sigma_{ij}^{(2),\{F,0\},\{1,\{H,0\},0\}}(z_1, z_2) &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{injm}(z_1) G_{mn}^{(1),\{H,0\},0}(z_1, z_{1+}) \\ &= \pm (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{nimj}(z_1)\end{aligned}\quad (2.161)$$

$$\int_{\mathcal{C}} dz_3 \sum_{pq} G_{mp}^{(0)}(z_1, z_3) \sum_{rs} w_{rpqs}(z_3) G_{sr}^{(0)}(z_3, z_{3+}) G_{qn}^{(0)}(z_3, z_{1+})$$

as well as

$$\begin{aligned}\Sigma_{ij}^{(2),\{F,0\},\{1,\{F,0\},0\}}(z_1, z_2) &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{injm}(z_1) G_{mn}^{(1),\{F,0\},0}(z_1, z_{1+}) \\ &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{nimj}(z_1)\end{aligned}\quad (2.162)$$

$$\int_{\mathcal{C}} dz_3 \sum_{pq} G_{mp}^{(0)}(z_1, z_3) \sum_{rs} w_{psqr}(z_3) G_{rs}^{(0)}(z_3, z_{3+}) G_{qn}^{(0)}(z_3, z_{1+}).$$

The corresponding components are all time-diagonal and read

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{H,0\},\{1,\{H,0\},0\},\delta}(t_1) \tag{2.163} \\
 &= (i\hbar)^2 \sum_{mn} w_{mijn}(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_{pq} G_{np}^{(0),>}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qm}^{(0),<}(t_3, t_1) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{np}^{(0),<}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qm}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{H,0\},\{1,\{F,0\},0\},\delta}(t_1) \tag{2.164} \\
 &= \pm (i\hbar)^2 \sum_{mn} w_{mijn}(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_{pq} G_{np}^{(0),>}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qm}^{(0),<}(t_3, t_1) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{np}^{(0),<}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qm}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{F,0\},\{1,\{H,0\},0\},\delta}(t_1) \tag{2.165} \\
 &= \pm (i\hbar)^2 \sum_{mn} w_{nimj}(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_{pq} G_{mp}^{(0),>}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qn}^{(0),<}(t_3, t_1) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{mp}^{(0),<}(t_1, t_3) \sum_{rs} w_{rpqs}(t_3) G_{sr}^{(0),<}(t_3, t_3) G_{qn}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{F,0\},\{1,\{F,0\},0\},\delta}(t_1) \tag{2.166} \\
 &= (i\hbar)^2 \sum_{mn} w_{nimj}(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_{pq} G_{mp}^{(0),>}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qn}^{(0),<}(t_3, t_1) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_{pq} G_{mp}^{(0),<}(t_1, t_3) \sum_{rs} w_{psqr}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{qn}^{(0),>}(t_3, t_1) \right).
 \end{aligned}$$

2.7.1.2.1 Diagonal basis For $w_{ijkl} = \delta_{il}\delta_{jk}w_{ij}$, the selfconsistent second-order selfenergy terms, cf. Eqs. (2.141) and (2.150), simplify to

$$\begin{aligned}
 & \Sigma_{ij}^{(2),2,0,\text{diagonal}}(z_1, z_2) \tag{2.167} \\
 &= \pm (i\hbar)^2 G_{ij}(z_1, z_2) \sum_s w_{is}(z_1) \sum_t G_{st}(z_1, z_2) G_{ts}(z_2, z_1) w_{tj}(z_2),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{ij}^{(2),1,1,\text{diagonal}}(z_1, z_2) \tag{2.168} \\
 &= (i\hbar)^2 \sum_p w_{ip}(z_1) \sum_n G_{in}(z_1, z_2) w_{nj}(z_2) G_{np}(z_2, z_1) G_{pj}(z_1, z_2),
 \end{aligned}$$

with the corresponding components

$$\begin{aligned}
 & \Sigma_{ij}^{(2),2,0,\text{diagonal},\gtrless}(t_1, t_2) \tag{2.169} \\
 &= \pm (i\hbar)^2 G_{ij}^{\gtrless}(t_1, t_2) \sum_s w_{is}(t_1) \sum_t G_{st}^{\gtrless}(t_1, t_2) G_{ts}^{\lesseqgtr}(t_2, t_1) w_{tj}(t_2)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),1,1,\text{diagonal},\gtrless}(t_1, t_2) \tag{2.170} \\
 &= (i\hbar)^2 \sum_p w_{ip}(t_1) \sum_n G_{in}^{\gtrless}(t_1, t_2) w_{nj}(t_2) G_{np}^{\lesseqgtr}(t_2, t_1) G_{pj}^{\gtrless}(t_1, t_2).
 \end{aligned}$$

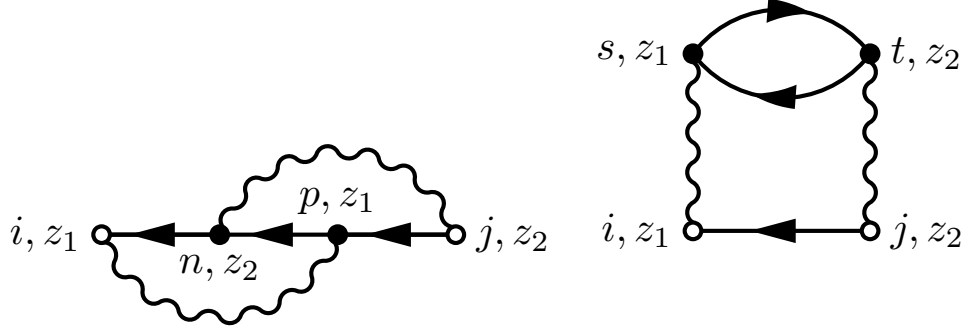


Figure 2.7: Selfconsistent second-order diagrams in diagonal basis. **Left:** Exchange diagram $\Sigma^{(2),1,1,\text{diagonal}}$. **Right:** Direct diagram, $\Sigma^{(2),2,0,\text{diagonal}}$.

The Feynman diagrams are shown in Fig. 2.7. The non-selfconsistent terms attain the form, cf. Eqs. (2.167) and (2.169),

$$\Sigma_{ij}^{(2),(2),2,0,0,\text{diagonal}}(z_1, z_2) \quad (2.171)$$

$$\equiv \Sigma_{ij}^{(2),2,0,\text{diagonal}}(z_1, z_2) (G \rightarrow G^{(0)})$$

and

$$\Sigma_{ij}^{(2),(2),1,0,1,\text{diagonal}}(z_1, z_2) \quad (2.172)$$

$$\equiv \Sigma_{ij}^{(2),1,1,\text{diagonal}}(z_1, z_2) (G \rightarrow G^{(0)})$$

as well as

$$\Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{diagonal}}(z_1, z_2) \quad (2.173)$$

$$= (\mathbf{i}\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} \sum_m w_{mi}(z_1)$$

$$\int_{\mathcal{C}} dz_3 \sum_p G_{mp}^{(0)}(z_1, z_3) G_{pm}^{(0)}(z_3, z_{1+}) \sum_r w_{rp}(z_3) G_{rr}^{(0)}(z_3, z_{3+})$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{H,0\},\{1,\{F,0\},0\},\text{diagonal}}(z_1, z_2) & (2.174) \\
 & = \pm (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} \sum_m w_{mi}(z_1) \\
 & \quad \int_{\mathcal{C}} dz_3 \sum_p G_{mp}^{(0)}(z_1, z_3) \sum_q w_{pq}(z_3) G_{pq}^{(0)}(z_3, z_{3+}) G_{qm}^{(0)}(z_3, z_{1+}).
 \end{aligned}$$

Further,

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{F,0\},\{1,\{H,0\},0\},\text{diagonal}}(z_1, z_2) & (2.175) \\
 & = \pm (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) w_{ij}(z_1) \\
 & \quad \int_{\mathcal{C}} dz_3 \sum_p G_{ip}^{(0)}(z_1, z_3) \sum_r w_{rp}(z_3) G_{rr}^{(0)}(z_3, z_{3+}) G_{pj}^{(0)}(z_3, z_{1+})
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{F,0\},\{1,\{F,0\},0\},\text{diagonal}}(z_1, z_2) & (2.176) \\
 & = (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) w_{ij}(z_1) \\
 & \quad \int_{\mathcal{C}} dz_3 \sum_p G_{ip}^{(0)}(z_1, z_3) \sum_q w_{pq}(z_3) G_{pq}^{(0)}(z_3, z_{3+}) G_{qj}^{(0)}(z_3, z_{1+}).
 \end{aligned}$$

The components read, cf. Eqs. (2.169) and (2.170),

$$\Sigma_{ij}^{(2),(2),2,0,0,\text{diagonal},\geq}(t_1, t_2) \equiv \Sigma_{ij}^{(2),2,0,\text{diagonal},\geq}(t_1, t_2) (G \rightarrow G^{(0)}), \quad (2.177)$$

$$\Sigma_{ij}^{(2),(2),1,0,1,\text{diagonal},\geq}(t_1, t_2) \equiv \Sigma_{ij}^{(2),1,1,\text{diagonal},\geq}(t_1, t_2) (G \rightarrow G^{(0)}) \quad (2.178)$$

as well as, cf. Eq. (2.163) to Eq. (2.167),

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{H,0\},\{1,\{H,0\},0\},\text{diagonal},\delta}(t_1) \tag{2.179} \\
 &= (i\hbar)^2 \delta_{ij} \sum_m w_{mi}(t_1) \left(\right. \\
 & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{mp}^{(0),>}(t_1, t_3) \sum_r w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pm}^{(0),<}(t_3, t_1) \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{mp}^{(0),<}(t_1, t_3) \sum_r w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pm}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{H,0\},\{1,\{F,0\},0\},\delta}(t_1) \tag{2.180} \\
 &= \pm (i\hbar)^2 \delta_{ij} \sum_m w_{mi}(t_1) \left(\right. \\
 & \quad \int_{t_0}^{t_1} dt_3 G_{mr}^{(0),>}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sm}^{(0),<}(t_3, t_1) \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 G_{mr}^{(0),<}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sm}^{(0),>}(t_3, t_1) \right).
 \end{aligned}$$

Further,

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{F,0\},\{1,\{H,0\},0\},\text{diagonal},\delta}(t_1, t_2) \tag{2.181} \\
 &= \pm (i\hbar)^2 w_{ji}(t_1) \left(\right. \\
 & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{ip}^{(0),>}(t_1, t_3) \sum_{rs} w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pj}^{(0),<}(t_3, t_1) \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{ip}^{(0),<}(t_1, t_3) \sum_{rs} w_{rp}(t_3) G_{rr}^{(0),<}(t_3, t_3) G_{pj}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{F,0\},\{1,\{F,0\},0\},\delta}(t_1) \tag{2.182} \\
 &= (i\hbar)^2 \sum_n w_{ji}(t_1) \left(\int_{t_0}^{t_1} dt_3 G_{ir}^{(0),<}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sj}^{(0),>}(t_3, t_1) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 G_{ir}^{(0),>}(t_1, t_3) \sum_{rs} w_{rs}(t_3) G_{rs}^{(0),<}(t_3, t_3) G_{sj}^{(0),<}(t_3, t_1) \right).
 \end{aligned}$$

2.7.1.2.2 Hubbard basis For the Hubbard basis, the selfconsistent second-order selfenergy contributions become

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,bosons}}(z_1, z_2) \tag{2.183} \\
 &= (i\hbar)^2 G_{i\alpha j\alpha}(z_1, z_2) U(z_1) \sum_{\epsilon} G_{i\epsilon j\epsilon}(z_1, z_2) G_{j\epsilon i\epsilon}(z_2, z_1) U(z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,bosons}}(z_1, z_2) \tag{2.184} \\
 &= (i\hbar)^2 U(z_1) G_{i\alpha j\alpha}(z_1, z_2) U(z_2) G_{j\alpha i\alpha}(z_2, z_1) G_{i\alpha j\alpha}(z_1, z_2),
 \end{aligned}$$

for bosons, and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,fermions}}(z_1, z_2) \tag{2.185} \\
 &= -(i\hbar)^2 G_{i\alpha j\alpha}(z_1, z_2) U(z_1) \sum_{\epsilon \neq \alpha} G_{i\epsilon j\epsilon}(z_1, z_2) G_{j\epsilon i\epsilon}(z_2, z_1) U(z_2)
 \end{aligned}$$

as well as

$$\Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,fermions}}(z_1, z_2) \equiv 0, \tag{2.186}$$

for fermions. The corresponding components read

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,bosons},\geq}(t_1, t_2) & \quad (2.187) \\ &= (\text{i}\hbar)^2 G_{i\alpha j\alpha}^{\geq}(t_1, t_2) U(t_1) \sum_{\epsilon} G_{i\epsilon j\epsilon}^{\geq}(t_1, t_2) G_{j\epsilon i\epsilon}^{\leq}(t_2, t_1) U(t_2) \end{aligned}$$

and

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,bosons},\geq}(t_1, t_2) & \quad (2.188) \\ &= (\text{i}\hbar)^2 U(t_1) G_{i\alpha j\alpha}^{\geq}(t_1, t_2) U(t_2) G_{j\alpha i\alpha}^{\leq}(t_2, t_1) G_{i\alpha j\alpha}^{\geq}(t_1, t_2), \end{aligned}$$

for bosons, and

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,fermions},\geq}(t_1, t_2) & \quad (2.189) \\ &= -(\text{i}\hbar)^2 G_{i\alpha j\alpha}^{\geq}(t_1, t_2) U(t_1) \sum_{\epsilon \neq \alpha} G_{i\epsilon j\epsilon}^{\geq}(t_1, t_2) G_{j\epsilon i\epsilon}^{\leq}(t_2, t_1) U(t_2) \end{aligned}$$

as well as

$$\Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,fermions},\geq}(t_1, t_2) \equiv 0, \quad (2.190)$$

for fermions. The non-selfconsistent contributions attain the form

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard,bosons}}(z_1, z_2) & \quad (2.191) \\ &\equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,bosons}}(z_1, z_2) (G \rightarrow G^{(0)}) \end{aligned}$$

and

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard,bosons}}(z_1, z_2) & \quad (2.192) \\ &\equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,bosons}}(z_1, z_2) (G \rightarrow G^{(0)}), \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{H,0\},\{1,\{H,0\},0\},\text{Hubbard,bosons}}(z_1, z_2) & (2.193) \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} \sum_{\epsilon} U(z_1) \\
 & \int_{\mathcal{C}} dz_3 \sum_p G_{i\epsilon p\epsilon}^{(0)}(z_1, z_3) G_{p\epsilon i\epsilon}^{(0)}(z_3, z_{1+}) \sum_{\zeta} U(z_3) G_{p\zeta p\zeta}^{(0)}(z_3, z_{3+})
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{H,0\},\{1,\{F,0\},0\},\text{Hubbard,bosons}}(z_1, z_2) & (2.194) \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} \sum_{\epsilon} U(z_1) \\
 & \int_{\mathcal{C}} dz_3 \sum_p G_{i\epsilon p\epsilon}^{(0)}(z_1, z_3) U(z_3) G_{p\epsilon p\epsilon}^{(0)}(z_3, z_{3+}) G_{p\epsilon i\epsilon}^{(0)}(z_3, z_{1+}).
 \end{aligned}$$

Further,

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{F,0\},\{1,\{H,0\},0\},\text{Hubbard,bosons}}(z_1, z_2) & (2.195) \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} U(z_1) \\
 & \int_{\mathcal{C}} dz_3 \sum_p G_{i\alpha p\alpha}^{(0)}(z_1, z_3) U(z_3) \sum_{\epsilon} G_{p\epsilon p\epsilon}^{(0)}(z_3, z_{3+}) G_{p\alpha i\alpha}^{(0)}(z_3, z_{1+})
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{F,0\},\{1,\{F,0\},0\},\text{Hubbard,bosons}}(z_1, z_2) & (2.196) \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} U(z_1) \\
 & \int_{\mathcal{C}} dz_3 \sum_p G_{i\alpha p\alpha}^{(0)}(z_1, z_3) U(z_3) G_{p\alpha p\alpha}^{(0)}(z_3, z_{3+}) G_{p\alpha i\alpha}^{(0)}(z_3, z_{1+}),
 \end{aligned}$$

for bosons, and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard,fermions}}(z_1, z_2) & (2.197) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,fermions}}(z_1, z_2) (G \rightarrow G^{(0)}) \end{aligned}$$

and

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard,fermions}}(z_1, z_2) & (2.198) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,fermions}}(z_1, z_2) (G \rightarrow G^{(0)}) \end{aligned}$$

as well as

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,fermions}}(z_1, z_2) & (2.199) \\ & = (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} \sum_{\epsilon \neq \alpha} U(z_1) \end{aligned}$$

$$\begin{aligned} & \int_{\mathcal{C}} dz_3 \sum_p G_{i\epsilon p\epsilon}^{(0)}(z_1, z_3) G_{p\epsilon i\epsilon}^{(0)}(z_3, z_{1+}) \sum_{\zeta \neq \epsilon} U(z_3) G_{p\zeta p\zeta}^{(0)}(z_3, z_{3+}), \\ & \Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard,fermions}}(z_1, z_2) \equiv 0 & (2.200) \end{aligned}$$

and

$$\Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,fermions}}(z_1, z_2) \equiv 0, \quad (2.201)$$

$$\Sigma_{i\alpha j\alpha}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard,fermions}}(z_1, z_2) \equiv 0, \quad (2.202)$$

for fermions. The components read

$$\begin{aligned} & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard,bosons},\geq}(t_1, t_2) & (2.203) \\ & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,bosons},\geq}(t_1, t_2) (G \rightarrow G^{(0)}), \end{aligned}$$

$$\Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard,bosons},\geq}(t_1, t_2) \quad (2.204)$$

$$\equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,bosons},\geq}(t_1, t_2) \left(G \rightarrow G^{(0)} \right),$$

$$\Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard,fermions},\geq}(t_1, t_2) \quad (2.205)$$

$$\equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,fermions},\geq}(t_1, t_2) \left(G \rightarrow G^{(0)} \right),$$

$$\Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard,fermions},\geq}(t_1, t_2) \quad (2.206)$$

$$\equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,fermions},\geq}(t_1, t_2) \left(G \rightarrow G^{(0)} \right)$$

as well as

$$\Sigma_{i\alpha j\alpha}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,bosons},\delta}(t_1, t_2) \quad (2.207)$$

$$= (i\hbar)^2 \delta_{ij} \sum_{\epsilon} U(t_1) \left($$

$$\int_{t_0}^{t_1} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),>}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),<}(t_3, t_1) \sum_{\zeta} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3)$$

$$+ \int_{t_1}^{t_0} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),<}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),>}(t_3, t_1) \sum_{\zeta} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \Big)$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{H,0\},\{1,\{F,0\},0\},\text{Hubbard,bosons},\delta}(t_1, t_2) \tag{2.208} \\
 &= (i\hbar)^2 \delta_{ij} \sum_{\epsilon} U(t_1) \left(\right. \\
 & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),>}(t_1, t_3) U(t_3) G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\epsilon i\alpha}^{(0),<}(t_3, t_1) \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),<}(t_1, t_3) U(t_3) G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\epsilon i\alpha}^{(0),>}(t_3, t_1) \right).
 \end{aligned}$$

Further,

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{F,0\},\{1,\{H,0\},0\},\text{Hubbard,bosons},\delta}(t_1, t_2) \tag{2.209} \\
 &= (i\hbar)^2 \delta_{ij} U(z_1) \left(\right. \\
 & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),>}(t_1, t_3) U(t_3) \sum_{\epsilon} G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),<}(t_3, t_1) \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),<}(t_1, t_3) U(t_3) \sum_{\epsilon} G_{p\epsilon p\epsilon}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{F,0\},\{1,\{F,0\},0\},\text{Hubbard,bosons},\delta}(t_1, t_2) \tag{2.210} \\
 &= (i\hbar)^2 \delta_{ij} U(t_1) \left(\right. \\
 & \quad \int_{t_0}^{t_1} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),>}(t_1, t_3) U(t_3) G_{p\alpha p\alpha}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),<}(t_3, t_1) \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\alpha p\alpha}^{(0),<}(t_1, t_3) U(t_3) G_{p\alpha p\alpha}^{(0),<}(t_3, t_3) G_{p\alpha i\alpha}^{(0),>}(t_3, t_1) \right)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),\{H,0\},\{1,\{H,0\},0\},\text{Hubbard,fermions},\delta}(t_1, t_2) \quad (2.211) \\
 &= (i\hbar)^2 \delta_{ij} \sum_{\epsilon \neq \alpha} U(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),>}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),<}(t_3, t_1) \sum_{\zeta \neq \epsilon} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\epsilon p\epsilon}^{(0),<}(t_1, t_3) G_{p\epsilon i\epsilon}^{(0),>}(t_3, t_1) \sum_{\zeta \neq \epsilon} U(t_3) G_{p\zeta p\zeta}^{(0),<}(t_3, t_3) \right).
 \end{aligned}$$

For spin-0 bosons and spin-1/2 fermions, respectively, the selfconsistent second-order contributions are given by

$$\begin{aligned}
 & \Sigma_{ij}^{(2),2,0,\text{Hubbard,bosons},0}(z_1, z_2) \quad (2.212) \\
 &= (i\hbar)^2 G_{ij}(z_1, z_2) U(z_1) G_{ij}(z_1, z_2) G_{ji}(z_2, z_1) U(z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(2),1,1,\text{Hubbard,bosons},0}(z_1, z_2) \quad (2.213) \\
 &= (i\hbar)^2 U(z_1) G_{ij}(z_1, z_2) U(z_2) G_{ji}(z_2, z_1) G_{ij}(z_1, z_2)
 \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{(2),2,0,\text{Hubbard,fermions},1/2}(z_1, z_2) \quad (2.214) \\
 &= -(i\hbar)^2 G_{i\downarrow(\uparrow)j\downarrow(\uparrow)}(z_1, z_2) U(z_1) G_{i\uparrow(\downarrow)j\uparrow(\downarrow)}(z_1, z_2) G_{j\uparrow(\downarrow)i\uparrow(\downarrow)}(z_2, z_1) U(z_2).
 \end{aligned}$$

The Feynman diagrams of the self-consistent second-order selfenergy contributions for spin-0 bosons and spin-1/2 fermions are depicted in Figs. 2.8 and 2.9. The

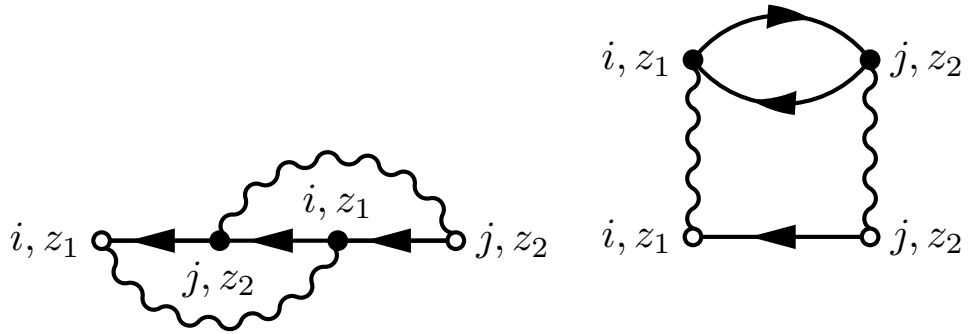


Figure 2.8: Selfconsistent second-order diagrams for spin-0 bosons in the Hubbard basis. **Left:** Exchange diagram $\Sigma^{(2),1,1,\text{Hubbard,bosons},0}$. **Right:** Direct diagram, $\Sigma^{(2),2,0,\text{Hubbard,bosons},0}$. Note that both diagrams coincide for the Hubbard basis.

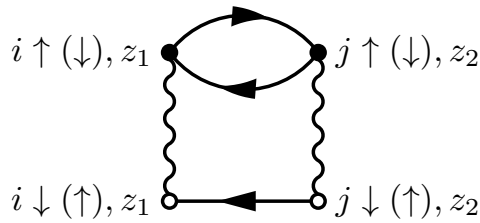


Figure 2.9: Selfconsistent second-order diagram for spin-1/2 fermions in the Hubbard basis, $\Sigma^{(2),2,0,\text{Hubbard,fermions},1/2}$.

corresponding components read

$$\begin{aligned} \Sigma_{ij}^{(2),2,0,\text{Hubbard,bosons},0,\geq}(t_1, t_2) & \quad (2.215) \\ &= (i\hbar)^2 G_{ij}^{\geq}(t_1, t_2) U(t_1) G_{ij}^{\geq}(t_1, t_2) G_{ji}^{\leq}(t_2, t_1) U(t_2) \end{aligned}$$

and

$$\begin{aligned} \Sigma_{ij}^{(2),1,1,\text{Hubbard,bosons},0,\geq}(t_1, t_2) & \quad (2.216) \\ &= (i\hbar)^2 U(t_1) G_{ij}^{\geq}(t_1, t_2) U(t_2) G_{ji}^{\leq}(t_2, t_1) G_{ij}^{\geq}(t_1, t_2) \end{aligned}$$

as well as

$$\begin{aligned} \Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{(2),2,0,\text{Hubbard,fermions},1/2,\geq}(t_1, t_2) & \quad (2.217) \\ &= -(i\hbar)^2 G_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{\geq}(t_1, t_2) U(t_1) G_{i\uparrow(\downarrow)j\uparrow(\downarrow)}^{\geq}(t_1, t_2) G_{j\uparrow(\downarrow)i\uparrow(\downarrow)}^{\leq}(t_2, t_1) U(t_2). \end{aligned}$$

For the non-selfconsistent terms, one has

$$\begin{aligned} \Sigma_{ij}^{(2),(2),2,0,0,\text{Hubbard,bosons},0}(z_1, z_2) & \quad (2.218) \\ &\equiv \Sigma_{ij}^{(2),2,0,\text{Hubbard,bosons},0}(z_1, z_2) (G \rightarrow G^{(0)}) \end{aligned}$$

and

$$\begin{aligned} \Sigma_{ij}^{(2),(2),1,0,1,\text{Hubbard,bosons},0}(z_1, z_2) & \quad (2.219) \\ &\equiv \Sigma_{ij}^{(2),1,1,\text{Hubbard,bosons},0}(z_1, z_2) (G \rightarrow G^{(0)}) \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,bosons},0}(z_1, z_2) & (2.220) \\
 & = \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard,bosons},0}(z_1, z_2) \\
 & = \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,bosons},0}(z_1, z_2) \\
 & = \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard,bosons},0}(z_1, z_2) \\
 & = (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} U(z_1) \\
 & \quad \int_{\mathcal{C}} dz_3 \sum_p G_{ip}^{(0)}(z_1, z_3) G_{pi}^{(0)}(z_3, z_{1+}) U(z_3) G_{pp}^{(0)}(z_3, z_{3+}),
 \end{aligned}$$

for spin-0 bosons, and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard,fermions},1/2}(z_1, z_2) & (2.221) \\
 & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,fermions},1/2}(z_1, z_2) (G \rightarrow G^{(0)})
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard,fermions},1/2}(z_1, z_2) & (2.222) \\
 & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,fermions},1/2}(z_1, z_2) (G \rightarrow G^{(0)})
 \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{i\uparrow j\uparrow}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,fermions}}(z_1, z_2) & (2.223) \\
 & = (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \delta_{ij} U(z_1) \\
 & \quad \int_{\mathcal{C}} dz_3 \sum_p G_{i\downarrow p\downarrow}^{(0)}(z_1, z_3) G_{p\downarrow i\downarrow}^{(0)}(z_3, z_{1+}) U(z_3) G_{p\uparrow p\uparrow}^{(0)}(z_3, z_{3+})
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{i\downarrow j\downarrow}^{(2),\{H,0\},\{1,\{H,0\},0\},\text{Hubbard,fermions}}(z_1, z_2) & (2.224) \\
 & = (i\hbar)^2 \delta_C(z_1, z_2) \delta_{ij} U(z_1) \\
 & \quad \int_C dz_3 \sum_p G_{i\uparrow p\uparrow}^{(0)}(z_1, z_3) G_{p\uparrow i\uparrow}^{(0)}(z_3, z_{1+}) U(z_3) G_{p\downarrow p\downarrow}^{(0)}(z_3, z_{3+}),
 \end{aligned}$$

for spin-1/2 fermions. The corresponding components read

$$\begin{aligned}
 & \Sigma_{ij}^{(2),(2),2,0,0,\text{Hubbard,bosons},0,\geq}(t_1, t_2) & (2.225) \\
 & \equiv \Sigma_{ij}^{(2),2,0,\text{Hubbard,bosons},0,\geq}(t_1, t_2) (G \rightarrow G^{(0)}),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{ij}^{(2),(2),1,0,1,\text{Hubbard,bosons},0,\geq}(t_1, t_2) & (2.226) \\
 & \equiv \Sigma_{ij}^{(2),1,1,\text{Hubbard,bosons},0,\geq}(t_1, t_2) (G \rightarrow G^{(0)}),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),(2),2,0,0,\text{Hubbard,fermions},1/2,\geq}(t_1, t_2) & (2.227) \\
 & \equiv \Sigma_{i\alpha j\alpha}^{(2),2,0,\text{Hubbard,fermions},1/2,\geq}(t_1, t_2) (G \rightarrow G^{(0)}),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{i\alpha j\alpha}^{(2),(2),1,0,1,\text{Hubbard,fermions},1/2,\geq}(t_1, t_2) & (2.228) \\
 & \equiv \Sigma_{i\alpha j\alpha}^{(2),1,1,\text{Hubbard,fermions},1/2,\geq}(t_1, t_2) (G \rightarrow G^{(0)})
 \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,bosons},0,\delta}(t_1, t_2) & (2.229) \\
 &= \Sigma_{ij}^{(2),\{\text{H},0\},\{1,\{\text{F},0\},0\},\text{Hubbard,bosons},0,\delta}(t_1, t_2) \\
 &= \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,bosons},0,\delta}(t_1, t_2) \\
 &= \Sigma_{ij}^{(2),\{\text{F},0\},\{1,\{\text{F},0\},0\},\text{Hubbard,bosons},0,\delta}(t_1, t_2) \\
 &= (i\hbar)^2 \delta_{ij} U(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_p G_{ip}^{(0),>}(t_1, t_3) G_{pi}^{(0),<}(t_3, t_1) U(t_3) G_{pp}^{(0),<}(t_3, t_3) \right. \\
 &\quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{ip}^{(0),<}(t_1, t_3) G_{pi}^{(0),>}(t_3, t_1) U(t_3) G_{pp}^{(0),<}(t_3, t_3) \right),
 \end{aligned}$$

for spin-0 bosons, and

$$\begin{aligned}
 & \Sigma_{i\uparrow j\uparrow}^{(2),\{\text{H},0\},\{1,\{\text{H},0\},0\},\text{Hubbard,fermions},1/2,\delta}(t_1, t_2) & (2.230) \\
 &= (i\hbar)^2 \delta_{ij} U(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_p G_{i\downarrow p\downarrow}^{(0),>}(t_1, t_3) G_{p\downarrow i\downarrow}^{(0),<}(t_3, t_1) U(t_3) G_{p\uparrow p\uparrow}^{(0),<}(t_3, t_3) \right. \\
 &\quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\downarrow p\downarrow}^{(0),<}(t_1, t_3) G_{p\downarrow i\downarrow}^{(0),>}(t_3, t_1) U(t_3) G_{p\uparrow p\uparrow}^{(0),<}(t_3, t_3) \right)
 \end{aligned}$$

as well as

$$\begin{aligned}
 & \Sigma_{i\downarrow j\downarrow}^{(2),\{H,0\},\{1,\{H,0\},0\},\text{Hubbard,fermions},1/2,\delta}(t_1, t_2) \\
 &= (i\hbar)^2 \delta_{ij} U(t_1) \left(\int_{t_0}^{t_1} dt_3 \sum_p G_{i\uparrow p\uparrow}^{(0),>}(t_1, t_3) G_{p\uparrow i\uparrow}^{(0),<}(t_3, t_1) U(t_3) G_{p\downarrow p\downarrow}^{(0),<}(t_3, t_3) \right. \\
 & \quad \left. + \int_{t_1}^{t_0} dt_3 \sum_p G_{i\uparrow p\uparrow}^{(0),<}(t_1, t_3) G_{p\uparrow i\uparrow}^{(0),>}(t_3, t_1) U(t_3) G_{p\downarrow p\downarrow}^{(0),<}(t_3, t_3) \right).
 \end{aligned} \tag{2.231}$$

2.7.1.3 Third-order terms

The structure of the selfconsistent third-order contributions to the selfenergy can again be deduced from Eq. (2.98). A total order of three can be achieved with the following classes,

$$\Sigma^{(3),3,0} = \Sigma^{\text{xc}}(W^{(3)}, \Gamma^{(0)}), \tag{2.232}$$

$$\Sigma^{(3),2,1} = \Sigma^{\text{xc}}(W^{(2)}, \Gamma^{(1)}), \tag{2.233}$$

$$\Sigma^{(3),1,2} = \Sigma^{\text{xc}}(W^{(1)}, \Gamma^{(2)}). \tag{2.234}$$

For the first class, in turn, one has to compute the possible contributions to $W^{(3)}$, which are

$$W^{(3),0,2} = W^{\text{screened}}(P^{(0)}, W^{(2)}), \tag{2.235}$$

$$W^{(3),1,1} = W^{\text{screened}}(P^{(1)}, W^{(1)}), \tag{2.236}$$

Using Eq. (2.101), one finds

$$\begin{aligned}
 & W_{ijkl}^{(3),0,2}(z_1, z_2) \\
 &= \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} (\pm i\hbar G_{np}(z_1, z_3) G_{qm}(z_3, z_1)) W_{pqkq}^{(2)}(z_3, z_2).
 \end{aligned} \tag{2.237}$$

Employing Eq. (2.138) yields

$$\begin{aligned}
 W_{ijkl}^{(3),0,2}(z_1, z_2) & \quad (2.238) \\
 &= \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} (\pm i\hbar G_{np}(z_1, z_3) G_{qm}(z_3, z_1)) \\
 & \quad \left(\pm i\hbar \sum_{rs} w_{prsq}(z_3) \sum_{tu} G_{st}(z_3, z_2) G_{ur}(z_2, z_3) w_{tjku}(z_2) \right).
 \end{aligned}$$

Evaluating and reordering, one has

$$\begin{aligned}
 W_{ijkl}^{(3),0,2}(z_1, z_2) & \quad (2.239) \\
 &= (i\hbar)^2 \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{np}(z_1, z_3) G_{qm}(z_3, z_1) \sum_{rs} w_{prsq}(z_3) \\
 & \quad \sum_{tu} G_{st}(z_3, z_2) G_{ur}(z_2, z_3) w_{tjku}(z_2).
 \end{aligned}$$

With this, the first term of the first third-order selfenergy class, $\Sigma^{(3),3,0}$, becomes

$$\begin{aligned}
 \Sigma_{ij}^{(3),\{3;0,2\},0}(z_1, z_2) & \quad (2.240) \\
 &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(3),0,2}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(0)}(z_4, z_2, z_3).
 \end{aligned}$$

Using Eq. (2.107), one has

$$\begin{aligned}
 \Sigma_{ij}^{(3),\{3;0,2\},0}(z_1, z_2) & \quad (2.241) \\
 &= (i\hbar)^3 \sum_{mn} G_{mn}(z_1, z_2) \sum_{rs} w_{irsm}(z_1) \int_{\mathcal{C}} dz_3 \sum_{tu} G_{st}(z_1, z_3) G_{ur}(z_3, z_1) \\
 & \quad \sum_{vw} w_{tvwu}(z_3) \sum_{xy} G_{wx}(z_3, z_2) G_{yv}(z_2, z_3) w_{xnjy}(z_2).
 \end{aligned}$$

For the second class of the interaction, $W^{(3),1,1}$, the first-order contribution to the polarization is needed, which is given by, cf. Eqs. (2.102) and (2.148),

$$\begin{aligned} P_{ijkl}^{(1)}(z_1, z_2) &= P_{ijkl}(z_1, z_2) \left(\Gamma^{(1)} \right) \\ &= \pm i\hbar \int_{\mathcal{C}} dz_3 \sum_m G_{im}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{nl}(z_4, z_1) \Gamma_{mjkn}^{(1)}(z_3, z_4, z_2). \end{aligned} \quad (2.242)$$

Employing Eq. (2.148), one arrives at

$$\begin{aligned} P_{ijkl}^{(1)}(z_1, z_2) & \\ &= \pm (i\hbar)^2 \int_{\mathcal{C}} dz_3 \sum_m G_{im}(z_1, z_3) \sum_n G_{nl}(z_3, z_1) \\ & \quad \sum_{pq} w_{mqnp}(z_3) G_{pk}(z_3, z_2) G_{jq}(z_2, z_3). \end{aligned} \quad (2.243)$$

Inserting this result back, one finds, using Eq. (2.101),

$$\begin{aligned} W_{ijkl}^{(3),1,1}(z_1, z_2) &= \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} P_{nqpm}^{(1)}(z_1, z_3) W_{pjkl}^{(1)}(z_3, z_2) \\ &= \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} \left(\pm (i\hbar)^2 \int_{\mathcal{C}} dz_4 \sum_r G_{nr}(z_1, z_4) \sum_s G_{sm}(z_4, z_1) \right. \\ & \quad \left. \sum_{tu} w_{rust}(z_4) G_{tp}(z_4, z_3) G_{qu}(z_3, z_4) \right) \delta_{\mathcal{C}}(z_3, z_2) w_{pjkl}(z_2). \end{aligned} \quad (2.244)$$

After reordering, one has

$$\begin{aligned} W_{ijkl}^{(3),1,1}(z_1, z_2) & \\ &= \pm (i\hbar)^2 \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_r G_{nr}(z_1, z_3) \sum_s G_{sm}(z_3, z_1) \\ & \quad \sum_{tu} w_{rust}(z_3) \sum_{pq} G_{tp}(z_3, z_2) G_{qu}(z_2, z_3) w_{pjkl}(z_2). \end{aligned} \quad (2.245)$$

With these results, the second term of the class $\Sigma^{(3),3,0}$ is found, using Eq. (2.98),

$$\begin{aligned} \Sigma_{ij}^{(3),\{3;1,1\},0}(z_1, z_2) & \quad (2.246) \\ &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(3),1,1}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(0)}(z_4, z_2, z_3). \end{aligned}$$

Using Eq. (2.107), one finds

$$\begin{aligned} \Sigma_{ij}^{(3),\{3;1,1\},0}(z_1, z_2) & \quad (2.247) \\ &= \pm (i\hbar)^3 \sum_{mn} G_{mn}(z_1, z_2) \sum_{rs} w_{irsm}(z_1) \int_{\mathcal{C}} dz_3 \sum_t G_{st}(z_1, z_3) \sum_u G_{ur}(z_3, z_1) \\ & \quad \sum_{vw} w_{twuv}(z_3) \sum_{xy} G_{vx}(z_3, z_2) G_{yw}(z_2, z_3) w_{xnjy}(z_2). \end{aligned}$$

Continuing with the second class $\Sigma^{(3),2,1}$, it is directly worked out by combining Eqs. (2.138) and (2.148),

$$\begin{aligned} \Sigma_{ij}^{(3),2,1}(z_1, z_2) &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(2)}(z_1, z_3) \quad (2.248) \\ & \quad \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(1)}(z_4, z_2, z_3). \end{aligned}$$

Inserting Eq. (2.148) yields

$$\begin{aligned} \Sigma_{ij}^{(3),2,1}(z_1, z_2) & \quad (2.249) \\ &= \pm (i\hbar)^3 \int_{\mathcal{C}} dz_3 \sum_{mrs} w_{irsm}(z_1) \sum_{tu} G_{st}(z_1, z_3) G_{ur}(z_3, z_1) \sum_{pq} w_{tpqu}(z_3) \\ & \quad \sum_n G_{mn}(z_1, z_2) \sum_{vw} w_{nwjv}(z_2) G_{vp}(z_2, z_3) G_{qw}(z_3, z_2). \end{aligned}$$

For the third class $\Sigma^{(3),1,2}$, the second-order contributions to the vertex $\Gamma^{(2)}$ have to be computed. The structural classes to consider are

$$\Gamma^{(2),1,1} = \Gamma\left(\delta\Sigma^{\text{xc},(1)}/\delta G, \Gamma^{(1)}\right), \quad (2.250)$$

$$\Gamma^{(2),2,0} = \Gamma\left(\delta\Sigma^{\text{xc},(2)}/\delta G, \Gamma^{(0)}\right). \quad (2.251)$$

For the single contribution to the class $\Gamma^{(2),1,1}$, one finds, employing Eqs. (2.144) and (2.148),

$$\begin{aligned} \Gamma_{ijkl}^{(2),1,1}(z_1, z_2, z_3) &= \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta\Sigma_{il}^{\text{xc},(1)}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\ &\quad \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pj kq}^{(1)}(z_6, z_7, z_3). \end{aligned} \quad (2.252)$$

Evaluating the derivative yields

$$\begin{aligned} \Gamma_{ijkl}^{(2),1,1}(z_1, z_2, z_3) & \quad (2.253) \\ &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{inlm}(z_1) \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_1, z_6) \\ &\quad \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_1) \Gamma_{pj kq}^{(1)}(z_6, z_7, z_3). \end{aligned}$$

Employing Eq. (2.148), one finds

$$\begin{aligned} \Gamma_{ijkl}^{(2),1,1}(z_1, z_2, z_3) & \quad (2.254) \\ &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{inlm}(z_1) \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_1, z_6) \\ &\quad \sum_q G_{qn}(z_6, z_1) \sum_{rs} w_{psqr}(z_6) G_{rk}(z_6, z_3) G_{js}(z_3, z_6). \end{aligned}$$

This enables the computation of $\Sigma^{(3),1,\{2;1,1\}}$ with Eqs. (2.98) and (2.106),

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;1,1\}}(z_1, z_2) & \quad (2.255) \\ &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1}(z_4, z_2, z_3) \\ &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1}(z_4, z_2, z_1). \end{aligned}$$

Using Eq. (2.254), one arrives at

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;1,1\}}(z_1, z_2) & \quad (2.256) \\ &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \sum_n G_{mn}(z_1, z_2) \sum_{rs} w_{nsjr}(z_2) \int_{\mathcal{C}} dz_3 \sum_t G_{rt}(z_2, z_3) \\ & \quad \sum_u G_{us}(z_3, z_2) \sum_{vw} w_{twuv}(z_3) G_{vp}(z_3, z_1) G_{qw}(z_1, z_3). \end{aligned}$$

The vertex class $\Gamma^{(2),2,0}$ has six members stemming from the derivatives with respect to each of the three Green functions in both second-order contributions to $\Sigma^{(2)}$, cf. Eqs. (2.141) and (2.150),

$$\Gamma^{(2),\{2;2,0\},0} = \Gamma\left(\delta\Sigma^{(2),2,0}/\delta G, \Gamma^{(0)}\right), \quad (2.257)$$

$$\Gamma^{(2),\{2;1,1\},0} = \Gamma\left(\delta\Sigma^{(2),1,1}/\delta G, \Gamma^{(0)}\right). \quad (2.258)$$

For the first terms, one finds

$$\begin{aligned} \Gamma_{ijkl}^{(2),\{2;2,0\},0}(z_1, z_2, z_3) &= \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta\Sigma_{il}^{(2),2,0}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\ & \quad \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pjkl}^{(0)}(z_6, z_7, z_3) \quad (2.259) \\ &= \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta\Sigma_{il}^{(2),2,0}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} G_{mk}(z_4, z_3) G_{jn}(z_3, z_5). \end{aligned}$$

Inserting Eq. (2.141), the term attains the form

$$\Gamma_{ijkl}^{(2),\{2;2,0\},0}(z_1, z_2, z_3) = \pm(i\hbar)^2 \int_{\mathcal{C}} dz_4 dz_5 \quad (2.260)$$

$$\sum_{mn} \frac{\delta \left(\sum_{pq} G_{pq}(z_1, z_2) \sum_{st} G_{st}(z_1, z_2) \sum_r w_{irsp}(z_1) \sum_u w_{tqlu}(z_2) G_{ur}(z_2, z_1) \right)}{\delta G_{mn}(z_4, z_5)}$$

$$G_{mk}(z_4, z_3) G_{jn}(z_3, z_5).$$

Evaluating the derivative, one has

$$\Gamma_{ijkl}^{(2),\{2;2,0\},0}(z_1, z_2, z_3) = \Gamma_{ijkl}^{(2),\{2;2,0\},0,a}(z_1, z_2, z_3) \quad (2.261)$$

$$+ \Gamma_{ijkl}^{(2),\{2;2,0\},0,b}(z_1, z_2, z_3) + \Gamma_{ijkl}^{(2),\{2;2,0\},0,c}(z_1, z_2, z_3),$$

with

$$\Gamma_{ijkl}^{(2),\{2;2,0\},0,a}(z_1, z_2, z_3) \quad (2.262)$$

$$= \pm(i\hbar)^2 \sum_{mn} \sum_{st} G_{st}(z_1, z_2) \sum_r w_{irsm}(z_1)$$

$$\sum_u w_{tnlu}(z_2) G_{ur}(z_2, z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2)$$

and

$$\Gamma_{ijkl}^{(2),\{2;2,0\},0,b}(z_1, z_2, z_3) \quad (2.263)$$

$$\pm(i\hbar)^2 \sum_{mn} \sum_{pq} G_{pq}(z_1, z_2) \sum_r w_{irmp}(z_1)$$

$$\sum_u w_{nqlu}(z_2) G_{ur}(z_2, z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2)$$

as well as

$$\begin{aligned}
 & \Gamma_{ijkl}^{(2),\{2;2,0\},0,c}(z_1, z_2, z_3) \\
 & \pm (i\hbar)^2 \sum_{mn} \sum_{pq} G_{pq}(z_1, z_2) \sum_{st} G_{st}(z_1, z_2) \\
 & w_{insp}(z_1) w_{tqlm}(z_2) G_{mk}(z_2, z_3) G_{jn}(z_3, z_1).
 \end{aligned} \tag{2.264}$$

Similarly, one finds

$$\begin{aligned}
 \Gamma_{ijkl}^{(2),\{2;1,1\},0}(z_1, z_2, z_3) &= \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{(2),1,1}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\
 & \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pjkl}^{(0)}(z_6, z_7, z_3).
 \end{aligned} \tag{2.265}$$

Inserting Eq. (2.150) yields

$$\begin{aligned}
 \Gamma_{ijkl}^{(2),\{2;1,1\},0}(z_1, z_2, z_3) &= (i\hbar)^2 \int_{\mathcal{C}} dz_4 dz_5 \\
 & \sum_{mn} \frac{\delta \left(\sum_{prs} w_{irsp}(z_1) \sum_q G_{pq}(z_1, z_2) \sum_{tu} w_{qult}(z_2) G_{tr}(z_2, z_1) G_{su}(z_1, z_2) \right)}{\delta G_{mn}(z_4, z_5)} \\
 & G_{mk}(z_4, z_3) G_{jn}(z_3, z_5),
 \end{aligned} \tag{2.266}$$

which, after evaluation of the derivative, yields

$$\begin{aligned}
 \Gamma_{ijkl}^{(2),\{2;1,1\},0}(z_1, z_2, z_3) &= \Gamma_{ijkl}^{(2),\{2;1,1\},0,a}(z_1, z_2, z_3) \\
 & + \Gamma_{ijkl}^{(2),\{2;1,1\},0,b}(z_1, z_2, z_3) + \Gamma_{ijkl}^{(2),\{2;1,1\},0,c}(z_1, z_2, z_3),
 \end{aligned} \tag{2.267}$$

with

$$\begin{aligned}
 & \Gamma_{ijkl}^{(2),\{2;1,1\},0,a}(z_1, z_2, z_3) & (2.268) \\
 &= (i\hbar)^2 \sum_{mn} \sum_{rs} w_{irsm}(z_1) \sum_{tu} w_{nult}(z_2) G_{tr}(z_2, z_1) \\
 & \quad G_{su}(z_1, z_2) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Gamma_{ijkl}^{(2),\{2;1,1\},0,b}(z_1, z_2, z_3) & (2.269) \\
 &+ (i\hbar)^2 \sum_{mn} \sum_{ps} w_{inps}(z_1) \sum_q G_{pq}(z_1, z_2) \sum_u w_{qulm}(z_2) \\
 & \quad G_{su}(z_1, z_2) G_{mk}(z_2, z_3) G_{jn}(z_3, z_1)
 \end{aligned}$$

as well as

$$\begin{aligned}
 & \Gamma_{ijkl}^{(2),\{2;1,1\},0,c}(z_1, z_2, z_3) & (2.270) \\
 &+ (i\hbar)^2 \sum_{mn} \sum_{pr} w_{irmp}(z_1) \sum_q G_{pq}(z_1, z_2) \sum_t w_{qnlm}(z_2) \\
 & \quad G_{tr}(z_2, z_1) G_{mk}(z_1, z_3) G_{jn}(z_3, z_2).
 \end{aligned}$$

With this result, the corresponding selfenergy terms can be computed,

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;2,0,a\}}(z_1, z_2) & (2.271) \\
 &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),2,0,a}(z_4, z_2, z_3) \\
 &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),2,0,a}(z_4, z_2, z_1).
 \end{aligned}$$

Inserting Eq. (2.262), one arrives at

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;2,0,a\}}(z_1, z_2) &= \pm (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \\ &\int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rsuv} G_{uv}(z_4, z_2) \sum_t w_{ntur}(z_4) \\ &\sum_w w_{vsjw}(z_2) G_{wt}(z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (2.272)$$

For the second term, one has

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;2,0,b\}}(z_1, z_2) \\ = i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),2,0,b}(z_4, z_2, z_1). \end{aligned} \quad (2.273)$$

Using Eq. (2.263) yields

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;2,0,b\}}(z_1, z_2) \\ = \pm (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tu} G_{tu}(z_4, z_2) \\ \sum_v w_{nvrt}(z_4) \sum_w w_{sujw}(z_2) G_{wv}(z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (2.274)$$

The third term is given by

$$\begin{aligned} \Sigma_{ij}^{(3),1,\{2;2,0,c\}}(z_1, z_2) \\ = i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),2,0,c}(z_4, z_2, z_1). \end{aligned} \quad (2.275)$$

With Eq. (2.264), one finds

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;2,0,c\}}(z_1, z_2) \tag{2.276} \\
 &= \pm (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tu} G_{tu}(z_4, z_2) \\
 & \quad \sum_{vw} G_{vw}(z_4, z_2) w_{nsvt}(z_4) w_{wujr}(z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_4).
 \end{aligned}$$

For the other class, one has

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,a\}}(z_1, z_2) \tag{2.277} \\
 &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}^{(1)}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1,a}(z_4, z_2, z_3) \\
 &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1,a}(z_4, z_2, z_1).
 \end{aligned}$$

Inserting Eq. (2.268) yields

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,a\}}(z_1, z_2) \tag{2.278} \\
 &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tu} w_{ntur}(z_4) \\
 & \quad \sum_{vw} w_{swjv}(z_2) G_{vt}(z_2, z_4) G_{uw}(z_4, z_2) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2).
 \end{aligned}$$

Similarly, the second term reads

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,b\}}(z_1, z_2) \tag{2.279} \\
 &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1,b}(z_4, z_2, z_1).
 \end{aligned}$$

With Eq. (2.269), one has

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,b\}}(z_1, z_2) \tag{2.280} \\
 &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tv} w_{nsvt}(z_4) \\
 & \quad \sum_u G_{tu}(z_4, z_2) \sum_w w_{uwjr}(z_2) G_{vw}(z_4, z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_4).
 \end{aligned}$$

For the third term, one finds

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,c\}}(z_1, z_2) \tag{2.281} \\
 &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(2),1,1,c}(z_4, z_2, z_1).
 \end{aligned}$$

Employing Eq. (2.270), one arrives at

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,c\}}(z_1, z_2) \tag{2.282} \\
 &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \sum_{rs} \sum_{tv} w_{nrvt}(z_4) \\
 & \quad \sum_u G_{tu}(z_4, z_2) \sum_w w_{usjw}(z_2) G_{wv}(z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_2).
 \end{aligned}$$

The \gtrsim -components of all third-order terms can be computed in a generic fashion, splitting all integrals at the points where the arguments of each Green function change their relative ordering on the contour. As an example, for $\Sigma_{ij}^{(3),1,\{2;2,0,b\}}(z_1, z_2)$, one has, cf. Eq. (2.74),

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;2,0,b\},<}(t_1, t_2) = \Sigma_{ij}^{(3),1,\{2;2,0,b\},<}(z_{1-}, z_{2+}) \tag{2.283} \\
 &= \pm (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_{1-}) \\
 & \quad \left(I_{mpq}^{1,<}(z_{1-}, z_{2+}) + I_{mpq}^{2,<}(z_{1-}, z_{2+}) + I_{mpq}^{3,<}(z_{1-}, z_{2+}) \right),
 \end{aligned}$$

with

$$I_{mpq}^{1,<}(z_{1-}, z_{2+}) = \int_{z_{0-}}^{z_{1-}} dz_4 \sum_n G_{mn}^>(z_{1-}, z_4) \quad (2.284)$$

$$\sum_{rs} \sum_{tu} G_{tu}^<(z_4, z_{2+}) \sum_v w_{nvrt}(z_4)$$

$$\sum_w w_{sujw}(z_{2+}) G_{wv}^>(z_{2+}, z_4) G_{rp}^<(z_4, z_{1-}) G_{qs}^<(z_{1-}, z_{2+})$$

and

$$I_{mpq}^{2,<}(z_{1-}, z_{2+}) = \int_{z_{1-}}^{z_{2+}} dz_4 \sum_n G_{mn}^<(z_{1-}, z_4) \quad (2.285)$$

$$\sum_{rs} \sum_{tu} G_{tu}^<(z_4, z_{2+}) \sum_v w_{nvrt}(z_4)$$

$$\sum_w w_{sujw}(z_{2+}) G_{wv}^>(z_{2+}, z_4) G_{rp}^>(z_4, z_{1-}) G_{qs}^<(z_{1-}, z_{2+})$$

as well as

$$I_{mpq}^{3,<}(z_{1-}, z_{2+}) = \int_{z_{2+}}^{z_{0+}} dz_4 \sum_n G_{mn}^<(z_{1-}, z_4) \quad (2.286)$$

$$\sum_{rs} \sum_{tu} G_{tu}^>(z_4, z_{2+}) \sum_v w_{nvrt}(z_4)$$

$$\sum_w w_{sujw}(z_{2+}) G_{wv}^<(z_{2+}, z_4) G_{rp}^>(z_4, z_{1-}) G_{qs}^<(z_{1-}, z_{2+}).$$

Transforming to real-time integrals,

$$\Sigma_{ij}^{(3),1,\{2;2,0,b\},<}(t_1, t_2) = \pm (i\hbar)^3 \sum_{mpq} w_{ipqm}(t_1) \quad (2.287)$$

$$\left(I_{mpq}^{1,<}(t_1, t_2) + I_{mpq}^{2,<}(t_1, t_2) + I_{mpq}^{3,<}(t_1, t_2) \right),$$

with

$$\begin{aligned}
 I_{mpq}^{1,<}(t_1, t_2) &= \int_{t_0}^{t_1} dt_4 \sum_n G_{mn}^>(t_1, t_4) \\
 &\sum_{rs} \sum_{tu} G_{tu}^<(t_4, t_2) \sum_v w_{nvrt}(t_4) \\
 &\sum_w w_{sujw}(t_2) G_{wv}^>(t_2, t_4) G_{rp}^<(t_4, t_1) G_{qs}^<(t_1, t_2)
 \end{aligned} \tag{2.288}$$

and

$$\begin{aligned}
 I_{mpq}^{2,<}(t_1, t_2) &= \int_{t_1}^{t_2} dt_4 \sum_n G_{mn}^<(t_1, t_4) \\
 &\sum_{rs} \sum_{tu} G_{tu}^<(t_4, t_2) \sum_v w_{nvrt}(t_4) \\
 &\sum_w w_{sujw}(t_2) G_{wv}^>(t_2, t_4) G_{rp}^>(t_4, t_1) G_{qs}^<(t_1, t_2)
 \end{aligned} \tag{2.289}$$

as well as

$$\begin{aligned}
 I_{mpq}^{3,<}(t_1, t_2) &= \int_{t_2}^{t_0} dt_4 \sum_n G_{mn}^<(t_1, t_4) \\
 &\sum_{rs} \sum_{tu} G_{tu}^>(t_4, t_2) \sum_v w_{nvrt}(t_4) \\
 &\sum_w w_{sujw}(t_2) G_{wv}^<(t_2, t_4) G_{rp}^>(t_4, t_1) G_{qs}^<(t_1, t_2).
 \end{aligned} \tag{2.290}$$

For the greater component, one finds

$$\begin{aligned}
 \Sigma_{ij}^{(3),1,\{2;2,0,b\},>}(t_1, t_2) &= \Sigma_{ij}^{(3),1,\{2;2,0,b\},>}(z_{1+}, z_{2-}) \\
 &= \pm(i\hbar)^3 \sum_{mpq} w_{ipqm}(z_{1+}) \\
 &\left(I_{mpq}^{1,>}(z_{1+}, z_{2-}) + I_{mpq}^{2,>}(z_{1+}, z_{2-}) + I_{mpq}^{3,>}(z_{1+}, z_{2-}) \right),
 \end{aligned} \tag{2.291}$$

with

$$I_{mpq}^{1,>}(z_{1+}, z_{2-}) = \int_{z_{0-}}^{z_{2-}} dz_4 \sum_n G_{mn}^{>}(z_{1+}, z_4) \quad (2.292)$$

$$\sum_{rs} \sum_{tu} G_{tu}^{<}(z_4, z_{2-}) \sum_v w_{nvrt}(z_4)$$

$$\sum_w w_{sujw}(z_{2-}) G_{wv}^{>}(z_{2-}, z_4) G_{rp}^{<}(z_4, z_{1+}) G_{qs}^{>}(z_{1+}, z_{2-})$$

and

$$I_{mpq}^{2,>}(z_{1+}, z_{2-}) = \int_{z_{2-}}^{z_{1+}} dz_4 \sum_n G_{mn}^{>}(z_{1+}, z_4) \quad (2.293)$$

$$\sum_{rs} \sum_{tu} G_{tu}^{>}(z_4, z_{2-}) \sum_v w_{nvrt}(z_4)$$

$$\sum_w w_{sujw}(z_{2-}) G_{wv}^{<}(z_{2-}, z_4) G_{rp}^{<}(z_4, z_{1+}) G_{qs}^{>}(z_{1+}, z_{2-})$$

as well as

$$I_{mpq}^{3,>}(z_{1+}, z_{2-}) = \int_{z_{1+}}^{z_{0+}} dz_4 \sum_n G_{mn}^{<}(z_{1+}, z_4) \quad (2.294)$$

$$\sum_{rs} \sum_{tu} G_{tu}^{>}(z_4, z_{2-}) \sum_v w_{nvrt}(z_4)$$

$$\sum_w w_{sujw}(z_{2-}) G_{wv}^{<}(z_{2-}, z_4) G_{rp}^{>}(z_4, z_{1+}) G_{qs}^{>}(z_{1+}, z_{2-}).$$

Transforming to real-time integrals,

$$\Sigma_{ij}^{(3),1,\{2;2,0,b\},>}(t_1, t_2) = \pm (i\hbar)^3 \sum_{mpq} w_{ipqm}(t_1) \quad (2.295)$$

$$\left(I_{mpq}^{1,>}(t_1, t_2) + I_{mpq}^{2,>}(t_1, t_2) + I_{mpq}^{3,>}(t_1, t_2) \right),$$

with

$$\begin{aligned}
 I_{mpq}^{1,>}(t_1, t_2) &= \int_{t_0}^{t_2} dt_4 \sum_n G_{mn}^>(t_1, t_4) \\
 &\sum_{rs} \sum_{tu} G_{tu}^<(t_4, t_2) \sum_v w_{nvrt}(t_4) \\
 &\sum_w w_{sujw}(t_2) G_{wv}^>(t_2, t_4) G_{rp}^<(t_4, t_1) G_{qs}^>(t_1, t_2)
 \end{aligned} \tag{2.296}$$

and

$$\begin{aligned}
 I_{mpq}^{2,>}(t_1, t_2) &= \int_{t_2}^{t_1} dt_4 \sum_n G_{mn}^>(t_1, t_4) \\
 &\sum_{rs} \sum_{tu} G_{tu}^>(t_4, t_2) \sum_v w_{nvrt}(t_4) \\
 &\sum_w w_{sujw}(t_2) G_{wv}^<(t_2, t_4) G_{rp}^<(t_4, t_1) G_{qs}^>(t_1, t_2)
 \end{aligned} \tag{2.297}$$

as well as

$$\begin{aligned}
 I_{mpq}^{3,>}(t_1, t_2) &= \int_{t_1}^{t_0} dt_4 \sum_n G_{mn}^<(t_1, t_4) \\
 &\sum_{rs} \sum_{tu} G_{tu}^>(t_4, t_2) \sum_v w_{nvrt}(t_4) \\
 &\sum_w w_{sujw}(t_2) G_{wv}^<(t_2, t_4) G_{rp}^>(t_4, t_1) G_{qs}^>(t_1, t_2).
 \end{aligned} \tag{2.298}$$

The additional non-selfconsistent diagrams are of either of the structures

$$\begin{aligned}
 \Sigma^{(3)}(G \longrightarrow G^{(0)}) &\quad (10 \text{ terms}) \\
 \Sigma^{(2)}(G^{(0)} \longrightarrow G^{(0)} \Sigma^{(1)} G^{(0)}) &\quad (6 \cdot 2 = 12 \text{ terms}) \\
 \Sigma^{\text{H}}/\Sigma^{\text{F}}(G^{(0)} \longrightarrow G^{(0)} \Sigma^{(2)} G^{(0)}) &\quad (2 \cdot 6 = 12 \text{ terms}) \\
 \Sigma^{\text{H}}/\Sigma^{\text{F}}(G^{(0)} \longrightarrow G^{(0)} \Sigma^{(1)} G^{(0)} \Sigma^{(1)} G^{(0)}) &\quad (2 \cdot 2 \cdot 2 = 8 \text{ terms})
 \end{aligned}$$

This makes a total of 42 non-selfconsistent third-order terms.

2.7.1.3.1 Diagonal basis In a diagonal basis, the selfconsistent third-order selfenergy contributions become

$$\begin{aligned}
 & \Sigma_{ij}^{(3),\{3;0,2\},0,\text{diagonal}}(z_1, z_2) & (2.299) \\
 & = (i\hbar)^3 G_{ij}(z_1, z_2) \sum_r w_{ir}(z_1) \int_{\mathcal{C}} dz_3 \sum_t G_{rt}(z_1, z_3) G_{tr}(z_3, z_1) \\
 & \quad \sum_v w_{tv}(z_3) \sum_x G_{vx}(z_3, z_2) G_{xv}(z_2, z_3) w_{xj}(z_2),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{ij}^{(3),\{3;1,1\},0,\text{diagonal}}(z_1, z_2) & (2.300) \\
 & = \pm (i\hbar)^3 G_{ij}(z_1, z_2) \sum_r w_{ir}(z_1) \int_{\mathcal{C}} dz_3 \sum_t G_{rt}(z_1, z_3) \sum_u G_{ur}(z_3, z_1) \\
 & \quad w_{tu}(z_3) \sum_x G_{tx}(z_3, z_2) G_{xu}(z_2, z_3) w_{xj}(z_2),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{ij}^{(3),2,1,\text{diagonal}}(z_1, z_2) & (2.301) \\
 & = \pm (i\hbar)^3 \int_{\mathcal{C}} dz_3 \sum_r w_{ir}(z_1) \sum_t G_{rt}(z_1, z_3) G_{tr}(z_3, z_1) \sum_p w_{tp}(z_3) \\
 & \quad \sum_n G_{in}(z_1, z_2) w_{nj}(z_2) G_{np}(z_2, z_3) G_{pj}(z_3, z_2),
 \end{aligned}$$

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1\},\text{diagonal}}(z_1, z_2) & (2.302) \\
 & = (i\hbar)^3 \sum_p w_{ip}(z_1) \sum_n G_{in}(z_1, z_2) w_{nj}(z_2) \int_{\mathcal{C}} dz_3 \sum_t G_{nt}(z_2, z_3) \\
 & \quad \sum_u G_{uj}(z_3, z_2) w_{tu}(z_3) G_{tp}(z_3, z_1) G_{pu}(z_1, z_3),
 \end{aligned}$$

$$\Sigma_{ij}^{(3),1,\{2;2,0,a\},\text{diagonal}}(z_1, z_2) \quad (2.303)$$

$$= \pm (i\hbar)^3 \sum_p w_{ip}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) \sum_{tv} G_{tv}(z_4, z_2) \\ w_{nt}(z_4) w_{vj}(z_2) G_{vt}(z_2, z_4) G_{np}(z_4, z_1) G_{pj}(z_1, z_2),$$

$$\Sigma_{ij}^{(3),1,\{2;2,0,b\},\text{diagonal}}(z_1, z_2) \quad (2.304)$$

$$= \pm (i\hbar)^3 \sum_p w_{ip}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) \sum_{rs} G_{nj}(z_4, z_2) \\ w_{nr}(z_4) w_{sj}(z_2) G_{sr}(z_2, z_4) G_{rp}(z_4, z_1) G_{ps}(z_1, z_2),$$

$$\Sigma_{ij}^{(3),1,\{2;2,0,c\},\text{diagonal}}(z_1, z_2) \quad (2.305)$$

$$= \pm (i\hbar)^3 \sum_p w_{ip}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) \sum_{rs} G_{nj}(z_4, z_2) \\ G_{sr}(z_4, z_2) w_{ns}(z_4) w_{rj}(z_2) G_{rp}(z_2, z_1) G_{ps}(z_1, z_4)$$

and

$$\Sigma_{ij}^{(3),1,\{2;1,1,a\},\text{diagonal}}(z_1, z_2) \quad (2.306)$$

$$= (i\hbar)^3 \sum_p w_{ip}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) \sum_{st} w_{nt}(z_4) \\ w_{sj}(z_2) G_{st}(z_2, z_4) G_{tj}(z_4, z_2) G_{np}(z_4, z_1) G_{ps}(z_1, z_2),$$

$$\Sigma_{ij}^{(3),1,\{2;1,1,b\},\text{diagonal}}(z_1, z_2) \quad (2.307)$$

$$= (i\hbar)^3 \sum_p w_{ip}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) \sum_{rs} w_{ns}(z_4) \\ G_{nr}(z_4, z_2) w_{rj}(z_2) G_{sj}(z_4, z_2) G_{rp}(z_2, z_1) G_{ps}(z_1, z_4),$$

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;1,1,c\},\text{diagonal}}(z_1, z_2) & (2.308) \\
 &= (i\hbar)^3 \sum_p w_{ip}(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) \sum_r w_{nr}(z_4) \\
 & \quad \sum_u G_{nu}(z_4, z_2) w_{uj}(z_2) G_{ur}(z_2, z_4) G_{rp}(z_4, z_1) G_{pj}(z_1, z_2).
 \end{aligned}$$

The corresponding components as well as the non-selfconsistent selfenergy contributions can be worked out in analogy to those in the non-diagonal basis. The diagrams of the selfconsistent third-order selfenergy contributions in a diagonal basis are shown in Fig. 2.10.

2.7.1.3.2 Hubbard basis For the Hubbard basis and the specialization to spin-0 bosons, the third-order selfenergy contributions separate into the two classes

$$\begin{aligned}
 & \Sigma_{ij}^{(3),\{3;0,2\},0,\text{bosons},0}(z_1, z_2) = \Sigma_{ij}^{(3),\{3;1,1\},0,\text{bosons},0}(z_1, z_2) & (2.309) \\
 &= \Sigma_{ij}^{(3),2,1,\text{bosons},0}(z_1, z_2) = \Sigma_{ij}^{(3),1,\{2;1,1\},\text{bosons},0}(z_1, z_2) \\
 &= \Sigma_{ij}^{(3),1,\{2;2,0,a\},\text{bosons},0}(z_1, z_2) = \Sigma_{ij}^{(3),1,\{2;2,0,b\},\text{bosons},0}(z_1, z_2) \\
 &= \Sigma_{ij}^{(3),1,\{2;1,1,a\},\text{bosons},0}(z_1, z_2) = \Sigma_{ij}^{(3),1,\{2;1,1,c\},\text{bosons},0}(z_1, z_2) \\
 &= (i\hbar)^3 G_{ij}(z_1, z_2) U(z_1) \int_{\mathcal{C}} dz_3 \sum_t G_{it}(z_1, z_3) G_{ti}(z_3, z_1) \\
 & \quad U(z_3) G_{tj}(z_3, z_2) G_{jt}(z_2, z_3) U(z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 & \Sigma_{ij}^{(3),1,\{2;2,0,c\},\text{bosons},0}(z_1, z_2) = \Sigma_{ij}^{(3),1,\{2;1,1,b\},\text{bosons},0}(z_1, z_2) & (2.310) \\
 &= (i\hbar)^3 U(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{in}(z_1, z_4) G_{nj}(z_4, z_2) \\
 & \quad G_{nj}(z_4, z_2) U(z_4) U(z_2) G_{ji}(z_2, z_1) G_{in}(z_1, z_4).
 \end{aligned}$$

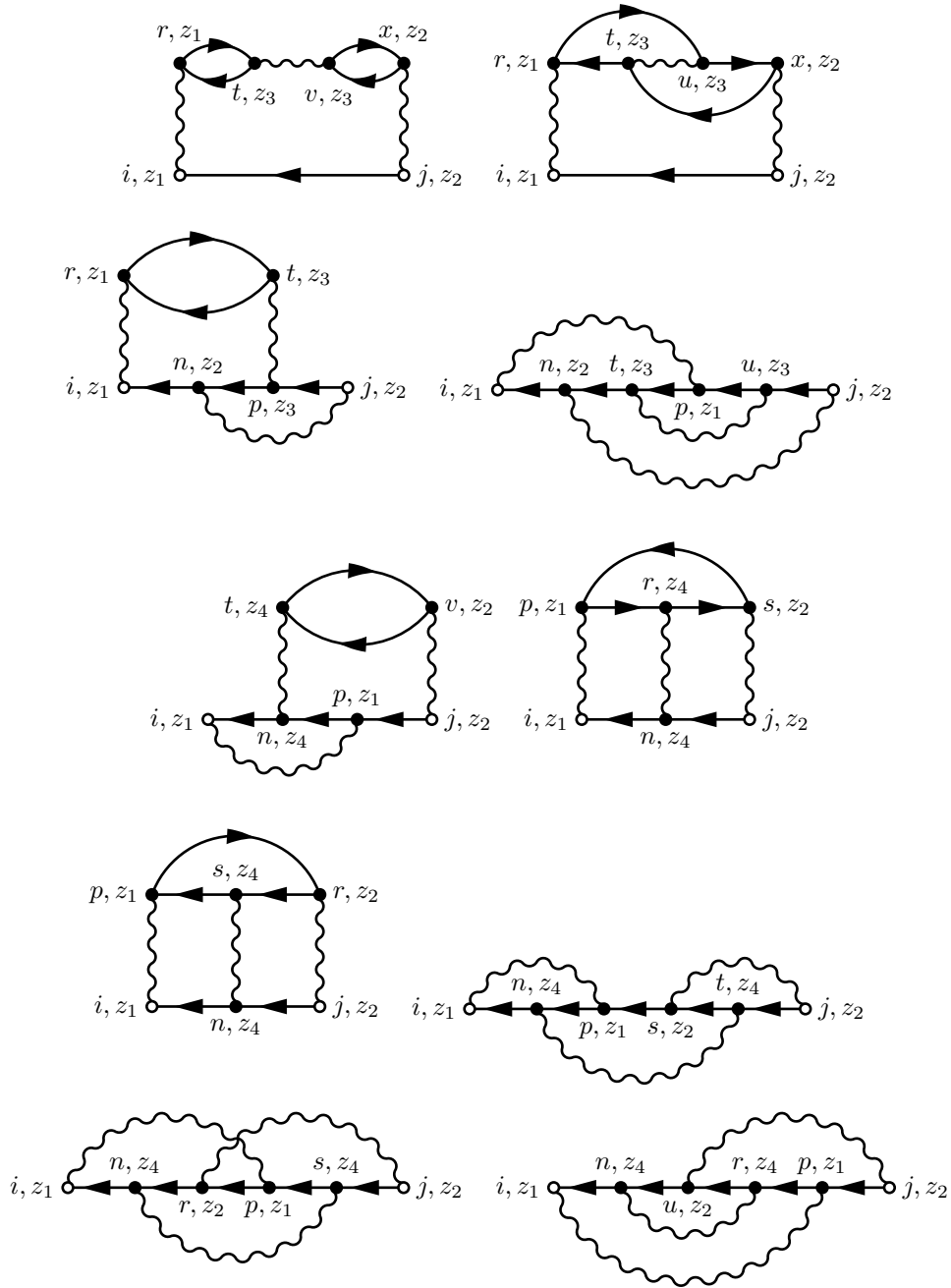


Figure 2.10: Third-order diagrams in diagonal basis from left to right. **First row:** $\Sigma^{(3),\{3;0,2\},0,\text{diagonal}}$, $\Sigma^{(3),\{3;1,1\},0,\text{diagonal}}$ **Second row:** $\Sigma^{(3),2,1,\text{diagonal}}$, $\Sigma^{(3),1,\{2;1,1\},\text{diagonal}}$ **Third row:** $\Sigma^{(3),1,\{2;2,0,a\},\text{diagonal}}$, $\Sigma^{(3),1,\{2;2,0,b\},\text{diagonal}}$ **Fourth row:** $\Sigma^{(3),1,\{2;2,0,c\},\text{diagonal}}$, $\Sigma^{(3),1,\{2;1,1,a\},\text{diagonal}}$ **Fifth row:** $\Sigma^{(3),1,\{2;1,1,b\},\text{diagonal}}$, $\Sigma^{(3),1,\{2;1,1,c\},\text{diagonal}}$.

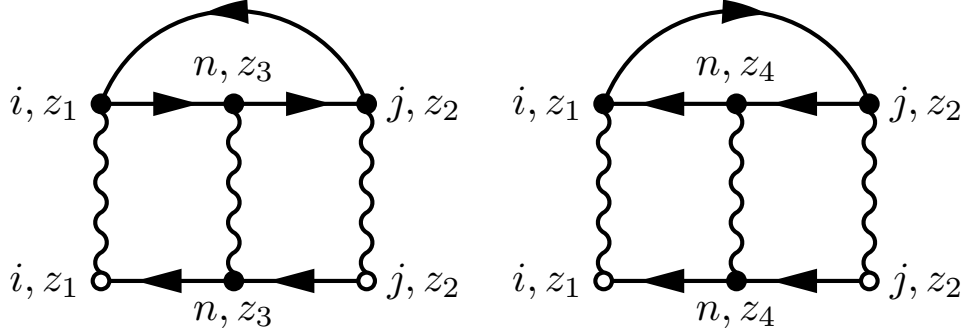


Figure 2.11: Third-order diagrams in the Hubbard basis for spin-0 bosons.

Left: First equivalence class of $\Sigma^{(3),\{3;0,2\},0,\text{diagonal}}$, $\Sigma^{(3),\{3;1,1\},0,\text{diagonal}}$, $\Sigma^{(3),2,1,\text{diagonal}}$, $\Sigma^{(3),1,\{2;1,1\},\text{diagonal}}$, $\Sigma^{(3),1,\{2;2,0,a\},\text{diagonal}}$, $\Sigma^{(3),1,\{2;2,0,b\},\text{diagonal}}$, $\Sigma^{(3),1,\{2;1,1,a\},\text{diagonal}}$ and $\Sigma^{(3),1,\{2;1,1,c\},\text{diagonal}}$. **Right:** Second equivalence class of $\Sigma^{(3),1,\{2;2,0,c\},\text{diagonal}}$ and $\Sigma^{(3),1,\{2;1,1,b\},\text{diagonal}}$.

The corresponding diagrams are shown in Fig. 2.11. For spin-1/2 fermions, only the terms $\Sigma^{(3),1,\{2;2,0,b\},\text{fermions},1/2}$ as well as $\Sigma^{(3),1,\{2;2,0,c\},\text{fermions},1/2}$ with

$$\Sigma_{i\uparrow j\uparrow}^{(3),1,\{2;2,0,b\},\text{fermions},1/2}(z_1, z_2) \quad (2.311)$$

$$= -(\text{i}\hbar)^3 U(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{i\uparrow n\uparrow}(z_1, z_4) G_{n\uparrow j\uparrow}(z_4, z_2) \\ U(z_4) U(z_2) G_{j\downarrow n\downarrow}(z_2, z_4) G_{n\downarrow i\downarrow}(z_4, z_1) G_{i\downarrow j\downarrow}(z_1, z_2),$$

$$\Sigma_{i\downarrow j\downarrow}^{(3),1,\{2;2,0,b\},\text{fermions},1/2}(z_1, z_2) \quad (2.312)$$

$$= -(\text{i}\hbar)^3 U(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{i\downarrow n\downarrow}(z_1, z_4) G_{n\downarrow j\downarrow}(z_4, z_2) \\ U(z_4) U(z_2) G_{j\uparrow n\uparrow}(z_2, z_4) G_{n\uparrow i\uparrow}(z_4, z_1) G_{i\uparrow j\uparrow}(z_1, z_2)$$

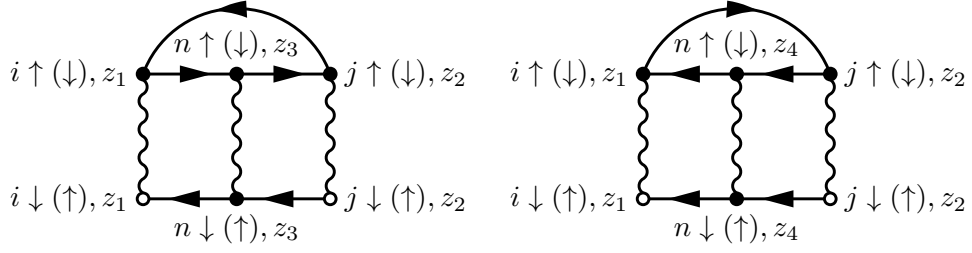


Figure 2.12: Third-order diagrams in Hubbard basis for spin-1/2 fermions.
Left: $\Sigma_{i\uparrow j\uparrow}^{(3),1,\{2;2,0,b\},\text{fermions},1/2}$. **Right:** $\Sigma_{i\downarrow j\downarrow}^{(3),1,\{2;2,0,c\},\text{fermions},1/2}$.

and

$$\Sigma_{i\uparrow j\uparrow}^{(3),1,\{2;2,0,c\},\text{fermions},1/2}(z_1, z_2) \quad (2.313)$$

$$= -(\mathrm{i}\hbar)^3 U(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{i\uparrow n\uparrow}(z_1, z_4) G_{n\uparrow j\uparrow}(z_4, z_2) \\ U(z_4) U(z_2) G_{n\downarrow j\downarrow}(z_4, z_2) G_{i\downarrow n\downarrow}(z_1, z_4) G_{j\downarrow i\downarrow}(z_2, z_1),$$

$$\Sigma_{i\downarrow j\downarrow}^{(3),1,\{2;2,0,c\},\text{fermions},1/2}(z_1, z_2) \quad (2.314)$$

$$= -(\mathrm{i}\hbar)^3 U(z_1) \int_{\mathcal{C}} dz_4 \sum_n G_{i\downarrow n\downarrow}(z_1, z_4) G_{n\downarrow j\downarrow}(z_4, z_2) \\ U(z_4) U(z_2) G_{n\uparrow j\uparrow}(z_2, z_4) G_{i\uparrow n\uparrow}(z_4, z_1) G_{j\uparrow i\uparrow}(z_1, z_2),$$

have non-zero contribution, cf. Fig. 2.12.

2.7.1.4 Higher-order terms

All terms of higher order than three can be generated similarly to the lower orders by computing all possible permutations of the quantities involved in Hedin's equations that lead to the desired total order. To achieve a structure suitable for a recursive algorithm, one starts by eliminating the polarization from Hedin's equations, yielding,

cf. Eq. (2.94) to Eq. (2.103),

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^H(z_1, z_2) + i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}(z_1, z_3) \quad (2.315)$$

$$\int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}(z_4, z_2, z_3),$$

$$W_{ijkl}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2) w_{ijkl}(z_1) \quad (2.316)$$

$$\begin{aligned} & \pm i\hbar \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} \int_{\mathcal{C}} dz_4 \sum_r G_{nr}(z_1, z_4) \\ & \int_{\mathcal{C}} dz_5 \sum_s G_{sm}(z_5, z_1) \Gamma_{rqpj}(z_4, z_5, z_3) W_{pjkl}(z_3, z_2) \end{aligned}$$

and

$$\Gamma_{ijkl}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl} \quad (2.317)$$

$$+ \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{\text{xc}}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6)$$

$$\int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Gamma_{pjkl}(z_6, z_7, z_3).$$

With this set of three coupled equations, the following recursive algorithm can be applied to calculate the N -th order selfenergy contributions:

1. Initialize $\Sigma^{(1)} = \Sigma^H$, cf. Eq. (2.315)
2. Initialize $W^{(1)} = w$, cf. Eq. (2.316)
3. Initialize $\Gamma = \Gamma^{(0)}$, cf. Eq. (2.317)
4. Loop over $n = 1 \dots N$:
 - If $n > 1$: Loop over all orders $m = (1 \dots (n - 1))$:
 - Loop over all selfenergy contributions $\Sigma^{(m)}$ of order m :

- Loop over all vertex contributions $\Gamma^{(n-1-m)}$ of order $n - 1 - m$:
- Calculate the new vertex contribution $\Gamma^{(n-1)}$ from $\Sigma^{(m)}$ and $\Gamma^{(n-1-m)}$ of order $m + n - 1 - m = n - 1$ via Eq. (2.317)
- If $n > 1$: Loop over all orders $m = (1 \dots (n - 1))$:
 - Loop over all contributions to the screened interaction $W^{(m)}$ of order m :
 - Loop over all vertex contributions $\Gamma^{(n-1-m)}$ of order $n - 1 - m$:
 - Calculate the new contribution to the screened interaction $W^{(n)}$ from w , $W^{(m)}$ and $\Gamma^{(n-1-m)}$ of order $1 + m + n - 1 - m = n$ via Eq. (2.316)
 - Loop over all orders $m = 1 \dots n$:
 - Loop over all contributions to the screened interaction $W^{(m)}$ of order m :
 - Loop over all vertex contributions $\Gamma^{(n-m)}$ of order $n - m$:
 - Calculate the new selfenergy contribution $\Sigma^{(n)}$ from $W^{(m)}$ and $\Gamma^{(n-m)}$ of order $m + n - m = n$ via Eq. (2.315)

A similar algorithm yielding the diagrams with respect to the bare interaction w can be deduced, substituting the full vertex Γ by the bare vertex Λ , cf. Eqs. (2.96) and (2.97). Further, the generation of the non-selfconsistent diagrams is straight forward by inclusion of the Dyson equation and additionally taking into account the order of the Green functions in the respective equations.

2.7.2 Resummation approaches

As an alternative to the perturbative expansion in terms of the interaction strength presented in Section 2.7.1, especially for larger interaction strength, this section deals with resummation techniques. The underlying idea is to take into consideration one or several classes of terms with a recursive structure which occur in all orders of the interaction based on physical intuition about their importance. Starting from the notion of the screened interaction W , the most natural choice is the GW

approximation [61] which centers around treating W exactly according to Eq. (2.99) while taking the screened vertex Γ only in zeroth order approximation. The resulting structure of the selfenergy approximation is discussed in the ensuing Section 2.7.2.2.

In contrast, the T -matrix approximation, another common resummation approach—existing in two flavors as the particle–particle T -matrix approximation and the electron-hole T -matrix approximation—treats the interaction only at the level of the bare interaction, but focuses instead on a good representation of the bare vertex functions Λ . Furthermore, several other approaches have been introduced, which mix screened and bare interaction [47]. An example for this group is the second-order screened exchange (SOSEX)-approximation [47, 79, 98], which takes the second-order diagrams exchange diagram, cf. Eq. (2.150), and replaces one of the bare interactions w by the screened interaction W . Doing that, the total complexity is still of $\mathcal{O}(N_t^3)$, since both, the determination of the selfenergy, the computation of the screened interaction according to Eq. (2.101) and the solution of the KBE, cf. Eqs. (2.66) and (2.67), scale as $\mathcal{O}(N_t^3)$.

Another possible way is to combine several approximations taking care about an eventual double counting. This strategy is pursued in the so called fluctuating exchange (FLEX)-approximation, which adds the diagrams of third and higher order of the GW approximation and both T -matrices to the second-order diagrams, which are taken only once. The FLEX approximation, which will be detailed in Section 2.7.2.5 can be seen as the starting term of the more sophisticated plaquet theory [99–105], where one uses coupled equations for the vertex functions in different channels. Before the GW -approximation, the T -matrix approximation and the FLEX-approximation will be detailed in Sections 2.7.2.2, 2.7.2.3 and 2.7.2.5, the Hartree and the Fock approximation for the two-particle Green function will be established in Section 2.7.2.1, since they will be used later.

2.7.2.1 Hartree and Fock approximation for $G^{(2)}$

In the following, two simple approximations for the two-particle Green function are defined which will be used to simplify expressions occurring in the resummation approaches. Those are the Hartree Green function $G^{(2),H}$ and the Fock Green function $G^{(2),F}$.

$G^{(2),\text{H}}$ approximates the two-particle Green function $G^{(2)}$ as

$$\begin{aligned} G_{ijkl}^{(2)}(t_1, t_2, t_3, t_4) & \quad (2.318) \\ & = G_{ijkl}^{(2),\text{H}}(t_1, t_2, t_3, t_4) := G_{ik}(t_1, t_3)G_{jl}(t_2, t_4), \end{aligned}$$

while $G^{(2),\text{F}}$ reads

$$\begin{aligned} G_{ijkl}^{(2)}(t_1, t_2, t_3, t_4) & \quad (2.319) \\ & = G_{ijkl}^{(2),\text{F}}(t_1, t_2, t_3, t_4) := \pm G_{il}(t_1, t_4)G_{jk}(t_2, t_3). \end{aligned}$$

In the resummation expansions in the following sections, both quantities enter mapped onto a single-particle quantity, G^{H} and G^{F} , respectively. These expressions follow by setting equal two time-arguments each and adding a dimensionality factor $i\hbar$. This leads to

$$\begin{aligned} G_{ijkl}^{\text{H}}(t_1, t_2) & := i\hbar G_{ijkl}^{(2),\text{H}}(t_1, t_1, t_2, t_2) & (2.320) \\ & = i\hbar G_{ik}(t_1, t_2)G_{jl}(t_1, t_2), \end{aligned}$$

while, for the Fock approximation, one has

$$\begin{aligned} G_{ijkl}^{\text{F}}(t_1, t_2) & = i\hbar G_{ijkl}^{(2),\text{F}}(t_1, t_2, t_1, t_2) & (2.321) \\ & = \pm i\hbar G_{il}(t_1, t_2)G_{jk}(t_2, t_1). \end{aligned}$$

The corresponding \gtrless -Keldysh components of Eqs. (2.320) and (2.321) are

$$G_{ijkl}^{\text{H},<}(t_1, t_2) = i\hbar G_{ik}^<(t_1, t_2)G_{jl}^<(t_1, t_2), \quad (2.322)$$

$$G_{ijkl}^{\text{H},>}(t_1, t_2) = i\hbar G_{ik}^>(t_1, t_2)G_{jl}^>(t_1, t_2) \quad (2.323)$$

as well as

$$G_{ijkl}^{\text{H,R}}(t_1, t_2) = i\hbar\Theta(t_1, t_2) \quad (2.324)$$

$$\left[G_{ik}^>(t_1, t_2)G_{jl}^>(t_1, t_2) - G_{ik}^<(t_1, t_2)G_{jl}^<(t_1, t_2) \right],$$

$$G_{ijkl}^{\text{H,A}}(t_1, t_2) = i\hbar\Theta(t_2, t_1) \quad (2.325)$$

$$\left[G_{ik}^<(t_1, t_2)G_{jl}^<(t_1, t_2) - G_{ik}^>(t_1, t_2)G_{jl}^>(t_1, t_2) \right]$$

and

$$G_{ijkl}^{\text{F,<}}(t_1, t_2) = \pm i\hbar G_{il}^<(t_1, t_2)G_{jk}^>(t_2, t_1), \quad (2.326)$$

$$G_{ijkl}^{\text{F,>}}(t_1, t_2) = \pm i\hbar G_{il}^>(t_1, t_2)G_{jk}^<(t_2, t_1) \quad (2.327)$$

as well as

$$G_{ijkl}^{\text{F,R}}(t_1, t_2) = \pm i\hbar\Theta(t_1, t_2) \quad (2.328)$$

$$\left[G_{il}^>(t_1, t_2)G_{jk}^<(t_2, t_1) - G_{il}^<(t_1, t_2)G_{jk}^>(t_2, t_1) \right],$$

$$G_{ijkl}^{\text{F,A}}(t_1, t_2) = \pm i\hbar\Theta(t_2, t_1) \quad (2.329)$$

$$\left[G_{il}^<(t_1, t_2)G_{jk}^>(t_2, t_1) - G_{il}^>(t_1, t_2)G_{jk}^<(t_2, t_1) \right].$$

2.7.2.2 *GW* approximation

The *GW* approximation solves Hedin's equation for the screened interaction W according to Eq. (2.101) with the zeroth order vertex $\Gamma^{(0)}$. The set of equations is given by the Dyson equation, cf. Eq. (2.91),

$$G_{ij}(z_1, z_2) = G_{ij}^{(0)}(z_1, z_2) \quad (2.330)$$

$$+ \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2),$$

the equation for the selfenergy, cf. Eq. (2.94)

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^{\text{xc}}(z_1, z_2), \quad (2.331)$$

with

$$\begin{aligned} \Sigma_{ij}^{\text{xc}}(z_1, z_2) &= i\hbar \int_{\mathcal{C}} dz_3 \sum_{mpq} W_{ipqm}(z_1, z_3) \\ &\int_{\mathcal{C}} dz_4 \sum_n G_{mn}(z_1, z_4) \Gamma_{nqpj}^{(0)}(z_4, z_2, z_3) \\ &= i\hbar \sum_{mp} W_{ipjm}(z_1, z_2) G_{mp}(z_1, z_2), \end{aligned} \quad (2.332)$$

the zeroth order polarization function, cf. Eq. (2.137),

$$P_{ijkl}(z_1, z_2) = P_{ijkl}^{(0)}(z_1, z_2) = \pm i\hbar G_{ik}(z_1, z_2) G_{jl}(z_2, z_1), \quad (2.333)$$

the zeroth order vertex, cf. Eq. (2.107),

$$\Gamma_{ijkl}(z_1, z_2, z_3) = \Gamma_{ijkl}^{(0)}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl} \quad (2.334)$$

and the screened interaction, cf. Eqs. (2.99) and (2.101),

$$W_{ijkl}(z_1, z_2) = \delta_{\mathcal{C}}(z_1, z_2) w_{ijkl}(z_1) + W_{ijkl}^{\text{screened}}(z_1, z_2), \quad (2.335)$$

with

$$\begin{aligned} W_{ijkl}^{\text{screened}}(z_1, z_2) & \\ &= \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} P_{nqpm}^{(0)}(z_1, z_3) W_{pj kq}(z_3, z_2) \\ &= \pm i\hbar \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{np}(z_1, z_3) G_{qm}(z_3, z_1) W_{pj kq}(z_3, z_2). \end{aligned} \quad (2.336)$$

To solve this set of equations, one has to determine the selfconsistent solution of Eq. (2.335). Thereto, it is more suitable to eliminate the singular bare interaction by

defining

$$\begin{aligned} W_{ijkl}^{\text{non-sing.}}(z_1, z_2) &= W_{ijkl}(z_1, z_2) - W_{ijkl}^{\text{bare}}(z_1, z_2) \\ &= W_{ijkl}(z_1, z_2) - \delta_{\mathcal{C}}(z_1, z_2) w_{ijkl}(z_1). \end{aligned} \quad (2.337)$$

With this, one arrives at

$$\begin{aligned} \Sigma_{ij}^{\text{GW}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + i\hbar \sum_{mp} W_{ipjm}(z_1, z_2) G_{mp}(z_1, z_2) \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + i\hbar \sum_{mp} w_{ipjm}(z_1) G_{mp}(z_1, z_{1+}) \delta_{\mathcal{C}}(z_1, z_2) \\ &\quad + i\hbar \sum_{mp} W_{ipjm}^{\text{non-sing.}}(z_1, z_2) G_{mp}(z_1, z_2). \end{aligned} \quad (2.338)$$

Using Eq. (2.108), the expression simplifies to

$$\begin{aligned} \Sigma_{ij}^{\text{GW}}(z_1, z_2) & \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) + i\hbar \sum_{mp} W_{ipjm}^{\text{non-sing.}}(z_1, z_2) G_{mp}(z_1, z_2) \\ &=: \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) + \Sigma_{ij}^{\text{GW,corr}}(z_1, z_2). \end{aligned} \quad (2.339)$$

For the screened interaction, one has

$$\begin{aligned} W_{ijkl}^{\text{non-sing.}}(z_1, z_2) & \\ &= \pm i\hbar \sum_{mn} w_{imnl}(z_1) \sum_{pq} G_{np}(z_1, z_2) G_{qm}(z_2, z_1) w_{pj kq}(z_2) \\ &\quad \pm i\hbar \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{np}(z_1, z_3) G_{qm}(z_3, z_1) W_{pj kq}^{\text{non-sing.}}(z_3, z_2). \end{aligned} \quad (2.340)$$

Using the definition of G^F in Eq. (2.321), Eq. (2.340) can be simplified to

$$\begin{aligned}
 W_{ijkl}^{\text{non-sing.}}(z_1, z_2) &= \sum_{mn} w_{imnl}(z_1) \sum_{pq} G_{nqmp}^F(z_1, z_2) w_{pjkq}(z_2) \\
 &+ \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{nqmp}^F(z_1, z_3) W_{pjkq}^{\text{non-sing.}}(z_3, z_2) \\
 &=: \Phi_{ijkl}^{GW}(z_1, z_2) \\
 &+ \sum_{mn} w_{imnl}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{nqmp}^F(z_1, z_3) W_{pjkq}^{\text{non-sing.}}(z_3, z_2).
 \end{aligned} \tag{2.341}$$

The components of the correlation part of Eq. (2.339) read

$$\Sigma_{ij}^{\text{GW,corr.},\geq}(t_1, t_2) = i\hbar \sum_{mp} W_{ipjm}^{\text{non-sing.},\geq}(t_1, t_2) G_{mp}^{\geq}(t_1, t_2). \tag{2.342}$$

For the components of Eq. (2.341), one finds

$$W_{ijkl}^{\text{non-sing.},\geq}(t_1, t_2) = \Phi_{ijkl}^{GW,\geq}(t_1, t_2) + \sum_{mn} w_{imnl}(t_1) \sum_{pq} \tag{2.343}$$

$$\begin{aligned}
 &\left(\int_{t_0}^{t_1} dt_3 G_{nqmp}^{\text{F,R}}(t_1, t_3) W_{pjkq}^{\text{non-sing.},\geq}(t_3, t_2) \right. \\
 &\left. + \int_{t_0}^{t_2} dt_3 G_{nqmp}^{\text{F},\geq}(t_1, t_3) W_{pjkq}^{\text{non-sing.},\text{A}}(t_3, t_2) \right),
 \end{aligned}$$

$$W_{ijkl}^{\text{non-sing.},\text{A}}(t_1, t_2) = \Phi_{ijkl}^{GW,\text{A}}(t_1, t_2) \tag{2.344}$$

$$+ \sum_{mn} w_{imnl}(t_1) \int_{t_1}^{t_2} dt_3 \sum_{pq} G_{nqmp}^{\text{F},\text{A}}(t_1, t_3) W_{pjkq}^{\text{non-sing.},\text{A}}(t_3, t_2)$$

and

$$\begin{aligned}
 W_{ijkl}^{\text{non-sing.,R}}(t_1, t_2) &= \Phi_{ijkl}^{GW, \text{R}}(t_1, t_2) \\
 &+ \sum_{mn} w_{imnl}(t_1) \int_{t_2}^{t_1} dt_3 \sum_{pq} G_{nqmp}^{\text{F,R}}(t_1, t_3) W_{pj kq}^{\text{non-sing.,R}}(t_3, t_2).
 \end{aligned} \tag{2.345}$$

2.7.2.2.1 Diagonal basis In a diagonal basis set, Eq. (2.341) simplifies to

$$\begin{aligned}
 W_{ijkl}^{\text{non-sing.,diag.}}(z_1, z_2) & \\
 &= \delta_{il} \delta_{jk} \sum_m w_{im}(z_1) \sum_p G_{mpmp}^{\text{F}}(z_1, z_2) w_{pj}(z_2) \\
 &+ \delta_{il} \sum_m w_{im}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{mpmq}^{\text{F}}(z_1, z_3) W_{pj kq}^{\text{non-sing.,diag.}}(z_3, z_2).
 \end{aligned} \tag{2.346}$$

Using Φ , one has

$$\begin{aligned}
 W_{ijkl}^{\text{non-sing.,diag.}}(z_1, z_2) & \\
 &= \delta_{il} \delta_{jk} \Phi_{ijji}^{GW, \text{diag.}}(z_1, z_2) \\
 &+ \delta_{il} \sum_m w_{im}(z_1) \int_{\mathcal{C}} dz_3 \sum_{pq} G_{mpmq}^{\text{F}}(z_1, z_3) W_{pj kq}^{\text{non-sing.,diag.}}(z_3, z_2).
 \end{aligned} \tag{2.347}$$

By iteration, it becomes evident that $W^{\text{non-sing.,diag.}}$ and $\Phi_{ijji}^{GW, \text{diag.}}$ are always of the structure

$$\begin{aligned}
 W_{ijkl}^{\text{non-sing.,diag.}}(z_1, z_2) & \\
 &= \delta_{il} \delta_{jk} W_{ijji}^{\text{non-sing.,diag.}}(z_1, z_2) =: \delta_{il} \delta_{jk} W_{ij}^{\text{non-sing.,diag.}}(z_1, z_2),
 \end{aligned} \tag{2.348}$$

$$\begin{aligned}
 \Phi_{ijkl}^{GW, \text{diag.}}(z_1, z_2) & \\
 &= \delta_{il} \delta_{jk} \Phi_{ijji}^{GW, \text{diag.}}(z_1, z_2) =: \delta_{il} \delta_{jk} \Phi_{ij}^{GW, \text{diag.}}(z_1, z_2).
 \end{aligned} \tag{2.349}$$

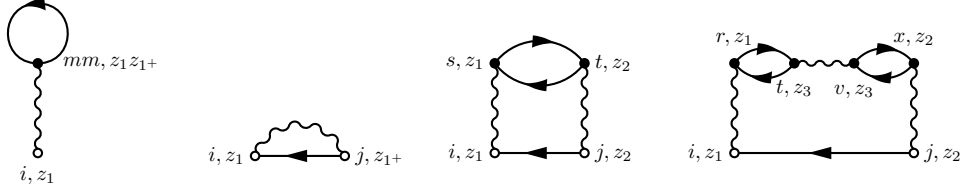


Figure 2.13: The first four terms of the GW -selfenergy in a diagonal basis.

With this, for a diagonal basis, Eq. (2.341) attains the form

$$\begin{aligned}
 W_{ij}^{\text{non-sing.,diag.}}(z_1, z_2) &= \Phi_{ij}^{GW,\text{diag.}}(z_1, z_2) \\
 &+ \sum_m w_{im}(z_1) \int_{\mathcal{C}} dz_3 \sum_p G_{mpmp}^{\text{F}}(z_1, z_3) W_{pj}^{\text{non-sing.,diag.}}(z_3, z_2).
 \end{aligned} \tag{2.350}$$

The selfenergy, cf. Eq. (2.339), reads

$$\begin{aligned}
 \Sigma_{ij}^{GW,\text{diag.}}(z_1, z_2) &= \Sigma_{ij}^{\text{diag.,H}}(z_1, z_2) + \Sigma_{ij}^{\text{diag.,F}}(z_1, z_2) \\
 &+ i\hbar W_{ij}^{\text{non-sing.,diag.}}(z_1, z_2) G_{ij}(z_1, z_2) \\
 &=: \Sigma_{ij}^{\text{diag.,H}}(z_1, z_2) + \Sigma_{ij}^{\text{diag.,F}}(z_1, z_2) + \Sigma_{ij}^{GW,\text{corr.,diag.}}(z_1, z_2).
 \end{aligned} \tag{2.351}$$

The first four terms of the GW -selfenergy are shown diagrammatically in Fig. 2.13. The relevant components read, cf. Eqs. (2.343), (2.344) and (2.345),

$$W_{ij}^{\text{non-sing.,diag.,}\geq}(t_1, t_2) = \Phi_{ij}^{GW,\text{diag.,}\geq}(t_1, t_2) + \sum_{mp} w_{im}(t_1) \tag{2.352}$$

$$\begin{aligned}
 &\left(\int_{t_0}^{t_1} dt_3 G_{mpmp}^{\text{F,R}}(t_1, t_3) W_{pj}^{\text{non-sing.,diag.,}\geq}(t_3, t_2) \right. \\
 &\left. + \int_{t_0}^{t_2} dt_3 G_{mpmp}^{\text{F,}\geq}(t_1, t_3) W_{pj}^{\text{non-sing.,diag.,A}}(t_3, t_2) \right),
 \end{aligned}$$

$$W_{ij}^{\text{non-sing.,diag.,A}}(t_1, t_2) = \Phi_{ij}^{GW, \text{diag.,A}}(t_1, t_2) \quad (2.353)$$

$$+ \sum_{mp} w_{im}(t_1) \int_{t_1}^{t_2} dt_3 G_{mpmp}^{\text{F,A}}(t_1, t_3) W_{pj}^{\text{non-sing.,diag.,A}}(t_3, t_2),$$

$$W_{ij}^{\text{non-sing.,diag.,R}}(t_1, t_2) = \Phi_{ij}^{GW, \text{diag.,R}}(t_1, t_2) \quad (2.354)$$

$$+ \sum_{mp} w_{im}(t_1) \int_{t_2}^{t_1} dt_3 G_{mpmp}^{\text{F,R}}(t_1, t_3) W_{pj}^{\text{non-sing.,diag.,R}}(t_3, t_2),$$

and, cf. Eq. (2.342),

$$\Sigma_{ij}^{GW, \text{corr.,diag.,}\geq}(t_1, t_2) = i\hbar W_{ij}^{\text{non-sing.,diag.,}\geq}(t_1, t_2) G_{ij}^{\geq}(t_1, t_2). \quad (2.355)$$

2.7.2.2.2 Hubbard basis In the Hubbard basis, cf. Section 2.3, the GW approximation attains the form

$$W_{i\alpha j\beta}^{\text{non-sing.,bosons}}(z_1, z_2) = U(z_1) \sum_{\epsilon} G_{i\epsilon j\epsilon}^{\text{F}}(z_1, z_2) U(z_2) \quad (2.356)$$

$$+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_{p\epsilon} G_{i\epsilon p\epsilon}^{\text{F}}(z_1, z_3) W_{p\epsilon j\beta}^{\text{non-sing.,bosons}}(z_3, z_2)$$

$$=: \Phi_{ij}^{GW, \text{bosons}}(z_1, z_2)$$

$$+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_{p\epsilon} G_{i\epsilon p\epsilon}^{\text{F}}(z_1, z_3) W_{p\epsilon j\beta}^{\text{non-sing.,bosons}}(z_3, z_2)$$

and

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{GW, \text{bosons}}(z_1, z_2) &= \Sigma_{i\alpha j\alpha}^{\text{H, bosons}}(z_1, z_2) + \Sigma_{i\alpha j\alpha}^{\text{F, bosons}}(z_1, z_2) \\ &\quad + i\hbar W_{i\alpha j\alpha}^{\text{non-sing.,bosons}}(z_1, z_2) G_{i\alpha j\alpha}(z_1, z_2) \\ &=: \Sigma_{i\alpha j\alpha}^{\text{H, bosons}}(z_1, z_2) + \Sigma_{i\alpha j\alpha}^{\text{F, bosons}}(z_1, z_2) \\ &\quad + \Sigma_{i\alpha j\alpha}^{GW, \text{corr.,bosons}}(z_1, z_2), \end{aligned} \quad (2.357)$$

for bosons. The components become

$$W_{i\alpha j\beta}^{\text{non-sing.,bosons},\geq}(t_1, t_2) = \Phi_{ij}^{GW, \text{bosons}, \geq}(t_1, t_2) \quad (2.358)$$

$$\begin{aligned} &+ U(t_1) \int_{t_0}^{t_1} dt_3 \sum_{p\epsilon} G_{i\epsilon p \epsilon i\epsilon p \epsilon}^{\text{F,R}}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,bosons},\geq}(t_3, t_2) \\ &+ U(t_1) \int_{t_0}^{t_2} dt_3 \sum_{p\epsilon} G_{i\epsilon p \epsilon i\epsilon p \epsilon}^{\text{F},\geq}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,bosons,A}}(t_3, t_2), \end{aligned}$$

$$W_{i\alpha j\beta}^{\text{non-sing.,bosons,A}}(t_1, t_2) = \Phi_{ij}^{GW, \text{bosons,A}}(t_1, t_2) \quad (2.359)$$

$$+ U(z_1) \int_{t_1}^{t_2} dt_3 \sum_{p\epsilon} G_{i\epsilon p \epsilon i\epsilon p \epsilon}^{\text{F,A}}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,bosons,A}}(t_3, t_2),$$

$$W_{i\alpha j\beta}^{\text{non-sing.,bosons,R}}(t_1, t_2) = \Phi_{ij}^{GW, \text{bosons,R}}(t_1, t_2) \quad (2.360)$$

$$+ U(z_1) \int_{t_2}^{t_1} dt_3 \sum_{p\epsilon} G_{i\epsilon p \epsilon i\epsilon p \epsilon}^{\text{F,R}}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,bosons,R}}(t_3, t_2)$$

and

$$\Sigma_{i\alpha j\alpha}^{GW, \text{corr.}, \text{bosons}, \geq}(t_1, t_2) \quad (2.361)$$

$$= i\hbar W_{i\alpha j\alpha}^{\text{non-sing.,bosons},\geq}(t_1, t_2) G_{i\alpha j\alpha}^{\geq}(t_1, t_2).$$

For the special case of spin-0 bosons, the relevant quantities read

$$W_{ij}^{\text{non-sing.,bosons,0}}(z_1, z_2) = U(z_1) G_{ijij}^{\text{F}}(z_1, z_2) U(z_2) \quad (2.362)$$

$$+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_p G_{ipip}^{\text{F}}(z_1, z_3) W_{pj}^{\text{non-sing.,bosons,0}}(z_3, z_2)$$

$$=: \Phi_{ij}^{GW, \text{bosons,0}}(z_1, z_2)$$

$$+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_p G_{ipip}^{\text{F}}(z_1, z_3) W_{pj}^{\text{non-sing.,bosons,0}}(z_3, z_2)$$

and

$$\begin{aligned}
 \Sigma_{ij}^{GW,\text{bosons},0}(z_1, z_2) &= \Sigma_{ij}^{\text{H},\text{bosons},0}(z_1, z_2) + \Sigma_{ij}^{\text{F},\text{bosons},0}(z_1, z_2) \\
 &\quad + i\hbar W_{ij}^{\text{non-sing.},\text{bosons},0}(z_1, z_2) G_{ij}(z_1, z_2) \\
 &=: \Sigma_{ij}^{\text{H},\text{bosons},0}(z_1, z_2) + \Sigma_{ij}^{\text{F},\text{bosons},0}(z_1, z_2) \\
 &\quad + \Sigma_{ij}^{GW,\text{corr.},\text{bosons},0}(z_1, z_2).
 \end{aligned} \tag{2.363}$$

The components become

$$\begin{aligned}
 W_{ij}^{\text{non-sing.},\text{bosons},0,\geq}(t_1, t_2) &= \Phi_{ij}^{GW,\text{bosons},0,\geq}(t_1, t_2) \\
 &\quad + U(t_1) \int_{t_0}^{t_1} dt_3 \sum_p G_{ipip}^{\text{F},\text{R}}(t_1, t_3) W_{pj}^{\text{non-sing.},\text{bosons},0,\geq}(t_3, t_2) \\
 &\quad + U(t_1) \int_{t_0}^{t_2} dt_3 \sum_p G_{ipip}^{\text{F},\geq}(t_1, t_3) W_{pj}^{\text{non-sing.},\text{bosons},0,\text{A}}(t_3, t_2),
 \end{aligned} \tag{2.364}$$

$$\begin{aligned}
 W_{ij}^{\text{non-sing.},\text{bosons},0,\text{A}}(t_1, t_2) &= \Phi_{ij}^{GW,\text{bosons},0,\text{A}}(t_1, t_2) \\
 &\quad + U(z_1) \int_{t_1}^{t_2} dt_3 \sum_p G_{ipip}^{\text{F},\text{A}}(t_1, t_3) W_{pj}^{\text{non-sing.},\text{bosons},0,\text{A}}(t_3, t_2),
 \end{aligned} \tag{2.365}$$

$$\begin{aligned}
 W_{ij}^{\text{non-sing.},\text{bosons},0,\text{R}}(t_1, t_2) &= \Phi_{ij}^{GW,\text{bosons},0,\text{R}}(t_1, t_2) \\
 &\quad + U(z_1) \int_{t_2}^{t_1} dt_3 \sum_p G_{ipip}^{\text{F},\text{R}}(t_1, t_3) W_{pj}^{\text{non-sing.},\text{bosons},0,\text{R}}(t_3, t_2)
 \end{aligned} \tag{2.366}$$

and

$$\begin{aligned}
 \Sigma_{ij}^{GW,\text{corr.},\text{bosons},0,\geq}(t_1, t_2) & \\
 &= i\hbar W_{ij}^{\text{non-sing.},\text{bosons},0,\geq}(t_1, t_2) G_{ij}^{\geq}(t_1, t_2).
 \end{aligned} \tag{2.367}$$

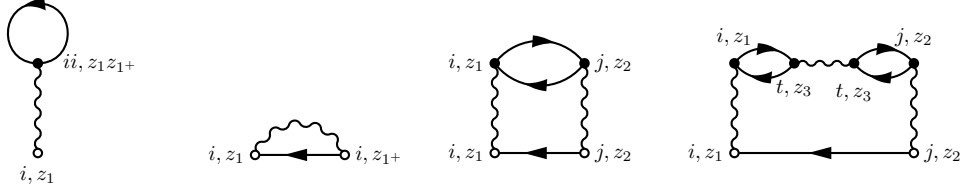


Figure 2.14: The first four terms of the GW -selfenergy in the Hubbard basis for spin-0 bosons.

The diagrammatic representation of the leading terms for spin-0 bosons in the Hubbard basis is shown in Fig. 2.14. For fermions, the equations attain the form

$$W_{i\alpha j\beta}^{\text{non-sing.,fermions}}(z_1, z_2) = \sum_{\epsilon \neq \{\alpha, \beta\}} U(z_1) G_{i\epsilon j\epsilon i\epsilon j\epsilon}^{\text{F}}(z_1, z_2) U(z_2) \quad (2.368)$$

$$+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_p \sum_{\epsilon \neq \alpha} G_{i\epsilon p\epsilon i\epsilon p\epsilon}^{\text{F}}(z_1, z_3) W_{p\epsilon j\beta}^{\text{non-sing.,fermions}}(z_3, z_2)$$

$$=: \Phi_{ij\alpha\beta}^{\text{GW,fermions}}(z_1, z_2)$$

$$+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_p \sum_{\epsilon \neq \alpha} G_{i\epsilon p\epsilon i\epsilon p\epsilon}^{\text{F}}(z_1, z_3) W_{p\epsilon j\beta}^{\text{non-sing.,fermions}}(z_3, z_2)$$

and

$$\Sigma_{i\alpha j\alpha}^{\text{GW,fermions}}(z_1, z_2) = \Sigma_{i\alpha j\alpha}^{\text{H,fermions}}(z_1, z_2) \quad (2.369)$$

$$+ i\hbar W_{i\alpha j\alpha}^{\text{non-sing.,fermions}}(z_1, z_2) G_{i\alpha j\alpha}(z_1, z_2),$$

with components

$$W_{i\alpha j\beta}^{\text{non-sing.,fermions}, \geq}(t_1, t_2) = \Phi_{ij\alpha\beta}^{\text{GW,fermions}, \geq}(t_1, t_2) \quad (2.370)$$

$$+ U(t_1) \int_{t_0}^{t_1} dt_3 \sum_p \sum_{\epsilon \neq \alpha} G_{i\epsilon p\epsilon i\epsilon p\epsilon}^{\text{F,R}}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,fermions}, \geq}(t_3, t_2)$$

$$+ U(t_1) \int_{t_0}^{t_2} dt_3 \sum_p \sum_{\epsilon \neq \alpha} G_{i\epsilon p\epsilon i\epsilon p\epsilon}^{\text{F}, \geq}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,fermions,A}}(t_3, t_2),$$

$$W_{i\alpha j\beta}^{\text{non-sing.,fermions,A}}(t_1, t_2) = \Phi_{ij\alpha\beta}^{GW,fermions,A}(t_1, t_2) \quad (2.371)$$

$$+U(z_1) \int_{t_1}^{t_2} dt_3 \sum_p \sum_{\epsilon \neq \alpha} G_{i\epsilon p \epsilon i \epsilon p \epsilon}^{F,A}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,fermions,A}}(t_3, t_2),$$

$$W_{i\alpha j\beta}^{\text{non-sing.,fermions,R}}(t_1, t_2) = \Phi_{ij\alpha\beta}^{GW,fermions,R}(t_1, t_2) \quad (2.372)$$

$$+U(z_1) \int_{t_2}^{t_1} dt_3 \sum_p \sum_{\epsilon \neq \alpha} G_{i\epsilon p \epsilon i \epsilon p \epsilon}^{F,R}(t_1, t_3) W_{p\epsilon j\beta}^{\text{non-sing.,fermions,R}}(t_3, t_2)$$

and

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{GW,corr.,fermions,\geq}(t_1, t_2) & \quad (2.373) \\ & = i\hbar W_{i\alpha j\alpha}^{\text{non-sing.,fermions,\geq}}(t_1, t_2) G_{i\alpha j\alpha}^{\geq}(t_1, t_2). \end{aligned}$$

For the special case of spin- $\frac{1}{2}$ -fermions, the equations for the screened interaction become

$$W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2}}(z_1, z_2) = U(z_1) G_{i\downarrow j\downarrow i\downarrow j\downarrow}^F(z_1, z_2) U(z_2) \quad (2.374)$$

$$+U(z_1) \int_{\mathcal{C}} dz_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^F(z_1, z_3) W_{m\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2}}(z_3, z_2)$$

$$=: \Phi_{ij\uparrow}^{GW,fermions,1/2}(z_1, z_2)$$

$$+U(z_1) \int_{\mathcal{C}} dz_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^F(z_1, z_3) W_{m\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2}}(z_3, z_2),$$

$$W_{i\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2}}(z_1, z_2) \quad (2.375)$$

$$= U(z_1) \int_{\mathcal{C}} dz_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^F(z_1, z_3) W_{m\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2}}(z_3, z_2),$$

$$\begin{aligned}
 W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions},1/2}(z_1, z_2) &= U(z_1) G_{i\uparrow j\uparrow i\uparrow j\uparrow}^{\text{F}}(z_1, z_2) U(z_2) \quad (2.376) \\
 &+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F}}(z_1, z_3) W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions},1/2}(z_3, z_2) \\
 &=: \Phi_{ij\downarrow}^{\text{GW,fermions},1/2}(z_1, z_2) \\
 &+ U(z_1) \int_{\mathcal{C}} dz_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F}}(z_1, z_3) W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions},1/2}(z_3, z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 W_{i\uparrow j\downarrow}^{\text{non-sing.,fermions},1/2}(z_1, z_2) \quad (2.377) \\
 = U(z_1) \int_{\mathcal{C}} dz_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F}}(z_1, z_3) W_{m\downarrow j\downarrow}^{\text{non-sing.,fermions},1/2}(z_3, z_2).
 \end{aligned}$$

The selfenergy reads

$$\begin{aligned}
 \Sigma_{i\uparrow j\uparrow}^{\text{GW,fermions},1/2}(z_1, z_2) \quad (2.378) \\
 = \Sigma_{i\uparrow j\uparrow}^{\text{H,fermions},1/2}(z_1, z_2) + i\hbar W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions},1/2}(z_1, z_2) G_{i\uparrow j\uparrow}(z_1, z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 \Sigma_{i\downarrow j\downarrow}^{\text{GW,fermions},1/2}(z_1, z_2) \quad (2.379) \\
 = \Sigma_{i\downarrow j\downarrow}^{\text{H,fermions},1/2}(z_1, z_2) + i\hbar W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions},1/2}(z_1, z_2) G_{i\downarrow j\downarrow}(z_1, z_2).
 \end{aligned}$$

The diagrammatic representation of the leading terms for spin-1/2 fermions in the Hubbard basis is shown in Fig. 2.15. One recognizes a special structure of these equations for spin- $\frac{1}{2}$ -fermions. The selfenergy $\left(\Sigma_{i\uparrow j\uparrow}^{\text{GW,fermions},1/2} / \Sigma_{i\downarrow j\downarrow}^{\text{GW,fermions},1/2} \right)$, which couples only contributions of the same spin, also directly depends only on the same-spin parts of the screened interaction $\left(W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions},1/2} G_{i\uparrow j\uparrow} / W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions},1/2} G_{i\downarrow j\downarrow} \right)$, cf. Eqs. (2.378) and (2.379). The same-spin screened interaction, in turn, depends on the screened interaction with different spin orienta-

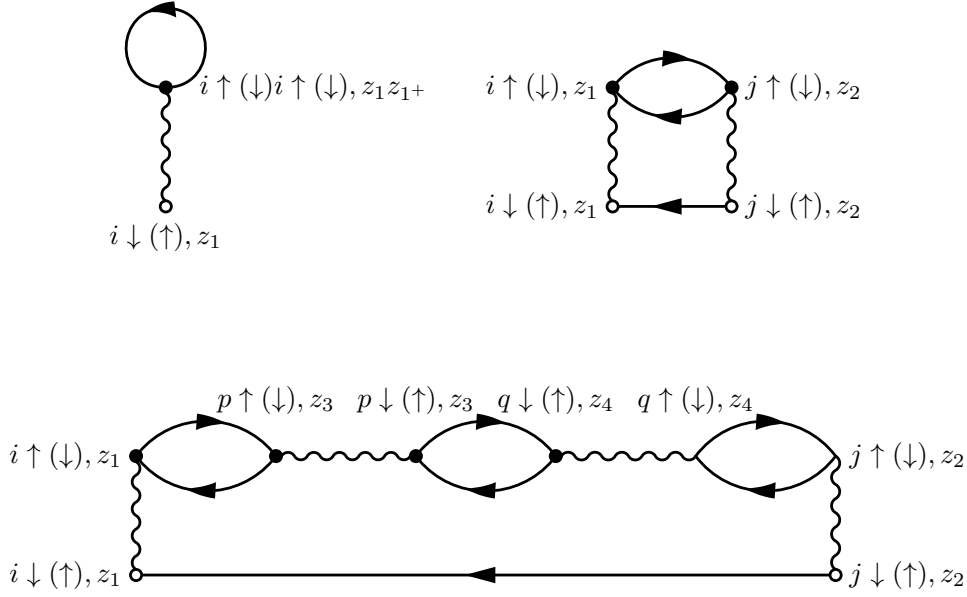


Figure 2.15: The first three terms of the GW -selfenergy in the Hubbard basis for spin-1/2 fermions.

tions $\left(W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2}} / W_{m\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2}} \right)$, which itself couples back to the same-spin part. The respective components read

$$W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2},\geq}(t_1, t_2) = \Phi_{ij\uparrow}^{GW, \text{fermions,1/2},\geq}(t_1, t_2) \quad (2.380)$$

$$\begin{aligned} &+U(t_1) \int_{t_0}^{t_1} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,R}}(t_1, t_3) W_{m\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2},\geq}(t_3, t_2) \\ &+U(t_1) \int_{t_0}^{t_2} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F},\geq}(t_1, t_3) W_{m\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2), \end{aligned}$$

$$W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2,A}}(t_1, t_2) = \Phi_{ij\uparrow}^{GW, \text{fermions,1/2,A}}(t_1, t_2) \quad (2.381)$$

$$+U(t_1) \int_{t_1}^{t_2} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,A}}(t_1, t_3) W_{m\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2),$$

$$W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2,R}}(t_1, t_2) = \Phi_{ij\uparrow}^{GW,\text{fermions,1/2,R}}(t_1, t_2) \quad (2.382)$$

$$+U(t_1) \int_{t_2}^{t_1} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,R}}(t_1, t_3) W_{m\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2,R}}(t_3, t_2),$$

$$W_{i\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2,\geq}}(t_1, t_2) \quad (2.383)$$

$$= U(t_1) \int_{t_0}^{t_1} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,R}}(t_1, t_3) W_{m\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2,\geq}}(t_3, t_2)$$

$$+U(t_1) \int_{t_0}^{t_2} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,\geq}}(t_1, t_3) W_{m\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2),$$

$$W_{i\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2,A}}(t_1, t_2) \quad (2.384)$$

$$= U(t_1) \int_{t_1}^{t_2} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,A}}(t_1, t_3) W_{m\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2),$$

$$W_{i\downarrow j\uparrow}^{\text{non-sing.,fermions,1/2,R}}(t_1, t_2) \quad (2.385)$$

$$= U(t_1) \int_{t_2}^{t_1} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,R}}(t_1, t_3) W_{m\uparrow j\uparrow}^{\text{non-sing.,fermions,1/2,R}}(t_3, t_2),$$

$$W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,\geq}}(t_1, t_2) = \Phi_{ij\downarrow}^{GW,\text{fermions,1/2,\geq}}(t_1, t_2) \quad (2.386)$$

$$+U(t_1) \int_{t_0}^{t_1} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,R}}(t_1, t_3) W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,\geq}}(t_3, t_2)$$

$$+U(t_1) \int_{t_0}^{t_2} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,\geq}}(t_1, t_3) W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2),$$

$$W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,A}}(t_1, t_2) = \Phi_{ij\downarrow}^{GW, \text{fermions,1/2,A}}(t_1, t_2) \quad (2.387)$$

$$+U(t_1) \int_{t_1}^{t_2} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,A}}(t_1, t_3) W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2),$$

$$W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,R}}(t_1, t_2) = \Phi_{ij\downarrow}^{GW, \text{fermions,1/2,R}}(t_1, t_2) \quad (2.388)$$

$$+U(t_1) \int_{t_2}^{t_1} dt_3 \sum_m G_{i\uparrow m\uparrow i\uparrow m\uparrow}^{\text{F,R}}(t_1, t_3) W_{m\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,R}}(t_3, t_2),$$

$$W_{i\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,\geq}}(t_1, t_2) \quad (2.389)$$

$$= U(t_1) \int_{t_0}^{t_1} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,R}}(t_1, t_3) W_{m\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,\geq}}(t_3, t_2)$$

$$+U(t_1) \int_{t_0}^{t_2} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,\geq}}(t_1, t_3) W_{m\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2)$$

and

$$W_{i\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,A}}(t_1, t_2) \quad (2.390)$$

$$= U_1 \int_{t_1}^{t_2} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,A}}(t_1, t_3) W_{m\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,A}}(t_3, t_2),$$

$$W_{i\uparrow j\downarrow}^{\text{non-sing.,fermions,1/2,R}}(t_1, t_2) \quad (2.391)$$

$$= U_1 \int_{t_2}^{t_1} dt_3 \sum_m G_{i\downarrow m\downarrow i\downarrow m\downarrow}^{\text{F,R}}(t_1, t_3) W_{m\downarrow j\downarrow}^{\text{non-sing.,fermions,1/2,R}}(t_3, t_2).$$

The components of the correlation selfenergy read

$$\Sigma_{i\uparrow j\uparrow}^{\text{GW,corr,fermions,\geq}}(t_1, t_2) \quad (2.392)$$

$$= i\hbar W_{i\uparrow j\uparrow}^{\text{non-sing.,fermions,\geq}}(t_1, t_2) G_{i\uparrow j\uparrow}^{\geq}(t_1, t_2)$$

and

$$\begin{aligned} & \Sigma_{i\downarrow j\downarrow}^{\text{GW,corr,fermions},\geq}(t_1, t_2) \\ &= i\hbar W_{i\downarrow j\downarrow}^{\text{non-sing.,fermions},\geq}(t_1, t_2) G_{i\downarrow j\downarrow}^{\geq}(t_1, t_2). \end{aligned} \quad (2.393)$$

2.7.2.3 T -matrices

In contrast to the GW -approximation, the T -matrix is an approximation, which takes only the bare interaction w into account and aims instead at a good approximation of the bare vertex function Λ . Thus, its constitutive equations are the Dyson equation,

$$\begin{aligned} G_{ij}(z_1, z_2) &= \\ & G_{ij}^{(0)}(z_1, z_2) + \int_{\mathcal{C}} dz_3 dz_4 \sum_{mn} G_{im}^{(0)}(z_1, z_3) \Sigma_{mn}(z_3, z_4) G_{nj}(z_4, z_2), \end{aligned} \quad (2.394)$$

the equation for the selfenergy, cf. Eqs. (2.94) and (2.96),

$$\Sigma_{ij}(z_1, z_2) = \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{xc}}(z_1, z_2), \quad (2.395)$$

with

$$\begin{aligned} & \Sigma_{ij}^{\text{xc}}(z_1, z_2) \\ &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \Lambda_{nqpj}(z_3, z_2, z_1). \end{aligned} \quad (2.396)$$

The bare vertex Λ is self-consistently given as the solution of

$$\begin{aligned} & \Lambda_{ijkl}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl} \\ & + \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} \int_{\mathcal{C}} dz_6 \sum_p G_{mp}(z_4, z_6) \\ & \int_{\mathcal{C}} dz_7 \sum_q G_{qn}(z_7, z_5) \Lambda_{pj kq}(z_6, z_7, z_3). \end{aligned} \quad (2.397)$$

If these equations are iterated ad infinitum, all selfenergy terms will be generated. To break the circular dependence between Eqs. (2.396) and (2.397), the T -matrix approximation starts by taking the bare vertex on the right-hand side of Eq. (2.397) only in zeroth order,

$$\Lambda_{ijkl}^{(0)}(z_1, z_2, z_3) = \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl}, \quad (2.398)$$

transforming it into

$$\begin{aligned} \Lambda_{ijkl}^{\text{closed}}(z_1, z_2, z_3) &= \delta_{\mathcal{C}}(z_1, z_{2+}) \delta_{\mathcal{C}}(z_3, z_2) \delta_{ik} \delta_{jl} \\ &+ \int_{\mathcal{C}} dz_4 dz_5 \sum_{mn} \frac{\delta \Sigma_{il}^{\text{closed}}(z_1, z_2)}{\delta G_{mn}(z_4, z_5)} G_{mk}(z_4, z_3) G_{jn}(z_3, z_5). \end{aligned} \quad (2.399)$$

To arrive at a closed equation, this result is used in Eq. (2.395), yielding

$$\begin{aligned} \Sigma_{ij}^{\text{closed}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{xc}}(z_1, z_2) \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \Lambda_{nqpj}^{\text{closed}}(z_3, z_2, z_1). \end{aligned} \quad (2.400)$$

Inserting Eq. (2.399), one has

$$\begin{aligned} \Sigma_{ij}^{\text{closed}}(z_1, z_2) &= \pm i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} w_{mijn}(z_1) G_{nm}(z_1, z_{1+}) \\ &+ i\hbar \sum_{mn} w_{injm}(z_1) G_{mn}(z_1, z_{1+}) \delta_{\mathcal{C}}(z_1, z_2) \\ &+ i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \end{aligned} \quad (2.401)$$

This term can be restructured to yield

$$\begin{aligned}
 & \Sigma_{ij}^{\text{closed}}(z_1, z_2) \tag{2.402} \\
 &= i\hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mn} G_{mn}(z_1, z_{1+}) (w_{injm}(z_1) \pm w_{nijm}(z_1)) \\
 &+ i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\
 &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).
 \end{aligned}$$

Using Eq. (2.108) again, one finds

$$\begin{aligned}
 & \Sigma_{ij}^{\text{closed}}(z_1, z_2) \tag{2.403} \\
 &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) + i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\
 &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).
 \end{aligned}$$

Taking the derivative with respect to G , one arrives at

$$\begin{aligned}
 & \frac{\delta \Sigma_{ij}^{\text{closed}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} = i\hbar \delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_1, z_6) \delta_{\mathcal{C}}(z_{1+}, z_7) (w_{iujt}(z_1) \pm w_{uijt}(z_1)) \\
 & \left(\frac{\delta \Sigma_{ij}^{\text{closed,a}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} + \frac{\delta \Sigma_{ij}^{\text{closed,b}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \right. \\
 & \left. + \frac{\delta \Sigma_{ij}^{\text{closed,c}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} + \frac{\delta \Sigma_{ij}^{\text{closed,d}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \right), \tag{2.404}
 \end{aligned}$$

with

$$\frac{\delta\Sigma_{ij}^{\text{closed,a}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \quad (2.405)$$

$$= i\hbar\delta_C(z_1, z_6) \sum_{pq} w_{ipqt}(z_1) \int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta\Sigma_{uj}^{\text{closed}}(z_7, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5),$$

$$\frac{\delta\Sigma_{ij}^{\text{closed,b}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \quad (2.406)$$

$$= i\hbar\delta_C(z_1, z_7) \sum_{mq} w_{iuqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \int_{\mathcal{C}} dz_5 \sum_s \frac{\delta\Sigma_{nj}^{\text{closed}}(z_3, z_2)}{\delta G_{ts}(z_6, z_5)} G_{qs}(z_1, z_5)$$

and

$$\frac{\delta\Sigma_{ij}^{\text{closed,c}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \quad (2.407)$$

$$= i\hbar\delta_C(z_1, z_6) \sum_{mp} w_{iptm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \int_{\mathcal{C}} dz_4 \sum_r \frac{\delta\Sigma_{nj}^{\text{closed}}(z_3, z_2)}{\delta G_{ru}(z_4, z_7)} G_{rp}(z_4, z_1)$$

as well as

$$\begin{aligned}
 & \frac{\delta \Sigma_{ij}^{\text{closed,d}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\
 &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\
 & \int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5) \delta G_{tu}(z_6, z_7)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).
 \end{aligned} \tag{2.408}$$

Neglecting $\frac{\delta \Sigma_{ij}^{\text{closed,d}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)}$ as an approximation, Eq. (2.404) becomes a closed equation for $\frac{\delta \Sigma^{\text{closed}}}{\delta G}$. The first iteration yields the second-order terms

$$\begin{aligned}
 & \frac{\delta \Sigma_{ij}^{\text{closed,(2)}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \approx \frac{\delta \Sigma_{ij}^{\text{closed,(2),a}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\
 & + \frac{\delta \Sigma_{ij}^{\text{closed,(2),b}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} + \frac{\delta \Sigma_{ij}^{\text{closed,(2),c}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)},
 \end{aligned} \tag{2.409}$$

with

$$\begin{aligned}
 & \frac{\delta \Sigma_{ij}^{\text{closed,(2),a}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_6) \delta_{\mathcal{C}}(z_2, z_7) \sum_{pq} w_{ipqt}(z_1) \\
 & \sum_{rs} (w_{usjr}(z_2) \pm w_{sujr}(z_2)) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2)
 \end{aligned} \tag{2.410}$$

and

$$\begin{aligned}
 & \frac{\delta \Sigma_{ij}^{\text{closed},(2),\text{b}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_7) \delta_{\mathcal{C}}(z_2, z_6) \sum_{mq} w_{iuqm}(z_1) \\
 & \quad \sum_n G_{mn}(z_1, z_2) \sum_s (w_{nsjt}(z_2) \pm w_{snjt}(z_2)) G_{qs}(z_1, z_2)
 \end{aligned} \tag{2.411}$$

as well as

$$\begin{aligned}
 & \frac{\delta \Sigma_{ij}^{\text{closed},(2),\text{c}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)} \\
 &= (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_6) \delta_{\mathcal{C}}(z_2, z_7) \sum_{mp} w_{iptm}(z_1) \\
 & \quad \sum_n G_{mn}(z_1, z_2) \sum_r (w_{nujr}(z_2) \pm w_{unjr}(z_2)) G_{rp}(z_2, z_1).
 \end{aligned} \tag{2.412}$$

Note that, for the first iteration, $\frac{\delta \Sigma_{ij}^{\text{closed},\text{d}}(z_1, z_2)}{\delta G_{tu}(z_6, z_7)}$ is exactly equal to zero, thus Eq. (2.409) is also exact up to second order in w . In the following, each of the three terms will be considered separately. To start with, one recognizes that all three terms yield the same first and second-order contributions to the selfenergy, which read

$$\Sigma_{ij}^{\text{closed},(1)}(z_1, z_2) = \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \tag{2.413}$$

$$\Sigma_{ij}^{\text{closed},(2)}(z_1, z_2) = (i\hbar)^2 \sum_{mpq} w_{ipqm}(z_1) \sum_n G_{mn}(z_1, z_2) \tag{2.414}$$

$$\sum_{rs} (w_{nsjr}(z_2) \pm w_{snjr}(z_2)) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2)$$

and agree with the exact first and second-order terms, already encountered in Eqs. (2.110), (2.141) and (2.150). The third-order contributions to Σ^{closed} from the

second-order terms in Eq. (2.409) are given by

$$\begin{aligned} \Sigma_{ij}^{\text{closed,(3),a}}(z_1, z_2) &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed,(2),a}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \end{aligned} \quad (2.415)$$

Inserting the second-order term yields

$$\begin{aligned} \Sigma_{ij}^{\text{closed,(3),a}}(z_1, z_2) &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\sum_{rs} \sum_{tu} w_{ntur}(z_3) \sum_{vw} (w_{swjv}(z_2) \pm w_{wsjv}(z_2)) \\ &G_{vt}(z_2, z_3) G_{uw}(z_3, z_2) G_{rp}(z_3, z_1) G_{qs}(z_1, z_2). \end{aligned} \quad (2.416)$$

For the second third-order selfenergy term, one has

$$\begin{aligned} \Sigma_{ij}^{\text{closed,(3),b}}(z_1, z_2) &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed,(2),b}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5). \end{aligned} \quad (2.417)$$

which evaluates to

$$\begin{aligned} \Sigma_{ij}^{\text{closed,(3),b}}(z_1, z_2) &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ &\sum_{rs} \sum_{tu} w_{nsut}(z_3) \sum_v G_{tv}(z_3, z_2) \sum_w (w_{vwjr}(z_2) \pm w_{wvjr}(z_2)) \\ &G_{uw}(z_3, z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_3). \end{aligned} \quad (2.418)$$

The third term reads

$$\begin{aligned}
 \Sigma_{ij}^{\text{closed,(3),c}}(z_1, z_2) &= i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \quad (2.419) \\
 &\int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} \frac{\delta \Sigma_{nj}^{\text{closed,(2),c}}(z_3, z_2)}{\delta G_{rs}(z_4, z_5)} G_{rp}(z_4, z_1) G_{qs}(z_1, z_5) \\
 &= (i\hbar)^3 \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3).
 \end{aligned}$$

Using the second-order result, one arrives at

$$\begin{aligned}
 \Sigma_{ij}^{\text{closed,(3),c}}(z_1, z_2) \quad (2.420) \\
 \sum_{rs} \sum_{tu} w_{nurt}(z_3) \sum_v G_{tv}(z_3, z_2) \sum_w (w_{vsjw}(z_2) \pm w_{svjw}(z_2)) \\
 G_{wu}(z_2, z_3) G_{rp}(z_3, z_1) G_{qs}(z_1, z_2).
 \end{aligned}$$

These terms and all higher-order contributions are completely determined by the knowledge of $\frac{\delta \Sigma^{\text{closed}}}{\delta G}$, cf. Eq. (2.404), which follows from the solution of Eq. (2.409).

For $\frac{\delta \Sigma_{ij}^{\text{closed,a}}}{\delta G}$, one has

$$\begin{aligned}
 K_{ijkl}^a(z_1, z_2, z_3, z_4) &:= \pm \frac{\delta \Sigma_{ik}^{\text{closed,a}}(z_1, z_3)}{\delta G_{lj}(z_4, z_2)} \quad (2.421) \\
 &= \pm i\hbar \delta_{\mathcal{C}}(z_1, z_3) \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_1, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)) \\
 &\quad \pm i\hbar \delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \\
 &\quad \int_{\mathcal{C}} dz_5 dz_6 \sum_{rs} \frac{\delta \Sigma_{jk}^{\text{closed}}(z_2, z_3)}{\delta G_{rs}(z_5, z_6)} G_{rp}(z_5, z_1) G_{qs}(z_1, z_6).
 \end{aligned}$$

where the kernel K has been introduced. Making the approximation

$$\frac{\delta \Sigma_{jk}^{\text{closed}}(z_2, z_3)}{\delta G_{rs}(z_5, z_6)} \approx \frac{\delta \Sigma_{jk}^{\text{closed,a}}(z_2, z_3)}{\delta G_{rs}(z_5, z_6)}, \quad (2.422)$$

one arrives at a closed equation for $K_{ijkl}^a(z_1, z_2, z_3, z_4)$,

$$\begin{aligned} K_{ijkl}^a(z_1, z_2, z_3, z_4) & \\ &= \pm i\hbar \delta_{\mathcal{C}}(z_1, z_3) \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)) \\ &\quad + i\hbar \delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \\ &\quad \int_{\mathcal{C}} dz_5 dz_6 \sum_{rs} K_{jskr}^a(z_2, z_6, z_3, z_5) G_{rp}(z_5, z_1) G_{qs}(z_1, z_6). \end{aligned} \quad (2.423)$$

Iterating this equation, starting from

$$\begin{aligned} K_{ijkl}^{a,(1)}(z_1, z_2, z_3, z_4) &= \\ &\pm i\hbar \delta_{\mathcal{C}}(z_1, z_3) \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)), \end{aligned} \quad (2.424)$$

one has

$$\begin{aligned} K_{ijkl}^{a,(2)}(z_1, z_2, z_3, z_4) &= i\hbar \delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \\ &\quad \int_{\mathcal{C}} dz_5 dz_6 \sum_{rs} K_{jskr}^{a,(1)}(z_2, z_6, z_3, z_5) G_{rp}(z_5, z_1) G_{qs}(z_1, z_6) \\ &= \pm (i\hbar)^2 \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_2, z_3) \sum_{pq} w_{ipql}(z_1) \\ &\quad \sum_{rs} (w_{jskr}(z_2) \pm w_{sjkr}(z_2)) G_{rp}(z_2, z_1) G_{qs}(z_1, z_2), \end{aligned} \quad (2.425)$$

$$K_{ijkl}^{a,(3)}(z_1, z_2, z_3, z_4) = i\hbar\delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \quad (2.426)$$

$$\begin{aligned} & \int_{\mathcal{C}} dz_5 dz_6 \sum_{rs} K_{jskr}^{a,(2)}(z_2, z_6, z_3, z_5) G_{rp}(z_5, z_1) G_{qs}(z_1, z_6) \\ &= \pm i\hbar\delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \\ & \sum_{rs} K_{jskr}^{a,(2)}(z_2, z_3, z_3, z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_3), \end{aligned}$$

$$K_{ijkl}^{a,(4)}(z_1, z_2, z_3, z_4) = i\hbar\delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \quad (2.427)$$

$$\begin{aligned} & \int_{\mathcal{C}} dz_5 dz_6 \sum_{rs} K_{jskr}^{a,(3)}(z_2, z_6, z_3, z_5) G_{rp}(z_5, z_1) G_{qs}(z_1, z_6) \\ &= i\hbar\delta_{\mathcal{C}}(z_1, z_4) \sum_{pq} w_{ipql}(z_1) \\ & \int_{\mathcal{C}} dz_6 \sum_{rs} K_{jskr}^{a,(3)}(z_2, z_6, z_3, z_2) G_{rp}(z_2, z_1) G_{qs}(z_1, z_6) \end{aligned}$$

and a similar structure for the higher orders. It is noteworthy that the computation of the fourth- and higher-order iterations are of complexity $\mathcal{O}(N_t^4)$, since, due to the appearance of $\delta_{\mathcal{C}}(z_1, z_4)$,

$$K_{ijkl}^{a,(N)}(z_1, z_2, z_3, z_4) = \delta_{\mathcal{C}}(z_1, z_4) K_{ijkl}^{a,(N)}(z_1, z_2, z_3, z_1), \quad (2.428)$$

and the right-hand side consists of one integral over an intermediate time, which limits the applicability of this approximation to very short time scales.

Turning to the second approximation involving $\frac{\delta\Sigma_{ij}^{\text{closed,b}}}{\delta G}$, cf. Eq. (2.409), one

arrives at

$$\begin{aligned}
 K_{ijkl}^{\text{b}}(z_1, z_2, z_3, z_4) &:= \pm \frac{\delta \Sigma_{ik}^{\text{closed,b}}(z_1, z_3)}{\delta G_{lj}(z_4, z_2)} \\
 &\approx \pm i \hbar \delta_{\mathcal{C}}(z_1, z_3) \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)) \\
 &\quad \pm i \hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mq} w_{ijqm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\quad \int_{\mathcal{C}} dz_6 \sum_s \frac{\delta \Sigma_{nk}^{\text{closed,b}}(z_5, z_3)}{\delta G_{ls}(z_4, z_6)} G_{qs}(z_1, z_6),
 \end{aligned} \tag{2.429}$$

which yields

$$\begin{aligned}
 K_{ijkl}^{\text{b}}(z_1, z_2, z_3, z_4) & \\
 &= \pm i \hbar \delta_{\mathcal{C}}(z_1, z_3) \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)) \\
 &\quad + i \hbar \delta_{\mathcal{C}}(z_1, z_2) \sum_{mq} w_{ijqm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\quad \int_{\mathcal{C}} dz_6 \sum_s K_{nskl}^{\text{b}}(z_5, z_6, z_3, z_4) G_{qs}(z_1, z_6).
 \end{aligned} \tag{2.430}$$

Iterating, starting again from

$$\begin{aligned}
 K_{ijkl}^{\text{b,(1)}}(z_1, z_2, z_3, z_4) & \\
 &= \pm i \hbar \delta_{\mathcal{C}}(z_1, z_3) \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)),
 \end{aligned} \tag{2.431}$$

one finds

$$\begin{aligned}
 K_{ijkl}^{b,(2)}(z_1, z_2, z_3, z_4) &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mq} w_{ijqm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\quad \int_{\mathcal{C}} dz_6 \sum_s K_{nskl}^{b,(1)}(z_5, z_6, z_3, z_4) G_{qs}(z_1, z_6) \\
 &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_3, z_4) \sum_{mq} w_{ijqm}(z_1) \sum_n G_{mn}(z_1, z_3) \\
 &\quad \sum_s K_{nskl}^{b,(1)}(z_3, z_3, z_3, z_3) G_{qs}(z_1, z_3)
 \end{aligned} \tag{2.432}$$

as well as

$$\begin{aligned}
 K_{ijkl}^{b,(3)}(z_1, z_2, z_3, z_4) &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \sum_{mq} w_{ijqm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\quad \int_{\mathcal{C}} dz_6 \sum_s K_{nskl}^{b,(2)}(z_5, z_6, z_3, z_4) G_{qs}(z_1, z_6) \\
 &= i\hbar\delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_3, z_4) \sum_{mq} w_{ijqm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\quad \sum_s K_{nskl}^{b,(2)}(z_5, z_5, z_3, z_3) G_{qs}(z_1, z_5)
 \end{aligned} \tag{2.433}$$

and similar in higher orders. The structure of this approximation is such that the computation of all terms lies within $\mathcal{O}(N_t^3)$, since one has, due to the two delta functions,

$$\begin{aligned}
 K_{ijkl}^{b,(N)}(z_1, z_2, z_3, z_4) &= \delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_3, z_4) K_{ijkl}^{b,(N)}(z_1, z_1, z_2, z_2) \\
 &=: \delta_{\mathcal{C}}(z_1, z_2) \delta_{\mathcal{C}}(z_3, z_4) K_{ijkl}^{b,(N)}(z_1, z_2),
 \end{aligned} \tag{2.434}$$

and one integration on the right-hand side. With this, one finds, cf. Eq. (2.433),

$$\begin{aligned}
 K_{ijkl}^b(z_1, z_3) &= \delta_C(z_1, z_3) K_{ijkl}^{b,(1)}(z_1, z_1) \\
 &+ \sum_{mq} w_{ijqm}(z_1) \int_C dz_5 \sum_{ns} G_{mqns}^H(z_1, z_5) K_{nskl}^b(z_5, z_3),
 \end{aligned} \tag{2.435}$$

where Eq. (2.320) has been used in the last line. To simplify the following expressions further, it is useful to introduce the non-singular kernel, cf. Eqs. (2.435) and (2.431) according to

$$\begin{aligned}
 K_{ijkl}^{b,\text{non-sing}}(z_1, z_2) &:= K_{ijkl}^b(z_1, z_2) - \delta_C(z_1, z_2) K_{ijkl}^{b,(1)}(z_1, z_1) \\
 &= K_{ijkl}^b(z_1, z_2) \mp i\hbar \delta_C(z_1, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)).
 \end{aligned} \tag{2.436}$$

It obeys, cf. Eq. (2.435),

$$\begin{aligned}
 K_{ijkl}^{b,\text{non-sing}}(z_1, z_2) &= \sum_{mq} w_{ijqm}(z_1) \int_C dz_5 \sum_{ns} G_{mqns}^H(z_1, z_5) \\
 &\quad \left\{ K_{nskl}^{b,\text{non-sing}}(z_5, z_2) \pm i\hbar \delta_C(z_5, z_2) (w_{nskl}(z_2) \pm w_{snkl}(z_2)) \right\} \\
 &= \pm i\hbar \sum_{mq} w_{ijqm}(z_1) \sum_{ns} G_{mqns}^H(z_1, z_2) (w_{nskl}(z_2) \pm w_{snkl}(z_2)) \\
 &\quad + \sum_{mq} w_{ijqm}(z_1) \int_C dz_5 \sum_{ns} G_{mqns}^H(z_1, z_5) K_{nskl}^{b,\text{non-sing}}(z_5, z_2).
 \end{aligned} \tag{2.437}$$

The corresponding selfenergy reads, cf. Eq. (2.403),

$$\begin{aligned}
 \Sigma_{ij}^{\text{closed,b}}(z_1, z_2) &= \Sigma_{ij}^H(z_1, z_2) + \Sigma_{ij}^F(z_1, z_2) \\
 &\quad \pm i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_C dz_3 \sum_n G_{mn}(z_1, z_3) \\
 &\quad \int_C dz_4 dz_5 \sum_{rs} K_{nsjr}^b(z_3, z_5, z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).
 \end{aligned} \tag{2.438}$$

Inserting the expression for K^b , one finds

$$\begin{aligned} \Sigma_{ij}^{\text{closed,b}}(z_1, z_2) & \quad (2.439) \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \pm i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\ & \quad \sum_{rs} G_{qs}(z_1, z_3) K_{nsjr}^b(z_3, z_2) G_{rp}(z_2, z_1), \end{aligned}$$

which, by insertion of Eq. (2.436), transforms to

$$\begin{aligned} \Sigma_{ij}^{\text{closed,b}}(z_1, z_2) & \quad (2.440) \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \pm \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_{nrs} G_{mqns}^{\text{H}}(z_1, z_3) \\ & \quad \left\{ K_{nsjr}^{\text{b,non-sing}}(z_3, z_2) \pm i\hbar \delta_{\mathcal{C}}(z_3, z_2) (w_{nsjr}(z_2) \pm w_{snjr}(z_2)) \right\} G_{rp}(z_2, z_1). \end{aligned}$$

After restructuring, one has

$$\begin{aligned} \Sigma_{ij}^{\text{closed,b}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \quad (2.441) \\ & \pm \left(\pm i\hbar \sum_{mpq} w_{ipqm}(z_1) \sum_{nrs} G_{mqns}^{\text{H}}(z_1, z_3) (w_{nsjr}(z_2) \pm w_{snjr}(z_2)) \right) \\ & + \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_{nrs} G_{mqns}^{\text{H}}(z_1, z_3) K_{nsjr}^{\text{b,non-sing}}(z_3, z_2) G_{rp}(z_2, z_1). \end{aligned}$$

Looking at Eq. (2.437), it is obvious that the right-hand side already contains the first iteration of the recursion equation and one simply has

$$\begin{aligned} \Sigma_{ij}^{\text{closed,b}}(z_1, z_2) & \quad (2.442) \\ &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \pm \sum_{pr} K_{ipjr}^{\text{b,non-sing}}(z_1, z_2) G_{rp}(z_2, z_1). \end{aligned}$$

With the definition

$$i\hbar T_{ijkl}^{\text{pp}}(z_1, z_2) := \pm K_{ijkl}^{\text{b,non-sing}}(z_1, z_2), \quad (2.443)$$

the coupled solution of, cf. Eqs. (2.437) and (2.442),

$$\begin{aligned}
 T_{ijkl}^{\text{PP}}(z_1, z_2) &= \sum_{mq} w_{ijqm}(z_1) \sum_{ns} G_{mqns}^{\text{H}}(z_1, z_2) (w_{nskl}(z_2) \pm w_{snkl}(z_2)) \\
 &+ \sum_{mq} w_{ijqm}(z_1) \sum_{ns} \int_{\mathcal{C}} dz_5 G_{mqns}^{\text{H}}(z_1, z_5) T_{nskl}^{\text{PP}}(z_5, z_2) \quad (2.444) \\
 &=: \Phi_{ijkl}^{\text{PP}}(z_1, z_2) + \sum_{mq} w_{ijqm}(z_1) \sum_{ns} \int_{\mathcal{C}} dz_5 G_{mqns}^{\text{H}}(z_1, z_5) T_{nskl}^{\text{PP}}(z_5, z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 \Sigma_{ij}^{\text{TPP}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \quad (2.445) \\
 &+ i\hbar \sum_{pr} T_{ipjr}^{\text{PP}}(z_1, z_2) G_{rp}(z_2, z_1)
 \end{aligned}$$

constitutes the so-called (particle–particle) T -matrix approximation . It relates to a similar quantity in scattering theory, which is called transfer matrix there. It describes an interacting scattering state of a system selfconsistently in terms of a free state of two particles which undergo infinitely many scattering events with each other, which can be resummed into the transfer matrix acting on the two particles. Looking at Eqs. (2.444) and (2.445), the same interpretation is possible, since G^{H} describes two particles and the scattering is governed by T^{PP} . The Keldysh components of the particle–particle T -matrix read

$$\begin{aligned}
 T_{ijkl}^{\text{PP}, \gtrless}(t_1, t_2) &= \sum_{mq} w_{ijqm}(t_1) \sum_{ns} G_{mqns}^{\text{H}, \gtrless}(t_1, t_2) (w_{nskl}(t_2) \pm w_{snkl}(t_2)) \\
 &+ \sum_{mq} w_{ijqm}(t_1) \sum_{ns} \quad (2.446) \\
 &\left(\int_{t_0}^{t_1} dt_5 G_{mqns}^{\text{H}, \text{R}}(t_1, t_5) T_{nskl}^{\text{PP}, \gtrless}(t_5, t_2) + \int_{t_0}^{t_2} dt_5 G_{mqns}^{\text{H}, \gtrless}(t_1, t_5) T_{nskl}^{\text{PP}, \text{A}}(t_5, t_2) \right).
 \end{aligned}$$

Introducing an abbreviation for the first term like for the GW approximation, one

has

$$T_{ijkl}^{\text{PP},\geq}(t_1, t_2) \quad (2.447)$$

$$=: \Phi_{ijkl}^{\text{PP},\geq} + \sum_{mq} w_{ijqm}(t_1) \sum_{ns}$$

$$\left(\int_{t_0}^{t_1} dt_5 G_{mqns}^{\text{H,R}}(t_1, t_5) T_{nskl}^{\text{PP},\geq}(t_5, t_2) + \int_{t_0}^{t_2} dt_5 G_{mqns}^{\text{H},\geq}(t_1, t_5) T_{nskl}^{\text{PP,A}}(t_5, t_2) \right),$$

$$T_{ijkl}^{\text{PP,A}}(t_1, t_2) = \sum_{mq} w_{ijqm}(t_1) \sum_{ns} G_{mqns}^{\text{H,A}}(t_1, t_2) (w_{nskl}(t_2) \pm w_{snkl}(t_2))$$

$$+ \sum_{mq} w_{ijqm}(t_1) \sum_{ns} \int_{t_1}^{t_2} dt_5 G_{mqns}^{\text{H,A}}(t_1, t_5) T_{nskl}^{\text{PP,A}}(t_5, t_2)$$

$$=: \Phi_{ijkl}^{\text{PP,A}}(t_1, t_2)$$

$$+ \sum_{mq} w_{ijqm}(t_1) \sum_{ns} \int_{t_1}^{t_2} dt_5 G_{mqns}^{\text{H,A}}(t_1, t_5) T_{nskl}^{\text{PP,A}}(t_5, t_2) \quad (2.448)$$

and

$$T_{ijkl}^{\text{PP,R}}(t_1, t_2) = \sum_{mq} w_{ijqm}(t_1) \sum_{ns} G_{mqns}^{\text{H,R}}(t_1, t_2) (w_{nskl}(t_2) \pm w_{snkl}(t_2))$$

$$+ \sum_{mq} w_{ijqm}(t_1) \sum_{ns} \int_{t_2}^{t_1} dt_5 G_{mqns}^{\text{H,R}}(t_1, t_5) T_{nskl}^{\text{PP,R}}(t_5, t_2)$$

$$=: \Phi_{ijkl}^{\text{PP,R}}(t_1, t_2)$$

$$+ \sum_{mq} w_{ijqm}(t_1) \sum_{ns} \int_{t_2}^{t_1} dt_5 G_{mqns}^{\text{H,R}}(t_1, t_5) T_{nskl}^{\text{PP,R}}(t_5, t_2). \quad (2.449)$$

For the components of the selfenergy, one has

$$\begin{aligned}\Sigma_{ij}^{T^{pp},\geq}(t_1, t_2) &= \Sigma_{ij}^{H,\geq}(t_1, t_2) + \Sigma_{ij}^{F,\geq}(t_1, t_2) \\ &+ i\hbar \sum_{pr} T_{ipjr}^{pp,\geq}(t_1, t_2) G_{rp}^{\leq}(t_2, t_1).\end{aligned}\quad (2.450)$$

2.7.2.3.1 Particle–particle T -matrix in a diagonal basis In a basis with diagonal interaction $w_{ijkl} = \delta_{il}\delta_{jk}w_{ij}$, Eq. (2.444) attains the form

$$\begin{aligned}T_{ijkl}^{pp,diag.}(z_1, z_2) &= w_{ij}(z_1) \left(G_{ijlk}^H(z_1, z_2) \pm G_{ijkl}^H(z_1, z_2) \right) w_{lk}(z_2) \\ &+ w_{ij}(z_1) \sum_{ns} \int_{\mathcal{C}} dz_5 G_{ijn s}^H(z_1, z_5) T_{n s k l}^{pp,diag.}(z_5, z_2).\end{aligned}\quad (2.451)$$

Again using Φ , one finds

$$\begin{aligned}T_{ijkl}^{pp,diag.}(z_1, z_2) &=: \Phi_{ijkl}^{pp,diag.}(z_1, z_2) \\ &+ w_{ij}(z_1) \sum_{ns} \int_{\mathcal{C}} dz_5 G_{ijn s}^H(z_1, z_5) T_{n s k l}^{pp,diag.}(z_5, z_2).\end{aligned}\quad (2.452)$$

The term for the selfenergy, corresponding to Eq. (2.445), reads

$$\begin{aligned}\Sigma_{ij}^{pp,diag.}(z_1, z_2) &= \Sigma_{ij}^{diag.,H}(z_1, z_2) + \Sigma_{ij}^{diag.,F}(z_1, z_2) \\ &+ i\hbar \sum_{pr} T_{ipjr}^{pp,diag.}(z_1, z_2) G_{rp}(z_2, z_1).\end{aligned}\quad (2.453)$$

The leading contributions to the selfenergy for a diagonal basis are shown in Fig. 2.16. The respective components are

$$\begin{aligned}T_{ijkl}^{pp,diag.,\geq}(t_1, t_2) &= \Phi_{ijkl}^{pp,diag.,\geq}(t_1, t_2) \\ &+ w_{ij}(t_1) \left(\int_{t_0}^{t_1} dt_5 \sum_{ns} G_{ijn s}^{H,R}(t_1, t_5) T_{n s k l}^{pp,diag.,\geq}(t_5, t_2) \right. \\ &\quad \left. + \int_{t_0}^{t_2} dt_5 G_{ijn s}^{H,\geq}(t_1, t_5) T_{n s k l}^{pp,diag.,A}(t_5, t_2) \right),\end{aligned}\quad (2.454)$$

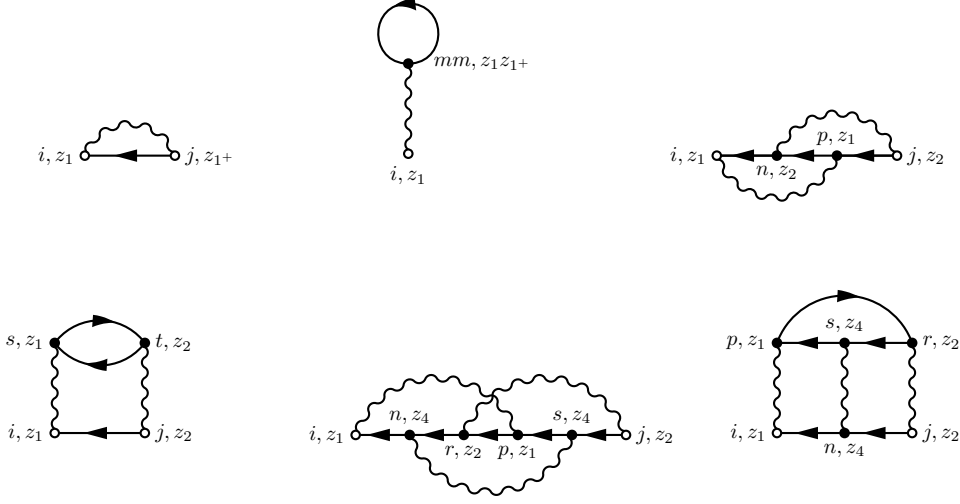


Figure 2.16: Leading terms of $\Sigma^{\text{pp,diag.}}$ in a diagonal basis.

$$T_{ijkl}^{\text{pp,diag.,A}}(t_1, t_2) = \Phi_{ijkl}^{\text{pp,diag.,A}}(t_1, t_2) \quad (2.455)$$

$$+ w_{ij}(t_1) \sum_{ns} \int_{t_1}^{t_2} dt_5 G_{ijn_s}^{\text{H,A}}(t_1, t_5) T_{n_skl}^{\text{pp,diag.,A}}(t_5, t_2),$$

$$T_{ijkl}^{\text{pp,diag.,R}}(t_1, t_2) = \Phi_{ijkl}^{\text{pp,diag.,R}}(t_1, t_2) \quad (2.456)$$

$$+ w_{ij}(t_1) \sum_{ns} \int_{t_2}^{t_1} dt_5 G_{ijn_s}^{\text{H,R}}(t_1, t_5) T_{n_skl}^{\text{pp,diag.,R}}(t_5, t_2)$$

and

$$\Sigma_{ij}^{\text{pp,diag.,}\geq}(t_1, t_2) = \Sigma_{ij}^{\text{H,diag.,}\geq}(t_1, t_2) + \Sigma_{ij}^{\text{F,diag.,}\geq}(t_1, t_2) \quad (2.457)$$

$$+ \sum_{pr} T_{ipjr}^{\text{pp,diag.,}\geq}(t_1, t_2) G_{rp}^{\leq}(t_2, t_1).$$

2.7.2.3.2 Particle–particle T -matrix in the Hubbard basis In the bosonic Hubbard basis, the particle–particle T -matrix reads

$$\begin{aligned}
 T_{i\alpha j\beta k\alpha l\beta}^{\text{pp,bosons}}(z_1, z_2) &= 2\delta_{ij}\delta_{kl}U(z_1)G_{i\alpha i\beta k\alpha k\beta}^{\text{H}}(z_1, z_2)U(z_2) \\
 &+ \delta_{ij}U(z_1)\sum_{ns}\int_{\mathcal{C}}dz_5G_{i\alpha i\beta n\alpha s\beta}^{\text{H}}(z_1, z_5)T_{n\alpha s\beta k\alpha l\beta}^{\text{pp,bosons}}(z_5, z_2) \\
 &=: \delta_{ij}\delta_{kl}\Phi_{i\alpha i\beta k\alpha k\beta}^{\text{pp,bosons}}(z_1, z_2) \\
 &+ \delta_{ij}U(z_1)\sum_{ns}\int_{\mathcal{C}}dz_5G_{i\alpha i\beta n\alpha s\beta}^{\text{H}}(z_1, z_5)T_{n\alpha s\beta k\alpha l\beta}^{\text{pp,bosons}}(z_5, z_2).
 \end{aligned} \tag{2.458}$$

For the selfenergy, one has

$$\begin{aligned}
 \Sigma_{i\alpha j\alpha}^{\text{pp,bosons}}(z_1, z_2) &= \Sigma_{i\alpha j\alpha}^{\text{H,bosons}}(z_1, z_2) + \Sigma_{i\alpha j\alpha}^{\text{F,bosons}}(z_1, z_2) \\
 &+ i\hbar\sum_{pr}\sum_{\epsilon}T_{i\alpha p\epsilon j\alpha r\epsilon}^{\text{pp,bosons}}(z_1, z_2)G_{r\epsilon p\epsilon}(z_2, z_1).
 \end{aligned} \tag{2.459}$$

From these equations it is evident that

$$\Phi_{i\alpha j\beta k\alpha l\beta}^{\text{pp,bosons}}(z_1, z_2) = \delta_{ij}\delta_{kl}\Phi_{i\alpha i\beta k\alpha k\beta}^{\text{pp,bosons}}(z_1, z_2) \tag{2.460}$$

implies

$$T_{i\alpha j\beta k\alpha l\beta}^{\text{pp,bosons}}(z_1, z_2) =: \delta_{ij}\delta_{kl}T_{ik\alpha\beta}^{\text{pp,bosons}}(z_1, z_2) \tag{2.461}$$

by iteration. Regarding the notation, one has to bear in mind that $T_{ik\alpha\beta}^{\text{pp,bosons}}$ and

$$G_{ik\alpha\beta}^{\text{H}} := G_{i\alpha i\beta k\alpha k\beta}^{\text{H}} \tag{2.462}$$

are quantities of all four spin-space orbitals $|i\alpha\rangle, |i\beta\rangle, |k\alpha\rangle, |k\beta\rangle$. With this, the equations become

$$\begin{aligned}
 T_{ik\alpha\beta}^{\text{pp,bosons}}(z_1, z_2) &= 2U(z_1)G_{ik\alpha\beta}^{\text{H}}(z_1, z_2)U(z_2) \\
 &+ U(z_1)\sum_n \int_{\mathcal{C}} dz_5 G_{in\alpha\beta}^{\text{H}}(z_1, z_5)T_{nk\alpha\beta}^{\text{pp,bosons}}(z_5, z_2) \\
 &= \Phi_{ik\alpha\beta}^{\text{pp,bosons}}(z_1, z_2) \\
 &+ U(z_1)\sum_n \int_{\mathcal{C}} dz_5 G_{in\alpha\beta}^{\text{H}}(z_1, z_5)T_{nk\alpha\beta}^{\text{pp,bosons}}(z_5, z_2)
 \end{aligned} \tag{2.463}$$

and

$$\begin{aligned}
 \Sigma_{i\alpha j\alpha}^{\text{pp,bosons}}(z_1, z_2) &= \Sigma_{i\alpha j\alpha}^{\text{H,bosons}}(z_1, z_2) + \Sigma_{i\alpha j\alpha}^{\text{F,bosons}}(z_1, z_2) \\
 &+ i\hbar \sum_{\epsilon} T_{ij\alpha\epsilon}^{\text{pp,bosons}}(z_1, z_2)G_{j\epsilon i\epsilon}(z_2, z_1).
 \end{aligned} \tag{2.464}$$

The components read

$$\begin{aligned}
 \Sigma_{i\alpha j\alpha}^{\text{pp,bosons},\geq}(t_1, t_2) &= \Sigma_{i\alpha j\alpha}^{\text{H,bosons},\geq}(t_1, t_2) + \Sigma_{i\alpha j\alpha}^{\text{F,bosons},\geq}(t_1, t_2) \\
 &+ i\hbar \sum_{\epsilon} T_{ij\alpha\epsilon}^{\text{pp,bosons},\geq}(t_1, t_2)G_{j\epsilon i\epsilon}^{\leq}(t_2, t_1)
 \end{aligned} \tag{2.465}$$

and

$$\begin{aligned}
 T_{ik\alpha\beta}^{\text{pp,bosons},\geq}(t_1, t_2) &= \Phi_{ik\alpha\beta}^{\text{pp,bosons},\geq}(t_1, t_2) + U(t_1)\sum_n \\
 &\left(\int_{t_0}^{t_1} dt_5 G_{in\alpha\beta}^{\text{H,R}}(t_1, t_5)T_{nk\alpha\beta}^{\text{pp},\geq}(t_5, t_2) + \int_{t_0}^{t_2} dt_5 G_{in\alpha\beta}^{\text{H},\geq}(t_1, t_5)T_{nk\alpha\beta}^{\text{pp,A}}(t_5, t_2) \right)
 \end{aligned} \tag{2.466}$$

as well as

$$T_{ik\alpha\beta}^{\text{pp,bosons,A}}(t_1, t_2) = \Phi_{ik\alpha\beta}^{\text{pp,bosons,A}}(t_1, t_2) + U(t_1) \sum_n \quad (2.467)$$

$$\int_{t_1}^{t_2} dt_5 G_{in\alpha\beta}^{\text{H,A}}(t_1, t_5) T_{nk\alpha\beta}^{\text{pp,A}}(t_5, t_2)$$

and

$$T_{ik\alpha\beta}^{\text{pp,bosons,R}}(t_1, t_2) = \Phi_{ik\alpha\beta}^{\text{pp,bosons,R}}(t_1, t_2) + U(t_1) \sum_n \quad (2.468)$$

$$\int_{t_2}^{t_1} dt_5 G_{in\alpha\beta}^{\text{H,R}}(t_1, t_5) T_{nk\alpha\beta}^{\text{pp,R}}(t_5, t_2).$$

In the case of spin-0 bosons, one has

$$T_{ik}^{\text{pp,bosons,0}}(z_1, z_2) = 2U(z_1) G_{ik}^{\text{H}}(z_1, z_2) U(z_2) \quad (2.469)$$

$$+ U(z_1) \sum_n \int_{\mathcal{C}} dz_5 G_{in}^{\text{H}}(z_1, z_5) T_{nk}^{\text{pp,bosons,0}}(z_5, z_2)$$

$$= \Phi_{ik}^{\text{pp,bosons,0}}(z_1, z_2)$$

$$+ U(z_1) \sum_n \int_{\mathcal{C}} dz_5 G_{in}^{\text{H}}(z_1, z_5) T_{nk}^{\text{pp,bosons,0}}(z_5, z_2)$$

and

$$\Sigma_{ij}^{\text{pp,bosons,0}}(z_1, z_2) = \Sigma_{ij}^{\text{H,bosons,0}}(z_1, z_2) + \Sigma_{ij}^{\text{F,bosons,0}}(z_1, z_2) \quad (2.470)$$

$$+ i\hbar T_{ij}^{\text{pp,bosons,0}}(z_1, z_2) G_{ji}(z_2, z_1).$$

The components are

$$\begin{aligned} \Sigma_{ij}^{\text{pp,bosons,0},\geq}(t_1, t_2) &= \Sigma_{ij}^{\text{H,bosons,0},\geq}(t_1, t_2) + \Sigma_{ij}^{\text{F,bosons,0},\geq}(t_1, t_2) \\ &+ i\hbar T_{ij}^{\text{pp,bosons,0},\geq}(t_1, t_2) G_{ji}^{\leq}(t_2, t_1) \end{aligned} \quad (2.471)$$

and

$$T_{ik}^{\text{pp,bosons},0,\geq}(t_1, t_2) = \Phi_{ik}^{\text{pp,bosons},0,\geq}(t_1, t_2) + U(t_1) \sum_n \quad (2.472)$$

$$\left(\int_{t_0}^{t_1} dt_5 G_{in}^{\text{H,R}}(t_1, t_5) T_{nk}^{\text{pp,bosons},0,\geq}(t_5, t_2) \right. \\ \left. + \int_{t_0}^{t_2} dt_5 G_{in}^{\text{H},\geq}(t_1, t_5) T_{nk}^{\text{pp,bosons},0,\text{A}}(t_5, t_2) \right),$$

$$T_{ik}^{\text{pp,bosons},0,\text{A}}(t_1, t_2) = \Phi_{ik}^{\text{pp,bosons},0,\text{A}}(t_1, t_2) + U(t_1) \sum_n \quad (2.473)$$

$$\int_{t_1}^{t_2} dt_5 G_{in}^{\text{H,A}}(t_1, t_5) T_{nk}^{\text{pp,bosons},0,\text{A}}(t_5, t_2),$$

$$T_{ik}^{\text{pp,bosons},0,\text{R}}(t_1, t_2) = \Phi_{ik}^{\text{pp,bosons},0,\text{R}}(t_1, t_2) + U(t_1) \sum_n \quad (2.474)$$

$$\int_{t_2}^{t_1} dt_5 G_{in}^{\text{H,R}}(t_1, t_5) T_{nk}^{\text{pp,bosons},0,\text{R}}(t_5, t_2).$$

The corresponding diagrams are shown in Fig. 2.17. For fermions, one has

$$\Sigma_{i\alpha j\alpha}^{\text{pp,fermions}}(z_1, z_2) = \Sigma_{i\alpha j\alpha}^{\text{H,fermions}}(z_1, z_2) \quad (2.475)$$

$$+ i\hbar \sum_{pr} \sum_{\epsilon} T_{iapej\alpha\epsilon}^{\text{pp,fermions}}(z_1, z_2) G_{repe}(z_2, z_1)$$

and

$$T_{i\alpha j\beta k\alpha l\beta}^{\text{pp,fermions}}(z_1, z_2) = U(z_1) \delta_{ij} \delta_{kl} \bar{\delta}_{\alpha\beta} \quad (2.476)$$

$$\left(G_{i\alpha i\beta k\beta k\alpha}^{\text{H}}(z_1, z_2) \delta_{\alpha\beta} - G_{i\alpha i\beta k\alpha k\beta}^{\text{H}}(z_1, z_2) \delta_{\alpha\alpha} \delta_{\beta\beta} \right) U(z_2)$$

$$+ U(z_1) \bar{\delta}_{\alpha\beta} \delta_{ij} \sum_{ns} \int_{\mathcal{C}} dz_5 G_{i\alpha i\beta n\alpha s\beta}^{\text{H}}(z_1, z_5) T_{n\alpha s\beta k\alpha l\beta}^{\text{pp,fermions}}(z_5, z_2).$$

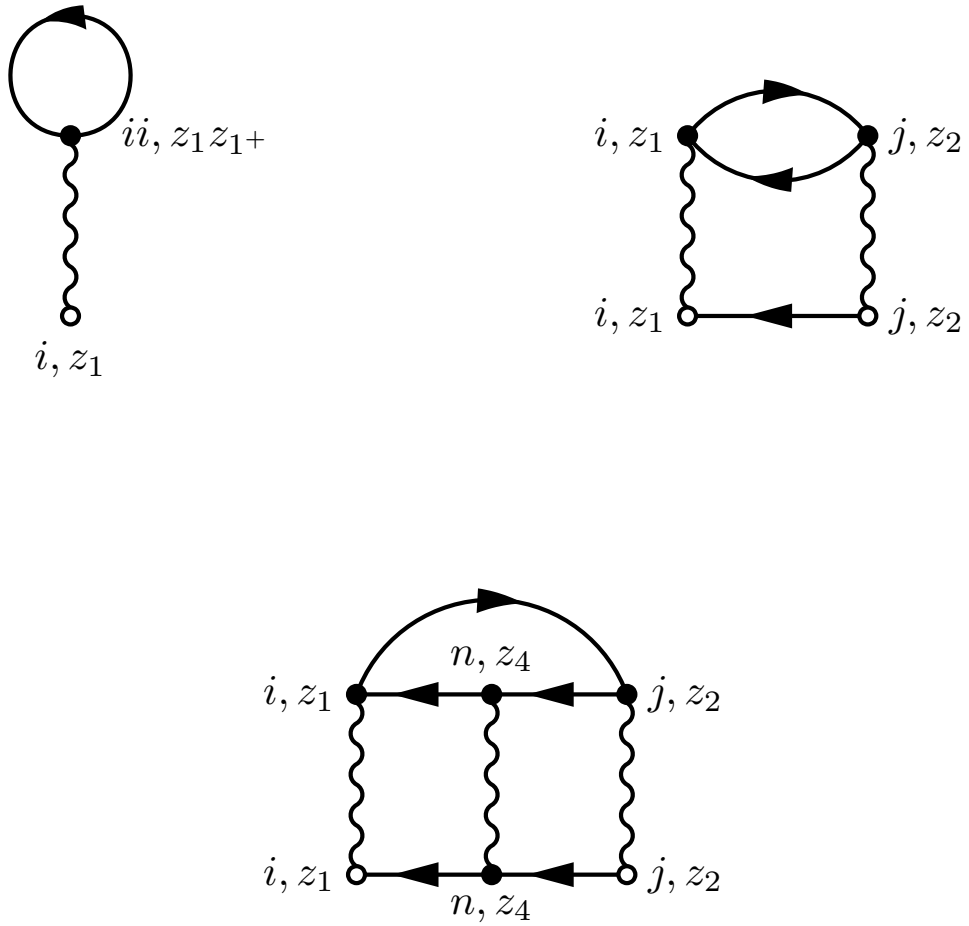


Figure 2.17: Leading terms of $\Sigma^{\text{pp,bosons},0}$ in the Hubbard basis for spin-0 bosons. Each term carries a factor of two.

Canceling the term equal to zero, one finds

$$\begin{aligned}
 T_{i\alpha j\beta k\alpha l\beta}^{\text{pp,fermions}}(z_1, z_2) & \quad (2.477) \\
 &= -U(z_1)\delta_{ij}\delta_{kl}\bar{\delta}_{\alpha\beta}G_{i\alpha i\beta k\alpha k\beta}^{\text{H}}(z_1, z_2)U(z_2) \\
 & \quad +U(z_1)\bar{\delta}_{\alpha\beta}\delta_{ij}\sum_{ns}\int_{\mathcal{C}}dz_5G_{i\alpha i\beta n\alpha s\beta}^{\text{H}}(z_1, z_5)T_{n\alpha s\beta k\alpha l\beta}^{\text{pp,fermions}}(z_5, z_2).
 \end{aligned}$$

Introducing Φ again, one arrives at

$$\begin{aligned}
 T_{i\alpha j\beta k\alpha l\beta}^{\text{pp,fermions}}(z_1, z_2) & \quad (2.478) \\
 &=: \bar{\delta}_{\alpha\beta}\delta_{ij}\delta_{kl}\Phi_{iik\alpha\beta}^{\text{pp,fermions}}(z_1, z_2) \\
 & \quad +U(z_1)\bar{\delta}_{\alpha\beta}\delta_{ij}\sum_{ns}\int_{\mathcal{C}}dz_5G_{i\alpha i\beta n\alpha s\beta}^{\text{H}}(z_1, z_5)T_{n\alpha s\beta k\alpha l\beta}^{\text{pp,fermions}}(z_5, z_2).
 \end{aligned}$$

Similar as for bosons, by iteration starting with

$$\begin{aligned}
 \Phi_{i\alpha j\beta k\alpha l\beta}^{\text{pp,fermions}}(z_1, z_2) & \quad (2.479) \\
 &= \bar{\delta}_{\alpha\beta}\delta_{ij}\delta_{kl}\Phi_{iik\alpha\beta}^{\text{pp,fermions}}(z_1, z_2) =: \bar{\delta}_{\alpha\beta}\delta_{ij}\delta_{kl}\Phi_{ik\alpha\neq\beta}^{\text{pp,fermions}}(z_1, z_2),
 \end{aligned}$$

the particle–particle T -matrix is also of the structure

$$\begin{aligned}
 T_{i\alpha j\beta k\alpha l\beta}^{\text{pp,fermions}}(z_1, z_2) & := \bar{\delta}_{\alpha\beta}\delta_{ij}\delta_{kl}T_{iik\alpha\beta}^{\text{pp,fermions}}(z_1, z_2) \quad (2.480) \\
 &=: \delta_{ij}\delta_{kl}\bar{\delta}_{\alpha\beta}T_{ik\alpha\neq\beta}^{\text{pp,fermions}}(z_1, z_2).
 \end{aligned}$$

The resulting equations read

$$T_{ik\alpha\neq\beta}^{\text{pp,fermions}}(z_1, z_2) = \Phi_{ik\alpha\neq\beta}^{\text{pp,fermions}}(z_1, z_2) \quad (2.481)$$

$$+ U(z_1) \sum_n \int_{\mathcal{C}} dz_5 G_{in\alpha\neq\beta}^{\text{H}}(z_1, z_5) T_{nk\alpha\neq\beta}^{\text{pp,fermions}}(z_5, z_2),$$

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{\text{pp,fermions}}(z_1, z_2) &= \Sigma_{i\alpha j\alpha}^{\text{H,fermions}}(z_1, z_2) \\ &+ i\hbar \sum_{\epsilon \neq \alpha} T_{ij\alpha\neq\epsilon}^{\text{pp,fermions}}(z_1, z_2) G_{j\epsilon i\epsilon}(z_2, z_1). \end{aligned} \quad (2.482)$$

The components are given by

$$\Sigma_{i\alpha j\alpha}^{\text{pp,fermions}, \geq}(t_1, t_2) = \Sigma_{i\alpha j\alpha}^{\text{H,fermions}, \geq}(t_1, t_2) \quad (2.483)$$

$$+ i\hbar \sum_{\epsilon \neq \alpha} T_{ij\alpha\neq\epsilon}^{\text{pp,fermions}, \geq}(t_1, t_2) G_{j\epsilon i\epsilon}^{\leq}(t_2, t_1)$$

and

$$T_{ik\alpha\neq\beta}^{\text{pp,fermions}, \geq}(t_1, t_2) = \Phi_{ik\alpha\neq\beta}^{\text{pp,fermions}, \geq}(t_1, t_2) + U(t_1) \sum_n \quad (2.484)$$

$$\begin{aligned} &\left(\int_{t_0}^{t_1} dt_5 G_{in\alpha\neq\beta}^{\text{H,R}}(t_1, t_5) T_{nk\alpha\neq\beta}^{\text{pp,fermions}, \geq}(t_5, t_2) \right. \\ &\quad \left. + \int_{t_0}^{t_2} dt_5 G_{in\alpha\neq\beta}^{\text{H}, \geq}(t_1, t_5) T_{nk\alpha\neq\beta}^{\text{pp,fermions,A}}(t_5, t_2) \right), \end{aligned}$$

$$T_{ik\alpha\neq\beta}^{\text{pp,fermions,A}}(t_1, t_2) = \Phi_{ik\alpha\neq\beta}^{\text{pp,fermions,A}}(t_1, t_2) \quad (2.485)$$

$$+ U(t_1) \sum_n \int_{t_1}^{t_2} dt_5 G_{in\alpha\neq\beta}^{\text{H,A}}(t_1, t_5) T_{nk\alpha\neq\beta}^{\text{pp,fermions,A}}(t_5, t_2)$$

and

$$T_{ik\alpha\neq\beta}^{\text{pp,fermions,R}}(t_1, t_2) = \Phi_{ik\alpha\neq\beta}^{\text{pp,fermions,A}}(t_1, t_2) \quad (2.486)$$

$$+U(t_1) \sum_n \int_{t_2}^{t_1} dt_5 G_{in\alpha\neq\beta}^{\text{H,R}}(t_1, t_5) T_{nk\alpha\neq\beta}^{\text{pp,fermions,R}}(t_5, t_2).$$

In the special case of spin- $\frac{1}{2}$ fermions, one has

$$\Phi_{ik\alpha\neq\beta}^{\text{pp,fermions,1/2}}(z_1, z_2) \quad (2.487)$$

$$= \Phi_{ik\beta\neq\alpha}^{\text{pp,fermions,1/2}}(z_1, z_2) =: \Phi_{ik}^{\text{pp,fermions,1/2}}(z_1, z_2),$$

$$G_{ik\alpha\neq\beta}^{\text{H}}(z_1, z_2) = G_{ik\beta\neq\alpha}^{\text{H}}(z_1, z_2) =: G_{ik}^{\text{H}}(z_1, z_2) \quad (2.488)$$

and, consequently,

$$T_{ik\alpha\neq\beta}^{\text{pp,fermions,1/2}}(z_1, z_2) \quad (2.489)$$

$$= T_{ik\beta\neq\alpha}^{\text{pp,fermions,1/2}}(z_1, z_2) =: T_{ik}^{\text{pp,fermions,1/2}}(z_1, z_2)$$

holds. With this, one arrives at

$$T_{ik}^{\text{pp,fermions,1/2}}(z_1, z_2) = \Phi_{ik}^{\text{pp,fermions,1/2}}(z_1, z_2) \quad (2.490)$$

$$+U(z_1) \sum_n \int_{\mathcal{C}} dz_5 G_{in}^{\text{H}}(z_1, z_5) T_{nk}^{\text{pp,fermions,1/2}}(z_5, z_2)$$

and

$$\Sigma_{i\uparrow j\uparrow}^{\text{pp,fermions,1/2}}(z_1, z_2) = \Sigma_{i\uparrow j\uparrow}^{\text{H,fermions,1/2}}(z_1, z_2) \quad (2.491)$$

$$+i\hbar T_{ij}^{\text{pp,fermions,1/2}}(z_1, z_2) G_{j\downarrow i\downarrow}(z_2, z_1)$$

as well as

$$\Sigma_{i\downarrow j\downarrow}^{\text{pp,fermions,1/2}}(z_1, z_2) = \Sigma_{i\downarrow j\downarrow}^{\text{H,fermions,1/2}}(z_1, z_2) \quad (2.492)$$

$$+i\hbar T_{ij}^{\text{pp,fermions,1/2}}(z_1, z_2) G_{j\uparrow i\uparrow}(z_2, z_1).$$

The components are given by

$$\begin{aligned} \Sigma_{i\uparrow j\uparrow}^{\text{pp,fermions},1/2,\geq}(t_1, t_2) &= \Sigma_{i\uparrow j\uparrow}^{\text{H,fermions},1/2,\geq}(t_1, t_2) \\ &+ i\hbar T_{ij}^{\text{pp,fermions},1/2,\geq}(t_1, t_2) G_{j\downarrow i\downarrow}^{\leq}(t_2, t_1) \end{aligned} \quad (2.493)$$

and

$$\begin{aligned} \Sigma_{i\downarrow j\downarrow}^{\text{pp,fermions},1/2,\geq}(t_1, t_2) &= \Sigma_{i\downarrow j\downarrow}^{\text{H,fermions},1/2,\geq}(t_1, t_2) \\ &+ i\hbar T_{ij}^{\text{pp,fermions},1/2,\geq}(t_1, t_2) G_{j\uparrow i\uparrow}^{\leq}(t_2, t_1) \end{aligned} \quad (2.494)$$

as well as

$$\begin{aligned} T_{ik}^{\text{pp,fermions},1/2,\geq}(t_1, t_2) &= \Phi_{ik}^{\text{pp,fermions},1/2,\geq}(t_1, t_2) \\ &+ U(t_1) \sum_n \int_{t_0}^{t_1} dt_5 G_{in}^{\text{H,R}}(t_1, t_5) T_{nk}^{\text{pp,fermions},1/2,\geq}(t_5, t_2) \\ &+ U(t_1) \sum_n \int_{t_0}^{t_2} dt_5 G_{in}^{\text{H},\geq}(t_1, t_5) T_{nk}^{\text{pp,fermions},1/2,\text{A}}(t_5, t_2), \end{aligned} \quad (2.495)$$

$$\begin{aligned} T_{ik}^{\text{pp,fermions},1/2,\text{A}}(t_1, t_2) &= \Phi_{ik}^{\text{pp,fermions},1/2,\text{A}}(t_1, t_2) \\ &+ U(t_1) \sum_n \int_{t_1}^{t_2} dt_5 G_{in}^{\text{H,A}}(t_1, t_5) T_{nk}^{\text{pp,fermions},1/2,\text{A}}(t_5, t_2) \end{aligned} \quad (2.496)$$

and

$$\begin{aligned} T_{ik}^{\text{pp,fermions},1/2,\text{R}}(t_1, t_2) &= \Phi_{ik}^{\text{pp,fermions},1/2,\text{R}}(t_1, t_2) \\ &+ U(t_1) \sum_n \int_{t_2}^{t_1} dt_5 G_{in}^{\text{H,R}}(t_1, t_5) T_{nk}^{\text{pp,fermions},1/2,\text{R}}(t_5, t_2). \end{aligned} \quad (2.497)$$

The diagrams are shown in Fig. 2.18.

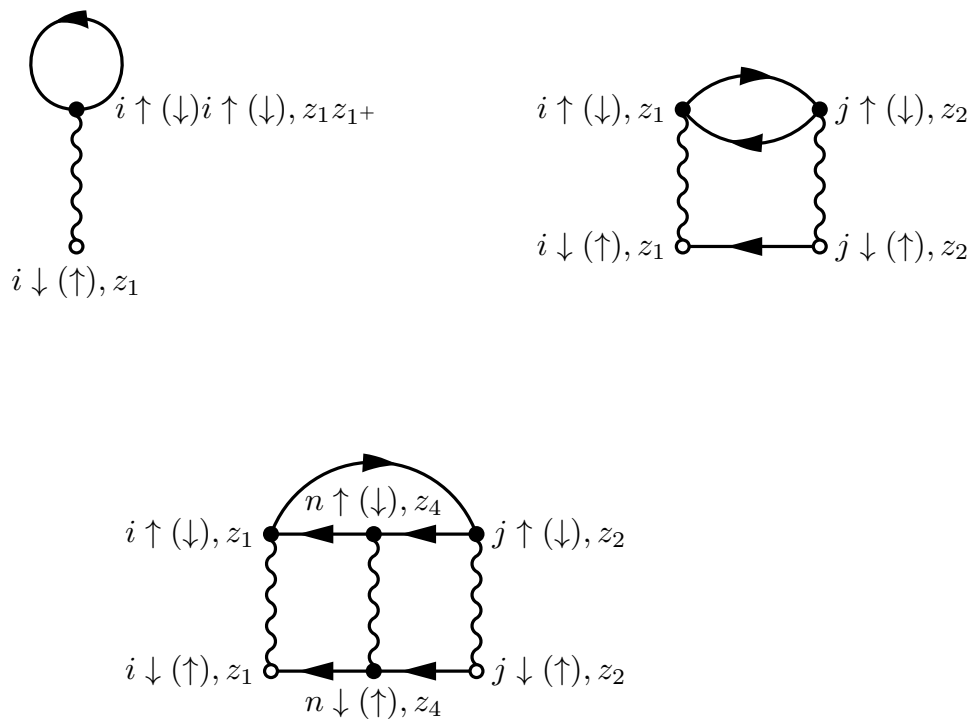


Figure 2.18: Leading terms of $\Sigma^{\text{pp,fermions},1/2}$ in the Hubbard basis for spin-1/2 fermions.

2.7.2.4 Particle–hole T -matrix approximation

Returning to Eq. (2.409) and taking the third approximation, one has

$$\begin{aligned}
 K_{ijkl}^c(z_1, z_2, z_3, z_4) & \tag{2.498} \\
 & := \pm \frac{\delta \Sigma_{ik}^{\text{closed},c}(z_1, z_3)}{\delta G_{lj}(z_4, z_2)} \\
 & \approx \pm i\hbar \delta_C(z_1, z_3) \delta_C(z_1, z_4) \delta_C(z_{1+}, z_2) \\
 & \quad (w_{ijkl}(z_1) \pm w_{jikl}(z_1)) \\
 & \quad \pm i\hbar \delta_C(z_1, z_4) \sum_{mp} w_{iplm}(z_1) \int_C dz_5 \sum_n G_{mn}(z_1, z_5) \\
 & \quad \int_C dz_6 \sum_r \frac{\delta \Sigma_{nk}^{\text{closed},c}(z_5, z_3)}{\delta G_{rj}(z_6, z_2)} G_{rp}(z_6, z_1).
 \end{aligned}$$

Evaluating the terms, one finds

$$\begin{aligned}
 K_{ijkl}^c(z_1, z_2, z_3, z_4) & \tag{2.499} \\
 & = \pm i\hbar \delta_C(z_1, z_3) \delta_C(z_1, z_4) \delta_C(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)) \\
 & \quad + i\hbar \delta_C(z_1, z_4) \sum_{mp} w_{iplm}(z_1) \int_C dz_5 \sum_n G_{mn}(z_1, z_5) \\
 & \quad \int_C dz_6 \sum_r K_{njk r}^c(z_5, z_2, z_3, z_6) G_{rp}(z_6, z_1).
 \end{aligned}$$

Iterating as before, starting with

$$\begin{aligned}
 K_{ijkl}^{c,(1)}(z_1, z_2, z_3, z_4) & \tag{2.500} \\
 & = \pm i\hbar \delta_C(z_1, z_3) \delta_C(z_1, z_4) \delta_C(z_{1+}, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)),
 \end{aligned}$$

one arrives at

$$\begin{aligned}
 K_{ijkl}^{c,(2)}(z_1, z_2, z_3, z_4) &= i\hbar\delta_{\mathcal{C}}(z_1, z_4) \sum_{mp} w_{iplm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\int_{\mathcal{C}} dz_6 \sum_r K_{njkr}^{c,(1)}(z_5, z_2, z_3, z_6) G_{rp}(z_6, z_1). \tag{2.501}
 \end{aligned}$$

Using the δ -structure of $K^{c,(1)}$, one arrives at

$$\begin{aligned}
 K_{ijkl}^{c,(2)}(z_1, z_2, z_3, z_4) &= i\hbar\delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_2, z_3) \sum_{mp} w_{iplm}(z_1) \sum_n G_{mn}(z_1, z_2) \\
 &\sum_r K_{njkr}^{c,(1)}(z_2, z_2, z_2, z_2) G_{rp}(z_2, z_1), \tag{2.502}
 \end{aligned}$$

$$\begin{aligned}
 K_{ijkl}^{c,(3)}(z_1, z_2, z_3, z_4) &= i\hbar\delta_{\mathcal{C}}(z_1, z_4) \sum_{mp} w_{iplm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\int_{\mathcal{C}} dz_6 \sum_r K_{njkr}^{c,(2)}(z_5, z_2, z_3, z_6) G_{rp}(z_6, z_1) \tag{2.503} \\
 &= i\hbar\delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_2, z_3) \sum_{mp} w_{iplm}(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{mn}(z_1, z_5) \\
 &\sum_r K_{njkr}^{c,(2)}(z_5, z_2, z_2, z_5) G_{rp}(z_5, z_1).
 \end{aligned}$$

The structure again stays the same for higher orders, so that this approximation lies within $\mathcal{O}(N_t^3)$ due to

$$\begin{aligned}
 K_{ijkl}^{c,(N)}(z_1, z_2, z_3, z_4) &= \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_2, z_3) K_{ijkl}^{c,(N)}(z_1, z_2, z_2, z_1) \\
 &=: \delta_{\mathcal{C}}(z_1, z_4) \delta_{\mathcal{C}}(z_2, z_3) K_{ijkl}^{c,(N)}(z_1, z_2), \tag{2.504}
 \end{aligned}$$

and one integration on the right-hand side. With this, one arrives at, cf. Eq. (2.498),

$$K_{ijkl}^c(z_1, z_2) = \delta_C(z_1, z_2) K_{ijkl}^{c,(1)}(z_1, z_1) + i\hbar \sum_{mp} w_{iplm}(z_1) \int_C dz_5 \sum_n G_{mn}(z_1, z_5) \sum_r K_{njkr}^c(z_5, z_2) G_{rp}(z_5, z_1). \quad (2.505)$$

To simplify, one again goes over to a non-singular kernel

$$\begin{aligned} K_{ijkl}^{c,\text{non-sing}}(z_1, z_2) &:= K_{ijkl}^c(z_1, z_2) - \delta_C(z_1, z_2) K_{ijkl}^{c,(1)}(z_1, z_1) \\ &= K_{ijkl}^c(z_1, z_2) \mp i\hbar \delta_C(z_1, z_2) (w_{ijkl}(z_1) \pm w_{jikl}(z_1)). \end{aligned} \quad (2.506)$$

This quantity obeys, cf. Eq. (2.503),

$$\begin{aligned} K_{ijkl}^{c,\text{non-sing}}(z_1, z_2) &= i\hbar \sum_{mp} w_{iplm}(z_1) \int_C dz_5 \sum_n G_{mn}(z_1, z_5) \sum_r G_{rp}(z_5, z_1) \\ &\quad \left\{ K_{njkr}^{c,\text{non-sing}}(z_5, z_2) \pm i\hbar \delta_C(z_5, z_2) (w_{njkr}(z_2) \pm w_{jnkr}(z_2)) \right\}. \end{aligned} \quad (2.507)$$

Restructuring, this implies

$$\begin{aligned} K_{ijkl}^{c,\text{non-sing}}(z_1, z_2) & \quad (2.508) \\ &= \pm (i\hbar)^2 \sum_{mp} w_{iplm}(z_1) \sum_n G_{mn}(z_1, z_2) \sum_r G_{rp}(z_2, z_1) \\ &\quad (w_{njkr}(z_2) \pm w_{jnkr}(z_2)) \\ &\quad + i\hbar \sum_{mp} w_{iplm}(z_1) \int_C dz_5 \sum_n G_{mn}(z_1, z_5) \sum_r G_{rp}(z_5, z_1) K_{njkr}^{c,\text{non-sing}}(z_5, z_2) \end{aligned}$$

and, finally,

$$\begin{aligned}
 K_{ijkl}^{\text{c,non-sing}}(z_1, z_2) & \quad (2.509) \\
 &= i\hbar \sum_{mp} w_{iplm}(z_1) \sum_{nr} G_{mrpn}^{\text{F}}(z_1, z_2) (w_{njkr}(z_2) \pm w_{jnkr}(z_2)) \\
 & \quad \pm \sum_{mp} w_{iplm}(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{mrpn}^{\text{F}}(z_1, z_5) K_{njkr}^{\text{c,non-sing}}(z_5, z_2),
 \end{aligned}$$

where in the last line, Eq. (2.321) has been used. With this, the selfenergy reads, cf. Eq. (2.403),

$$\begin{aligned}
 \Sigma_{ij}^{\text{closed,c}}(z_1, z_2) &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \quad (2.510) \\
 & \quad \pm i\hbar \sum_{mpq} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_n G_{mn}(z_1, z_3) \\
 & \quad \int_{\mathcal{C}} dz_4 dz_5 \sum_{rs} K_{nsjr}^{\text{c}}(z_3, z_5, z_2, z_4) G_{rp}(z_4, z_1) G_{qs}(z_1, z_5).
 \end{aligned}$$

Using Eq. (2.506), one arrives at

$$\begin{aligned}
 \Sigma_{ij}^{\text{closed,c}}(z_1, z_2) & \quad (2.511) \\
 &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \\
 & \quad \pm i\hbar \sum_{mpqs} w_{ipqm}(z_1) G_{qs}(z_1, z_2) \sum_{nr} \int_{\mathcal{C}} dz_3 G_{mn}(z_1, z_3) G_{rp}(z_3, z_1) \\
 & \quad \left\{ K_{nsjr}^{\text{c,non-sing}}(z_3, z_2) \pm i\hbar \delta_{\mathcal{C}}(z_3, z_2) (w_{nsjr}(z_2) \pm w_{snjr}(z_2)) \right\}.
 \end{aligned}$$

Evaluating further, one finds

$$\begin{aligned}
 & \Sigma_{ij}^{\text{closed,c}}(z_1, z_2) \tag{2.512} \\
 &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \pm \sum_{qs} G_{qs}(z_1, z_2) \\
 & \quad \left(i\hbar \sum_{pm} w_{ipqm}(z_1) \sum_{rn} G_{mrpn}^{\text{F}}(z_1, z_2) (w_{nsjr}(z_2) \pm w_{snjr}(z_2)) \right. \\
 & \quad \left. \pm \sum_{pm} w_{ipqm}(z_1) \int_{\mathcal{C}} dz_3 \sum_{rn} G_{mrpn}^{\text{F}}(z_1, z_3) K_{nsjr}^{\text{c,non-sing}}(z_3, z_2) \right).
 \end{aligned}$$

Like for the particle–particle T -matrix, the right-hand side already contains the first iteration of Eq. (2.509) and, thus, one can simplify

$$\begin{aligned}
 & \Sigma_{ij}^{\text{closed,c}}(z_1, z_2) \tag{2.513} \\
 &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) \pm \sum_{qs} G_{qs}(z_1, z_2) K_{isjq}^{\text{c,non-sing}}(z_1, z_2).
 \end{aligned}$$

Defining

$$i\hbar T_{ijkl}^{\text{eh}}(z_1, z_2) := \pm K_{ijkl}^{\text{c,non-sing}}(z_1, z_2), \tag{2.514}$$

and solving Eqs. (2.509) and (2.513), one has

$$\begin{aligned}
 & T_{ijkl}^{\text{ph}}(z_1, z_2) = \pm \sum_{mp} w_{iplm}(z_1) \sum_{nr} G_{mrpn}^{\text{F}}(z_1, z_2) (w_{njkr}(z_2) \pm w_{jnkr}(z_2)) \\
 & \quad \pm \sum_{mp} w_{iplm}(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{mrpn}^{\text{F}}(z_1, z_5) T_{njkr}^{\text{ph}}(z_5, z_2) \tag{2.515} \\
 & =: \Phi_{ijkl}^{\text{ph}}(z_1, z_2) \\
 & \quad \pm \sum_{mp} w_{iplm}(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{mrpn}^{\text{F}}(z_1, z_5) T_{njkr}^{\text{ph}}(z_5, z_2)
 \end{aligned}$$

and

$$\begin{aligned} \Sigma_{ij}^{T^{\text{ph}}} (z_1, z_2) & \quad (2.516) \\ &= \Sigma_{ij}^{\text{H}} (z_1, z_2) + \Sigma_{ij}^{\text{F}} (z_1, z_2) + i\hbar \sum_{qs} G_{qs} (z_1, z_2) T_{isjq}^{\text{ph}} (z_1, z_2), \end{aligned}$$

which is the so-called (particle–hole) T -matrix approximation. In contrast to the particle–particle T -matrix, which describes the recurrent scattering of a pair of particles, the particle–hole T -matrix describes the scattering of a particle–hole pair. The Keldysh components of the particle–hole T -matrix read

$$\begin{aligned} T_{ijkl}^{\text{ph},\gtrless} (t_1, t_2) &= \Phi_{ijkl}^{\text{ph},\gtrless} (t_1, t_2) \\ &\pm \sum_{mp} w_{iplm} (t_1) \sum_{nr} \quad (2.517) \end{aligned}$$

$$\left(\int_{t_0}^{t_1} dt_5 G_{mrpn}^{\text{F,R}} (t_1, t_5) T_{njkr}^{\text{ph},\gtrless} (t_5, t_2) + \int_{t_0}^{t_2} dt_5 G_{mrpn}^{\text{F},\gtrless} (t_1, t_5) T_{njkr}^{\text{ph,A}} (t_5, t_2) \right),$$

$$T_{ijkl}^{\text{ph,A}} (t_1, t_2) = \Phi_{ijkl}^{\text{ph,A}} (t_1, t_2) \quad (2.518)$$

$$\pm \sum_{mp} w_{iplm} (t_1) \sum_{nr} \int_{t_1}^{t_2} dt_5 G_{mrpn}^{\text{H,A}} (t_1, t_5) T_{njkr}^{\text{ph,A}} (t_5, t_2),$$

and

$$T_{ijkl}^{\text{ph,R}} (t_1, t_2) = \Phi_{ijkl}^{\text{ph,R}} (t_1, t_2) \quad (2.519)$$

$$\pm \sum_{mp} w_{iplm} (t_1) \sum_{nr} \int_{t_2}^{t_1} dt_5 G_{mrpn}^{\text{H,R}} (t_1, t_5) T_{njkr}^{\text{ph,R}} (t_5, t_2).$$

For the components of the selfenergy, one has

$$\Sigma_{ij}^{\text{ph},\gtrless} (t_1, t_2) \quad (2.520)$$

$$= \Sigma_{ij}^{\text{H},\gtrless} (t_1, t_2) + \Sigma_{ij}^{\text{F},\gtrless} (t_1, t_2) + \sum_{qs} G_{qs}^{\gtrless} (t_1, t_2) T_{isjq}^{\text{ph},\gtrless} (t_1, t_2).$$

2.7.2.4.1 Particle-hole T -matrix in a diagonal basis For diagonal basis sets with $w_{ijkl} = \delta_{il}\delta_{jk}w_{ij}$, Eqs. (2.515) and (2.516) become

$$\begin{aligned}
 T_{ijkl}^{\text{ph,diag.}}(z_1, z_2) & \quad (2.521) \\
 &= \pm w_{il}(z_1) \left(\delta_{jk} \sum_n G_{inln}^{\text{F}}(z_1, z_2) w_{nj}(z_2) \pm G_{ijlk}^{\text{F}}(z_1, z_2) w_{jk}(z_2) \right) \\
 & \quad \pm w_{il}(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{irln}^{\text{F}}(z_1, z_5) T_{njkr}^{\text{ph,diag.}}(z_5, z_2) \\
 &=: \Phi_{ijkl}^{\text{ph,diag.}}(z_1, z_2) \pm w_{il}(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{irln}^{\text{F}}(z_1, z_5) T_{njkr}^{\text{ph,diag.}}(z_5, z_2)
 \end{aligned}$$

and

$$\begin{aligned}
 \Sigma_{ij}^{\text{ph,diag.}}(z_1, z_2) & \quad (2.522) \\
 &= \Sigma_{ij}^{\text{H}}(z_1, z_2) + \Sigma_{ij}^{\text{F}}(z_1, z_2) + i\hbar \sum_{qs} G_{qs}(z_1, z_2) T_{isjq}^{\text{ph,diag.}}(z_1, z_2).
 \end{aligned}$$

The components are

$$\begin{aligned}
 T_{ijkl}^{\text{ph,diag.,}\geq}(t_1, t_2) &= \Phi_{ijkl}^{\text{ph,diag.,}\geq}(t_1, t_2) \pm w_{il}(t_1) \sum_{nr} & (2.523) \\
 & \left(\int_{t_0}^{t_1} dt_5 G_{irln}^{\text{F,R}}(t_1, t_5) T_{njkr}^{\text{ph,diag.,}\geq}(t_5, t_2) \right. \\
 & \left. + \int_{t_0}^{t_2} dt_5 G_{irln}^{\text{F,\geq}}(t_1, t_5) T_{njkr}^{\text{ph,diag.,A}}(t_5, t_2) \right),
 \end{aligned}$$

$$\begin{aligned}
 T_{ijkl}^{\text{ph,diag.,A}}(t_1, t_2) &= \Phi_{ijkl}^{\text{ph,diag.,A}}(t_1, t_2) & (2.524) \\
 & \pm w_{il}(t_1) \sum_{nr} \int_{t_1}^{t_2} dt_5 G_{irln}^{\text{F,A}}(t_1, t_5) T_{njkr}^{\text{ph,diag.,A}}(t_5, t_2)
 \end{aligned}$$

and

$$\begin{aligned}
 T_{ijkl}^{\text{ph,diag.,R}}(t_1, t_2) &= \Phi_{ijkl}^{\text{ph,diag.,R}}(t_1, t_2) \\
 &\pm w_{il}(t_1) \sum_{nr} \int_{t_2}^{t_1} dt_5 G_{irln}^{\text{F,R}}(t_1, t_5) T_{njkr}^{\text{ph,diag.,R}}(t_5, t_2).
 \end{aligned} \tag{2.525}$$

For the components of the selfenergy, one has

$$\begin{aligned}
 \Sigma_{ij}^{\text{ph,diag.,}\gtrless}(t_1, t_2) &= \Sigma_{ij}^{\text{H,diag.,}\gtrless}(t_1, t_2) + \Sigma_{ij}^{\text{F,diag.,}\gtrless}(t_1, t_2) \\
 &+ i\hbar \sum_{qs} G_{qs}^{\gtrless}(t_1, t_2) T_{isjq}^{\text{ph,diag.,}\gtrless}(t_1, t_2).
 \end{aligned} \tag{2.526}$$

The diagrammatic representation of the first terms of the particle–hole T -matrix is given in Fig. 2.19.

2.7.2.4.2 Particle–hole T -matrix in the Hubbard basis For the bosonic Hubbard basis, the particle–hole T -matrix reads

$$\begin{aligned}
 T_{\alpha j \beta k \alpha l \beta}^{\text{ph,bosons}}(z_1, z_2) & \\
 &= \delta_{il} \delta_{jk} U(z_1) \left(\delta_{\alpha\beta} G_{\alpha j \alpha i \alpha j \alpha}^{\text{F}}(z_1, z_2) + G_{\alpha j \beta i \beta j \alpha}^{\text{F}}(z_1, z_2) \right) U(z_2) \\
 &+ \delta_{il} U(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{i \alpha r \beta i \beta n \alpha}^{\text{F}}(z_1, z_5) T_{n \alpha j \beta k \alpha r \beta}^{\text{ph,bosons}}(z_5, z_2).
 \end{aligned} \tag{2.527}$$

Introducing Φ as before, one finds

$$\begin{aligned}
 T_{\alpha j \beta k \alpha l \beta}^{\text{ph,bosons}}(z_1, z_2) & \\
 &=: \delta_{il} \delta_{jk} \Phi_{\alpha j \beta i \alpha j \beta}^{\text{ph,bosons}}(z_1, z_2) \\
 &+ \delta_{il} U(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{i \alpha r \beta i \beta n \alpha}^{\text{F}}(z_1, z_5) T_{n \alpha j \beta k \alpha r \beta}^{\text{ph,bosons}}(z_5, z_2).
 \end{aligned} \tag{2.528}$$

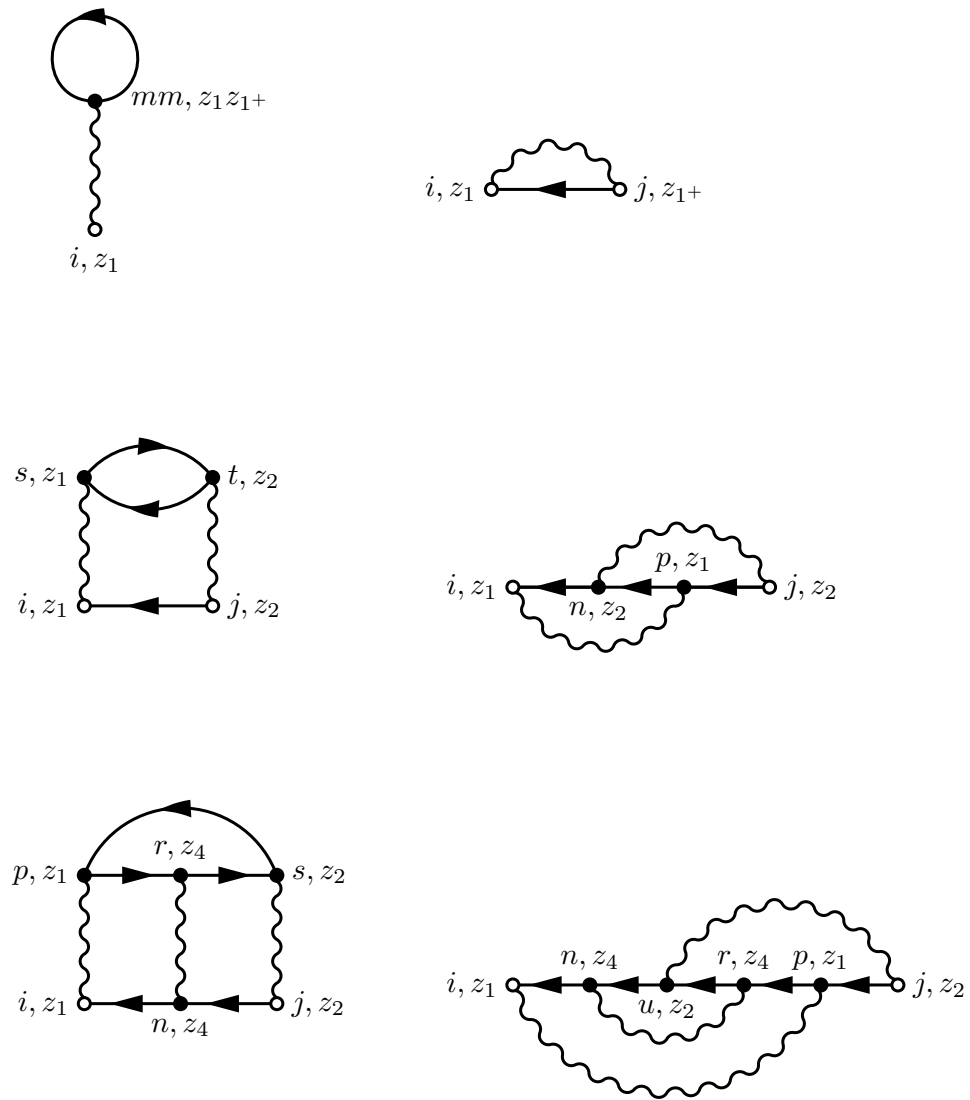


Figure 2.19: The first six terms of the particle-hole T -matrix selfenergy in a diagonal basis.

By iteration, starting from

$$\begin{aligned} \Phi_{i\alpha j\beta k\alpha l\beta}^{\text{ph,bosons}}(z_1, z_2) & \quad (2.529) \\ &= \delta_{il} \delta_{jk} \Phi_{i\alpha j\beta j\alpha i\beta}^{\text{ph,bosons}}(z_1, z_2) =: \delta_{il} \delta_{jk} \Phi_{ij\alpha\beta}^{\text{ph,bosons}}(z_1, z_2), \end{aligned}$$

it is evident that the particle-hole T -matrix is also of the structure

$$\begin{aligned} T_{i\alpha j\beta k\alpha l\beta}^{\text{ph,bosons}}(z_1, z_2) & \quad (2.530) \\ &= \delta_{il} \delta_{jk} T_{i\alpha j\beta j\alpha i\beta}^{\text{ph,bosons}}(z_1, z_2) =: \delta_{il} \delta_{jk} T_{ij\alpha\beta}^{\text{ph,bosons}}(z_1, z_2). \end{aligned}$$

The governing equation becomes

$$\begin{aligned} T_{ij\alpha\beta}^{\text{ph,bosons}}(z_1, z_2) &= \Phi_{ij\alpha\beta}^{\text{ph,bosons}}(z_1, z_2) & (2.531) \\ &+ U(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{i\alpha n\beta i\beta n\alpha}^{\text{F}}(z_1, z_5) T_{nj\alpha\beta}^{\text{ph,bosons}}(z_5, z_2). \end{aligned}$$

The resulting selfenergy reads

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{\text{ph,bosons}}(z_1, z_2) &= \Sigma_{i\alpha j\alpha}^{\text{H,bosons}}(z_1, z_2) + \Sigma_{i\alpha j\alpha}^{\text{F,bosons}}(z_1, z_2) \\ &+ i\hbar \sum_{\epsilon} G_{i\epsilon j\epsilon}(z_1, z_2) T_{ij\alpha\epsilon}^{\text{ph}}(z_1, z_2). \end{aligned} \quad (2.532)$$

The components are given by

$$\begin{aligned} \Sigma_{i\alpha j\alpha}^{\text{ph,bosons},\geq}(t_1, t_2) &= \Sigma_{i\alpha j\alpha}^{\text{H,bosons},\geq}(t_1, t_2) + \Sigma_{i\alpha j\alpha}^{\text{F,bosons},\geq}(t_1, t_2) \\ &+ i\hbar \sum_{\epsilon} G_{i\epsilon j\epsilon}^{\geq}(t_1, t_2) T_{ij\alpha\epsilon}^{\text{ph},\geq}(t_1, t_2), \end{aligned} \quad (2.533)$$

$$T_{ij\alpha\beta}^{\text{ph,bosons},\geq}(t_1, t_2) = \Phi_{ij\alpha\beta}^{\text{ph,bosons},\geq}(t_1, t_2) \quad (2.534)$$

$$+U(t_1) \left(\int_{t_0}^{t_1} dt_5 \sum_n G_{i\alpha n \beta i \beta n \alpha}^{\text{F,R}}(t_1, t_5) T_{nj\alpha\beta}^{\text{ph,bosons},\geq}(t_5, t_2) \right. \\ \left. + \int_{t_0}^{t_2} dt_5 \sum_n G_{i\alpha n \beta i \beta n \alpha}^{\text{F},\geq}(t_1, t_5) T_{nj\alpha\beta}^{\text{ph,bosons,A}}(t_5, t_2) \right),$$

$$T_{ij\alpha\beta}^{\text{ph,bosons,A}}(t_1, t_2) = \Phi_{ij\alpha\beta}^{\text{ph,bosons,A}}(t_1, t_2) \quad (2.535)$$

$$+U(t_1) \int_{t_1}^{t_2} dt_5 \sum_n G_{i\alpha n \beta i \beta n \alpha}^{\text{F,A}}(t_1, t_5) T_{nj\alpha\beta}^{\text{ph,bosons,A}}(t_5, t_2)$$

and

$$T_{ij\alpha\beta}^{\text{ph,bosons,R}}(t_1, t_2) = \Phi_{ij\alpha\beta}^{\text{ph,bosons,R}}(t_1, t_2) \quad (2.536)$$

$$+U(t_1) \int_{t_2}^{t_1} dt_5 \sum_n G_{i\alpha n \beta i \beta n \alpha}^{\text{F,R}}(t_1, t_5) T_{nj\alpha\beta}^{\text{ph,bosons,R}}(t_5, t_2).$$

For spin-0 bosons, the equations simplify to

$$T_{ij}^{\text{ph,bosons,0}}(z_1, z_2) = \Phi_{ij}^{\text{ph,bosons,0}}(z_1, z_2) \quad (2.537)$$

$$+U(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{in in}^{\text{F}}(z_1, z_5) T_{nj}^{\text{ph,bosons,0}}(z_5, z_2)$$

and

$$\Sigma_{ij}^{\text{ph,bosons,0}}(z_1, z_2) = \Sigma_{ij}^{\text{H,bosons,0}}(z_1, z_2) + \Sigma_{ij}^{\text{F,bosons,0}}(z_1, z_2) \\ + i\hbar G_{ij}(z_1, z_2) T_{ij}^{\text{ph,bosons,0}}(z_1, z_2). \quad (2.538)$$

The components are given by

$$\Sigma_{ij}^{\text{ph,bosons,0},\geq}(t_1, t_2) = \Sigma_{ij}^{\text{H,bosons,0},\geq}(t_1, t_2) + \Sigma_{ij}^{\text{F,bosons,0},\geq}(t_1, t_2) \\ + i\hbar G_{ij}^{\geq}(t_1, t_2) T_{ij}^{\text{ph,bosons,0},\geq}(t_1, t_2), \quad (2.539)$$

$$T_{ij}^{\text{ph,bosons},0,\geq}(t_1, t_2) = \Phi_{ij}^{\text{ph,bosons},0,\geq}(t_1, t_2) \quad (2.540)$$

$$\begin{aligned} &+ U(t_1) \left(\int_{t_0}^{t_1} dt_5 \sum_n G_{inin}^{\text{F,R}}(t_1, t_5) T_{nj}^{\text{ph,bosons},0,\geq}(t_5, t_2) \right. \\ &\quad \left. + \int_{t_0}^{t_2} dt_5 \sum_n G_{inin}^{\text{F},\geq}(t_1, t_5) T_{nj}^{\text{ph,bosons},0,\text{A}}(t_5, t_2) \right), \end{aligned}$$

$$T_{ij}^{\text{ph,bosons},0,\text{A}}(t_1, t_2) = \Phi_{ij}^{\text{ph,bosons},0,\text{A}}(t_1, t_2) \quad (2.541)$$

$$+ U(t_1) \int_{t_1}^{t_2} dt_5 \sum_n G_{inin}^{\text{F,A}}(t_1, t_5) T_{nj}^{\text{ph,bosons},0,\text{A}}(t_5, t_2)$$

and

$$T_{ij}^{\text{ph,bosons},0,\text{R}}(t_1, t_2) = \Phi_{ij}^{\text{ph,bosons},0,\text{R}}(t_1, t_2) \quad (2.542)$$

$$+ U(t_1) \int_{t_2}^{t_1} dt_5 \sum_n G_{inin}^{\text{F,R}}(t_1, t_5) T_{nj}^{\text{ph,bosons},0,\text{R}}(t_5, t_2).$$

The leading terms of the corresponding diagrams are shown in Fig. 2.20. For fermionic particles and holes, the particle–hole T -matrix satisfies

$$T_{i\alpha j\beta k\alpha l\beta}^{\text{eh,fermions}}(z_1, z_2) = \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} U(z_1) \quad (2.543)$$

$$\begin{aligned} &\left(-\delta_{\alpha\beta} G_{i\alpha j\alpha i\alpha j\alpha}^{\text{F}}(z_1, z_2) + G_{i\alpha j\beta i\beta j\alpha}^{\text{F}}(z_1, z_2) \right) U(z_2) \\ &- \delta_{il} \bar{\delta}_{\alpha\beta} U(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{i\alpha r\beta i\beta n\alpha}^{\text{F}}(z_1, z_5) T_{n\alpha j\beta k\alpha r\beta}^{\text{eh,fermions}}(z_5, z_2). \end{aligned}$$

Evaluating the terms, one has

$$T_{i\alpha j\beta k\alpha l\beta}^{\text{eh,fermions}}(z_1, z_2) \quad (2.544)$$

$$\begin{aligned} &= \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} U(z_1) G_{i\alpha j\beta i\beta j\alpha}^{\text{F}}(z_1, z_2) U(z_2) \\ &- \delta_{il} \bar{\delta}_{\alpha\beta} U(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{i\alpha r\beta i\beta n\alpha}^{\text{F}}(z_1, z_5) T_{n\alpha j\beta k\alpha r\beta}^{\text{eh,fermions}}(z_5, z_2), \end{aligned}$$

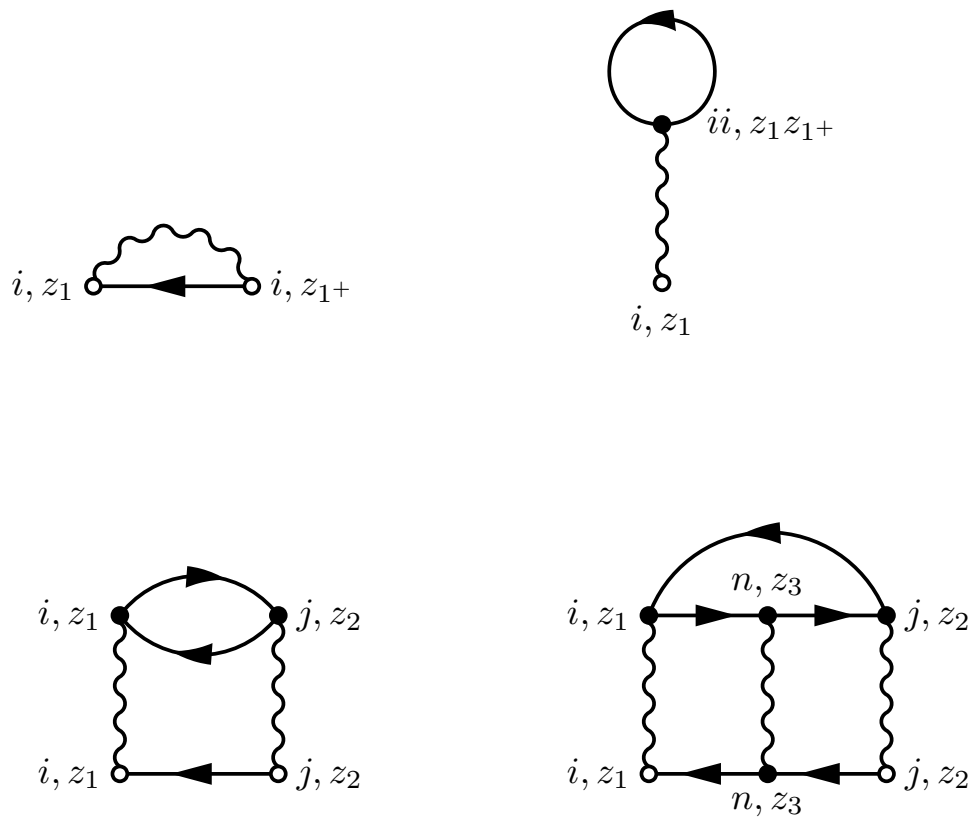


Figure 2.20: Leading terms of $\Sigma^{\text{ph,bosons},0}$ in the Hubbard basis for spin-0 bosons. Each term carries a factor of two.

which, with the introduction of Φ , becomes

$$\begin{aligned}
 T_{i\alpha j\beta k\alpha l\beta}^{\text{eh,fermions}}(z_1, z_2) & \quad (2.545) \\
 & =: \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} \Phi_{i\alpha j\beta i\alpha j\beta}^{\text{eh,fermions}}(z_1, z_2) \\
 & \quad - \delta_{il} \bar{\delta}_{\alpha\beta} U(z_1) \int_{\mathcal{C}} dz_5 \sum_{nr} G_{i\alpha r\beta i\beta n\alpha}^{\text{F}}(z_1, z_5) T_{n\alpha j\beta k\alpha r\beta}^{\text{eh,fermions}}(z_5, z_2).
 \end{aligned}$$

Again by iteration, starting from

$$\begin{aligned}
 \Phi_{i\alpha j\beta k\alpha l\beta}^{\text{eh,fermions}}(z_1, z_2) & \quad (2.546) \\
 & = \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} \Phi_{i\alpha j\beta j\alpha i\beta}^{\text{eh,fermions}}(z_1, z_2) =: \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} \Phi_{ij\alpha\neq\beta}^{\text{eh,fermions}}(z_1, z_2),
 \end{aligned}$$

$$\begin{aligned}
 T_{i\alpha j\beta k\alpha l\beta}^{\text{eh,fermions}}(z_1, z_2) & \quad (2.547) \\
 & = \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} T_{i\alpha j\beta j\alpha i\beta}^{\text{eh,fermions}}(z_1, z_2) =: \delta_{il} \delta_{jk} \bar{\delta}_{\alpha\beta} T_{ij\alpha\neq\beta}^{\text{eh,fermions}}(z_1, z_2)
 \end{aligned}$$

follows. With this, Eq. (2.545) simplifies to

$$\begin{aligned}
 T_{ij\alpha\neq\beta}^{\text{eh,fermions}}(z_1, z_2) & = \Phi_{ij\alpha\neq\beta}^{\text{eh,fermions}}(z_1, z_2) \quad (2.548) \\
 & \quad - U(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{i\alpha n\beta i\beta n\alpha}^{\text{F}}(z_1, z_5) T_{nj\alpha\neq\beta}^{\text{eh,fermions}}(z_5, z_2).
 \end{aligned}$$

The corresponding selfenergy becomes

$$\begin{aligned}
 \Sigma_{i\alpha j\alpha}^{\text{eh,fermions}}(z_1, z_2) & = \Sigma_{i\alpha j\alpha}^{\text{H,fermions}}(z_1, z_2) \\
 & \quad + i\hbar \sum_{\epsilon\neq\alpha} G_{i\epsilon j\epsilon}(z_1, z_2) T_{ij\alpha\neq\epsilon}^{\text{eh,fermions}}(z_1, z_2). \quad (2.549)
 \end{aligned}$$

The components read

$$T_{ij\alpha\neq\beta}^{\text{eh,fermions},\geq}(t_1, t_2) = \Phi_{ij\alpha\neq\beta}^{\text{eh,fermions},\geq}(t_1, t_2) \quad (2.550)$$

$$\begin{aligned} & -U(t_1) \left(\int_{t_0}^{t_1} dt_5 \sum_n G_{i\alpha n, \beta i \beta n \alpha}^{\text{F,R}}(t_1, t_5) T_{nj\alpha\neq\beta}^{\text{eh,fermions},\geq}(t_5, t_2) \right. \\ & \left. \int_{t_0}^{t_2} dt_5 \sum_n G_{i\alpha n, \beta i \beta n \alpha}^{\text{F},\geq}(t_1, t_5) T_{nj\alpha\neq\beta}^{\text{eh,fermions,A}}(t_5, t_2) \right), \end{aligned}$$

$$T_{ij\alpha\neq\beta}^{\text{eh,fermions,A}}(t_1, t_2) = \Phi_{ij\alpha\neq\beta}^{\text{eh,fermions,A}}(t_1, t_2) \quad (2.551)$$

$$-U(t_1) \int_{t_1}^{t_2} dt_5 \sum_n G_{i\alpha n, \beta i \beta n \alpha}^{\text{F,A}}(t_1, t_5) T_{nj\alpha\neq\beta}^{\text{eh,fermions,A}}(t_5, t_2),$$

$$T_{ij\alpha\neq\beta}^{\text{eh,fermions,R}}(t_1, t_2) = \Phi_{ij\alpha\neq\beta}^{\text{eh,fermions,R}}(t_1, t_2) \quad (2.552)$$

$$-U(t_1) \int_{t_2}^{t_1} dt_5 \sum_n G_{i\alpha n, \beta i \beta n \alpha}^{\text{F,R}}(t_1, t_5) T_{nj\alpha\neq\beta}^{\text{eh,fermions,R}}(t_5, t_2).$$

For the selfenergy, the components read

$$\Sigma_{i\alpha j\alpha}^{\text{eh,fermions},\geq}(t_1, t_2) = \Sigma_{i\alpha j\alpha}^{\text{H,fermions},\geq}(t_1, t_2) \quad (2.553)$$

$$+i\hbar \sum_{\epsilon \neq \alpha} G_{i\epsilon j\epsilon}^{\geq}(t_1, t_2) T_{ij\alpha\neq\epsilon}^{\text{eh,fermions},\geq}(t_1, t_2).$$

For spin- $\frac{1}{2}$ fermions, one has

$$\begin{aligned} T_{ij\uparrow\downarrow}^{\text{eh,fermions},1/2}(z_1, z_2) &= T_{ij\downarrow\uparrow}^{\text{eh,fermions},1/2}(z_1, z_2) =: T_{ij}^{\text{eh,fermions},1/2}(z_1, z_2) \\ &= \Phi_{ij}^{\text{eh,fermions},1/2}(z_1, z_2) \end{aligned} \quad (2.554)$$

$$-U(z_1) \int_{\mathcal{C}} dz_5 \sum_n G_{in}^{\text{F}}(z_1, z_5) T_{nj}^{\text{eh,fermions},1/2}(z_5, z_2).$$

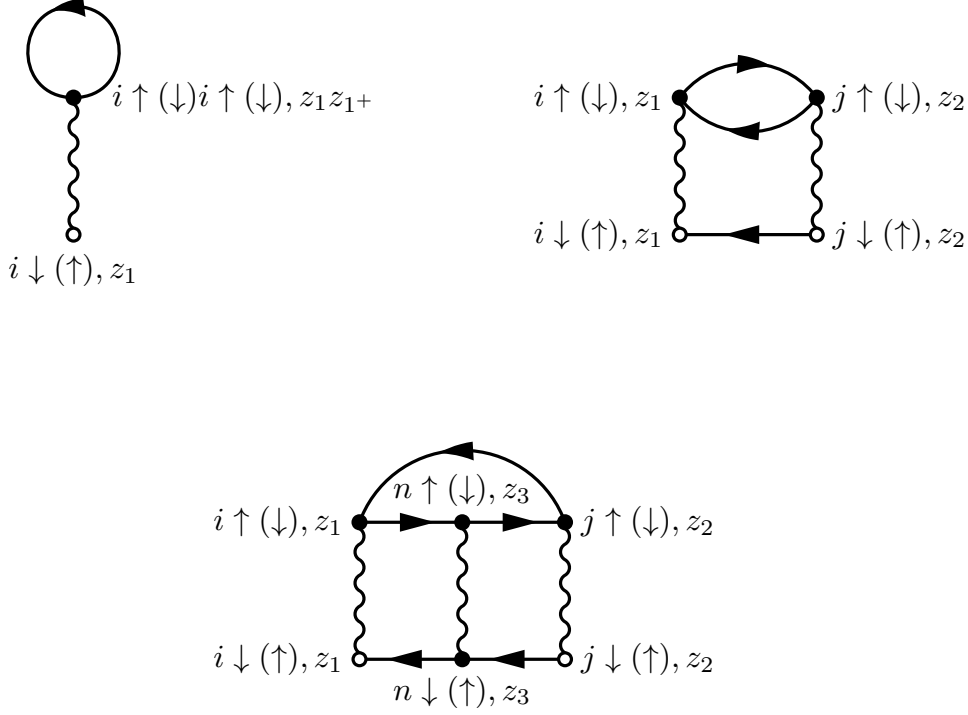


Figure 2.21: Leading terms of $\Sigma^{\text{eh,fermions},1/2}$ in the Hubbard basis for spin-1/2 fermions.

where one defines

$$\Phi_{ij}^{\text{eh,fermions},1/2}(z_1, z_2) \quad (2.555)$$

$$:= \Phi_{ij\uparrow\downarrow}^{\text{eh,fermions},1/2}(z_1, z_2) = \Phi_{ij\downarrow\uparrow}^{\text{eh,fermions},1/2}(z_1, z_2),$$

$$G_{in}^{\text{F}}(z_1, z_2) := G_{i\uparrow n\downarrow i\downarrow n\uparrow}^{\text{F}}(z_1, z_2) = G_{i\downarrow n\uparrow i\uparrow n\downarrow}^{\text{F}}(z_1, z_2). \quad (2.556)$$

The selfenergy reads

$$\begin{aligned} \Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{\text{eh,fermions},1/2}(z_1, z_2) &= \Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{\text{H,fermions},1/2}(z_1, z_2) \\ &+ i\hbar G_{i\uparrow(\downarrow)j\uparrow(\downarrow)}(z_1, z_2) T_{ij}^{\text{eh,fermions},1/2}(z_1, z_2). \end{aligned} \quad (2.557)$$

The first terms of the diagrammatic representation is shown in Fig. 2.21. The

components are

$$T_{ij}^{\text{eh,fermions},1/2,\geq}(t_1, t_2) = \Phi_{ij}^{\text{eh,fermions},1/2,\geq}(t_1, t_2) \quad (2.558)$$

$$-U(t_1) \left(\int_{t_0}^{t_1} dt_5 \sum_n G_{in}^{\text{F,R}}(t_1, t_5) T_{nj}^{\text{eh,fermions},1/2,\geq}(t_5, t_2) \right. \\ \left. \int_{t_0}^{t_2} dt_5 \sum_n G_{in}^{\text{F},\geq}(t_1, t_5) T_{nj}^{\text{eh,fermions},1/2,\text{A}}(t_5, t_2) \right),$$

$$T_{ij}^{\text{eh,fermions},1/2,\text{A}}(t_1, t_2) = \Phi_{ij}^{\text{eh,fermions},1/2,\text{A}}(t_1, t_2) \quad (2.559)$$

$$-U(t_1) \int_{t_1}^{t_2} dt_5 \sum_n G_{in}^{\text{F,A}}(t_1, t_5) T_{nj}^{\text{eh,fermions},1/2,\text{A}}(t_5, t_2),$$

$$T_{ij}^{\text{eh,fermions},1/2,\text{R}}(t_1, t_2) = \Phi_{ij}^{\text{eh,fermions},1/2,\text{R}}(t_1, t_2) \quad (2.560)$$

$$-U(t_1) \int_{t_2}^{t_1} dt_5 \sum_n G_{in}^{\text{F,R}}(t_1, t_5) T_{nj}^{\text{eh,fermions},1/2,\text{R}}(t_5, t_2).$$

For the selfenergy, the relevant components read

$$\Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{\text{eh,fermions},1/2,\geq}(t_1, t_2) = \Sigma_{i\downarrow(\uparrow)j\downarrow(\uparrow)}^{\text{H,fermions},1/2,\geq}(t_1, t_2) \quad (2.561)$$

$$+i\hbar G_{i\uparrow(\downarrow)j\uparrow(\downarrow)}^{\geq}(t_1, t_2) T_{ij}^{\text{eh,fermions},1/2,\geq}(t_1, t_2).$$

2.7.2.5 Fluctuating exchange approximation

The idea behind the fluctuating exchange approximation (FLEX) goes along the same line as both flavors of the T -matrix and the GW -approximation but takes into account the diagrams from all three without consideration of cross-terms between different approximations. To avoid double-counting, the common first-order and second-order terms are subtracted twice. Thereby, the resulting FLEX selfenergy becomes

$$\Sigma^{\text{FLEX}} = \Sigma^{\text{GW}} + \Sigma^{\text{T}^{\text{pp}}} + \Sigma^{\text{T}^{\text{eh}}} - 2(\Sigma^{\text{H}} + \Sigma^{\text{F}} + \Sigma^{(2)}). \quad (2.562)$$

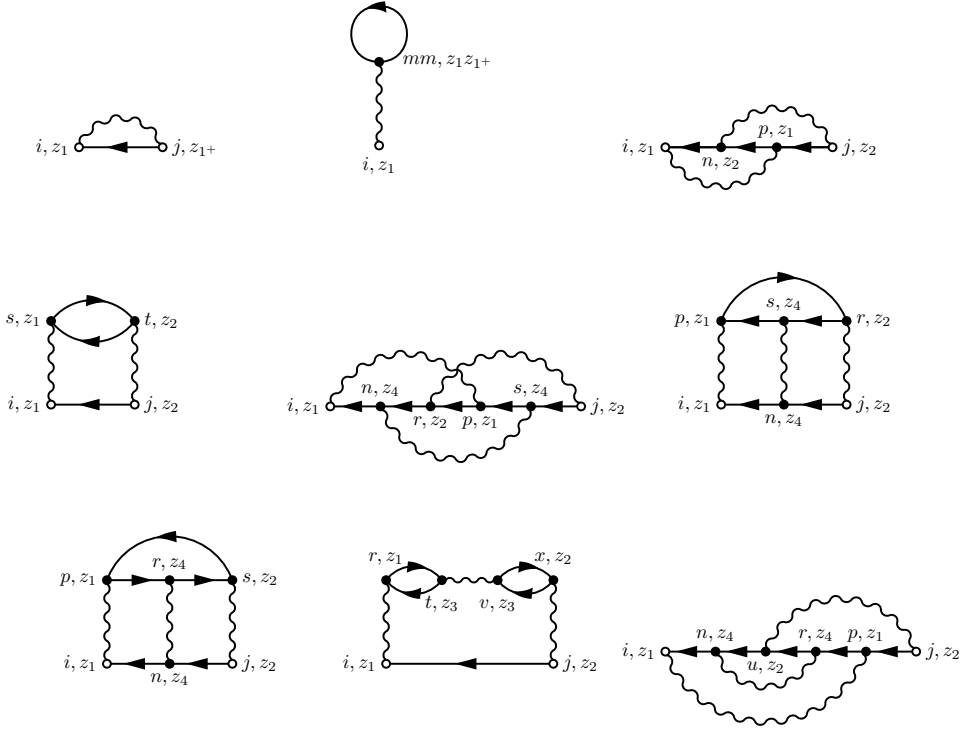


Figure 2.22: Leading terms of $\Sigma^{\text{FLEX,diag.}}$ in a diagonal basis.

The diagrammatic representation of the leading terms for a diagonal basis, and for spin-0 bosons as well as spin-1/2 fermions in the Hubbard basis are shown in Figs. 2.22 and 2.23 and Fig. 2.24, respectively.

2.8 The Generalized Kadanoff–Baym Ansatz

To compute the time-dependent single-particle Green functions, either the KBE, cf. Eqs. (2.66) and (2.67), or the Dyson equation, cf. Eq. (2.91) have to be solved, which both scale cubic with respect to the time arguments. An approximate way to transform the scaling to a quadratic one, has been proposed by Lipavský *et al.* and was named Generalized Kadanoff–Baym ansatz, for details about the derivation see [62] by Lipavský and [91, 93, 94, 106]. The approximation starts from an exact

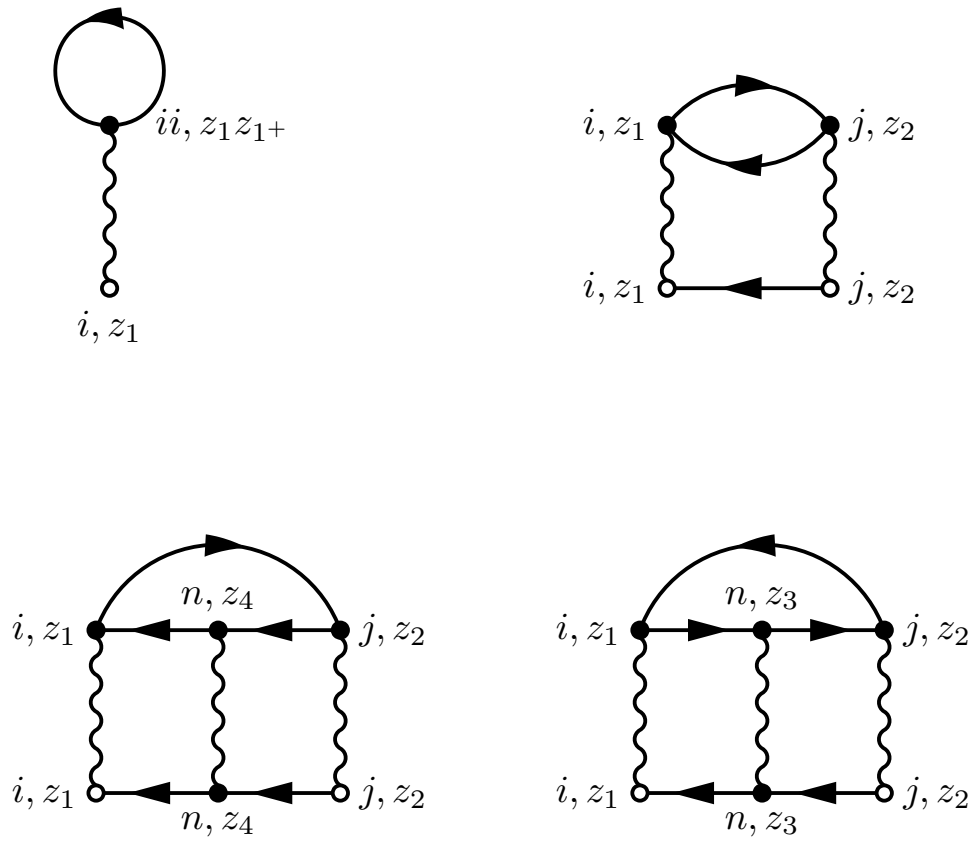


Figure 2.23: Leading terms of $\Sigma^{\text{FLEX, bosons}, 0}$ in the Hubbard basis for spin-0 bosons.

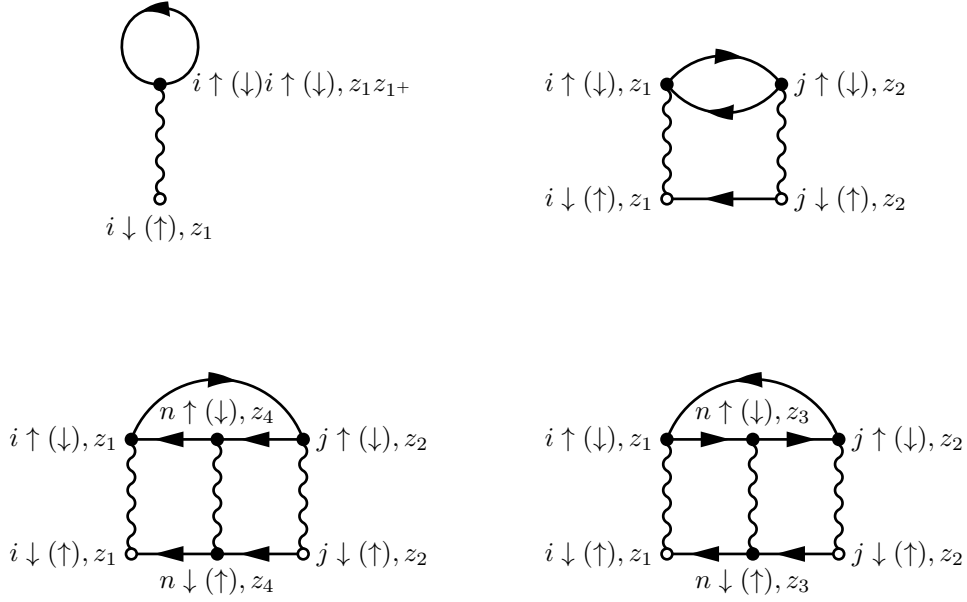


Figure 2.24: Leading terms of $\Sigma^{\text{FLEX,fermions},1/2}$ in the Hubbard basis for spin-1/2 fermions.

reformulation of the Dyson equation, the less-component of which reads

$$\begin{aligned}
 G_{ij}^<(t_1, t_2) = & -i\hbar \sum_k G_{ik}^{\text{R}}(t_1, t_2) G_{kj}^<(t_2, t_2) \\
 & + \int_{t_2}^{t_1} dt_3 \int_{t_0}^{t_2} dt_4 \sum_{kl} G_{ik}^{\text{R}}(t_1, t_3) \Sigma_{kl}^<(t_3, t_4) G_{lj}^{\text{A}}(t_4, t_2) \\
 & + \int_{t_2}^{t_1} dt_3 \int_{t_0}^{t_2} dt_4 \sum_{kl} G_{ik}^{\text{R}}(t_1, t_3) \Sigma_{kl}^{\text{R}}(t_3, t_4) G_{lj}^<(t_4, t_2) \\
 & + i\hbar G_{ik}^<(t_1, t_1) G_{kj}^{\text{A}}(t_1, t_2) \\
 & - \int_{t_0}^{t_1} dt_3 \int_{t_1}^{t_2} dt_4 \sum_{kl} G_{ik}^{\text{R}}(t_1, t_3) \Sigma_{kl}^<(t_3, t_4) G_{lj}^{\text{A}}(t_4, t_2) \\
 & - \int_{t_0}^{t_1} dt_3 \int_{t_1}^{t_2} dt_4 \sum_{kl} G_{ik}^<(t_1, t_3) \Sigma_{kl}^{\text{A}}(t_3, t_4) G_{lj}^{\text{A}}(t_4, t_2),
 \end{aligned} \tag{2.563}$$

and analog for the greater component. The GKBA approximates these terms by only retaining the non-integral contributions, which can be considered a simultaneous perturbative expansion of G with respect to Σ and to the spectral structure conveyed by the off-diagonal elements of both quantities. It reads,

$$\begin{aligned}
 G_{ij}^{\geq}(t_1, t_2) & \tag{2.564} \\
 &= -i\hbar \sum_k \left(G_{ik}^R(t_1, t_2) G_{kj}^{\geq}(t_2, t_2) + G_{ik}^{\geq}(t_1, t_1) G_{kj}^A(t_1, t_2) \right) \\
 &= \sum_k A_{ik}(t_1, t_2) \left(\Theta(t_1, t_2) G_{kj}^{\geq}(t_2, t_2) + \Theta(t_2, t_1) G_{kj}^{\geq}(t_1, t_1) \right),
 \end{aligned}$$

where, in the second line, the spectral function

$$A_{ij}(t_1, t_2) = i\hbar \left(G_{ij}^>(t_1, t_2) - G_{ij}^<(t_1, t_2) \right) \tag{2.565}$$

has been introduced. The approximated \geq -components are used in the right-hand sides of the KBE, which, thereby, need to be only propagated along the time-diagonal. To achieve the overall reduction to quadratic scaling, though, the GKBA has to be accompanied by a second-order selfenergy and another approximation concerning the retarded and advanced components, which, unapproximated, obey equations of similar complexity to the original KBE, i.e., with cubic scaling. In this work, the propagators, and with that the spectral function, will be approximated on the HF level. Another possibility, employed in [39], is to use approximate correlated propagators. The GKBA has several important benefits: It preserves the causal structure of the KBE and it conserves important constants of motion, whenever the chosen selfenergy approximation does [73]. Further, it cures certain damping induced artifacts for small systems [51, 72], an example of which will be further explored in Section 3.3.

2.9 Interacting initial state

To compute the time-evolution of the single-particle Green function according to Eqs. (2.66) and (2.67), the initial state represented by $G(t_0, t_0)$ has to be calculated. It is determined by the environment of the system. If the system is isolated,

i.e., is described by a pure state, $G(t_0, t_0)$ is the fully interacting initial state. For a system embedded into a bath with which it exchanges particles or energy, the initial state is strongly influenced by the equilibrium between degrees of freedom of the system and the bath. Under the assumption that the interaction between the both is weak and dominantly uncorrelated a suitable ensemble, for instance the canonical or grand canonical ensemble, determines the occupation of the energy levels in the initial state of the system. For both cases of systems, whether connected to a bath or isolated, there exist several methodologies to generate the interacting initial state, some of which will be detailed in the next sections including the method of adiabatic switch-on of the interaction in Section 2.9.2, which is used throughout this work.

2.9.1 Contour extension to finite temperatures

One possibility to include the description of the interacting initial state, in equilibrium with a bath or isolated, was originally proposed by *Matsubara* [107]. He proposed augmenting the original contour, comprised of a forward and a backward branch \mathcal{C}^+ , \mathcal{C}^- , by a “vertical” branch \mathcal{C}^M of complex time arguments ranging along the imaginary axis from z_0 to $z_0 - i\hbar\beta$, where β is the inverse temperature of the bath or equal to ∞ for an isolated system at zero temperature. The reasoning behind this can be understood by considering the following observations for quantum systems in contact with an environment. The simplest way to treat the interaction of the system with the environment is statistically, assigning bath-induced weights w_n of finding the system in one of its states $|n\rangle$. With this, the ensemble average of an observable $\hat{O}(t_0)$ can be defined as

$$O(t_0) = \sum_n w_n \langle n | \hat{O}(t_0) | n \rangle. \quad (2.566)$$

Note that Eq. (2.566) is a natural generalization of a pure state $|n\rangle = |\Psi_0\rangle$, to which it reduces if $w_n = 1$ only for $|\Psi_0\rangle$ and $w_n = 0$ else. With Eq. (2.566), the statistical density matrix operator $\hat{\rho}$ can be defined,

$$\hat{\rho} = \sum_n w_n |n\rangle \langle n|, \quad (2.567)$$

with which Eq. (2.566) can be rewritten as

$$O(t_0) = \text{Tr}[\hat{\rho}\hat{O}(t_0)]. \quad (2.568)$$

The trace Tr is to be understood as acting on the full Fock space $\mathcal{F}_\sigma^{\mathcal{H}}$. For the grand canonical ensemble (GCE), which describes a system which exchanges energy (characterized by inverse temperature β) and particles (characterized by the chemical potential μ) with its environment, the density matrix operator $\hat{\rho}$ reads

$$\hat{\rho} = \frac{\exp(-\beta\hat{H}_M)}{Z}, \quad (2.569)$$

with the corresponding Hamiltonian

$$\hat{H}_M = \hat{H} - \mu\hat{N} \quad (2.570)$$

and the partition function

$$Z^{\text{GCE}} = \text{Tr}[\exp(-\beta\hat{H}_M)]. \quad (2.571)$$

For the GCE, Eq. (2.568) becomes

$$O(t_0) = \frac{\text{Tr}[\exp(-\beta\hat{H}_M)\hat{O}(t_0)]}{Z^{\text{GCE}}}. \quad (2.572)$$

With this result, Eq. (2.45) can be specialized to

$$O(z) = \frac{\text{Tr}[\exp(-\beta\hat{H}_M)\hat{\mathcal{T}}_C\left\{\exp\left(\frac{1}{i\hbar}\int_C dz_3 \hat{H}(z_3)\hat{O}(z)\right)\right\}]}{\text{Tr}[\exp(-\beta\hat{H}_M)]}. \quad (2.573)$$

Using

$$\hat{\mathcal{T}}_C\left\{\exp\left(\frac{1}{i\hbar}\int_C dz_3 \hat{H}(z_3)\right)\right\} = \hat{1}, \quad (2.574)$$

and introducing the vertical part of the contour \mathcal{C}^M running from z_0 to $z_0 - i\hbar\beta$ with the identity

$$\exp(-\beta\hat{H}_M) = \exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}^M}\hat{H}_M\right), \quad (2.575)$$

we arrive at

$$O(z) = \frac{\text{Tr}\left[\exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}^M}\hat{H}_M\right)\hat{\mathcal{T}}_{\mathcal{C}}\left\{\exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}}dz_3\hat{H}(z_3)\right)\hat{O}(z)\right\}\right]}{\text{Tr}\left[\exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}^M}\hat{H}_M\right)\hat{\mathcal{T}}_{\mathcal{C}}\left\{\exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}}dz_3\hat{H}(z_3)\right)\right\}\right]}. \quad (2.576)$$

From this structure, Matsubara's idea can be directly derived. If one defines

$$\hat{H}|_{\mathcal{C}^M} \equiv \hat{H}_M, \quad \hat{O}|_{\mathcal{C}^M} \equiv \hat{O}(t_0) \quad (2.577)$$

and redefines the contour \mathcal{C} as

$$\mathcal{C} = \mathcal{C}^- \oplus \mathcal{C}^+ \oplus \mathcal{C}^M, \quad (2.578)$$

so that every point on the vertical track is defined as later than all points on the forward and backward branches, Eq. (2.576) can be recast as

$$O(z) = \frac{\text{Tr}\left[\hat{\mathcal{T}}_{\mathcal{C}}\left\{\exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}}dz_3\hat{H}(z_3)\right)\hat{O}(z)\right\}\right]}{\text{Tr}\left[\hat{\mathcal{T}}_{\mathcal{C}}\left\{\exp\left(-\frac{i}{\hbar}\int_{\mathcal{C}}dz_3\hat{H}(z_3)\right)\right\}\right]}. \quad (2.579)$$

The corresponding contour is depicted in Fig. 2.25. With this, definition (2.579) correctly reproduces the time-dependent expectation values in accordance with Eq. (2.45) for $z \in \mathcal{C}^- \oplus \mathcal{C}^+$ and the ensemble average for $z \in \mathcal{C}^M$ agreeing with Eq. (2.572). Note though that this treatment of the system–bath interaction is only valid for times smaller than its relaxation time as the bath only directly influences the initial state and not any time-dependent excitations during the propagation [52].

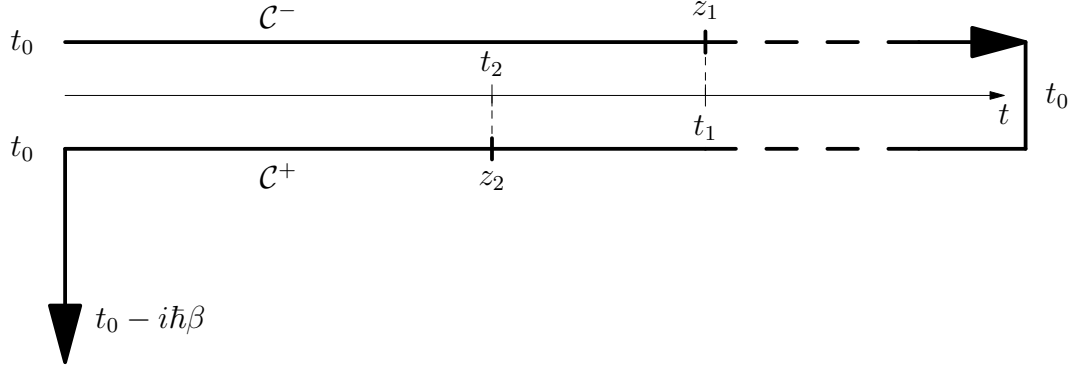


Figure 2.25: Matsubara contour \mathcal{C} extended to the imaginary axis. The forward-branch \mathcal{C}^- spans from the initial time t_0 to ∞ , bends and leads back to t_0 along the backward \mathcal{C}^+ -branch. Then it spans along the imaginary branch \mathcal{C}^M to $t_0 - i\hbar\beta$, where β is the inverse temperature.

2.9.2 Adiabatic switch-on of interactions

If one is mainly interested in the evolution of isolated systems described by a pure state, a suitable procedure is the generation of the non-interacting state of the system, which is known for most systems and a subsequent sufficiently slow ramp-up of the interaction strength from zero to the desired value. Provided the *Gell-Mann-Low theorem* holds [108], which assures the existence of some limites, and the non-interacting ground state is non-degenerate, it follows that the state of the system after switch-on of the interaction is an eigenstate of the fully interacting Hamiltonian. It remains to be checked—e.g., by comparison with other methods—that it is the groundstate. Under the adiabatic switching protocol, the Hamiltonian of Eq. (2.16) is replaced by

$$\hat{H}^{\text{AS}}(t) = \underbrace{\sum_{mn} h_{mn} \hat{c}_m^\dagger \hat{c}_n}_{\hat{H}^0} + \underbrace{\frac{1}{2} f^{\text{AS}}(t) \sum_{mnpq} w_{mnpq} \hat{c}_m^\dagger \hat{c}_n^\dagger \hat{c}_p \hat{c}_q}_{\hat{W}^{\text{AS}}(t)} \quad (2.580)$$

$$+ \underbrace{\sum_{mn} f_{mn}(t) \hat{c}_m^\dagger \hat{c}_n}_{\hat{F}(t)},$$

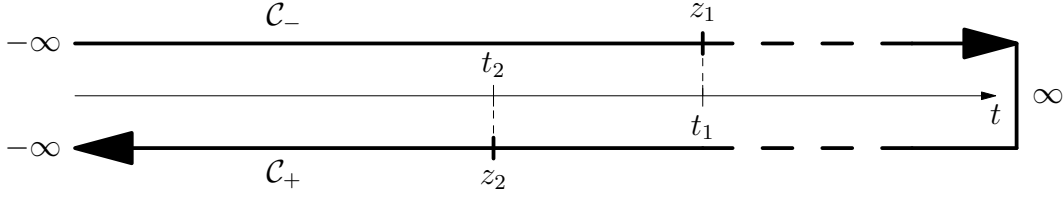


Figure 2.26: Schwinger–Keldysh contour \mathcal{C}^{AS} with adiabatic switch-on of the interactions. The starting and end point is now $-\infty$.

where the monotonically increasing switching function $f^{\text{AS}} : \mathbb{R} \rightarrow [0, 1]$ satisfies

$$\lim_{t \rightarrow -\infty} f^{\text{AS}}(t) = 0, \quad f^{\text{AS}}(t) = 1 \quad \text{for } t \geq t_0. \quad (2.581)$$

To achieve a high fidelity of the final state the switch-on process has to be performed slow enough and as smooth as possible. Here, the use of the function [109]

$$f_{\text{AS}}^{\tau, t_{\text{H}}}(t) = \exp\left(-\frac{A_{t_{\text{H}}}^{\tau}}{t_1/(2t_{\text{H}})} \exp\left(\frac{B_{t_{\text{H}}}^{\tau}}{t_1/(2t_{\text{H}})} - 1\right)\right),$$

$$B_{t_{\text{H}}}^{\tau} = \frac{t_{\text{H}}}{\tau \ln 2} - \frac{1}{2}, \quad (2.582)$$

$$A_{t_{\text{H}}}^{\tau} = \frac{\ln 2}{2} \exp\left(2B_{t_{\text{H}}}^{\tau}\right),$$

is superior compared to an approach based on a Fermi function, since it provides a very small relative change for values near the beginning and the end of the switch-on process. The free parameters τ and t_{H} , the half-time, control the steepness and the duration of the switch-on. Using the adiabatic-switching methodology, the time-contour attains the form depicted in Fig. 2.26.

3 Numerical simulations—Applications to lattice systems

This chapter discusses some applications of the approximation strategies detailed in Chapter 2. All simulations described in this chapter have been performed for spin-1/2 fermions in the Hubbard model, cf. Section 2.3, for zero temperature. After providing an overview of the algorithm for the numerical solution of the KBE in Section 3.1, results for the correlated ground-state of Hubbard nano-clusters are presented in Section 3.2. The ground-state energy and spectral function are used as benchmarks to compare the performance of the selfenergy approximations presented in Section 2.7 for different filling factors and interaction strengths. Subsequently, in Section 3.3, the behavior of the approximation strategies in the simulation of the time-dependent response of Hubbard clusters to external excitations is studied. A special focus lies on excitations that strongly drive the system out of equilibrium. There, the occurrence of a particular weakness of selfconsistent approaches, the so-called correlation-induced damping [51], is analyzed for all approximations and it is demonstrated how it can be mostly overcome by application of the GKBA, in Section 3.3.

3.1 Algorithm for the solution of the Kadanoff–Baym equations

This section gives an overview of the algorithm to calculate the solution of the KBE, cf. Eqs. (2.89) and (2.90), for spin-1/2 fermions. Both equations need to be equipped with the initial value $G^{\gtrless}(t_0, t_0)$, which is the Green function of the correlated initial state. This Green function, in turn, is generated from that of the ideal ground state, $G^{(0),\gtrless}$, via the adiabatic switching method described in Section 2.9.2. The \gtrless -components of the ideal Green function directly follow from the ideal one-particle

density matrix $n^{(0)}$ via the relation

$$G_{ij}^{(0),<} = -\frac{1}{i\hbar} n_{ji}^{(0)}, \quad (3.1)$$

$$G_{ij}^{(0),>} = \frac{1}{i\hbar} (\delta_{ij} - n_{ji}^{(0)}), \quad (3.2)$$

where the second equations follows from the more general relation for an arbitrary time t ,

$$G_{ij}^{>}(t, t) = \frac{1}{i\hbar} \delta_{ij} + G_{ij}^{<}(t, t). \quad (3.3)$$

Since, here, only zero-temperature applications are considered, the ideal fermionic density matrix can be found by diagonalization of the single-particle part of the Hamiltonian, \hat{H}^0 , cf. Eq. (2.16). The density matrix $n^{\hat{H}^0}$ in the eigenbasis of \hat{H}^0 is diagonal and, for N particles, reads (sorted by the eigenvalues, starting from the smallest eigenvalue)

$$n_{ij}^{\hat{H}^0} = \delta_{ij} \begin{cases} 1 & \text{if } i \leq N \\ 0 & \text{else} \end{cases}, \quad (3.4)$$

which, after retransformation into the Hubbard basis, yields the ideal density matrix $n_{ji}^{(0)}$ and, via Eqs. (3.1) and (3.2), the components of the ideal Green function. Using $G_{ij}^{(0),\geq}$ as initial values, following Eq. (2.580), the KBE are propagated along both time-directions simultaneously switching on the interaction with the switching function, cf. Eq. (2.582), i.e., the solutions of

$$\begin{aligned} & \sum_l \left[i\hbar \frac{d}{dt_1} \delta_{il} - h_{il}(t_1) \right] G_{lj}^{\geq}(t_1, t_2) \\ &= \sum_l \int_{t_s}^{t_1} dt_3 \left[\Sigma_{il}^{>}(t_1, t_3) - \Sigma_{il}^{<}(t_1, t_3) \right] G_{lj}^{\geq}(\bar{t}, t') \\ &+ \sum_l \int_{t_s}^{t_2} dt_3 \Sigma_{il}^{\geq}(t_1, t_3) \left(G_{lj}^{<}(\bar{t}, t') - G_{lj}^{>}(\bar{t}, t') \right), \end{aligned} \quad (3.5)$$

and

$$\begin{aligned}
 & \sum_l G_{il}^{\geq}(t_1, t_2) \left[-i\hbar \frac{\overleftarrow{d}}{dt_2} \delta_{lj} - h_{lj}(t_2) \right] \\
 &= \sum_l \int_{t_s}^{t_1} dt_3 \left[G_{il}^>(t_1, t_3) - G_{il}^<(t_1, t_3) \right] \Sigma_{lj}^{\geq}(t_3, t_2) \\
 &+ \sum_l \int_{t_s}^{t_2} dt_3 G_{il}^{\geq}(t_1, t_3) \left(\Sigma_{lj}^<(t_3, t_2) - \Sigma_{lj}^>(t_3, t_2) \right),
 \end{aligned} \tag{3.6}$$

for all values $t_1, t_2 \in [t_s, t_0]$, are computed, where t_s is the starting time of the adiabatic switching. The interaction matrix in the selfenergy terms for the chosen approximation, on the right-hand sides are replaced by, cf. Section 2.7,

$$w_{ijkl} \longrightarrow f_{\text{AS}}^{\tau, t_{\text{H}}}(t) w_{ijkl}, \tag{3.7}$$

where the switching parameters t_{H} and τ are chosen such that the resulting state is converged with respect to the relevant observables. In practice, values of $\tau = 19.0 J^{-1}$ and $t_{\text{H}} = 25.0 J^{-1}$ have been found sufficient for all calculations. After the switching has taken place, the system is prepared in the correlated ground state¹ described by $G^{\geq}(t_0, t_0)$. The information about the correlations in the system is encoded in the values of the Green functions for all time-points during the switching. That is why all integrals occurring in the solution of the KBE for physically relevant times have to extend along the whole time-plane including the adiabatic switching part, i.e., Eqs. (3.5) and (3.6) have to be used also for $t_1, t_2 > t_0$. It has to be noted that any time-dependent excitation of the system has to occur after the switching is finished and that the values of G with at least one argument in the switching region cannot be used for the determination of observables, as detailed in Section 3.1.1. For the numerical solution of the KBE, standard approaches for the solution of ordinary differential equations (ODEs), like Runge–Kutta methods [110], can be employed upon appropriately discretizing the two-time plane. Further, an integration routine for the right-hand sides of Eqs. (3.5) and (3.6) is necessary. Here, the approach

¹As already pointed out in Section 2.9.2, it has to be checked externally, e.g., by comparison with other methods, that the final state of the adiabatic switching is indeed the ground-state.

detailed in [59] has been employed for all calculations. As a general note, the use of higher-order methods for the solution of the ODEs and the integrals, i.e., methods where the error scales with a large power of the time step such that time steps of the order of 10^{-2} to 10^{-1} are possible, is especially advisable to achieve performance and accuracy, since the right-hand sides of the KBE are numerically very expensive.

3.1.1 Observables

This section briefly describes how important physical observables can be obtained from the time-dependent Green functions and additionally from the right-hand sides of the KBE, cf. Eqs. (3.5) and (3.6), the so-called collision integrals. As detailed in the Eq. (3.1), the less-component of the Green function of the interacting ground-state is directly linked to the density matrix. This relation also holds true for the time-dependent density matrix $n_{ij}(t)$, which describes the single-particle response of system subjected to a time-dependent excitation, reading

$$G_{ij}^<(t, t) = -\frac{1}{i\hbar} n_{ji}(t). \quad (3.8)$$

Apart from the time-dependent occupations of the Hubbard sites, which are given by the diagonal elements of the time-dependent density matrix, it also permits the calculation of several energy contributions:

- the kinetic energy,

$$E_{\text{kin}}(t) = \text{Re} \left(\sum_{mn} h_{mn} n_{nm}(t) \right), \quad (3.9)$$

- the energy induced by a time-dependent excitation $f_{mn}(t)$,

$$E_{\text{ex}}(t) = \text{Re} \left(\sum_{mn} f_{mn}(t) n_{nm}(t) \right), \quad (3.10)$$

– and the interaction energy,

$$\begin{aligned}
 E_{\text{int}}(t) &= -\frac{i\hbar}{2} \sum_{kl} \int_{t_0}^t d\bar{t} \left[\Sigma_{kl}^>(t, \bar{t}) - \Sigma_{kl}^<(t, \bar{t}) \right] G_{lk}^<(\bar{t}, t) \\
 &\quad + \sum_{kl} \int_{t_0}^t d\bar{t} \Sigma_{kl}^<(t, \bar{t}) \left[G_{lk}^<(\bar{t}, t) - G_{lk}^>(\bar{t}, t) \right] \\
 &= -\frac{i\hbar}{2} \sum_{kl} \int_{t_0}^t d\bar{t} \Sigma_{kl}^>(t, \bar{t}) G_{lk}^<(\bar{t}, t) - \Sigma_{kl}^<(t, \bar{t}) G_{lk}^>(\bar{t}, t),
 \end{aligned} \tag{3.11}$$

which originates from the trace over the right-hand side of Eq. (2.89), the collision integral.

Going beyond the time-diagonal of the Green function, one can use the information encoded in the off-diagonal values to gain insight into the $(N + 1)$ - and $(N - 1)$ spaces by means of the single-particle spectral function, already encountered in Eq. (2.565). If an N -particle system is prepared in the groundstate $|\Psi_0^{(N)}\rangle$ with energy $E_0^{(N)}$ (or any other N -particle energy eigenstate), e.g., via adiabatic switching, and afterwards propagated without additional excitations, the greater/less-components of the two-time Green functions obey

$$G_{ji}^<(t_1, t_2) = \tag{3.12}$$

$$\mp i\hbar \sum_m Q_m(j) Q_m^*(i) \exp\left(\frac{1}{i\hbar} (E_m^{(N-1)} - E_0^{(N)}) (t_2 - t_1)\right),$$

$$G_{ji}^>(t_1, t_2) = \tag{3.13}$$

$$i\hbar \sum_m P_m(j) P_m^*(i) \exp\left(\frac{1}{i\hbar} (E_m^{(N+1)} - E_0^{(N)}) (t_1 - t_2)\right),$$

where the amplitudes $Q_m(i)$, $P_m(i)$ are defined as

$$P_m(i) = \langle \Psi_0^{(N)} | \hat{c}_i | \Psi_m^{(N+1)} \rangle, \tag{3.14}$$

$$Q_m(i) = \langle \Psi_m^{(N-1)} | \hat{c}_i | \Psi_0^{(N)} \rangle. \tag{3.15}$$

They are the overlap matrix elements of the $(N - 1)$ - and $(N + 1)$ -particle states of energy E_m with the state which originates from removing/adding one particle in the i -th basis state from/to the N -particle state. By Fourier transforming and via the knowledge of $E_0^{(N)}$, the $(N - 1)$ - and $(N + 1)$ -particle energies can be determined from the propagation of two-time Green function of the N -particle system.

In addition to these single-particle quantities, via the collision integral, the time-dependent double-occupations $n_i^{(2)}(t)$, i.e., the conditional probabilities of an electron occupying a spin-orbital on a Hubbard site, while another electron occupies the corresponding orbital with different spin orientation at the same site, can be computed as

$$n_i^{(2)}(t) = \frac{1}{2U} \sum_l \int_{t_0}^t d\bar{t} \Sigma_{il}^>(t, \bar{t}) G_{li}^<(\bar{t}, t) - \Sigma_{il}^<(t, \bar{t}) G_{li}^>(\bar{t}, t), \quad (3.16)$$

which becomes obvious taking into account the relation between the selfenergy and the two-particle Green function, cf. Eqs. (2.64) and (2.66).

3.2 Interacting ground-state and spectral functions

In this section, numerical results of the interacting ground-state energies of the 6-site Hubbard model are presented. The performance with respect to filling level and interaction strength of the selfenergy approximation schemes introduced in Section 2.7 is measured via comparison with exact calculations. Following the adiabatic switching algorithm of Section 2.9.2, the systems are initially prepared in the non-interacting ground-state for $N = 1, 2, 3$ particles, i.e., filling levels $n = 0.17$, $n = 0.33$ and $n = 0.5$. Using the switching function (2.582) with parameters $\tau = 19.0 J^{-1}$ and $t_H = 25.0 J^{-1}$, ensuing, the interaction U is ramped-up to final values $U = 0.1, 0.5, 1.0, 2.0$. In Table 3.1, the selfenergy approximations used are listed.

Starting with $U = 0.1$, which is a very small interaction strength, the results for $N = 1, 2, 3$ are listed in Tables (3.2), (3.3) and (3.4). For all three filling factors, the Hartree results differ from the exact results in the third decimal place, while all methods going beyond Hartree agree up to the fourth decimal place. This can be explained by the fact that the Hartree approximation is only correct up to the first order in the interaction strength, while all other methods agree up to the second-order

method name	method
H	Hartree approximation: $\Sigma = \Sigma^H$
SOA	Second-order approximation: $\Sigma = \Sigma^{(2)}$
TOA	Third-order approximation: $\Sigma = \Sigma^{(3)}$
TPP	Particle-particle T -matrix approximation: $\Sigma = \Sigma^{T^{pp}}$
TEH	Electron-hole T -matrix approximation: $\Sigma = \Sigma^{T^{eh}}$
GWA	GW -approximation: $\Sigma = \Sigma^{GW}$
FLEX	Fluctuating exchange approximation: $\Sigma = \Sigma^{FLEX}$

Table 3.1: Method names

method	$E_{gs}[J]$
H	-0.533604
TPP	-0.534067
Exact	-0.534073
TOA	-0.534075
FLEX	-0.534076
SOA	-0.534084
GWA	-0.534084
TEH	-0.534093

Table 3.2: Ground-state energies

$$N_s = 6, N_\uparrow = 1, N_\downarrow = 1, U = 0.1$$

method	$E_{\text{gs}}[J]$
H	-2.642487
TPP	-2.643354
Exact	-2.643367
TOA	-2.643367
FLEX	-2.643368
SOA	-2.643376
GWA	-2.643376
TEH	-2.643390

Table 3.3: Ground-state energies
 $N_s = 6, N_{\uparrow} = 2, N_{\downarrow} = 2, U = 0.1$

method	$E_{\text{gs}}[J]$
H	-6.837918
TPP	-6.839299
Exact	-6.839331
TOA	-6.839331
SOA	-6.839331
GWA	-6.839331
FLEX	-6.839334
TEH	-6.839363

Table 3.4: Ground-state energies
 $N_s = 6, N_{\uparrow} = 3, N_{\downarrow} = 3, U = 0.1$

method	$E_{\text{gs}}[J]$
H	-0.44956
TPP	-0.45981
TOA	-0.46048
Exact	-0.46065
FLEX	-0.46129
SOA	-0.46164
GWA	-0.46181
TEH	-0.46293

Table 3.5: Ground-state energies
 $N_s = 6, N_\uparrow = 1, N_\downarrow = 1, U = 0.5$

in the interaction with each other and the exact solution. For both smaller-than-half filling factors, the results of the non-Hartree methods behave similarly. The best results, which agree up to at least 5 decimal places with the exact result, are achieved by the third-order and the FLEX approximations, which are both correct up the third order in the interaction strength. Covering only one of the two third-order selfenergy contributions, the particle-particle and electron-hole T -matrix, respectively, do not improve the result significantly over the use of the second order approximation (SOA) for $n = 0.33$, although, for $n = 0.17$, the particle-particle T -matrix is better than the electron-hole T -matrix, since the latter contributes less as the electronic density is comparatively small. For $U = 0.1$, the GW approximation shows no difference to the SOA results, since both approximations only differ in the fourth order, as the GWA has no third order diagram, cf. Eq. (2.392). For half-filling $n = 0.5$, all non-Hartree methods, which are also called correlated methods, apart from the T -matrices agree with each other and with the exact solution up to 5 decimal places. This is explained by the so-called particle-hole symmetry in the Hubbard model [57], which only occurs at half-filling and leads to the exact cancellation of electron-hole and particle-particle T -matrix terms in uneven orders of the interaction and equality of these terms in even orders. Therefore, for half-filling, SOA and TOA yield exactly the same results and agree with GWA and FLEX up the fourth order in the interaction.

For the increased but still small interaction strength $U = 0.5$, the results for $N = 1, 2, 3$ are shown in Tables (3.5), (3.6) and (3.7). Here, the Hartree results differ already in the second decimal place from the exact result. All correlated

method	$E_{\text{gs}}[J]$
H	-2.35948
TPP	-2.37963
TOA	-2.38093
Exact	-2.38107
FLEX	-2.38174
SOA	-2.38208
GWA	-2.38226
TEH	-2.38400

Table 3.6: Ground-state energies
 $N_s = 6, N_{\uparrow} = 2, N_{\downarrow} = 2, U = 0.5$

method	$E_{\text{gs}}[J]$
H	-6.23792
TPP	-6.26949
TOA	-6.27285
SOA	-6.27285
Exact	-6.27322
GWA	-6.27347
FLEX	-6.27471
TEH	-6.27741

Table 3.7: Ground-state energies
 $N_s = 6, N_{\uparrow} = 3, N_{\downarrow} = 3, U = 0.5$

method	$E_{\text{gs}}[J]$
H	-0.34718
TPP	-0.38291
TOA	-0.38545
Exact	-0.38810
SOA	-0.39472
FLEX	-0.39685
GWA	-0.39723
TEH	-0.40535

Table 3.8: Ground-state energies
 $N_s = 6, N_{\uparrow} = 1, N_{\downarrow} = 1, U = 1$

methods agree with the exact result in this decimal place. Compared to the $U = 0.1$ results, only the TOA stays close to the exact solution, all other methods show more pronounced deviations. For $n = 0.16$, FLEX and TPP yield comparably good results, TEH is worse compared to its particle-particle counterpart and GWA is worse than the SOA. For $n = 0.33$, FLEX becomes better than TPP, showing the increasing importance of the third-order electron-hole contribution. For half-filling, the GWA result is the closest to the exact solution, tightly followed by the equal results of the SOA and TOA. This gives a first hint that, at $U = 0.5$, the fourth and possibly higher-order terms gain influence, although among the approximations containing fourth-order and higher terms, only the GWA gives improved energies compared to second/third-order perturbative results.

For the higher interaction strengths $U = 1.0$ and $U = 2.0$, the results are shown in Tables (3.8), (3.9) and (3.10) and Tables (3.11), (3.12) and (3.13), respectively. Compared to the results for $U = 0.5$, the relative order of the performance stays the same, but the absolute differences to the exact results increase. Summarizing the results for the ground-state energies, it is evident that, for non-half filling, the TOA outperforms all other perturbative and non-perturbative selfenergy approximations, at least in the covered range of $U = 0.1 \dots 2.0$. For half-filling, the best results can be obtained from the *GW* approximation.

Considering another important quantity of the correlated initial state, which goes beyond the description of the lowest energy level is the single-particle spectral function, as introduced in Section 3.1.1. For an N -particle system, it shows the

method	$E_{\text{gs}}[J]$
H	-2.00967
TPP	-2.08369
TOA	-2.09182
Exact	-2.09367
SOA	-2.10058
GWA	-2.10357
FLEX	-2.10424
TEH	-2.11746

Table 3.9: Ground-state energies

$$N_s = 6, N_{\uparrow} = 2, N_{\downarrow} = 2, U = 1$$

method	$E_{\text{gs}}[J]$
H	-5.48791
TPP	-5.60173
TOA	-5.62356
SOA	-5.62356
Exact	-5.62889
GWA	-5.63259
FLEX	-5.64923
TEH	-5.66104

Table 3.10: Ground-state energies

$$N_s = 6, N_{\uparrow} = 3, N_{\downarrow} = 3, U = 1$$

method	$E_{\text{gs}}[J]$
H	-0.14939
TPP	-0.26319
TOA	-0.26738
Exact	-0.28820
SOA	-0.32514
GWA	-0.35068
FLEX	-0.36059
TEH	-0.39065

Table 3.11: Ground-state energies

$$N_s = 6, N_{\uparrow} = 1, N_{\downarrow} = 1, U = 2$$

method	$E_{\text{gs}}[J]$
H	-1.31891
TPP	-1.57367
TOA	-1.61455
Exact	-1.63342
SOA	-1.67092
GWA	-1.71303
FLEX	-1.76167
TEH	-1.80334

Table 3.12: Ground-state energies
 $N_s = 6, N_{\uparrow} = 2, N_{\downarrow} = 2, U = 2$

method	$E_{\text{gs}}[J]$
H	-3.98791
TPP	-4.36896
TOA	-4.48569
SOA	-4.48569
Exact	-4.54631
GWA	-4.58604
FLEX	-4.71630
TEH	-4.73547

Table 3.13: Ground-state energies
 $N_s = 6, N_{\uparrow} = 3, N_{\downarrow} = 3, U = 2$

transition energies into the $(N - 1)$ -particle as well as the $(N + 1)$ -particle system, i.e., the single-particle removal and addition energies. The removal energies are carried by the off-timedagonal values of $G^<$, while the addition energies are similarly encoded in $G^>$. They can be made visible by transforming into relative and center-of-mass time coordinates and afterwards Fourier transforming with respect to the relative time coordinate. Comparing with Eqs. (3.12) and (3.13), one expects peaks at the energy levels of $(N \pm 1)$ -particle systems shifted by the ground-state energy of the N -particle system. For the six-site Hubbard system of interaction strength $U = 1$, the ability of the different selfenergy approximations is studied for the three filling factors $n = 0.17, 0.33, 0.5$. The results are compared with exact excitation spectra of the relevant $(N \pm 1)$ -particle systems, which in turn are generated by excitation with a δ -kick and subsequent Fourier transform of the time-dependent density evolution.

For $n = 0.17$, the results are shown in Fig. 3.1. The frequency axis of the spectrum is shifted such that all removal energies, corresponding to $G^<$, have negative values while the addition energies, corresponding to $G^>$, have positive energies. Since the spectrum of the $(N - 1)$ -particle system only contains one spin-up or spin-down particle² it has no interaction effects and, thus, is ideal. This corresponds to the less-part of the spectrum having only one spectral line which matches the exact result (blue line) for every approximation including Hartree(-Fock). Analyzing the greater part of the spectrum which belongs to the system with two particles of one spin-direction and one particle of the other, one can separate two sets of spectral lines. The three spectral lines belonging to the lowest addition energies are in exact agreement throughout all approximations including Hartree and, thus, indicate mostly uncorrelated states. The position of the peak for the next higher addition energy begins to differ between the approximations. The best agreement with the exact solution is reached by the GWA followed by SOA, TEH and HF. The positions for TPP and FLEX are slightly shifted to lower energies. For TOA, the peak position cannot be easily distinguished with the shown spectral resolution, but the knee-structure within the left slope of the peak for the next higher energy suggests that the accuracy is comparable to that of the other approximations. Unlike

²As the fermionic Hubbard Hamiltonian contains no terms which are different for up or down spin-orientation, a system with N spin-up and M spin-down particles behaves like the system with M spin-up particles and N spin-down particles.

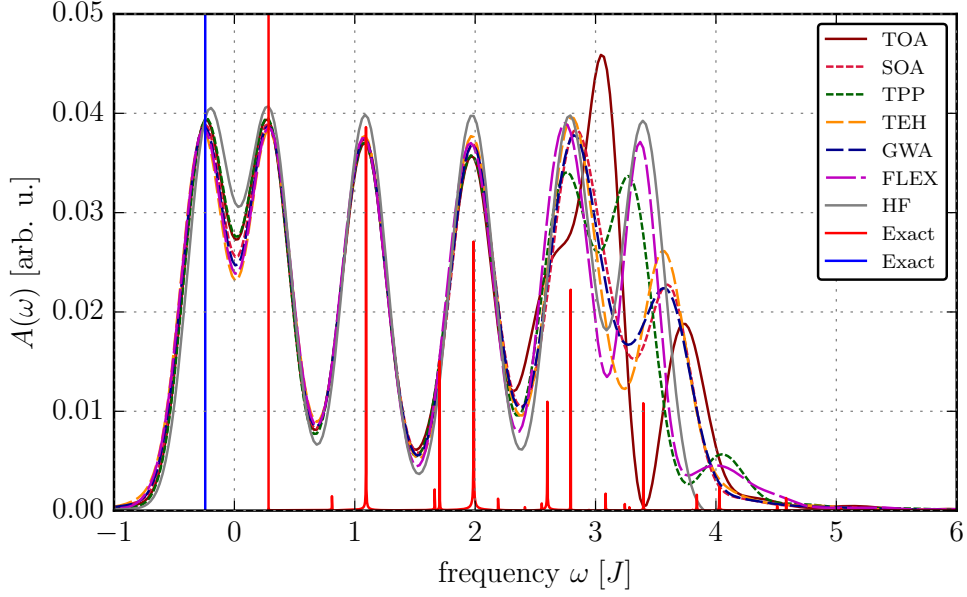


Figure 3.1: 6-site Hubbard cluster with $U = 1$ at one-sixth filling. Spectral function generated from different selfenergy approximations: brown full line: third-order approximation (TOA), crimson dashed line: second-order approximation (SOA), green dashed line: particle–particle T -matrix (TPP), yellow dashed line: electron–hole T -matrix (TEH, blue dashed line: GW approximation (GWA), purple semi-dashed line: fluctuating exchange approximation (FLEX), gray full line: Hartree–Fock approximation (HF). For comparison: Exact excitation spectra of the systems with $N^\uparrow = 1, N^\downarrow = 0$ (blue) and $N^\uparrow = 2, N^\downarrow = 1$ (red). The spectra are shifted such that $E = 0$ lies in the center between the highest removal energy and the lowest addition energy.

any other tested approximation, though, the TOA is able to show the energy level just above $\omega = 3$. The next-higher energy level at $\omega \approx 3.3$ is best captured by the FLEX approximation followed by TPP, which slightly shifts to lower energies. The SOA, GWA and the TEH show this peak shifted to higher energies. For the TOA, it remains questionable if the peak at $\omega \approx 3.8$ is to be attributed to exact energy level at $\omega \approx 3.3$ or if it shows the energy level at $\omega \approx 3.9$. The level just above $\omega = 4$ is only shown by the TPP and FLEX approximations, which indicates that these states embody a high degree of correlation. Summing up the findings for one-sixth filling, the best overall results are achieved by the TPP and FLEX approximation, while the latter is slightly better. In addition, the TOA shows energy levels which are not captured by any other approximation.

For $n = 0.33$, the results are shown in Fig. 3.2. Two removal energy levels with a large amplitude and one with a small amplitude are visible. It is noteworthy that the system the removal energies of the one-third filled Hubbard cluster connect to, i.e., that of two and one particle of both spin-directions, respectively, is the same the addition energies of the one-sixth filled cluster connect to. Comparing with the right part of Fig. 3.1, one immediately recognizes that the shown energy levels are not the same. For $n = 0.33$, the destination energy levels are levels 1, 2 and 6, while, for $n = 0.17$, the levels 1, 3, 6 and higher levels are reached. Thus, the combined information of both fillings can be used to gain insight into the energy spectrum of the in-between system with a difference of one particle to both. Concerning the quality of the approximations for the removal energy levels, all approximation agree with each other and with the exact solution, indicating that the states belonging to the removal energies are mainly uncorrelated. For the addition energies, the same is true for the first two levels. Starting from just above $\omega = 2$, there are many close-lying energy levels in the range up to $\omega \approx 4$, which renders a attribution to the different approximations difficult. In general, confirming the trend found for $n = 0.17$, the FLEX approximation yields results which show very good agreement with exact energy levels, while the TOA reveals correct energy levels not found with the other approximations.

Turning to the results for half-filling, shown in Fig. 3.3, one immediately recognizes two peculiarities of this setup. First, the removal and addition part of the spectrum is symmetric with respect to $E = 0$. This is, again, due to the occurrence of particle–hole symmetry [57]. Second, comparing the quality of the different approximations,

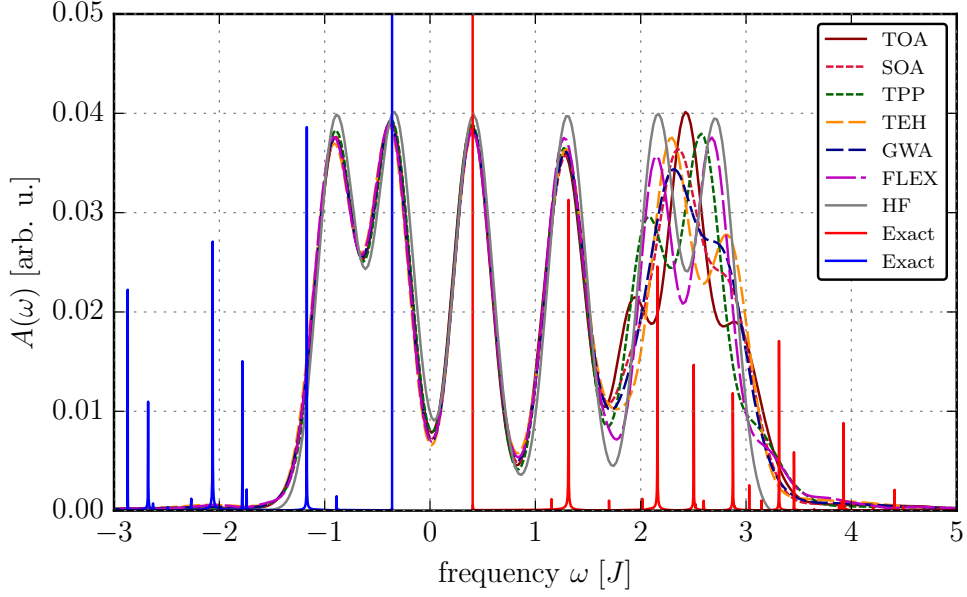


Figure 3.2: 6-site Hubbard cluster with $U = 1$ at one-third filling. Spectral function generated from different selfenergy approximations: brown full line: third-order approximation (TOA), crimson dashed line: second-order approximation (SOA), green dashed line: particle–particle T -matrix (TPP), yellow dashed line: electron–hole T -matrix (TEH, blue dashed line: GW approximation (GWA), purple semi-dashed line: fluctuating exchange approximation (FLEX), gray full line: Hartree–Fock approximation (HF). For comparison: Excitation spectra of the systems with $N^\uparrow = 2, N^\downarrow = 1$ (blue) and $N^\uparrow = 3, N^\downarrow = 2$ (red). The spectra are shifted such that $E = 0$ lies in the center between the highest removal energy and the lowest addition energy.

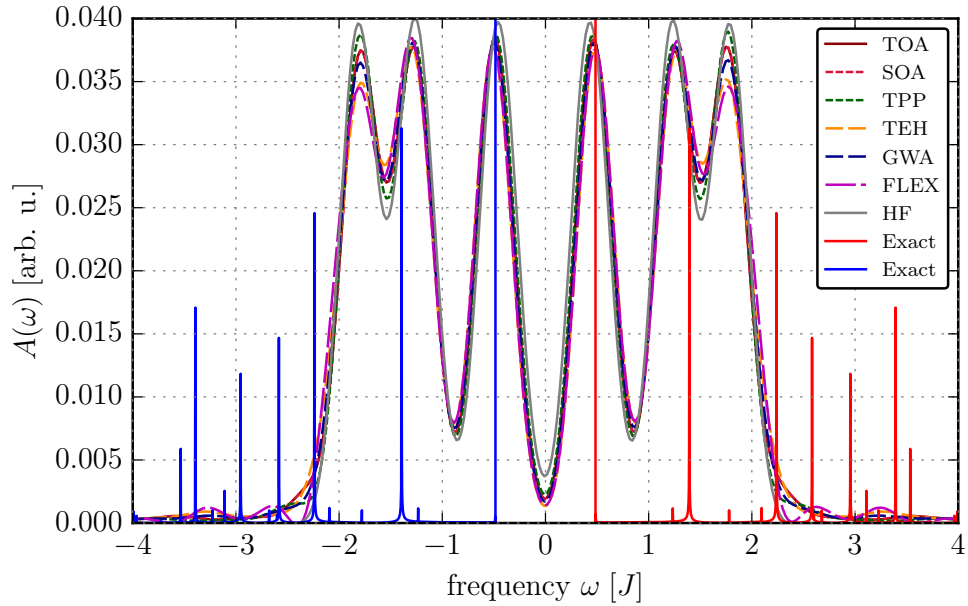


Figure 3.3: 6-site Hubbard cluster with $U = 1$ at half filling. Spectral function generated from different selfenergy approximations: brown full line: third-order approximation (TOA), crimson dashed line: second-order approximation (SOA), green dashed line: particle–particle T -matrix (TPP), yellow dashed line: electron–hole T -matrix (TEH, blue dashed line: GW approximation (GWA), purple semi-dashed line: fluctuating exchange approximation (FLEX), gray full line: Hartree–Fock approximation (HF). For comparison: Excitation spectra of the systems with $N^\uparrow = 3$, $N^\downarrow = 2$ (blue) and $N^\uparrow = 4$, $N^\downarrow = 3$ (red). The spectra are shifted such that $E = 0$ lies in the center between the highest removal energy and the lowest addition energy.

one can discern only minor differences at energy levels farther away from $E = 0$, which are most pronounced for the FLEX approximation. As a special note, the good performance of the Hartree approximation for the spectral function indicates that the use of the GKBA with Hartree propagators is justified for half-filling and explains the excellent results that could be achieved [33, 72, 94]. Summarizing the ability of NEGF methods to describe the spectral function of Hubbard clusters, one can state that the overall agreement for small to medium interaction strength is good and especially via combination of different approximation methods as well as probing from both systems with adjacent number of particles, one can gain a large part of the spectral information.

3.3 Time-dependent excitations

This section deals with the application of the correlated selfenergy approximations described in Section 2.7 to small Hubbard clusters which are driven to non-equilibrium by strong sudden quenches of the on-site potential. A deficiency of correlated selfenergy approximations is the occurrence of a correlation-induced damping (CID) in selfconsistent NEGF simulations of small Hubbard clusters, which has been first described by *von Friesen et al.* in [51] and the follow-up paper [90]. Here, the dependence of this phenomenon on the choice of selfenergy approximation is studied and it is shown that it can be mostly overcome by application of the GKBA. CID has been found occurring in simulations of systems subjected to a strong and sudden switch-on of an excitation f , when a selfconsistent selfenergy approximation is used. Accordingly, the time-dependent excitation matrix elements f_{ij} are chosen as, cf. Eq. (2.29),

$$f_{ij}(t) = \Theta(t, t_0) \delta_{ij} \delta_{i1} w_0, \quad (3.17)$$

which corresponds to a sudden switch-on of an onsite potential of strength w_0 on the first site $i = 1$ at $t_1 = t_0$. This excitation, initially, drives a depletion of this site which is followed by a subsequent oscillation of the electronic density throughout the system. For the case of the half-filled Hubbard dimer, i.e. comprising two sites, an interaction of $U = 1$ and excitation strength of $w_0 = 5.0$, the time-evolution of the density on the first site is shown in Fig. 3.4, published in [72], where the exact results

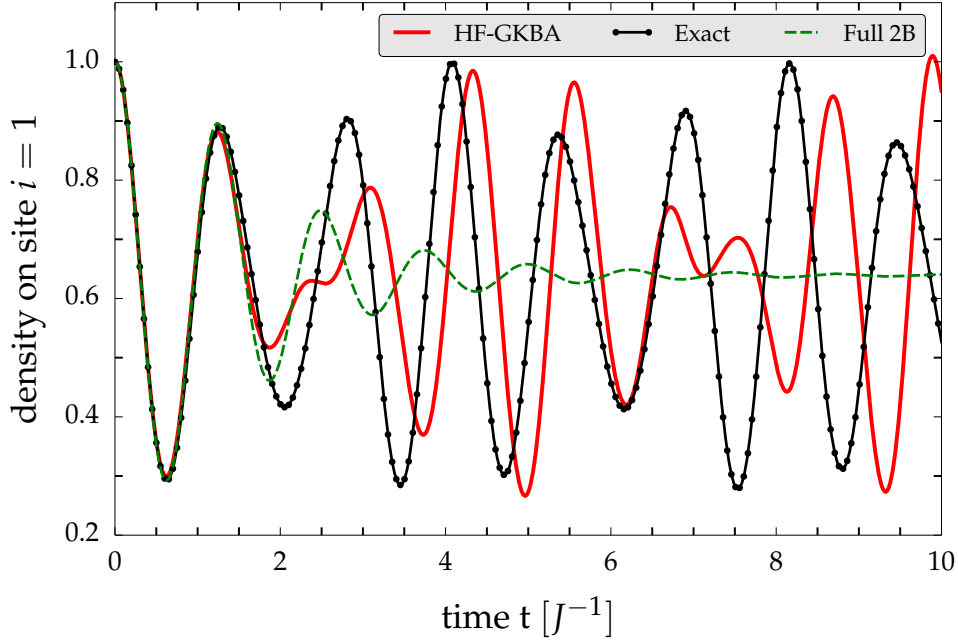


Figure 3.4: Half-filled Hubbard dimer for $U = 1$. Density evolution on the first site following a sudden switch-on of an onsite potential on the first site $i = 1$ of strength $w_0 = 5.0$. Black line with dots: exact results, green dashed line: Selfconsistent solution of the KBE with second-order selfenergy approximation (Full 2B), red full line: Application of the GKBA with HF propagators and second-order selfenergy approximation. Published in [72].

are compared to results obtained from a selfconsistent solution with and without additionally employing the GKBA with HF propagators (Full 2B/HF-GKBA). As predicted, the exact solution shows a periodic oscillation of the density between the two sites after an initial depletion of the first site. Comparing the result of the fully selfconsistent solution of the KBE with second order selfenergy to the exact results, one can see a reasonably good agreement with the exact solution only up to about two inverse hopping amplitudes, after which it quickly damps and reaches an artificial steady-state. As the authors of [51] have checked and has been confirmed in [72], this behavior is not a numerical artifact but rather intrinsic to the approximate selfconsistent solution of the KBE. To reduce the level of selfconsistency and still approximately retain the influence of correlations, it is natural to apply the GKBA

with HF propagators as described in 2.8. The corresponding results in Fig. 3.4 show that the GKBA in combination with the second-order approximation for the selfenergy indeed cures the artificial damping and qualitatively agrees with the exact solution. The quantitative agreement, though, can only be considered satisfactory for the first five oscillation periods up to 6 inverse hopping amplitudes. To achieve a better agreement with the exact results—apart from the loss of the numerical advantage of the GKBA in combination with a second-order approximation, as explained in Section 2.8—the GKBA can be combined with any other other higher-order and non-perturbative selfenergy approximation described in Section 2.7. By combination with the particle–particle T -matrix approximation, cf. Section 2.7.2.3, the GKBA can reach a very good qualitative agreement with exact results, as can be seen in Fig. 3.5, where the same setup as in Fig. 3.4 is studied. As one can immediately see, the GKBA with the particle–particle T -matrix approximation is in excellent agreement with the exact results for the whole simulation time. In contrast, the full solution of the KBE with the particle–particle T -matrix is quickly damped like the full second-order approximation. This makes the GKBA a very good solution to tackle the problem of CID. As the authors of [90] have reported in great detail, the occurrence of CID for correlated selfenergy approximations crucially depends on the chosen system parameters and chosen approximation.

For the case of the four-site fermionic Hubbard model with one quarter filling, an interaction strength of $U = 1.5$ and a switch-on excitation of strength $w_0 = 5.0$, *Friesen et. al.* reported the particle–particle T -matrix to show very good agreement with the exact solution, while the GW -approximation showed a much worse agreement. Here, the same setup is studied with all methods detailed in Section 2.7. One finds that the methods can be categorized into three groups based on the amount of CID occurring. The three most damped methods, which quickly fail to reproduce the exact result are the electron-hole T -matrix, the GW -approximation and the second-order selfenergy approximation, shown in Fig. 3.6. For all three methods, the damping sets in after the second oscillation and the amplitude quickly drops to roughly one third of the exact amplitude. For the fluctuating exchange approximation and the similarly constructed approximation combining only the electron–hole and the particle–particle T -matrix, the results are shown in Fig. 3.7. Here, one notices only a slight damping and the overall agreement with the exact results is improved compared to the first group of strongly damped approximations. The methods

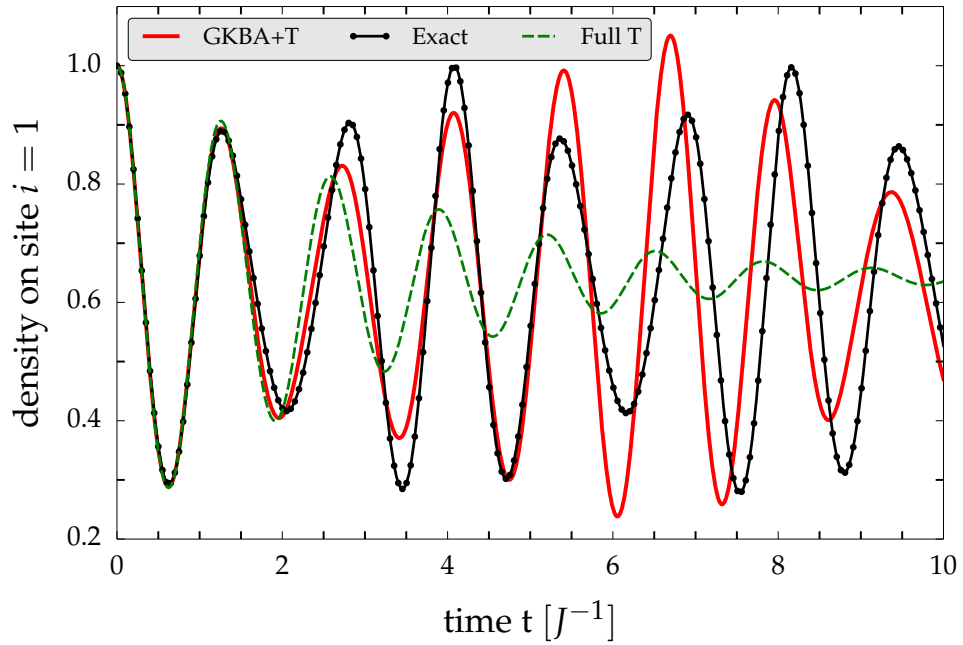


Figure 3.5: Half-filled Hubbard dimer for $U = 1$. Density evolution on the first site following a sudden switch-on of an onsite potential on the first site $i = 1$ of strength $w_0 = 5.0$. Black line with dots: exact results, green dashed line: Selfconsistent solution of the KBE with particle–particle selfenergy approximation (Full T), red full line: Application of the GKBA with HF propagators and particle–particle T -matrix selfenergy approximation. Published in [72].

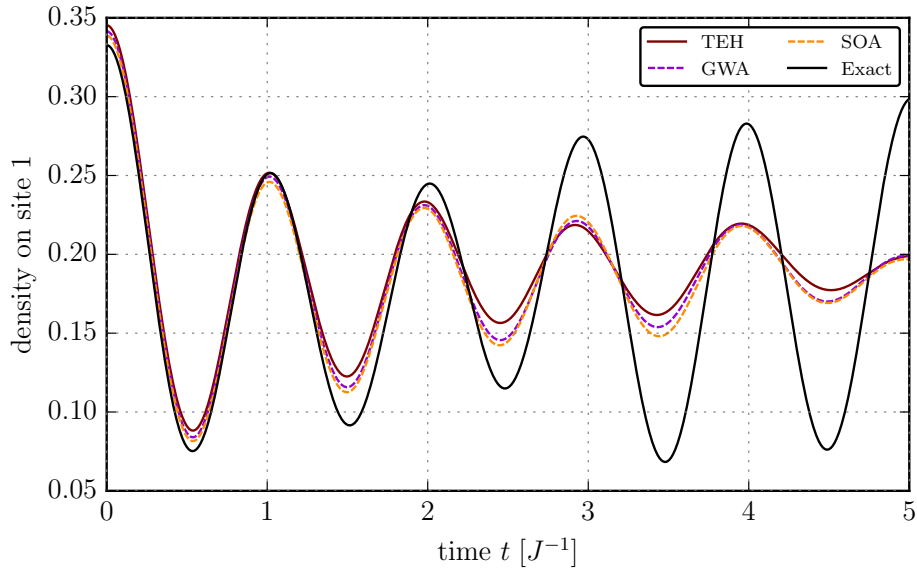


Figure 3.6: One quarter-filled four-site Hubbard dimer for $U = 1.5$. Density evolution of the first site following a sudden switch-on of an onsite potential on the first site $i = 1$ of strength $w_0 = 5.0$. Strongly damped methods. Brown solid line: electron-hole T -matrix (TEH), purple dashed line: GW -approximation (GWA), yellow dashed line: second-order selfenergy approximation (SOA), black solid line: exact result.

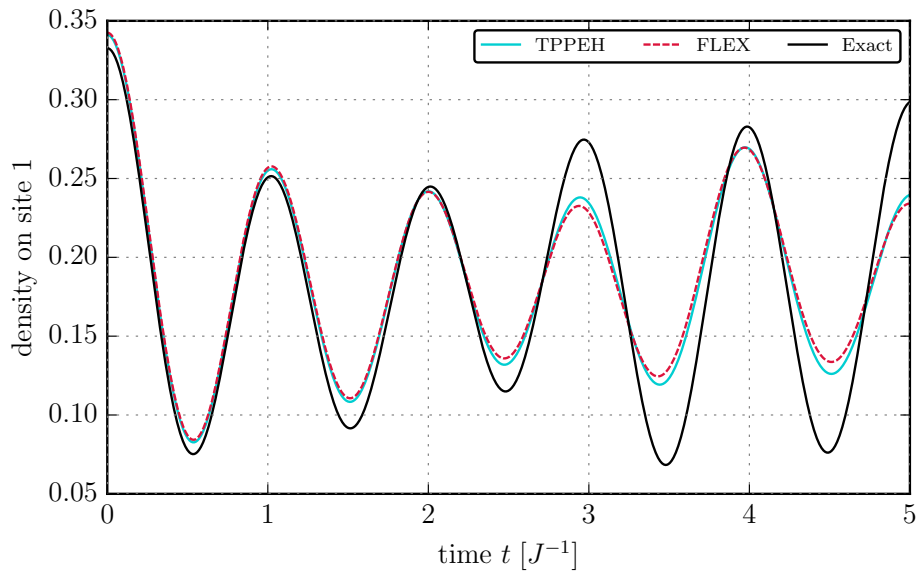


Figure 3.7: One quarter-filled four-site Hubbard dimer for $U = 1.5$. Density evolution of the first site following a sudden switch-on of an onsite potential on the first site $i = 1$ of strength $w_0 = 5.0$. Weakly damped methods. Turquoise solid line: Combination of the electron-hole and the particle-particle T -matrices (TPPEH), red dashed line: fluctuating exchange approximation (FLEX), black line: exact result.

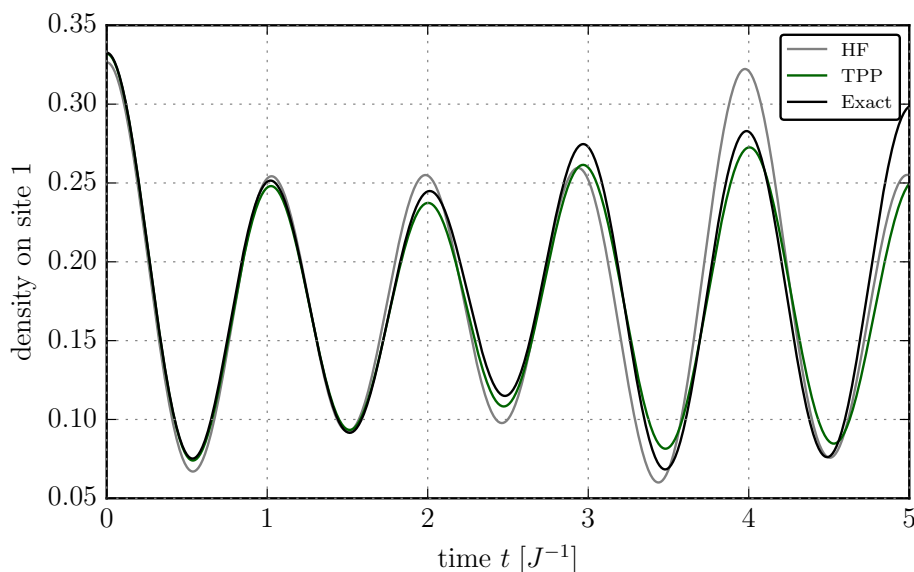


Figure 3.8: One quarter-filled four-site Hubbard dimer for $U = 1.5$. Density evolution of the first site following a sudden switch-on of an onsite potential on the first site $i = 1$ of strength $w_0 = 5.0$. Undamped methods. Green solid line: particle–particle T -matrix (TPP), gray solid line: Hartree(–Fock) approximation, black line: exact result.

without any conceivable CID are the particle–particle T -matrix and, by construction, the uncorrelated Hartree(–Fock) approximation. The corresponding results are shown in Fig. 3.8. Both methods are in good agreement with the exact result, but the quality of the T -matrix approximation is not reached with the uncorrelated Hartree approximation.

Concluding this part, it has been shown that, for the interacting groundstate, the order-by-order expansion with respect to the interaction strength yields good results already with the second-order approximation and significantly improves to excellent results taking the third-order terms into account. The non-perturbative expansions like both T -matrix approximations and GW or combination of several non-perturbative approximations cannot reach the same quality of results. Concerning the single-particle spectrum, both, perturbative and non-perturbative methods, yield good results and especially with the combination of the results for all available

methods, most of the spectral information can be computed. For time-dependent processes involving strong excitations, the GKBA has been found to be a valuable tool to mitigate correlation-induced damping. Together with the particle–particle T -matrix, which has shown to produce excellent results in full calculations for lower filling factors, it yields a density evolution which is close to the exact solution for all filling factors. With the great variety of available methods, covered in Section 2.7 with and without application of the GKBA, a suitable toolset is available to study systems of arbitrary dimension and large particle numbers, where no exact methods are available.

4 Conclusion

In this thesis, a detailed overview of approximation strategies for the single-particle selfenergy within the framework of nonequilibrium Green functions has been presented. The expressions for the selfenergy have been directly deduced from the exact set of coupled equations of motion and are given in the most general basis representation. Additionally, for the special cases of a basis, in which the interaction is diagonal, as well as for the fermionic and bosonic Hubbard basis with a scalar interaction, the corresponding selfenergy terms with Keldysh components have been derived. The studied approximations include non-perturbative as well as perturbative approaches with respect to the orders of the interaction strength. The latter have been studied up to the third order, which, as has been shown in Section 2.7, can be computed with the same numerical scaling as the second-order terms and are therefore strictly preferable. The non-perturbative selfenergy approximations studied—involving resummations of infinite partial series—are based on the particle–particle as well as the particle–hole T -matrix approximation, the screened interaction in the GW -approximation and, for the fluctuating exchange approximation, involves the combination of the terms from both T -matrices and GW .

To assert the quality of the different approximations, they have been applied to the calculation of the interacting ground-state as well as the density-response to sudden potential quenches in Hubbard nano-clusters for different filling factors and interaction strengths. For the interacting ground-state, the best results could be obtained for the perturbative approaches, i.e., the second-order and especially the third-order approximations, the latter being applied for the first time to the Hubbard model in this thesis. For small and medium filling, the ground-state energies computed with the TOA show by far the best agreement with exact reference calculations and it outperforms all previously applied approximations. For half-filling, though, the TOA exactly agrees with the SOA due to particle–hole symmetry and, consequently, yields no improvement over it. Here, the implementation of the fourth-order terms, following

the algorithm presented in Section 2.7.1.4, could achieve significant improvements, like it has been done successfully for homogeneous systems by *Gebhard et. al.* in [57]. One important obstacle to the application of the fourth-order terms, though, is the numerical downside of a quartic scaling with the propagation time, which will probably limit the applicability to small system sizes and short propagation times. If achievable, though, it opens the way to many new approximation strategies and resummations starting from the fourth order terms similar to the (third-order) T -matrices. Furthermore, the equations for the screened interaction W , cf. Eq. (2.101), and the polarization function P , cf. Eq. (2.102), can be solved exactly in fourth order for a given approximation of the vertex function.

Going beyond the ground-state energies by analyzing the spectral properties of Hubbard nano-clusters with the single-particle spectral function, the correctness of the approximations in the full two-time plane has been tested. Here, the best results could be achieved with the FLEX approximation which yields very good results for all filling factors. Additionally, the TOA shows single-particle energy transitions which are not contained in any other approximation. Thus, by taking into account the full set of approximation methods, most of the relevant energy levels of the systems differing by one particle from the analyzed system can be determined.

Finally, the performance of the different selfenergies in a time-dependent setup, where a Hubbard cluster is existed by a strong inhomogeneous potential quench, has been measured. Here, the problem of correlation induced damping had been found occurring in selfconsistent calculations depending on the filling factor and interaction as well as excitation strenght by *Friesen et al.* [51]. For a one quarter-filled setup, in this thesis, all the results of Friesen et al. could be confirmed and additionally it could be shown that the electron-hole T -matrix—like the SOA and GW —experiences strong damping, while the FLEX approximation as well as the combination of both flavors of the T -matrix show only some amount of damping. In contrast, for this small filling factor, the particle-particle T -matrix and HF yield completely undamped results, while the T -matrix gives the best overall agreement with the exact solution. For half-filling, though, all tested approximation quickly show a strong damping and, therefore, are unusable already after only a few oscillation periods. Here, the application of the GKBA can accomplish a dramatic improvement, which has been shown in this thesis. Together with the simple second-order approximation, it already gives a good qualitative agreement, which can be further improved by the

use of the particle–particle T -matrix with the GKBA. This combination allows the computation of density responses to strong and sudden excitations, which are in excellent agreement with the exact results and show no correlation-induced damping. In conclusion, with the presented selfenergy approximation strategies and the GKBA, the NEGF approach is very well suited not only for the application to the Hubbard model or similar lattice models, but also for application to spatially delocalized systems like nuclear collision physics or electronic structure calculations, where the correct description of correlations is crucial and exact methods fail due to the large number of particles.

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Diploma thesis

- [111] S. Hermanns, “Nonequilibrium Green’s function approach to Hubbard nano-clusters using the generalized Kadanoff–Baym ansatz,” diploma thesis (Christian-Albrechts-Universität zu Kiel, Aug. 2012).

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Scientific career



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Selbstständigkeitserklärung

Hiermit versichere ich, dass diese Dissertationsschrift, abgesehen von der Beratung durch den Betreuer, Herrn Prof. Dr. Michael Bonitz, nach Inhalt und Form meine eigene Arbeit ist.

Weiterhin erkläre ich, dass die vorliegende Arbeit weder ganz noch zum Teil bereits einer anderen Stelle im Rahmen eines Prüfungsverfahrens vorgelegen hat, sowie in dieser Form weder veröffentlicht noch zur Veröffentlichung eingereicht worden ist.

Die im Rahmen meiner Arbeit entstandenen wissenschaftlichen Publikation in Fachzeitschriften sind auf Seite 199 aufgeführt.

Des weiteren versichere ich, dass die Arbeit unter Einhaltung der Regeln guter wissenschaftlicher Praxis der Deutschen Forschungsgemeinschaft¹ verfasst wurde.

Norderstedt, den

¹Deutsche Forschungsgemeinschaft, *Vorschläge zur Sicherung guter wissenschaftlicher Praxis. Empfehlungen der Kommission Selbstkontrolle in der Wissenschaft*, WILEY-VCH Verlag GmbH, Weinheim (1998)