

Theory of extended two-particle Green's functions

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A general theory of extended two-particle Green's functions constructed from orthonormal extended states is presented. Three types of fermionic propagators are considered that allow the description of a wide range of two-particle processes in non-relativistic many-body systems: the extended particle-hole, particle-particle, and hole-hole Green's functions. Each member of the considered class of two-particle propagators fulfils a Dyson equation and defines a well-behaved two-particle self energy in analogy to the single-particle Green's function of traditional many-body theory. Besides presenting a general formalism for the unified treatment of the different extended two-particle Green's functions we discuss several formal properties on the example of the extended particle-hole Green's function. Particular emphasis is also given to the significance of the static part of the two-particle self energies because it carries the leading terms in perturbation theoretic approximations. A physical interpretation of the static part of the particle-particle self energy, which serves as an exact optical potential for two-particle scattering, is given for the example of Coulomb-interacting fermions. In analogy the particle-hole self energy can be understood as a scattering potential for particle-hole projectiles.

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I. INTRODUCTION

Effective or *optical potentials* have proven to be a powerful tool for investigating excitations of single-particle nature in many-body systems. These include ionisation (or knockout reactions), attachment, and single-particle scattering. Besides the phenomenological approaches there have been numerous theoretical derivations of physically equivalent, yet mathematically distinct single-particle potentials. The basic, unifying idea behind all optical potentials is that in a many-body system with a great number of degrees of freedom the motion of a single (or very few) particles can be described by a single- (or few-) particle Schrödinger equation while an effective or optical potential takes account of influences by the motion of the remaining particles. Especially the potential derived by Feshbach projection [1-3], on the one hand, in contrast to the self energy or mass operator of the single-particle Green's function [4-6], on the other hand, have seen wide applications in the fields of nuclear, atomic, and molecular physics. There have also been comparative investigations of the properties of these and other possible approaches from the practical [7] and the more formal point of view [8,9], respectively. The advantages of the Green's functions approach over the other competitors in the field are manifold. We want to mention especially the fact, that the single-particle Green's function can be seen as the resolvent of an effective Hamiltonian in the complete single-particle Hilbert space, regardless whether the many-body system is fully correlated or not. This is important since it allows a perturbation theoretical expansion of the effective Hamiltonian which is constituted by the single-particle kinetic energy and the self energy. Effective Hamiltonians of the Feshbach type, however, may only be defined restricted to subspaces of the single-particle Hilbert space in the case of non or only partially interacting systems and are thus not directly amenable to a perturbation theoretical treatment [8].

Looking at two-particle type excitations, some features of the theory of single-particle processes remain the same whereas others change. By two-particle type excitations we mean double-attachment and scattering by compound projectiles, on the one hand, but also particle-number conserving (neutral) excitations of the particle-hole type like excitons and collective vibrations of nuclei, on the other hand. Also two-particle removal processes can be treated by a similar formalism. One of the difficulties that arise in the theoretical description is that the fundamental two-particle Green's functions do not fulfil Dyson's equation but instead are governed by the much more complicated Bethe-Salpeter equation. Thus there is no direct access to an optical potential in the usual sense and using the Bethe-Salpeter kernel instead gives rise to many problems since it depends on three independent time or energy variables.

Recently, however, we succeeded in defining an extended particle-particle Green's function that fulfils a Dyson equation [10]. We could also show that the extended propagator possesses a well-behaved self energy that serves as an optical potential for scattering with two-particle projectiles. In the present work we will present a more general ansatz that leads to a manifold of effective two-particle Hamiltonians and corresponding Green's functions. The formal ansatz we use will also show clearly the underlying concepts that lead to a well-behaved Dyson equation. We will develop a theoretical framework that allows to treat three different types of extended Green's functions on the same footing, which will allow for the description of two-particle, two-hole, and particle-hole type excitations. It is interesting to note, that the suggested extended particle-hole Green's functions contain the (standard) polarisation propagator [11] and thus it is possible to derive the well-known random-phase approximation (RPA) as a special approximation to the particle-hole self energy. In general, however, approximations to the extended Green's functions lead to non-standard schemes. The same is also true for the extended two-particle and two-hole Green's functions, which contain the common particle-particle propagator [11].

We also want to mention that a Dyson-equation approach for propagators like the polarisation and the particle-particle propagator has been formulated and used to derive a self-consistent extension of the RPA, also called cluster-Hartree-Fock approximation, that has been applied in the fields of plasma and nuclear physics [12–14]. This formalism, however, has similar problems like Feshbach's theory and does not yield a universal, well-behaved optical potential because the two-particle space has to be restricted in order to make the approach well-defined [14].

The main goal of this paper is the construction of two-particle propagators that fulfil a Dyson equation in the unrestricted two-particle space. The reasons for being interested in a Dyson equation are manifold:

- First of all the Dyson equation defines an optical potential and the concept of an optical potential as a physical entity is an intuitively appealing concept. We already mentioned the advantages of Green's function optical potentials over Feshbach-type optical potentials. One major technical advantage of using optical potentials in numerical calculations is that the scattering problem can be separated from the many-body problem and the latter can be treated using bound-state techniques. However, also in purely bound state applications like the calculation of ionisation or excitation energies, the concept of an optical potential remains advantageous. When the self energy is approximated within a given scheme and then the Dyson equation utilised to construct the propagator, the "scattering problem" is solved exactly and the only approximation has been made

in the potential. Speaking in terms of perturbation theory, this idea manifests itself in the fact that Dyson's equation produces diagrams of infinite order for the propagator even if the self energy is only approximated to finite order. When instead also the "scattering problem" is solved only to a given order, an additional error is introduced. And it is a well-known fact in atomic and molecular physics that Møller-Plesset perturbation theory [15] performs very badly on excited states although it is the most direct (even size-consistent) way to approximate excitation energies in a perturbation theoretic framework. It has even been shown that the Møller-Plesset perturbation series may diverge in numerical calculations on single-determinant dominated atomic and molecular systems if extended basis sets are used [16].

- Also the case of one-particle Hamiltonians deserves particular attention. When the Hamiltonian of the system is a one-particle operator, i. e. no two-body forces are present but only external or mean fields, the self energy of the single-particle Green's function becomes an energy independent, first order quantity [11,10] (We will show that the same is true for the extended two-particle Green's function we are going to construct). Thus the first order approximation to the self energy is already the exact solution. Approximating instead the propagator directly, i. e. without using Dyson's equation, the perturbation expansion extends to infinite order (unless, of course, a diagonalising single-particle basis is chosen).
- Another point that we derive from experience in numerical calculations is that the static diagrams in the Feynman-Dyson series for the single-particle Green's function [11] generally do not give a well-converging perturbation series. They have to be renormalised. A much better approximation for the static self energy results by calculating it from the dynamic part of the self energy as described, e. g., in Ref. [17]. When approximating the particle propagator directly, this way of renormalising the static diagrams is not accessible. Using well-adapted algorithms [18], also the numerical evaluation of the self energy is not slower than the direct approximation of the propagator, since the same number of matrix elements has to be calculated. None the less, successful approximation schemes for bound state properties to the one-particle Green's function that avoid Dyson's equation have been reported in the literature (see, e. g. [19,20] and references cited therein).
- In a recent publication [21], we have shown that already the simplest approximation to the self energy of the extended particle-hole propagator yields a well-behaved, hermitian approximation scheme that removes

drawbacks of the RPA, which derives from the traditional polarisation propagator. A perturbation theoretical analysis as well as a simple model case could show that higher order corrections to the excitation energies deriving from ground state correlation are consistently taken into account in the first order self energy in contrast to non-Dyson approximations like the Tamm-Dancoff approximation (TDA) [11] or the RPA.

This paper is organised as follows: A rigorous and formal introduction into the basic formalism used throughout this paper is given in Chapter II. The reader who is not so much interested in the formal aspects of the theory may skip this Chapter in first reading. In the rest of the paper many of the concepts are explained in a less rigorous fashion and references to the formal definitions are given. In Chapter III we define the three different types of extended two-particle Green's functions. We derive Dyson's equation and define the self energies for these propagators in an analogous way to Ref. [10], but in a generalised formalism. Chapter IV is devoted to the formal properties of the extended propagators, focusing on the example of the extended particle-hole Green's function. We will mainly be concerned with the consequences of the introduction of "unphysical" components in the extended Green's functions necessary to fulfil Dyson's equation (Sec. IV A–IV B). In Sec. IV C the general analytic structure of the extended particle-hole Green's function for complex arguments is discussed before defining the extended Green's functions for real arguments in Sec. IV D. Properties of the self energy are discussed in Chapter V. We show two simple approximations for the particle-hole self energy that lead to approximation schemes for excitation energies and transition moments of finite Fermi systems. In Chapter VI we adopt a different point of view by viewing the static self energy as a scattering potential in a system of fermions interacting by Coulomb force. For the sake of comparison, we briefly review the Green's function's and Feshbach's optical potentials for single-particle scattering in Sec. VI A before looking at the explicit expressions for the static two-particle and particle-hole self energy (Sec. VI B and VI C). Appendix A gives a definition of an abstract Hilbert space introduced in Chapter II and the two Appendices B and C contain formulas for the static self energy discussed in Chapter VI.

II. BASIC FORMALISM

Many of the algebraic properties of the single-particle Green's function, in particular Dyson's equation, are transferable to two-particle propagators if they are constructed starting from an orthonormal set of "primary" states. In this paper we will construct propagators $\mathcal{G}(\omega)$ with the help of the "extended

states" $|A, B\rangle$ defined in this Section. The peculiar property of these states is that they are "orthonormal" if A and B are chosen canonical particle creation or destruction operators. The extended Green's functions can then be defined in the following way:

$$\mathcal{G}(\omega) = (A, B | \frac{1}{\omega - \tilde{H}} | A', B').$$

The round brackets indicate the so-called μ -product which is a generalisation of the usual Hilbert space inner product with an indefinite metric. The "extended operator" \tilde{H} takes the role of an excitation energy operator which lives, like the extended states $|A, B\rangle$, in an "extended Hilbert space" \mathcal{Y} . These objects will be defined rigorously in this chapter in a very formal manner. In first reading these formal definitions may well be skipped.

The abstract formalism introduced in this chapter builds the fundament of the theory of extended two-particle Green's functions. Our approach is very general in order to allow for a unified treatment of the different species of extended Green's functions discussed in the main part of this paper. Since the discussed propagators can be applied to a wide variety of physical situations, the emphasis of this chapter lies on the unifying mathematical structure. The formalism is developed simultaneously for (projectile) particles of fermionic and bosonic character. We will define the general extended states which serve to define the primary or "model" space of the extended Green's functions. We also define the μ -product under which the previously defined extended states fulfil peculiar orthonormality conditions. Finally we introduce a canonical extension of common Fock-space operators and super-operators to the space of the extended states.

A. Extended States

Definition Let $|\psi\rangle$ and $|\varphi\rangle$ be normalised many-particle states, i. e. elements of the physical Fock space with $\langle\psi|\psi\rangle = \langle\varphi|\varphi\rangle = 1$, and let $Q = 1 - |\psi\rangle\langle\psi|$ denote the orthogonal projector onto the complement of $\{|\psi\rangle\}$. For linear Fock-space operators A and B we define the **extended state** $|A, B\rangle$ by the vector

$$|A, B\rangle = \begin{pmatrix} QAB|\psi\rangle \\ \langle\psi|ABQ \\ \langle\varphi|A \otimes \langle\psi|B \mp \langle\varphi|B \otimes \langle\psi|A \\ A|\varphi\rangle \otimes \langle\psi|B \mp B|\varphi\rangle \otimes \langle\psi|A \end{pmatrix}, \quad (1)$$

where the upper sign is appropriate for operators A and B with fermionic character and the lower sign for operators of bosonic character.

Properties

- The extended state $|A, B\rangle$ is linear in A and B .
- If the operators A and B anti-commute (commute) the extended state $|A, B\rangle$ is anti-symmetric (symmetric) under permutation of A and B :

$$|A, B\rangle = \mp |B, A\rangle \quad \text{if} \quad [A, B]_{\pm} = 0. \quad (2)$$

The square bracket $[\cdot, \cdot]_{\pm}$ denotes the usual anti-commutator (commutator). Again, the upper (lower) sign applies in the fermionic (bosonic) case.

- An inner product for extended states can be constructed by the following rules which are the canonic rules for direct sums and tensor product states [22] (c. f. Ref. [10]). For a direct sum the inner products of the components add:

$$\left\langle \left(\begin{array}{c} |A\rangle \\ \langle B| \end{array} \right), \left(\begin{array}{c} |C\rangle \\ \langle D| \end{array} \right) \right\rangle = \langle A|C\rangle + \langle D|B\rangle. \quad (3)$$

Here, the second component was chosen a “bra” state. This is understood as the particular element of the dual space to the corresponding space for “kets” according to the Riesz theorem [22].

For tensor product states the inner products of the components multiply:

$$(|A\rangle \otimes |B\rangle, |C\rangle \otimes |D\rangle) = \langle A|C\rangle \langle B|D\rangle. \quad (4)$$

Examples involving the extended states (1) will be given later [Eq. (10)].

- The extended states $|A, B\rangle$ are elements of a Hilbert space denoted by \mathcal{Y} that is constructed by direct sums and tensor products from the component spaces and possesses the inner product introduced above. Strictly speaking, the extended states $|A, B\rangle$ can be elements of a Hilbert space only if all components have finite norm, like usual in quantum mechanics. In the following example we define the Hilbert space \mathcal{Y} relevant for the extended particle-hole Green’s function. For the other propagators, the appropriate space \mathcal{Y} can be constructed in a completely analogous manner. A convenient formal definition of \mathcal{Y} for the general case is given in App. A. It is important to realise that the space \mathcal{Y} is in general *not* isomorphic to any subspace of the fermion or boson Fock-space. This is because the tensor products in the third and fourth component in (1) do not fulfil the symmetry requirements of the Pauli principle.

Example Choosing both reference states $|\psi\rangle$ and $|\varphi\rangle$ equal to the N particle ground state $|\Psi_0^N\rangle$ of a fermionic system, the definition of the so-called extended particle-hole states becomes

$$|a_r^\dagger, a_s\rangle = \begin{pmatrix} Qa_r^\dagger a_s |\Psi_0^N\rangle \\ \langle \Psi_0^N | a_r^\dagger a_s Q \\ \langle \Psi_0^N | a_r^\dagger \otimes \langle \Psi_0^N | a_s - \langle \Psi_0^N | a_s \otimes \langle \Psi_0^N | a_r^\dagger \\ a_r^\dagger |\Psi_0^N\rangle \otimes \langle \Psi_0^N | a_s - a_s |\Psi_0^N\rangle \otimes \langle \Psi_0^N | a_r^\dagger \end{pmatrix}. \quad (5)$$

These are elements of a Hilbert space \mathcal{Y} which is the direct sum of four subspaces related to the four entries of the above defined column vector. The first component $Qa_r^\dagger a_s |\Psi_0^N\rangle$ is element of the physical N fermion Hilbert space \mathcal{H}^N (excluding the ground state due to Q) and can be understood as an approximate particle-hole type excitation. The second entry $\langle \Psi_0^N | a_r^\dagger a_s Q$ is a “bra” state and thus an element of the dual space \mathcal{H}^{N*} of the N particle space. This second entry can also be seen as an approximate excited state but the “hole” and “particle” role of the indices r and s has interchanged. Each of the remaining two entries is the direct sum of tensor product states of “bras” or “kets” in the $N-1$ and $N+1$ particle Hilbert spaces, e. g. $\langle \Psi_0^N | a_r^\dagger \otimes \langle \Psi_0^N | a_s \in \mathcal{H}^{(N-1)*} \otimes \mathcal{H}^{(N+1)*}$. For the present example, the full composite space \mathcal{Y} is consequently described by

$$\begin{aligned} \mathcal{Y} = \mathcal{H}^N \oplus \mathcal{H}^{N*} \oplus \mathcal{H}^{(N-1)*} \otimes \mathcal{H}^{(N+1)*} \oplus \mathcal{H}^{(N+1)*} \otimes \mathcal{H}^{(N-1)*} \\ \oplus \mathcal{H}^{(N+1)} \otimes \mathcal{H}^{(N+1)*} \oplus \mathcal{H}^{(N-1)} \otimes \mathcal{H}^{(N-1)*}. \end{aligned} \quad (6)$$

The construction of a basis of this space by sums and products of Slater determinantal basis sets of the component spaces is trivial. Obviously the dimension of the composite Hilbert space \mathcal{Y} is considerably enlarged in comparison with the physical N particle space \mathcal{H}^N , which contains all particle-number conserving excitations. The expression (6), however, only allows a rather rough estimate of the actual dimension of the relevant space for which it gives an upper bound. The minimal space needed is certainly smaller because symmetries may reduce the relevant spaces drastically. E. g. the fact that both reference states were chosen equal in Eq. (5) allows to replace the third component of the extended states by $\sqrt{2}\langle \Psi_0^N | a_r^\dagger \otimes \langle \Psi_0^N | a_s$, which spares the component $\mathcal{H}^{(N+1)*} \otimes \mathcal{H}^{(N-1)*}$ from the direct sum constituting the space \mathcal{Y} in Eq. (6). Also symmetries of the physical system may lead to a reduced dimensionality. For an exact but non-constructive definition of the minimal space needed, we again refer the reader to App. A.

A possible way to construct a basis for the Hilbert space \mathcal{Y} may also be the definition of operator sets \mathcal{A} and \mathcal{B} , such that the set of states $\{|A, B\rangle \mid A \in \mathcal{A}, B \in \mathcal{B}\}$ span the Hilbert space \mathcal{Y} . In the context of traditional one- and two-particle propagators of many-body theory, such complete operator manifolds have been found [23] and used for deriving approximation schemes (see e. g. [24] and references cited therein). In the present context, however, such a construction seems difficult because of the complicated nature of the extended states $|A, B\rangle$. It is certainly an interesting open question whether a convenient construction can be found.

- *Linear operators on the space \mathcal{Y}* are, in general, 4×4 matrices of operators. In this paper, however, we will restrict ourselves to diagonal matrix operators that do not mix the different components of the space \mathcal{Y} . Such a diagonal matrix operator O is determined by specifying the operators O_i that act in the different component spaces of \mathcal{Y} . We denote

$$O = \text{diag}(O_1, O_2, O_3, O_4). \quad (7)$$

In a dual space the operator acts “from the right”. E. g. for the second component we have

$$[O|A, B\rangle]_2 = \langle\psi|ABQO_2. \quad (8)$$

Note that there is no canonic way to define the application of a general Fock-space operator to an element of the space \mathcal{Y} . We will see later how to construct so-called extended operators that operate in the space \mathcal{Y} from Fock-space operators.

B. The μ -product

The *inner product* (scalar product) $\langle \cdot, \cdot \rangle$ in the Hilbert space \mathcal{Y} follows from the canonical rules for inner products of direct sums and tensor products of Hilbert spaces like mentioned above. We use common Dirac notation for matrix elements $\langle Y|O|Z\rangle$ of an operator O and vectors $|Y\rangle$ and $|Z\rangle$ in the Hilbert space \mathcal{Y} .

Definition The μ -product between two states $|Y\rangle, |Z\rangle \in \mathcal{Y}$ is given by the matrix element $\langle Y|\mu|Z\rangle$ where $\mu = \text{diag}(1, -1, 1, \pm 1)$ is called the metric operator. Again, here and in the following, the upper sign refers to the fermionic case and the lower to the bosonic case. For extended states of the form (1) we introduce the following shorthand notation for the μ -product:

$$(A, B | C, D) = \langle |A, B\rangle, \mu | C, D \rangle. \quad (9)$$

Properties

- Note that the metric operator μ commutes with all diagonal operators in the space \mathcal{Y} .
- The “metric” induced by the μ -product is indefinite which means that $\langle Y | \mu | Y \rangle$ need not be positive but can also be negative or zero even if $|Y\rangle$ is not the null-vector.
- The μ -product of the extended states $|A, B\rangle$ and $|C, D\rangle$ evaluates (by the canonic rules discussed above) to

$$\begin{aligned} (A, B | C, D) = & \langle \psi | [B^\dagger A^\dagger, CD]_- | \psi \rangle \\ & + \langle \varphi | [C, A^\dagger]_\pm | \varphi \rangle \langle \psi | DB^\dagger | \psi \rangle + \langle \varphi | [D, B^\dagger]_\pm | \varphi \rangle \langle \psi | CA^\dagger | \psi \rangle \\ & + \langle \varphi | [C, B^\dagger]_\pm | \varphi \rangle \langle \psi | DA^\dagger | \psi \rangle + \langle \varphi | [D, A^\dagger]_\pm | \varphi \rangle \langle \psi | CB^\dagger | \psi \rangle. \end{aligned} \quad (10)$$

This expression simplifies further in the case when the anti-commutators (commutators) of any pair of the operators A^\dagger , B^\dagger , C , and D simply are complex numbers:

$$(A, B | C, D) = [A^\dagger, C]_\pm [B^\dagger, D]_\pm \mp [A^\dagger, D]_\pm [B^\dagger, C]_\pm. \quad (11)$$

Note that this result is independent of the states $|\psi\rangle$ and $|\varphi\rangle$.

Example Let a_r^\dagger (a_r) denote the creation (destruction) operator for a single fermion and let the canonical anti-commutation relations be fulfilled ($[a_r^\dagger, a_s]_+ = \delta_{rs}$, etc.). We then find that the extended states $|a_r^\dagger, a_s\rangle$ are “normalised” and “orthogonal” with respect to the μ -product:

$$(a_r^\dagger, a_s | a_{r'}^\dagger, a_{s'}) = \delta_{rr'} \delta_{ss'}. \quad (12)$$

Definition A set of states $\{|Y_I\rangle\}_I \subset \mathcal{Y}$ is called μ -orthonormal if

$$\langle Y_I | \mu | Y_J \rangle = \pm \delta_{IJ}, \quad (13)$$

where the sign is left indeterminate (in the fermionic as well as in the bosonic case).

Notes

- A μ -orthonormal set of states is necessarily linear independent.

- A countable set of linearly independent states $\{|\tilde{Y}_I\rangle\}_I$ with μ -norm other than zero can in general be μ -orthonormalised following the Gram-Schmidt construction procedure.
- Throughout the paper we are using both the μ -product notation indicated by round brackets and common Dirac notation of the inner product indicated by angular brackets like usual. While the μ -product notation in particular allows for an elegant handling of super-operator expansions, the foremost advantage of the Dirac notation is to stress the Hilbert space nature of the formalism which allows for an intuitive understanding of basis set expansions and matrix representations.

C. Super-operators

The specification “super-operator” is common in quantum chemical and physical literature for linear mappings of Fock-space operators. It is very helpful to transfer this concept to the extended states $|A, B\rangle$ and define the application of super-operators by the action on the operators A and B . We will see later how this definition helps for a compact notation of iterated equations of motion and perturbation expansions. In certain cases, however, the action of a super-operator is fully equivalent to the action of an operator in the Hilbert space \mathcal{Y} . The alternative concept of \mathcal{Y} -space operators allows to introduce approximations by finite basis set representations of operators in a well-defined and lucid way.

We will only use super-operators constructed in the following way:

Definition Given a Fock-space operator U , we define \hat{U} by the linear mapping of an operator A onto the commutator of U with A :

$$\hat{U}(A) = [U, A]_- . \quad (14)$$

We call \hat{U} the **super-operator associated with the operator U** . The application of the super-operator \hat{U} to the extended state $|A, B\rangle$ (for arbitrary operators A and B) is defined as follows:

$$\begin{aligned} \hat{U}|A, B\rangle &= |\hat{U}(A), B\rangle + |A, \hat{U}(B)\rangle \\ &= |[U, A]_-, B\rangle + |A, [U, B]_-\rangle . \end{aligned} \quad (15)$$

Example Let $a_r^{(\dagger)}$ be a fermionic operator as above and let $v = \sum_{ij} v_{ij} a_i^\dagger a_j$ be a one-particle operator. Then

$$(a_r^\dagger, a_s | \hat{v} | a_{r'}^\dagger, a_{s'}) = v_{rr'} \delta_{ss'} - v_{s's} \delta_{rr'} \quad (16)$$

describes a matrix element that is determined only by the operator v and the single-particle basis while it is independent of the states $|\psi\rangle$ and $|\varphi\rangle$.

Properties If the states $|\psi\rangle$ and $|\varphi\rangle$ are eigenstates of the self-adjoint operator U with respective eigenvalues u_ψ and u_φ then applying the super-operator \hat{U} is equivalent to applying the diagonal operator

$$\check{U} = \text{diag}(U - u_\psi, u_\psi - U, u_\varphi - U \otimes 1 + u_\psi - 1 \otimes U, U \otimes 1 - u_\varphi + u_\psi - 1 \otimes U). \quad (17)$$

We illustrate the statement $\hat{U}|A, B\rangle = \check{U}|A, B\rangle$ by looking at the second component where

$$\begin{aligned} [\check{U}|A, B]_2 &= \langle\psi|ABQ(u_\psi - U) = \langle\psi|UABQ - \langle\psi|ABQU \\ &= \langle\psi|[U, AB]Q = [\hat{U}|A, B]_2 \end{aligned} \quad (18)$$

holds because Q commutes with U .

Definition We call \check{U} the **extended operator associated with the self-adjoint (Fock-space) operator U** .

Notes

- The symbols $\hat{}$ and $\check{}$ are understood as operations that map a Fock-space operator onto the corresponding super-operator and Y-space operator, respectively.
- A Y-space operator corresponding to the super-operator \hat{U} generally exists only if $|\psi\rangle$ and $|\varphi\rangle$ are eigenstates of the operator U and not for operators without this property.
- The operations $\hat{}$ and $\check{}$ are linear in the sense that if the operator U is a linear combination of Fock-space operators V and W

$$U = aV + bW \quad (19)$$

with complex numbers a and b then

$$\hat{U} = a\hat{V} + b\hat{W} \quad (20)$$

holds for the associated super-operators. If further $|\psi\rangle$ and $|\varphi\rangle$ are eigenstates of V and W then also

$$\check{U} = a\check{V} + b\check{W} \quad (21)$$

holds for the associated extended operators.

- It is easily seen that the extended operator \check{U} associated with a self-adjoint operator U is also self-adjoint:

$$\langle |A, B\rangle, \mu \check{U} |C, D\rangle \rangle = \langle \check{U} |A, B\rangle, \mu |C, D\rangle \rangle. \quad (22)$$

The same “holds” for the super-operator associated with a self-adjoint operator.

III. EFFECTIVE TWO-PARTICLE DESCRIPTION WITH ORTHONORMAL STATES

In the preceding section a self-contained introduction to the abstract formalism related to the extended states and the μ -product with rigorous definitions has been given but many properties will also be explained in the text. In this chapter we will show how a Dyson equation can be derived and a self energy defined upon the extended two-particle Green’s functions. This derivation has already been shown in Ref. [10] for the example of the extended particle-particle Green’s function. It is repeated here for the sake of self-containedness and also because the present formalism is more general including different types of fermionic two-particle Green’s functions as well as bosonic two-particle Green’s functions. Reviewing the derivation of Dyson’s equation in the abstract formalism also shows clearly the underlying concepts.

A. Extended two-particle Green’s functions

The particular choice of the operators A and B used for constructing the extended states $|A, B\rangle$ define the nature of the propagator while the choice of the Hamiltonian and the reference state $|\psi\rangle$ contained in the definition (1), define the physical system under investigation. In the following we will discuss three cases of Green’s functions which are very similar from the formal point of view but allow for the description of different physical situations.

- (a) The **extended particle-hole Green’s function** is defined by

$$\mathcal{G}_{rs,r's'}^{(ph)}(\omega) = (a_r^\dagger, a_s | \frac{1}{\omega - \check{H}} | a_{r'}^\dagger, a_{s'}), \quad (23)$$

and contains information related to particle-number conserving excitations and linear response properties. It is constructed with the states $|Y_{rs}^{(ph)}\rangle = |a_r^\dagger, a_s\rangle$ which we call **extended particle-hole states**.

(b) The **extended particle-particle Green's function** is defined by

$$\mathcal{G}_{rs,r's'}^{(pp)}(\omega) = (a_r^\dagger, a_s^\dagger | \frac{1}{\omega - \tilde{H}} | a_{r'}^\dagger, a_{s'}^\dagger), \quad (24)$$

and may be used for describing two-particle attachment or scattering processes. It is constructed using the **extended particle-particle states** $|Y_{rs}^{(pp)}\rangle = |a_r^\dagger, a_s^\dagger\rangle$.

(c) The **extended hole-hole Green's function** is defined by

$$\mathcal{G}_{rs,r's'}^{(hh)}(\omega) = (a_r, a_s | \frac{1}{\omega - \tilde{H}} | a_{r'}, a_{s'}), \quad (25)$$

and allows the description of two-particle removal processes like atomic or molecular Auger decay. The corresponding **extended hole-hole states** are $|Y_{rs}^{(hh)}\rangle = |a_r, a_s\rangle$.

Here, the operators a_r^\dagger and a_r denote canonical fermionic single-particle creation and destruction operators, respectively. We are not going to discuss bosonic two-particle Green's functions here further but most of the discussion in this chapter applies to bosons as well.

A preliminary justification for the classification given for the Green's functions and extended states is provided by the fact that the first or **physical component** of the defining vector of the extended state $|A, B\rangle$ is related to the state $AB|\psi\rangle$ [see definition (1)]. In this paper we will choose the reference state $|\psi\rangle$ to describe the exact ground state $|\Psi_0^N\rangle$ of an interacting N -fermion system. The physical component of the extended states $|Y_{rs}^{(ph)}\rangle$, $|Y_{rs}^{(pp)}\rangle$, and $|Y_{rs}^{(hh)}\rangle$ therefore describes states with N , $N+2$, and $N-2$ particles, respectively. The remaining components of the extended state $|A, B\rangle$ relate to different physical situations and we will classify them as **unphysical components**. They should be regarded as useful additives for achieving the particular algebraic properties presented in the following. Their nature and their importance upon approximate solutions will be discussed in later chapters.

The set of states $\{|Y_{rs}\rangle\}$, where the indices r and s are both taken from the full set of single-particle indices, will be called **primary set of states** which spans the so-called **model space**. For each of the three choices this set of states is μ -orthonormal (in the sense of Sec. II B) since the following orthonormality relations hold:

$$(a_r^\dagger, a_s | a_{r'}^\dagger, a_{s'}) = \delta_{rr'} \delta_{ss'}, \quad (26)$$

$$(a_r^\dagger, a_s^\dagger | a_{r'}^\dagger, a_{s'}^\dagger) = (a_r, a_s | a_{r'}, a_{s'}) = \delta_{rr'} \delta_{ss'} - \delta_{rs'} \delta_{sr'}. \quad (27)$$

These relations follow directly from the formal property (11) of the extended states $|A, B\rangle$.

Note that these equations can also be written without resuming to the μ -product notation indicated by the round brackets. Instead one can use common Dirac notation of the inner product in the Hilbert space \mathcal{Y} which is indicated by the use of angular brackets like usual. In this case the metric operator μ (defined in Sec. IIB) appears explicitly and, e.g., Eq. (26) becomes

$$\langle Y_{rs}^{(ph)} | \mu | Y_{r's'}^{(ph)} \rangle = \delta_{rr'} \delta_{ss'}. \quad (28)$$

In the following we will use both notations because each has its own advantages.

In the orthonormality relations (26) and (27), a difference occurs between the particle-hole case (a), on the one hand, and the cases of two-particle attachment (b) or removal (c), on the other hand. In the latter case Eq. (27) shows antisymmetry upon interchanging the single-particle indices r and s or r' and s' . The antisymmetry with respect to the interchange of single-particle labels applies to the extended states $|Y_{rs}^{(pp)}\rangle$ and $|Y_{rs}^{(hh)}\rangle$ as well (as shown in Sec. IIA). As a consequence, the primary set of states $\{|Y_{rs}\rangle\}$ for the choices (b) and (c) spans a model space which is isomorphous to the antisymmetrised Hilbert space of two indistinguishable fermions. In the particle-hole case (a), however, the symmetry is broken and the primary set $\{|Y_{rs}^{(ph)}\rangle\}$ now spans a model space which is isomorphous to the physical space of two distinguishable particles.

The primary states $|Y_{rs}\rangle$ as defined above are elements of an extended Hilbert space \mathcal{Y} . This point has been discussed in Sec. II where special attention is given to the choice (a) as an example. Within the space \mathcal{Y} , the role of a generalised **excitation energy operator** is taken by the extended operator \check{H} associated with the common Fock-space Hamiltonian H of the system as defined in Sec. IIC. Indeed, Eq. (17) shows that the operator \check{H} acts on the physical component of the states $|Y_{rs}\rangle$ as $H - E_0^N$, where E_0^N is the energy eigenvalue of the N -particle ground state $|\Psi_0^N\rangle$ of the system. Therefore \check{H} can be said to measure the energy of the system relative to the N -particle ground state energy.

The extended two-particle propagators can now be understood as projections of the resolvent of the excitation energy operator \check{H} onto the primary states $|Y_{rs}\rangle$. Without specifying the particular choice [(a), (b), or (c)] we may define the general **extended two-particle Green's function** $\underline{\underline{\mathcal{G}}}(\omega)$ as a function of the frequency variable ω and a matrix with two-particle indices (rs) by the matrix elements

$$\mathcal{G}_{rs,r's'}(\omega) = \langle Y_{rs} | \frac{\mu}{\omega - \check{H}} | Y_{r's'} \rangle. \quad (29)$$

This definition has before been written in the equivalent notation involving the μ -product for each case separately.

B. Dyson equation and self energy

We will now derive a Dyson equation by expressing the inverse matrix of the extended two-particle Green's function $\mathcal{G}_{rs,r's'}(\omega)$ by a matrix representation of the extended operator \check{H} . We already mentioned that the primary set of states $\{|Y_{rs}\rangle\}$ spans a subspace (the model space) of the Hilbert space \mathcal{Y} . Since the states $\{|Y_{rs}\rangle\}$ are μ -orthonormal they are also linearly independent and thus form a basis of this subspace. Here and in the following the set of pairs of single-particle indices (r, s) has to be restricted to $r > s$ for the pp and hh cases (b) and (c) where the states $|Y_{rs}\rangle$ are antisymmetric under permutation of r and s . No restriction applies in the ph case (a). The primary set of states $\{|Y_{rs}\rangle\}$ can now be extended to a complete basis $\{|Q_J\rangle\} \supset \{|Y_{rs}\rangle\}$ of the Hilbert space \mathcal{Y} . We may further demand that the states $|Q_J\rangle$ are μ -orthonormal:

$$\langle Q_I | \mu | Q_J \rangle = \pm \delta_{IJ}. \quad (30)$$

As a consequence of the indefinite nature of the metric μ , basis states with negative norm appear. We now define the diagonal overlap matrix $\underline{\underline{\mu}}$ by

$$[\underline{\underline{\mu}}]_{IJ} := \langle Q_I | \mu | Q_J \rangle, \quad (31)$$

and the basis set representation $\underline{\underline{H}}$ of the extended operator \check{H} with the matrix elements

$$[\underline{\underline{H}}]_{IJ} := \langle Q_I | \mu \check{H} | Q_J \rangle. \quad (32)$$

A block structure is imposed onto $\underline{\underline{H}}$ by the division of the basis $\{|Q_J\rangle\}$ into the primary set of states $\{|Y_{rs}\rangle\}$ and the rest:

$$\underline{\underline{H}} = \begin{pmatrix} \underline{\underline{H}}_{aa} & \underline{\underline{H}}_{ab} \\ \underline{\underline{H}}_{ba} & \underline{\underline{H}}_{bb} \end{pmatrix}. \quad (33)$$

The primary block $\underline{\underline{H}}_{aa}$, in particular, is just the part of the matrix representation of the operator \check{H} that corresponds to the states $\{|Y_{rs}\rangle\}$:

$$[\underline{\underline{H}}_{aa}]_{rs,r's'} = \langle Y_{rs} | \mu \check{H} | Y_{r's'} \rangle. \quad (34)$$

Now the extended Green's function $\underline{\underline{\mathcal{G}}}(\omega)$ can be expressed as the "upper left corner" of an inverse matrix:

$$\underline{\underline{\mathcal{G}}}(\omega) = \left[\frac{1}{\omega \underline{\underline{\mu}} - \underline{\underline{H}}} \right]_{aa}. \quad (35)$$

This equation expresses the fact that the extended Green's function $\underline{\underline{\mathcal{G}}}(\omega)$ is the projection of an operator resolvent onto a set of μ -orthonormal states [10]. Note that the matrix $\underline{\underline{H}}$ is hermitian if the Hamiltonian H of the many-body system is hermitian (which is assumed throughout this paper). By matrix partitioning we can write for the inverse of the Green's function

$$[\underline{\underline{\mathcal{G}}}(\omega)]^{-1} = \omega \underline{\underline{1}} - \underline{\underline{H}}_{aa} - \underline{\underline{H}}_{ab} \frac{1}{\omega \underline{\underline{\mu}}_{bb} - \underline{\underline{H}}_{bb}} \underline{\underline{H}}_{ba}. \quad (36)$$

This equation is the main result of the present considerations. In order to define the two-particle self energy $\underline{\underline{S}}(\omega)$ and for establishing the connection to the familiar form of Dyson's equation we adopt a perturbation theoretical view where a convenient single-particle description (e. g. the Hartree-Fock approximation) defines the zeroth order. We will see later that the coupling blocks $\underline{\underline{H}}_{ab}$ and $\underline{\underline{H}}_{ba}$ vanish in a single-particle approximation. Consequently the extended Green's function is the proper resolvent of the zeroth order primary block $\underline{\underline{H}}_{aa}^{(0)}$ which can be understood as an operator in the physical two-particle space:

$$\underline{\underline{\mathcal{G}}}^{(0)}(\omega) = \frac{1}{\omega \underline{\underline{1}} - \underline{\underline{H}}_{aa}^{(0)}}. \quad (37)$$

Introducing the **two-particle self energy**

$$\underline{\underline{S}}(\omega) = \underline{\underline{H}}_{aa} - \underline{\underline{H}}_{aa}^{(0)} + \underline{\underline{H}}_{ab} \frac{1}{\omega \underline{\underline{\mu}}_{bb} - \underline{\underline{H}}_{bb}} \underline{\underline{H}}_{ba}, \quad (38)$$

Eq. (36) can be rewritten into

$$\underline{\underline{\mathcal{G}}}(\omega) = \frac{1}{\omega \underline{\underline{1}} - \underline{\underline{H}}_{aa}^{(0)} - \underline{\underline{S}}(\omega)}. \quad (39)$$

Rearranged it takes on the familiar form of a **Dyson equation**:

$$\underline{\underline{\mathcal{G}}}(\omega) = \underline{\underline{\mathcal{G}}}^{(0)}(\omega) + \underline{\underline{\mathcal{G}}}^{(0)}(\omega) \underline{\underline{S}}(\omega) \underline{\underline{\mathcal{G}}}(\omega). \quad (40)$$

C. Static and dynamic self energy

The self energy $\underline{\underline{S}}(\omega)$ has a similar analytic structure to the common self energy [25,26] of the single-particle Green's function [11] in having single poles

and branch cuts on the real axis corresponding to the eigenvalue spectrum of the block \underline{H}_{bb} . For high energies ω (far outside the eigenvalue spectrum of the Hamiltonian) the self energy $\underline{S}(\omega)$ has a finite limit. It is called the **static self energy** $\underline{S}(\infty)$ and consists of the higher-order contributions to the primary block \underline{H}_{aa} :

$$\underline{S}(\infty) = \underline{H}_{aa} - \underline{H}_{aa}^{(0)}. \quad (41)$$

This equation yields a closed expression for the static self energy. The physical significance is to account for interactions and exchange phenomena between the two test particles (or holes) and the (static) particle density of isolated N -particle system. Also the additional (unphysical) components of the extended states take some effect here as well. The discussion of the static self energy and its physical significance will be the main objective of the rest of this paper.

The remaining ω -dependent part of the self energy is called **dynamic self energy** $\underline{M}(\omega)$:

$$\underline{M}(\omega) = \underline{S}(\omega) - \underline{S}(\infty) = \underline{H}_{ab} \frac{1}{\omega \underline{\mu}_{bb} - \underline{H}_{bb}} \underline{H}_{ba}. \quad (42)$$

This part takes account for dynamic correlation between the test particles and the finite system and is necessary for the complete description of two particle excitation processes. Of course, also here the unphysical components of the extended states enter.

Adopting the three choices for the extended states $|Y_{rs}\rangle$ from the beginning of this Chapter, we get three different types of two-particle self energies. Before we will concentrate on discussing in how far these self energies are useful for an effective two-particle description of diverse many-body phenomena in the remaining Chapters of this paper, we will briefly touch an alternative formal approach.

D. Super-operator expansions

So far we have used the picture of operators like \check{H} and μ , acting on states like $|Y_{rs}\rangle$ and $|Q_I\rangle$ in the Hilbert space \mathcal{Y} . For developing perturbation theoretic expansions, however, it is useful to use the complementary concept of super-operators acting on Fock-space operators as defined in Sec. IIC. Using the super-operator \hat{H} , the definition for the extended particle-hole Green's function of Eq. (23) can be written as

$$\mathcal{G}_{rs,r's'}^{(ph)}(\omega) = (a_r^\dagger, a_s | \frac{1}{\omega - \hat{H}} | a_r^\dagger, a_{s'}). \quad (43)$$

The “superoperator resolvent” $\frac{1}{\omega - \hat{H}}$ is defined by the usual series expansion and the application of \hat{H} on the extended states $|a_r^\dagger, a_{s'}\rangle$ has been defined by Eq. (15). Perturbation expansions of the super-operator resolvent in combination with perturbation expansions of the reference states give easy access to perturbation expansions of the Green’s function and the self energy. In the case of the single-particle Green’s function this has been carried out explicitly by Kutzelnigg and Mukherjee [27]. They could show that the common Feynman-Dyson perturbation expansion can be obtained in this manner without using Wick’s theorem. They also gave appropriate perturbation expansions for multi-determinantal zeroth order reference states. Their techniques can be applied to the extended Green’s functions in an analogous manner. The justification for the expansions cannot be given in the same way as in Ref. [27] because the mathematical concepts they use for the eigenvalue spectra of super-operators cannot be directly transferred to the extended two particle Green’s functions. Instead one would have to use the equivalence between the super-operator \hat{H} and the extended operator \check{H} (see Sec. II C). Here we do not want to elaborate this point further because the main goal of this paper does not lie in the development of perturbation theoretic expansions.

We will now continue with discussing some properties including the pole structure and a first order approximation to the self energy for the case of the extended particle-hole Green’s function. Previously we have treated the particle-particle Green’s function for which the self energy is an exact optical potential of elastic two-particle scattering [10]. In the last Chapter of this paper we will then concentrate on the physical interpretation of the static self energy as a scattering potential in the particle-particle and the particle-hole case.

IV. FORMAL PROPERTIES OF THE EXTENDED PROPAGATORS

We now want to discuss several formal properties of the extended states, the Green’s functions, and the self energies that were defined in the preceding section by Eqs. (23) – (25) and (38). In particular, we consider the meaning of the components of the extended states and the consequences the extensions have for degeneracies of the extended states and the analytic structure of the Green’s functions. We also discuss two simple first-order approximations to the self energy. In order to be definite, we restrict ourselves to the particle-hole case [choice (a) of Sec. III] in this chapter although most of the features considered appear in an analogous fashion for the other cases as well. Several properties of the extended particle-particle Green’s function and its self energy have already been discussed in Ref. [10].

We consider a fairly general system of indistinguishable fermions interacting by two-body forces and possibly with static external fields. In order to allow perturbation theory, we split the Hamiltonian H into two parts as usual: $H = H_o + H_1$. The one-particle operator $H_o = \sum_i \varepsilon_i a_i^\dagger a_i$ defines the zeroth order of perturbation theory and is characterised by the diagonalising single-particle basis $\{|\varphi_i\rangle\}$ and single-particle energies $\{\varepsilon_i\}$. The residual interaction $H_1 = v + V$ generally contains contributions of a one-particle operator v and the two-body interaction V :

$$v = \sum_{i,j} v_{ij} a_i^\dagger a_j, \quad (44)$$

$$V = \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k. \quad (45)$$

When using the Møller-Plesset partitioning of the Hamiltonian, the zeroth order Hamiltonian H_o is defined by the Hartree-Fock approximation. For a nondegenerate ground state the matrix elements v_{ij} of the one-particle part of the interaction in Eq. (44) are then given by

$$v_{ij}^{HF} = - \sum_k n_k V_{ik[jk]}. \quad (46)$$

Here $V_{rs[r's']} = V_{rsr's'} - V_{r'ss'r'}$ denotes the anti-symmetrised matrix element of the two-body interaction and n_r is the occupation number of the orbital $|\varphi_r\rangle$ in the zeroth order ground state Slater determinant $|\Phi_0^N\rangle$.

A. Extended particle-hole states

The extended states $|Y_{rs}^{(ph)}\rangle$ that appear in the definition of the extended particle-hole Green's function $\mathcal{G}_{rs,r's'}^{(ph)}(\omega)$ of Eq. (23) are given by

$$|Y_{rs}^{(ph)}\rangle = |a_r^\dagger, a_s\rangle = \begin{pmatrix} Q a_r^\dagger a_s |\Psi_0^N\rangle \\ \langle \Psi_0^N | a_r^\dagger a_s Q \\ \langle \varphi | a_r^\dagger \otimes \langle \Psi_0^N | a_s - \langle \varphi | a_s \otimes \langle \Psi_0^N | a_r^\dagger \\ a_r^\dagger |\varphi\rangle \otimes \langle \Psi_0^N | a_s - a_s |\varphi\rangle \otimes \langle \Psi_0^N | a_r^\dagger \end{pmatrix}, \quad (47)$$

where the choice of the Fock-space vector $|\varphi\rangle$ is arbitrary for the general algebra of the last section. For the following discussion of formal properties it is not very important either. We will discuss the freedom of choice for the secondary reference states $|\varphi\rangle$ in Sec. VIB. The operator Q is a projector that projects onto the orthogonal complement of the primary reference state $|\Psi_0^N\rangle$.

The first component $Q a_r^\dagger a_s |\Psi_0^N\rangle$ of the extended particle-hole state $|Y_{rs}^{(ph)}\rangle$ determines the physical situations that we want to describe namely particle

number conserving excitations of the system. The other components are only necessary to fulfil the orthonormality relation (26) that was crucial for the derivation of Dyson's equation in Sec. IIIB. The μ -orthonormality of the extended states is peculiar in two respects: firstly, because it extends over the full index space of two independent single-particle indices and secondly because it holds completely independent of the reference states $|\Phi_0^N\rangle$ and $|\varphi\rangle$. Thus the orthonormality persists through all orders of perturbation theory.

In order to understand how orthonormality is achieved it is useful to take a look at the zeroth order of the extended particle-hole states where the role of the single components can easily be understood:

$$|Y_{rs}^{(ph)}\rangle^{(0)} = \begin{pmatrix} Q^{(0)} a_r^\dagger a_s |\Phi_0^N\rangle \\ \langle \Phi_0^N | a_r^\dagger a_s Q^{(0)} \\ \langle \Phi_0^N | a_r^\dagger \otimes \langle \Phi_0^N | a_s - \langle \Phi_0^N | a_s \otimes \langle \Phi_0^N | a_r^\dagger \\ a_r^\dagger |\Phi_0^N\rangle \otimes \langle \Phi_0^N | a_s - a_s |\Phi_0^N\rangle \otimes \langle \Phi_0^N | a_r^\dagger \end{pmatrix} \begin{matrix} \leftarrow ph \\ \leftarrow hp \\ \leftarrow hp \\ \leftarrow pp, hh \end{matrix} \quad (48)$$

On the right a classification of the contributing entries is given which refers to the character of the single particle indices. We classify an index r as a particle index (p) if it refers to a single particle orbital $\varphi_r(x)$ which is vacant (virtual) in the Slater determinant $|\Phi_0^N\rangle$. Conversely a hole index (h) labels an occupied orbital in $|\Phi_0^N\rangle$. Accordingly the first component of $|Y_{rs}^{(ph)}\rangle^{(0)}$ in Eq. (48) is classified ph because it contributes only if r is a particle and s is a hole index. Correspondingly the second and third component vanish if the index pair (r, s) is of another type than hp , and so on.

We can now interpret the role of the components of the extended state $|Y_{rs}^{(ph)}\rangle$ in the following way: According to the orthonormality relation (28), the extended states have always the μ -norm 1. Since the first (and physical) component contributes in zeroth order only for ph index pairs, the other components (the extensions) have to take over in the remaining cases. The second component of the extended state of Eq. (47) or Eq. (48) is a kind of symmetric partner of the first component (which is also present in the polarisation propagator of traditional many-body theory). On its own, it leads to a negative contribution to the μ -product $\langle Y_{rs}^{(ph)} | \mu | Y_{r's'}^{(ph)} \rangle$ because the metric μ introduces a minus sign for the second component:

$$\mu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (49)$$

The third component of the extended state $|Y_{rs}^{(ph)}\rangle$ then takes the part of overcompensating this contribution, securing a positive " μ -norm". This means

that two components contribute for hp index pairs. Consequently there exist also linear independent partners to the Y -states $|Y_{rs}^{(ph)}\rangle$ with negative μ -norm. We will see later that these states, which we call K -states, are in zeroth-order degenerate to the Y -states and contribute to the dynamic part of the self energy. The fourth component of the primary states $|Y_{rs}^{(ph)}\rangle$ contributes in the remaining cases of pp and hh index pairs and contains tensor product states like the third component does.

At first sight it may seem strange to have an indefinite metric, on the one hand, and overcompensation of the negative contributions by the third component, on the other hand. The reason for this peculiar mechanism to achieve the orthonormality relation (28) independent of the reference states is that the contribution of the first component of the extended state $|Y_{rs}^{(ph)}\rangle$ to the μ -product $\langle Y_{rs}^{(ph)} | \mu | Y_{r's'}^{(ph)} \rangle$ contains a two-particle density of the ground state

$$\langle \Psi_0^N | a_s^\dagger a_r Q a_{r'}^\dagger a_{s'} | \Psi_0^N \rangle = \langle \Psi_0^N | a_s^\dagger a_r a_{r'}^\dagger a_{s'} | \Psi_0^N \rangle - \langle \Psi_0^N | a_s^\dagger a_r | \Psi_0^N \rangle \langle \Psi_0^N | a_{r'}^\dagger a_{s'} | \Psi_0^N \rangle. \quad (50)$$

The second component gives rise to another two-particle density that is subtracted due to the minus sign in the metric, yielding the commutator $[a_s^\dagger a_r, a_{r'}^\dagger a_{s'}] = a_{s'} a_s^\dagger \delta_{rr'} + a_r a_{r'}^\dagger \delta_{ss'}$. Thus the two-particle densities are reduced to single-particle densities that are compensated for by the third and fourth component.

B. The generalised excitation energy operator \check{H}

The operator \check{H} appears in the definitions of the extended Green's functions $\mathcal{G}_{rs,r's'}(\omega)$ in Eq. (29) and the matrix \underline{H} in Eq. (32) that builds the self energy $\underline{S}(\omega)$. For a simple single-component propagator, its place is usually taken by the difference of the common (Fock-space) Hamiltonian H of the system with the ground state energy E_0^N . This operator measures the excitation energy with respect to the N -particle ground state $|\Psi_0^N\rangle$. The operator \check{H} , which will be called the extended operator associated to H or generalised excitation energy operator, presents a suitable generalisation for the extended Green's functions. Since the extended Green's functions derive from the four-component states $|Y_{rs}\rangle$, the operator \check{H} is a 4×4 matrix. For the particle-hole Green's function, the proper choice is, according to Eq. (17), given by

$$\check{H} = \begin{pmatrix} H - E_0^N & 0 & 0 & 0 \\ 0 & E_0^N - H & 0 & 0 \\ 0 & 0 & A & 0 \\ 0 & 0 & 0 & B \end{pmatrix}, \quad (51)$$

with

$$A = E_\varphi - H \otimes 1 + E_0^N - 1 \otimes H, \quad (52)$$

$$B = H \otimes 1 - E_\varphi + E_0^N - 1 \otimes H. \quad (53)$$

Here, E_φ is the eigenvalue of the Hamiltonian H that belongs to the reference state $|\varphi\rangle$. We will characterise the operator \check{H} explicitly by its eigenstates and eigenvalues at the end of this subsection.

The matrix element of \check{H} that acts on the first and physical component of the extended states $|Y_{rs}\rangle$ indeed measures the excitation energy. The particular choice of the other components can best be motivated by the derivation via the super-operator \hat{H} of Sec. II C. The super-operator associated to the Hamiltonian operator H is denoted by \hat{H} and acts on the extended states by giving the commutator of the Hamiltonian with the canonic operators a_r^\dagger and a_s :

$$\hat{H}|a_r^\dagger, a_s\rangle = |[H, a_r^\dagger]_-, a_s\rangle + |a_r^\dagger, [H, a_s]_-\rangle. \quad (54)$$

Under the condition that the reference state $|\varphi\rangle$ is an eigenstate of the Hamiltonian H , the super-operator \hat{H} can be replaced by the associated extended operator denoted by \check{H} and given by Eq. (51):

$$\check{H}|a_r^\dagger, a_s\rangle = \hat{H}|a_r^\dagger, a_s\rangle. \quad (55)$$

While the concept of the (Hilbert space) operator \check{H} has the advantage of giving the possibility to interpret \underline{H} of Eq. (32) as a matrix representation of a common operator, the equivalent formulation with the super-operator \hat{H} is an appealing alternative concept. Not only does it present a simple and unified way to define a generalisation of excitation energy operator for all families of extended Green's functions covered in this paper, but it also simplifies perturbation theoretic expansions. Super-operator expansions have also been a popular tool for deriving approximation schemes in traditional propagator theory for many decades [28,29]. The practical advantage emerges in the present context when the Hamiltonian is split into zeroth order and interaction parts

$$\hat{H}|a_r^\dagger, a_s\rangle = \hat{H}_0|a_r^\dagger, a_s\rangle + \hat{H}_1|a_r^\dagger, a_s\rangle, \quad (56)$$

because the first term is very simple to evaluate regardless of approximations or particular choices for the reference states $|\Psi_0^N\rangle$ and $|\varphi\rangle$ in Eq. (47):

$$\hat{H}_0|a_r^\dagger, a_s\rangle = (\varepsilon_r - \varepsilon_s)|a_r^\dagger, a_s\rangle. \quad (57)$$

The difference of single particle energies $\varepsilon_r - \varepsilon_s$ appears here as a kind of "eigenvalue". As a first step towards a physical interpretation of the states $|Y_{rs}^{(ph)}\rangle = |a_r^\dagger, a_s\rangle$ one can thus say that the index r has something to do with a test particle and s with a test hole that are probing the system. Without interaction the test particles move freely and are correctly characterised by the difference of single-particle energies $\varepsilon_r - \varepsilon_s$.

Equation (57) holds for arbitrary reference states but becomes a proper eigenvalue equation when taking the Slater determinant $|\Phi_0^N\rangle$ as the reference state in Eq. (47), which means that the extended state $|Y_{rs}^{(ph)}\rangle = |a_r^\dagger, a_s\rangle$ is replaced by its zeroth order $|Y_{rs}^{(ph)}\rangle^{(0)}$ of Eq. (48). In this case the super-operator \check{H}_0 can be replaced by its corresponding extended operator $\check{H}^{(0)}$ (c. f. Sec. II C) which is the zeroth order of the operator \check{H} :

$$\check{H}^{(0)}|Y_{rs}^{(ph)}\rangle^{(0)} = (\varepsilon_r - \varepsilon_s)|Y_{rs}^{(ph)}\rangle^{(0)}. \quad (58)$$

In fact, the zeroth order extended states are eigenstates of the zeroth order excitation energy operator. Note that in contrast to the super-operator \check{H} , the perturbation expansion of the extended operator \check{H} contributes in all orders because the ground state energy E_0^N is a general function of the interaction strength.

Finally we want to give the explicit diagonal representation of the extended operator \check{H} in the form

$$\check{H} = \sum_q \omega_q |q\rangle\langle q|, \quad (59)$$

thereby characterising its eigenvectors $|q\rangle$ and eigenvalues ω_q . Assuming no degeneracies between the physically distinct component spaces, the eigenvectors of \check{H} are single-component states in the 4-component Y -space, as can be seen from Eqs. (51) to (53). Thus the projectors $|q\rangle\langle q|$ onto the eigenstates are proportional to the 4×4 projection matrices \underline{P}_i where all elements are zero except for the element in the i th row and the i th column, which is one. For example

$$\underline{P}_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (60)$$

Choosing for the secondary reference state $|\varphi\rangle = |\Psi_0^N\rangle$, we can now write Eq. (59) explicitly as

$$\check{H} = \sum_\nu (E_\nu^N - E_0^N) \left(\overleftarrow{|\Psi_\nu^N\rangle} \right) \left(\overrightarrow{\langle\Psi_\nu^N|} \right) \underline{P}_1$$

$$\begin{aligned}
& + \sum_{\nu} (E_0^N - E_{\nu}^N) \left(\overleftarrow{\langle \Psi_{\nu}^N |} \right) \left(\overrightarrow{|\Psi_{\nu}^N \rangle} \right) \underline{\underline{P}}_2 \\
& + \sum_{\kappa, \mu} (2E_0^N - E_{\kappa}^{N-1} - E_{\mu}^{N+1}) \left(\overleftarrow{\langle \Psi_{\kappa}^{N-1} |} \otimes \overleftarrow{\langle \Psi_{\mu}^{N+1} |} \right) \left(\overrightarrow{|\Psi_{\kappa}^{N-1} \rangle} \otimes \overrightarrow{|\Psi_{\mu}^{N+1} \rangle} \right) \underline{\underline{P}}_3 \\
& + \left\{ \sum_{\mu, \lambda} (E_{\mu}^{N+1} - E_{\lambda}^{N+1}) \left(\overleftarrow{\langle \Psi_{\mu}^{N+1} |} \otimes \overleftarrow{\langle \Psi_{\lambda}^{N+1} |} \right) \left(\overrightarrow{|\Psi_{\mu}^{N+1} \rangle} \otimes \overrightarrow{|\Psi_{\lambda}^{N+1} \rangle} \right) \right. \\
& \left. + \sum_{\kappa, \sigma} (E_{\kappa}^{N-1} - E_{\sigma}^{N-1}) \left(\overleftarrow{\langle \Psi_{\kappa}^{N-1} |} \otimes \overleftarrow{\langle \Psi_{\sigma}^{N-1} |} \right) \left(\overrightarrow{|\Psi_{\kappa}^{N-1} \rangle} \otimes \overrightarrow{|\Psi_{\sigma}^{N-1} \rangle} \right) \right\} \underline{\underline{P}}_4 \quad (61)
\end{aligned}$$

Here, we generalised the notation $|q\rangle\langle q|$ for a projection operator onto the “ket” state $|q\rangle$ to $\left(\overleftarrow{|q\rangle} \right) \left(\overrightarrow{\langle q|} \right)$ because not all of the eigenstates of \check{H} are ket vectors but some are bra vectors $\langle p|$ or tensor product states $\langle p| \otimes \langle q|$. Of course, it is also possible to project onto tensor product states like $\langle p| \otimes \langle q|$. We use arrows in our notation for this projection operator

$$\mathcal{P} = \left(\overleftarrow{\langle p| \otimes \langle q|} \right) \left(\overrightarrow{|p\rangle \otimes |q\rangle} \right),$$

in order to indicate the relevant directions for forming inner products. In the present example, operating \mathcal{P} on a product state $\langle a| \otimes \langle b|$ yields

$$\mathcal{P}(\langle a| \otimes \langle b|) = \langle a|p\rangle \langle b|q\rangle (\langle p| \otimes \langle q|),$$

which is again a product state proportional to $\langle p| \otimes \langle q|$. The inner products $\langle a|p\rangle \langle b|q\rangle$ here form the proportionality constant.

The sums in Eq. (61) always run over the complete sets of eigenvectors of the corresponding Hilbert spaces. The sums over ν , in particular, run over all exact states with N particles, μ and λ label the $N+1$, and κ and σ the $N-1$ particle states. As already mentioned in the discussion of the Hilbert space \mathcal{Y} of Eq. (6), symmetry considerations may reduce the number of states that actually couple to the primary states. Along with a reduced Hilbert space \mathcal{Y} , then also less terms are needed in the diagonal representation (61) of the extended operator \check{H} .

The eigenvalue spectrum of the extended operator \check{H} contained in Eq. (61) determines the pole structure of the extended Green’s function and will be discussed in the following paragraph.

C. The analytic structure of the extended particle-hole Green’s function

The analytic structure of the particle-hole Green’s function $\underline{\underline{G}}^{(ph)}(\omega)$ as a function of the complex variable ω is governed by single poles and branch cuts

at the eigenvalue spectrum of the generalised excitation energy operator \check{H} . This can be seen easily by inserting the (Y-space) complete set of eigenvectors $|q\rangle$ of this operator with eigenvalues ω_q into the definition of $\underline{\underline{G}}^{(ph)}(\omega)$ [Eq. (29) or (23)]:

$$\mathcal{G}_{rs,r's'}^{(ph)}(\omega) = \sum_q \frac{\langle Y_{rs}^{(ph)} | q \rangle m_q \langle q | Y_{r's'}^{(ph)} \rangle}{\omega - \omega_q}. \quad (62)$$

Here, $m_q = \pm 1$ are the eigenvalues of the metric operator μ .

The eigenvectors $|q\rangle$ and eigenvalues ω_q corresponding to the four components of the Hilbert space Y have already been listed explicitly in Eq. (61) for $|\varphi\rangle = |\Psi_0^N\rangle$ and assuming finite basis Hilbert spaces. In general, the eigenvalue spectrum ω_q leads by Eq. (62) to single poles and branch cuts of the extended Green's function. The overlaps $\langle q | Y_{r's'}^{(ph)} \rangle$ may vanish, however, when due to symmetry properties the components of $|Y_{rs}^{(ph)}\rangle$ decouple from classes of excitations of a given particle number. In this case the corresponding eigenvalues do not appear in the pole structure of the Green's function.

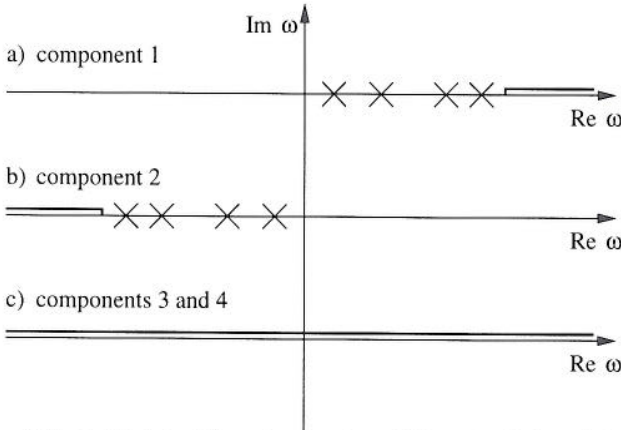


FIG. 1. Sketch of the pole structure of the extended particle-hole Green's function $\underline{\underline{G}}(\omega)$ in the complex omega plane. Crosses correspond to single poles and thick lines to branch cuts. Part a) shows the poles corresponding to the first component of the extended states $|Y_{rs}^{(ph)}\rangle$, which are given by the physical excitation energies of the system. Since excitations from the ground state are considered, all energies are non-negative. The start of the branch cut marks the threshold for ionisation of a particle. Part b) shows the poles and cuts that are introduced by the second component. They are the same as for the first component, mirrored at the imaginary axis. The contributions of the third and fourth component are shown in part c). In general they yield a cut along the whole real axis.

Figure 1 shows a schematic plot of the eigenvalue spectrum of \check{H} and therefore the pole structure of $\mathcal{G}^{(ph)}(\omega)$ for the first, second, and the additional components. The eigenvalues ω_q that derive from the physical, first component of \check{H} are the exact (discrete and continuous) excitation energies $E_q^N - E_0^N$ of the N particle system under study. Since E_0^N is the ground state energy, these energies are positive or possibly zero in the case of a degenerate ground state. There are usually some discrete eigenvalues corresponding to bound excited states but above the threshold energy for ionisation of one particle, the excitation spectrum is continuous. The second component of \check{H} mirrors the excitation spectrum of the first component to negative values. The parts of the spectrum that are contributed by the additional third and fourth component of the extended operator \check{H} are more difficult to interpret. Through these components, the eigenvalue spectrum of the $N + 1$ and the $N - 1$ particle system are introduced as can be seen from Eq. (61). In particular the 4th component of \check{H} introduces the energy differences $(E_\mu^{N+1} - E_\lambda^{N+1})$ and $(E_\kappa^{N-1} - E_\sigma^{N-1})$. Since the spectrum of the Hamiltonian H in $N \pm 1$ -particle systems will generally be unbounded from above showing a continuous spectrum at the top end, we may conclude that the spectrum of the last component of the generalised excitation energy operator \check{H} comprises the full real axis. This can already be seen in zeroth order where the primary states $|Y_{rs}^{(ph)}\rangle^{(0)}$ have the eigenvalues $\varepsilon_r - \varepsilon_s$. Since r and s can be chosen to denote virtual or scattering orbitals with arbitrary, positive energy, the difference $\varepsilon_r - \varepsilon_s$ can adopt any real value.

D. The extended Green's function for real arguments

In order to define the extended Green's function $\underline{\mathcal{G}}(\omega)$ for real arguments, the branch cuts introduced by the eigenvalue spectrum of \check{H} have to be moved away from the real axis. Commonly this is achieved by introducing a positive infinitesimal η with the option of performing the limit $\eta \rightarrow 0^+$ after all formal manipulations. In this way a **retarded or advanced extended Green's function** may be defined by $\underline{\mathcal{G}}(E \pm i\eta)$ where E now serves as a real energy variable. The concept of retarded or advanced Green's functions is traditionally associated with the properties of the Fourier transforms into time space representation. The Fourier transform from the variable E to t can be performed by using the residue theorem and yields a time space function which contributes only for $t > 0$ or $t < 0$ according to the sign of $i\eta$ [11].

The formal definition (29) of the extended Green's function implies a sum of propagators according to the different components of the extended state's vector. The terms introduced by the product states can be transformed into convolutions of single-particle propagators if we resort to real energies. For

the retarded version of the extended particle-hole Green's function $\mathcal{G}_{rs,r's'}^{(ph)}(\omega)$ defined by Eq. (23) we get:

$$\begin{aligned} \mathcal{G}_{rs,r's'}^{(ph)}(E + i\eta) = & \Pi_{rs,r's'}^{ph}(E + i\eta) - \Pi_{rs,r's'}^{hp}(E + i\eta) \\ & + \frac{1}{i} \left\{ \langle \varphi | a_{r'}^\dagger \frac{1}{E - E_\varphi + H + i\eta} a_r | \varphi \rangle * \langle \Psi_0^N | a_{s'} \frac{1}{E - E_o + H + i\eta} a_s^\dagger | \Psi_0^N \rangle \right. \\ & + \langle \Psi_0^N | a_{r'}^\dagger \frac{1}{E - E_o + H + i\eta} a_r | \Psi_0^N \rangle * \langle \varphi | a_{s'} \frac{1}{E - E_\varphi + H + i\eta} a_s^\dagger | \varphi \rangle \\ & + \langle \varphi | a_r \frac{1}{E - H + E_\varphi + i\eta} a_{r'}^\dagger | \varphi \rangle * \langle \Psi_0^N | a_{s'} \frac{1}{E - E_o + H + i\eta} a_s^\dagger | \Psi_0^N \rangle \\ & \left. + \langle \Psi_0^N | a_{r'}^\dagger \frac{1}{E - E_o + H + i\eta} a_r | \Psi_0^N \rangle * \langle \varphi | a_s^\dagger \frac{1}{E - H + E_\varphi + i\eta} a_{s'} | \varphi \rangle \right\}. \quad (63) \end{aligned}$$

The asterisk * denotes convolution with respect to E defined by

$$f(E) * g(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE' f(E') g(E - E'). \quad (64)$$

The particle-hole part $\Pi_{rs,r's'}^{ph}(\omega)$ and the hole-particle part $\Pi_{rs,r's'}^{hp}(\omega)$ of the well-known polarisation propagator [11] are defined by

$$\Pi_{rs,r's'}^{ph}(\omega) = \langle \Psi_0^N | a_s^\dagger a_r \frac{Q}{\omega - H + E_0^N} a_{r'}^\dagger a_{s'} | \Psi_0^N \rangle, \quad (65)$$

$$\Pi_{rs,r's'}^{hp}(\omega) = \langle \Psi_0^N | a_{r'}^\dagger a_{s'} \frac{Q}{\omega - E_0^N + H} a_s^\dagger a_r | \Psi_0^N \rangle. \quad (66)$$

Another possibility for defining the Green's functions for real energies is to distribute different $i\eta$'s or different signs for $i\eta$ among the components of the propagator. This is, e. g., the case for the so-called time-ordered Green's functions of traditional many-body theory [11]. In our formalism, this can be achieved by adding $i\eta$ s with the chosen sign to each component of the generalised excitation energy operator \tilde{H} of Eq. (51). This has the effect that the eigenvalue spectrum of the different components of this operator is shifted into the complex plane and consequently the argument ω of the extended Green's function may be chosen real. In the extended particle-particle Green's function of reference [10], e. g., we have chosen the signs of $i\eta$ such that the physical (in this case pp) component carries a positive sign while all others carry negative signs. For the Fourier transformed time space function this has the consequence that for positive times only the physical component contributes which allows the correct description of scattering processes.

So far we have discussed the pole structure of the extended particle-hole Green's function, which is given by the eigenvalue spectrum of the generalised

excitation energy operator \check{H} . The self energy formally has a similar analytic structure to the extended Green's function but poles and cuts appear at different energies. The connection between the pole structure of the Green's function and its self energy is, of course, established by Dyson's equation (39). Before discussing the energy dependence of the self energy, however, we first want to consider the lowest order approximation to the self energy in which it represents a static, energy independent quantity.

V. PROPERTIES OF THE SELF ENERGY

According to Eq. (42) the extended self energy can be written as the sum of a uniquely determined static, energy independent part $\underline{\underline{S}}(\infty)$ and the so-called dynamic part $\underline{\underline{M}}(\omega)$:

$$\underline{\underline{S}}(\omega) = \underline{\underline{S}}(\infty) + \underline{\underline{M}}(\omega). \quad (67)$$

While the dynamic part is of second order, the static self energy $\underline{\underline{S}}(\infty)$ contributes in first order. For brevity we will discuss only the particle-hole self energy in this chapter. In contrast to the single-particle Green's function where the first order of the self energy upon Hartree-Fock vanishes, the first order of the particle-hole self energy yields an interesting, nontrivial model for the extended particle-hole Green's function.

After looking at the static self energy part and its special role for one-particle potentials, we will briefly touch upon the meaning and the structure of the dynamic particle-hole self energy part. In the following we will then discuss the first order of the static part as the simplest non-trivial approximation to the particle-hole self energy in more detail. The rest of this chapter is devoted to another simple approximation of the self energy where additionally to the first order of the static self energy, also part of the dynamic self energy is taken into account, which leads to the RPA approximation.

A. The static part

According to Eqs. (41) and (34) the static self energy $\underline{\underline{S}}(\infty)$ is given by the primary block $\underline{\underline{H}}_{aa}$ of the matrix $\underline{\underline{H}}$ of Eq. (33) minus its zeroth order part. An explicit expression can be found with the help of the super-operator formalism and using the definition of the extended states (47):

$$\begin{aligned} [\underline{\underline{H}}_{aa}]_{rs,r's'} &= (a_r^\dagger, a_s | \hat{H} | a_{r'}^\dagger, a_{s'}') \\ &= \langle \Psi_0^N | [a_s^\dagger a_r, [H, a_{r'}^\dagger a_{s'}']] | \Psi_0^N \rangle \end{aligned}$$

$$\begin{aligned}
& + \langle \varphi | \{ [H, a_{r'}^\dagger], a_r \} | \varphi \rangle \langle \Psi_0^N | a_{s'} a_s^\dagger | \Psi_0^N \rangle \\
& + \delta_{rr'} \langle \Psi_0^N | [H, a_{s'}] a_s^\dagger | \Psi_0^N \rangle \\
& + \langle \Psi_0^N | [H, a_{r'}^\dagger] a_r | \Psi_0^N \rangle \delta_{ss'} \\
& + \langle \Psi_0^N | a_r a_{r'}^\dagger | \Psi_0^N \rangle \langle \varphi | \{ [H, a_{s'}], a_s^\dagger \} | \varphi \rangle.
\end{aligned} \tag{68}$$

For the one-particle part $H_0 + v$ of the Hamiltonian $H = H_0 + v + V$ this expression yields a very simple result:

$$(a_r^\dagger, a_s | \hat{H}_0 + \hat{v} | a_{r'}^\dagger, a_{s'}') = \delta_{rr'} \delta_{ss'} (\varepsilon_r - \varepsilon_s) + v_{rr'} \delta_{ss'} - v_{s's} \delta_{rr'}. \tag{69}$$

In the special case of systems without real two-body potentials V , where only interactions with external potentials or mean fields are considered, this is the exact solution for the primary block \underline{H}_{aa} , which determines the self energy. Since the dynamic self energy vanishes in this case, as will be shown shortly, the self energy is energy independent and given by

$$S_{rsr's'} = v_{rr'} \delta_{ss'} - v_{s's} \delta_{rr'}. \tag{70}$$

Note that this exact solution for the self energy is of first order and completely independent of the many-body system's ground state $|\Psi_0^N\rangle$ or the secondary reference state $|\varphi\rangle$. The matrix \underline{H}_{aa} of Eq. (69) can obviously be diagonalised by an appropriate choice of single-particle orbitals and then takes the form of the zeroth order part $\delta_{rr'} \delta_{ss'} (\varepsilon_r - \varepsilon_s)$. Thus the self energy of Eq. (70) describes particle-hole excitations in a system of independent particles. The unphysical components present in the extended states $|Y_{rs}^{(ph)}\rangle$ here serve to circumvent Pauli's exclusion principle because Eqs. (69) and (70) allow excitations from any orbital to any other orbital, regardless of their occupation in the many-body state $|\Psi_0^N\rangle$. The same behaviour with respect to one-particle Hamiltonians of the self energy becoming an energy-independent, first-order quantity and the lifting of the Pauli principle is also shown by the other extended two-particle Green's functions and the traditional single-particle Green's function.¹ The reason for this behaviour can be traced back to two features of the present theory: the construction from orthonormal states and the fact that the excitation energy operator \check{H} is equivalent to the super-operator \hat{H} , which leads to commutators. This can be seen when considering that the associated super-operator \hat{A} to a general single-particle operator $A = \sum_{ij} a_i^\dagger a_j A_{ij}$ maps the primary states $|Y_{rs}^{(ph)}\rangle$ onto linear combinations of primary states:

¹The case of the extended particle-particle Green's function in comparison with the single-particle Green's function has already been discussed in Ref. [10]

$$\begin{aligned}\hat{A}|Y_{rs}^{(ph)}\rangle &= |[A, a_r^\dagger]_-, a_s) + |a_r^\dagger, [A, a_s]_-) \\ &= \sum_{kl} (A_{rk}\delta_{sl} - A_{ls}\delta_{rk})|Y_{kl}^{(ph)}\rangle.\end{aligned}\quad (71)$$

Thus, the overlaps with basis states of the orthogonal complement of the primary set $|Q_I\rangle \in \{|Y_{rs}^{(ph)}\rangle\}^\perp$ vanish:

$$\langle Q_I | \mu \hat{A} | Y_{rs}^{(ph)} \rangle = 0, \quad (72)$$

and so do the off-diagonal blocks \underline{H}_{ab} and \underline{H}_{ba} . In the case of a single-particle Hamiltonian, thus, the self energy indeed is purely static and yields the exact energy eigenvalues of particle-hole type excitations while higher excitation classes like two-particle-two-hole excitations decouple completely.

In the more general case of a correlated system, the dynamic self energy does not vanish and thus the eigenvalues of the primary block \underline{H}_{aa} are generally not the exact excitation energies.

B. The dynamic particle-hole self energy

The dynamic self energy $\underline{\mathcal{M}}(\omega)$ as a function of the complex energy variable ω has an analytic structure which is very similar to that of the extended Green's function $\underline{\mathcal{G}}(\omega)$ discussed earlier (Sec. IV C). We have defined the self energy by matrix partitioning of the matrix \underline{H} of Eq. (33) which yields the expression (42) for the dynamic part. From this formula it can be seen that the dynamic self energy has single poles or branch cuts where the denominator of (42) becomes singular:

$$\det(\omega \underline{\mu}_{bb} - \underline{H}_{bb}) = 0. \quad (73)$$

By introducing a similarity transformation which simultaneously diagonalises the matrices $\underline{\mu}_{bb}$ and \underline{H}_{bb} , Eq. (42) can be cast into the form of Eq. (62). The difference is that the poles and cuts of the Green's function $\underline{\mathcal{G}}(\omega)$ appear at the generalised eigenvalues of the whole matrix \underline{H} while the pole structure of the self energy is given by the generalised eigenvalues of the block \underline{H}_{bb} only. The relation to the eigenvalue spectra of the block \underline{H}_{bb} and the full matrix \underline{H} depends much on the coupling blocks \underline{H}_{ab} and $\underline{H}_{ba} = \underline{H}_{ab}^\dagger$.

In the limiting case of vanishing coupling $\underline{H}_{ab} = 0$, the eigenvalue spectrum of \underline{H}_{bb} is a subset of the spectrum of \underline{H} . At the same time, however, the dynamic self energy part vanishes and the self energy becomes ω -independent. This happens, e. g. if the Hamiltonian is a single-particle operator and does not contain true two-particle forces but only external forces or mean fields as discussed in the last paragraph.

In the more general case of a fully correlated system all higher excitations couple. If the coupling is weak enough, however, the diagonal zeroth order of the matrix \underline{H} may give a good guess for the poles of the self energy. Of course, the coupling affects the poles by eventually lifting degeneracies and shifting the poles like discussed in the case of the single-particle Green's function in reference [25]. Similar to the full extended Green's function $\underline{G}(\omega)$, physical as well as unphysical poles appear. Like before, the physical poles caused by excited states of the system appear at positive energies. They lie above a threshold energy where double excitation ($2p-2h$) becomes possible. Another threshold for double excitation into the continuum indicates the lower border of the physical branch cut of the dynamic self energy. The dynamic self energy also contains diverse poles and cuts originating in the unphysical component of the extended state vectors (47). In particular the so-called K -states that will be discussed in the next paragraph give rise to poles of the dynamic self energy which are in zeroth order degenerate to eigenvalues of the primary block \underline{H}_{aa} . This, however, concerns only the negative energy part of the spectrum. The existence of the degenerate K -states can be traced back to the degeneracy of the second and third component – both unphysical – of the extended states $|Y_{rs}^{(ph)}\rangle$ in Eq. (48). I. e., these two degenerate unphysical components are mixed in the zeroth order Y -states. Taking the K -states into account additionally to the primary Y -states, leads to a minimal extension of the primary block \underline{H}_{aa} which allows the degenerate components to decouple. Interestingly the first order Hartree-Fock based approximation to this extended primary block $\underline{H}_{aa}^{\text{ext}(1)}$ yields the well known RPA. We will show this by presenting a universal unitary transformation which transforms the extended eigenvalue problem to the RPA after discussing the first-order approximation to the static self energy.

At this point we would briefly like to mention that the self energy $\underline{S}(\omega)$ of Eq. (38) is fully specified by the Dyson equation (39) or (40) only for energies ω where the Green's function $\underline{G}(\omega)$ can be inverted. Capuzzi and Mahaux have shown for the case of the single-particle Green's function that the self energy can be modified at isolated zeros of the Green's function and still satisfy the Dyson equation [9]. These modifications may be used to tailor dispersion relations for the self energy parts, however, they do not have physical implications. The arguments of Ref. [9] apply also to the extended two-particle Green's functions.

C. The zeroth-order degenerate states $|K_{an}^{(ph)}\rangle$

We are now going to discuss one example of states that lie outside the model space of the primary Y -states. These states, called K -states, play a special

role because they are in zeroth order degenerate with states of the primary space and also couple to the primary space in first order. The remaining states outside the primary space are generally not degenerate to the Y -states although accidental degeneracies may still occur.

We already remarked earlier that for a particular index pair (r, s) only certain components of the zeroth order states $|Y_{rs}^{(ph)}\rangle^{(0)}$ of Eq. (48) contribute according to the classification of the indices as p or h . For hp indices two components of the extended states contribute at the same time and naturally have the same (zeroth order) energies because the extended states are zeroth order eigenstates of the excitation energy operator. Therefore a linear independent, degenerate combination of the two components exists. A suitable choice for these states is given by

$$|K_{\alpha n}^{(ph)}\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \left(\langle \Phi_0^N | a_\alpha^\dagger \otimes \langle \Phi_0^N | a_n - \langle \Phi_0^N | a_n \otimes \langle \Phi_0^N | a_\alpha^\dagger \right) \\ 0 \end{pmatrix}, \quad (74)$$

where the indices α and n stand for occupied (h) and virtual (p) orbitals, respectively. It is readily verified that the states $|K_{\alpha n}^{(ph)}\rangle$ fulfil the following orthonormality relations (with α, α' occupied, n, n' virtual, and r and s arbitrary):

$$\langle K_{\alpha n}^{(ph)} | \mu | Y_{rs}^{(ph)} \rangle^{(0)} = \langle Y_{rs}^{(ph)} |^{(0)} \mu | K_{\alpha n}^{(ph)} \rangle = 0, \quad (75)$$

$$\langle K_{\alpha n}^{(ph)} | \mu | K_{\alpha' n'}^{(ph)} \rangle = -\delta_{\alpha\alpha'} \delta_{nn'}. \quad (76)$$

The states $|K_{\alpha n}^{(ph)}\rangle$ are obviously elements of the composite Hilbert space \mathcal{Y} but they lie outside of the (zeroth order) primary space spanned by the states $\{|Y_{rs}^{(ph)}\rangle^{(0)}\}$. Thus the “degenerate states” $\{|K_{\alpha n}^{(ph)}\rangle\}$ (which we also call K -states) contribute to the dynamic, ω -dependent part $\underline{\mathcal{M}}(\omega)$ of the self energy $\underline{\mathcal{S}}(\omega)$ of Eq. (42) whereas the primary states $\{|Y_{rs}^{(ph)}\rangle\}$ define the static self energy part $\underline{\mathcal{S}}(\infty)$.

The zeroth order degeneracy of K and Y -states is lifted in the spectral representation of the fully interacting Green’s function. The exact eigenstates decouple to yield N -particle states in the second component and tensor products of $N-1$ and $N+1$ -particle states in the third component. We will come back to discuss the meaning of the degenerate states $|K_{\alpha n}^{(ph)}\rangle$ in connection with the lowest order of the static self energy $\underline{\mathcal{S}}(\infty)$ in Sec. V.

Apart from the K -states there are other zeroth-order states outside the primary space that couple to Y -states. These are made up from higher excitations of the components of the zeroth-order Y -states of Eq. (48). E. g., there are states with a two-particle-two-hole configuration $a_n^\dagger a_{n'}^\dagger a_{\alpha'} a_\alpha |\Phi_0^N\rangle$ in

the first or in the second component, states with a tensor product of a two-hole-one-particle with a particle configuration in the third component, etc. All these states contribute in second order to the dynamic self energy and higher excitations contribute in higher orders to the self energy, like it is the case for the single-particle Green's function.

For completeness we would like to remark that the K -states can also be written as extended states of the form $|A, B\rangle$ according to definition (1). For convenience we introduce the particle number operator $N^{\text{Op}} = \sum_i a_i^\dagger a_i$ and define $m = (N^{\text{Op}} - N)^2 + 1$, where N is the number of particles in the state $|\Psi_0^N\rangle$. Then the K -states can be written as $|K_{\alpha n}^{(ph)}\rangle = \sqrt{2} |a_\alpha^\dagger, a_n m^{-1}\rangle^{(0)}$.

D. First order self energy

The first order of the particle-hole self energy is readily obtained from the expression (68) by replacing the reference states $|\Psi_0^N\rangle$ and $|\varphi\rangle$ by their zeroth orders $|\Phi_0^N\rangle$ and $|\varphi^{(0)}\rangle$, respectively, and by considering the interaction part \hat{H}_1 of the associated super-operator \hat{H} . We obtain

$$\left[\underline{\underline{H}}_{aa}^{(1)} \right]_{rs, r's'} = (a_r^\dagger, a_s | \hat{H}_1 | a_{r'}^\dagger, a_s') \left| \begin{array}{c} |\Psi_0^N\rangle \rightarrow |\Phi_0^N\rangle \\ |\varphi\rangle \rightarrow |\varphi^{(0)}\rangle \end{array} \right. \quad (77)$$

In a recent publication we have investigated this first order approximation to the particle-hole self energy for the choice $|\varphi\rangle = |\Psi_0^N\rangle$ for the reference state $|\varphi\rangle$ and starting from a Hartree-Fock zeroth order [21]. This particular approximation to the particle-hole self energy is referred to as **First Order Static Excitation Potential (FOSEP)**. In terms of the matrix elements of the Hamiltonian the FOSEP approximation of the primary block $\underline{\underline{H}}_{aa}$ reads

$$\left[\underline{\underline{H}}_{aa}^{\text{FOSEP}} \right]_{rs, r's'} = (\varepsilon_r - \varepsilon_s) \delta_{rr'} \delta_{ss'} + V_{rs'[sr']} (\bar{n}_r n_s - n_r \bar{n}_s) (\bar{n}_{r'} n_{s'} - n_{r'} \bar{n}_{s'}). \quad (78)$$

Here, n_r denotes the occupation number of the orbital with index r in the ground state Slater determinant $|\Phi_0^N\rangle$, while $\bar{n}_r = 1 - n_r$ is the anti-occupation number. The eigenvalues of this hermitian matrix yield approximations for the excitation energies of the system under study while the eigenvectors can be used to approximate transition moments. Since the FOSEP approximation has been studied in detail in reference [21], we will only summarise the most important properties in this paragraph.

The matrix that has to be diagonalised $\underline{\underline{H}}_{aa}^{\text{FOSEP}}$ has the dimension of the primary space like discussed in Chapter III. It is labelled by pairs of indices which comprise the full set of single-particle orbitals each. Like it has been

done before, the index pairs can be classified as hh , ph , hp , and pp with respect to the occupation of the orbitals in the ground state Slater determinant $|\Phi_0^N\rangle$. This classification superposes a four by four block structure to the matrix $\underline{\underline{H}}_{aa}^{\text{FOSEP}}$. It can be seen easily from Eq. (78) that the hh - hh and the pp - pp blocks are diagonal and decouple from the rest:

$$\left[\underline{\underline{H}}_{aa}^{\text{FOSEP}} \right] = \begin{pmatrix} * & 0 & 0 & 0 \\ 0 & * & * & 0 \\ 0 & * & * & 0 \\ 0 & 0 & 0 & * \end{pmatrix} \begin{matrix} \leftarrow hh \\ \leftarrow ph \\ \leftarrow hp \\ \leftarrow pp \end{matrix} \quad (79)$$

Since the zeroth order extended states $|a_r^\dagger, a_s\rangle^{(0)}$ of Eq. (48) that are used as basis give physical contributions only in the ph part of the index space, the decoupled hh and pp blocks do not have to be considered and a matrix eigenvalue problem comprising the ph and hp blocks remains:

$$\underline{\underline{M}}^{\text{FOSEP}} \underline{x} = \omega \underline{x}, \quad (80)$$

$$\text{with } \underline{\underline{M}}^{\text{FOSEP}} = \underline{\underline{H}}_{aa}^{\text{FOSEP}} \Big|_{ph \text{ and } hp \text{ blocks}} \quad (81)$$

The resulting eigenvectors have to be classified into so-called **physical** and **unphysical eigenvectors** according to the association with the zeroth order ph or hp states. Usually the physical eigenvalues are positive and well separated from the negative, unphysical ones.

The FOSEP approximation has to be compared with two other well-known first order approximation schemes, the Tamm-Dancoff approximation (TDA) [11,30] and the random phase approximation (RPA) [31,32,11,30]. The TDA leads to a hermitian eigenvalue problem of half the dimension of FOSEP. In fact the upper left (ph - ph) block of the FOSEP matrix $\underline{\underline{M}}^{\text{FOSEP}}$ coincides with the matrix that is diagonalised in the TDA. In this respect FOSEP can be seen as an extension of the TDA. The same holds for the RPA which has the same matrix size as FOSEP but poses a non-hermitian eigenvalue problem. Thus instabilities, which are avoided in FOSEP, can occur in the RPA and lead to complex eigenvalues.

The TDA for excitation energies yields the difference between the energies of the Hartree-Fock ground state and excited states which are correlated by single-excitation configuration interaction (SCI). A perturbation theoretical analysis shows that the TDA energies are consistent in first order with Rayleigh-Schrödinger perturbation theory and contain part of the second order correlation of the excited states [33]. FOSEP also shows these features and additionally takes into account part of the second order ground state correlation while the RPA proves inconsistent by containing second order ground state

correlation with the wrong sign. From the second order analysis it can thus be concluded that the FOSEP energies will generally lie above the TDA energies due to consideration of ground state correlation while the RPA energies will be lower.

These findings are also supported by the results of a simple, exactly solvable model (Hubbard model for H_2) where the ground state is correlated while the singly excited states are not [21]. For this model, the RPA yields bad results collapsing to complex eigenvalues for certain choices of the model parameters while the FOSEP approximation even gives the exact excitation energies.

Some numerical tests on small molecules have been performed by F. Tarantelli [34], which also support the perturbation theoretical results. While in most cases FOSEP yields comparable results to the RPA, there are examples, like the lowest (triplet) excitation energy of Ethylene (C_2H_4), where the RPA fails by one order of magnitude while FOSEP yields a reasonable approximation of the experimental value improving considerably upon the TDA. This situation resembles the results on the earlier mentioned Hubbard model of H_2 .

The FOSEP method can also be used to calculate approximate transition moments. For a given transition operator T , the transition moment $\langle \Psi_m | T | \Psi_0^N \rangle$ is defined by the matrix element of T between the exact excited state $|\Psi_m\rangle$ and the ground state $|\Psi_0^N\rangle$. Analysing this approximation by perturbation theory shows that the FOSEP approximation yields a consistent first-order description. So does the RPA while the TDA transition moments only describe the zeroth order correctly. One point that is often brought up in favour of the RPA is that it exactly preserves the equivalence of the length and the velocity forms of the transition moments of the dipole operator. It is indeed an unusual feature for a perturbation theory based approximation scheme to preserve this equivalence because it is not fulfilled in the Hartree-Fock approximation, which defines the zeroth order. Introducing the usual perturbation parameter in the Hamiltonian by $H = H_0 + \lambda H_1$, we see that the perturbation expansion for the difference Δ_m between the length and the velocity forms does not vanish identically as a function of λ but only disappears for $\lambda = 1$. The FOSEP approximation consistently describes this behaviour through first order and a discrepancy to the exact function $\Delta_m(\lambda)$ of second order remains. The RPA to the function $\Delta_m(\lambda)$ is in principle of the same first order quality but possesses the peculiar property to vanish exactly for $\lambda = 1$ when the transition moments are computed using a complete single-particle basis [35]. This property can be regarded unique to the RPA. Indeed, Hansen and Bouman [36] have shown that the RPA equations with their special non-hermitian structure may be derived from a configuration interaction representation of the ground and excited state wave function, requiring conditions which are a straightforward generalisation of the equivalence of the

length and the velocity forms.

E. First order extended eigenvalue problem and RPA

We consider the same first order approximation to the primary block \underline{H}_{aa} which defines the FOSEP approximation taking additionally into account the coupling to the K -states defined by Eq. (74). Considering the states $|K_{an}^{(ph)}\rangle$ as a minimal extension of the primary set of extended states $\{|Y_{rs}^{(ph)}\rangle\}$ we get additionally the block \underline{H}_{bb} and the coupling blocks \underline{H}_{ab} and \underline{H}_{ba} . The matrix elements up to first order are given by

$$[\underline{H}_{ba}]_{\alpha m, rs}^{(1)} = \langle K_{\alpha m}^{(ph)} | \mu \hat{H} | Y_{rs}^{(ph)} \rangle^{(0)} = -\sqrt{2} V_{\alpha s[rm]} (n_r - n_s), \quad (82)$$

$$[\underline{H}_{bb}]_{\alpha m, \alpha' m'}^{(0)+(1)} = -\delta_{\alpha\alpha'} \delta_{mm'} (\varepsilon_\alpha - \varepsilon_m) - 2V_{\alpha m'[\alpha' m]}. \quad (83)$$

Taking into account the block structure of the \underline{H}_{aa} block which is approximated by $\underline{H}^{\text{FOSEP}}$ of Eqs. (78) and (79), it can be seen that the pp - pp and the hh - hh blocks of the primary part do not couple to the K -states. Thus the structure of the present approximation to the matrix \underline{H} is as follows:

$$\underline{H}^{\text{ext}} = \begin{pmatrix} * & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & * \\ 0 & * & * & 0 & * \\ 0 & 0 & 0 & * & 0 \\ 0 & * & * & 0 & * \end{pmatrix} \begin{matrix} \leftarrow hh \\ \leftarrow ph \\ \leftarrow hp \\ \leftarrow pp \\ \leftarrow K(hp) \end{matrix}. \quad (84)$$

Dropping the non-coupling hh and pp rows and columns we are left with a 3×3 matrix of square blocks of the same dimension which can be written in the following way:

$$\underline{M}^{\text{ext}} = \begin{pmatrix} \underline{\varepsilon}^{ph} + \underline{V} & \underline{W} & \sqrt{2}\underline{W} \\ \underline{W} & -\underline{\varepsilon}^{ph} + \underline{V} & \sqrt{2}\underline{V} \\ \sqrt{2}\underline{W} & \sqrt{2}\underline{V} & \underline{\varepsilon}^{ph} + 2\underline{V} \end{pmatrix} \begin{matrix} \leftarrow ph \\ \leftarrow hp \\ \leftarrow K(hp) \end{matrix}. \quad (85)$$

Here the zeroth order matrix $\underline{\varepsilon}^{ph}$ and the first order coupling blocks \underline{V} , \underline{W} are defined by their matrix elements:

$$[\underline{\varepsilon}^{ph}]_{n\alpha, m\beta} = \delta_{nm} \delta_{\alpha\beta} (\varepsilon_n - \varepsilon_\alpha), \quad (86)$$

$$[\underline{V}]_{n\alpha, m\beta} = V_{n\beta[\alpha m]}, \quad (87)$$

$$[\underline{W}]_{n\alpha, m\beta} = -V_{nm[\alpha\beta]}. \quad (88)$$

The representation (85) of the extended FOSEP matrix follows directly from Eqs. (78), (82), and (83) by renumbering the rows and columns of the blocks in the hp and the $K(hp)$ row and under the assumption that the matrix elements of the two-body interaction V_{ijkl} are real and thus $V_{ijkl} = V_{klij}$.

The corresponding eigenvalue problem for the matrix $\underline{\underline{M}}^{\text{ext}}$ that remains reads

$$\underline{\underline{M}}^{\text{ext}} \underline{x} = \omega \underline{\underline{S}} \underline{x}, \quad (89)$$

where the diagonal overlap matrix $\underline{\underline{S}}$ is given by the proper part of the matrix $\underline{\underline{\mu}}$ of Eq. (31) which reads in block matrix notation

$$\underline{\underline{S}} = \begin{pmatrix} \underline{1} & 0 & 0 \\ 0 & \underline{1} & 0 \\ 0 & 0 & -\underline{1} \end{pmatrix} \begin{array}{l} \leftarrow ph \\ \leftarrow hp \\ \leftarrow K(hp) \end{array}. \quad (90)$$

The eigenvalue problem (89) can be transformed without changing the eigenvalues with the help of an orthonormal transformation with respect to the metric $\underline{\underline{S}}$:

$$\underline{\underline{T}}^\dagger \underline{\underline{S}} \underline{\underline{T}} = \underline{\underline{S}}. \quad (91)$$

With the help of the inverse matrix

$$\underline{\underline{T}}^{-1} = \underline{\underline{S}}^{-1} \underline{\underline{T}}^\dagger \underline{\underline{S}}, \quad (92)$$

Eq. (89) can be reformulated to yield

$$\underline{\underline{T}}^\dagger \underline{\underline{M}}^{\text{ext}} \underline{\underline{T}} \underline{\underline{T}}^{-1} \underline{x} = \omega \underline{\underline{T}}^\dagger \underline{\underline{S}} \underline{\underline{T}} \underline{\underline{T}}^{-1} \underline{x}. \quad (93)$$

Introducing

$$\underline{\underline{M}}' = \underline{\underline{T}}^\dagger \underline{\underline{M}}^{\text{ext}} \underline{\underline{T}}, \quad (94)$$

$$\underline{x}' = \underline{\underline{T}}^{-1} \underline{x}, \quad (95)$$

we obtain the transformed equation

$$\underline{\underline{M}}' \underline{x}' = \omega \underline{\underline{S}} \underline{x}'. \quad (96)$$

The particular choice

$$\underline{\underline{T}} = \begin{pmatrix} \underline{1} & 0 & 0 \\ 0 & \sqrt{2}\underline{1} & \underline{1} \\ 0 & \underline{1} & -\sqrt{2}\underline{1} \end{pmatrix} \begin{array}{l} \leftarrow ph \\ \leftarrow hp \\ \leftarrow K(hp) \end{array} \quad (97)$$

of the transformation matrix applied to the eigenvalue problem (89) leads to a further decoupling in the secular matrix

$$\underline{\underline{M}}^{\text{ext}} = \begin{pmatrix} \underline{\underline{\varepsilon}}^{ph} + \underline{\underline{V}} & 0 & -\underline{\underline{W}} \\ 0 & -\underline{\underline{\varepsilon}}^{ph} & 0 \\ -\underline{\underline{W}} & 0 & \underline{\underline{\varepsilon}}^{ph} + \underline{\underline{V}} \end{pmatrix}. \quad (98)$$

Dropping the decoupled central row and column, the following 2×2 block matrix eigenvalue problem remains:

$$\begin{pmatrix} \underline{\underline{\varepsilon}}^{ph} + \underline{\underline{V}} & -\underline{\underline{W}} \\ -\underline{\underline{W}} & \underline{\underline{\varepsilon}}^{ph} + \underline{\underline{V}} \end{pmatrix} \underline{\underline{x}}'' = \omega \begin{pmatrix} \frac{1}{0} & 0 \\ 0 & -\frac{1}{0} \end{pmatrix} \underline{\underline{x}}''. \quad (99)$$

This is identical to the RPA eigenvalue problem which has been presented in similar notation in Refs. [21] and [37]. A thorough comparison to the FOSEP approximation has been made in Ref. [21].

Concluding, we have shown that the present approximation $\underline{\underline{H}}_{aa}^{\text{ext}}$ to the matrix $\underline{\underline{H}}$ leads to the RPA. In terms of the self energy, the present approach consists of a first order static part of the self energy like in the FOSEP approximation and additionally to that part of the dynamic self energy comprising the K -states which are in zeroth order degenerate to parts of the primary (static) block.

It can also be shown that an approximation of the transition moments with the physical solutions of the $\underline{\underline{H}}^{\text{ext}}$ eigenvalue problem yields the RPA for the transition moments. The transition moments thus have all the RPA properties like, e. g., the exact equivalence of length and velocity form.

VI. STATIC SCATTERING POTENTIALS

In this chapter we will further discuss the static self energy of the extended two-particle Green's function. We have shown in a previous paper that the self energy of this propagator is an optical potential for elastic scattering of two-particle projectiles [10]. It is a well known fact that optical potentials are non-unique [8]. Thus it is useful to investigate the properties of a given optical potential critically from the formal, practical, and intuitive point of view. In the following we will try to illuminate the physical significance of the static self energy by viewing it as a static scattering potential. A strong analogy can here be drawn from the well established Green's function optical potential for single-particle scattering, which we will start with. We also compare with the alternative description by Feshbach's optical potential. The discussion of single-particle optical potentials then helps us to identify terms of the particle-particle self energy. Considering Coulomb-interacting particles and presenting

the static self energy in position space allows us to motivate the important terms in the static part of the optical potentials. Finally, the interpretation of the static self energy in the light of a scattering potential will also be transferred to the particle-hole self energy.

A. Optical potentials for single-particle scattering

We begin with the physical situation of scattering a single particle off an N -particle target in its ground state $|\Psi_0^N\rangle$. All particles are indistinguishable fermions and we only consider the elastic scattering channel where the out-asymptotes leave the target in its ground state. The influences of the interaction of the projectile particle with the many-body target can be accounted for by a so-called optical potential [3] that is a potential in the single-particle space and allows one to solve single-particle scattering equations that still give the exact results with all many-body effects included. This optical potential has to be non-local in order to describe exchange phenomena and has to depend on the energy of the incident particles in order to correctly describe the many-body interactions which can lead to resonances. Furthermore the optical potential is in general a non-hermitian operator in order to take account of the loss of scattering amplitude into inelastic channels.

1. Green's function optical potential

It has been shown by Bell and Squires [4] that the self energy $\underline{\Sigma}(\omega)$ of the single-particle Green's function represents an exact optical potential for elastic single-particle scattering. In an analogous way to Sec. III, the usual Dyson equation defining the single-particle self energy can be derived by a projection onto the span of the orthonormal primary set of states [26,9]

$$|Y_p^{(G)}\rangle = \begin{pmatrix} a_p^\dagger |\Psi_0^N\rangle \\ \langle \Psi_0^N | a_p \end{pmatrix}. \quad (100)$$

The formal analogy between the derivation of Dyson's equation for the single-particle Green's function and the extended two-particle Green's functions has been the original motivation for the construction of the present two-particle formalism and is discussed in detail in Ref. [10]. Here we only want to mention that the definition of the Green's function (29) and the expressions for the inverse Green's function (36) and the self energy (38) hold as well for the single-particle Green's function $G_{pq}(\omega)$ and self energy $\Sigma_{pq}(\omega)$ when the states $|Y_p^{(G)}\rangle$ replace the extended states $|Y_{rs}\rangle$ and the metric μ is replaced by unity.

Thus, the single-particle Green's function $\underline{\underline{G}}(\omega)$ can be written as the resolvent of an energy-dependent effective Hamiltonian:

$$\underline{\underline{G}}(\omega) = \frac{1}{\omega \underline{\underline{1}} - \underline{\underline{H}}_{aa}^{(G)(0)} - \underline{\underline{\Sigma}}(\omega)}. \quad (101)$$

We will now take a closer look at the static part of the Green's function optical Hamiltonian

$$\mathcal{R}_{pq}^{(G)} := \left[\underline{\underline{H}}_{aa}^{(G)(0)} \right]_{pq} + \Sigma_{pq}(\infty) = \langle \Psi_0^N | \left[a_p \left[H, a_q^\dagger \right]_- \right]_+ | \Psi_0^N \rangle. \quad (102)$$

The commutators of the creation and destruction operators with the Hamiltonian H are readily evaluated and we are left with the expression

$$\mathcal{R}_{pq}^{(G)} = \varepsilon_p \delta_{pq} + v_{pq} + \mathcal{V}_{pq}^{(G)} \quad (103)$$

for the static part of the Green's function optical Hamiltonian. The first two terms on the right hand side are easily interpreted as the influence of the single-particle part of the Hamiltonian like the kinetic energy and external forces on the projectile particle. The third term

$$\begin{aligned} \mathcal{V}_{pq}^{(G)} &= \langle \Psi_0^N | \left[a_p \left[V, a_q^\dagger \right]_- \right]_+ | \Psi_0^N \rangle \\ &= \sum_{kl} V_{pk[ql]} \rho_{lk} \end{aligned} \quad (104)$$

accounts for two-body interactions between the projectile and the target particles. The single-particle density ρ_{ij} is defined by

$$\rho_{ij} = \langle \Psi_0^N | a_j^\dagger a_i | \Psi_0^N \rangle. \quad (105)$$

This two-body interaction part of the static self energy becomes even more intuitive, when we consider a local interaction potential and transform the formulas into position space. Take, e. g., Coulomb interacting electrons where the matrix elements read

$$V_{r_1 r_2 r'_1 r'_2} = \frac{\delta_{r_1 r'_1} \delta_{r_2 r'_2}}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (106)$$

in position-space representation. The indices $r = (\mathbf{r}, \sigma)$ are composed of the spatial part \mathbf{r} and spin part σ and adequately the delta function becomes $\delta_{rr'} := \delta(\mathbf{r} - \mathbf{r}') \delta_{\sigma\sigma'}$.

In position space the interaction part of the static Green's function optical Hamiltonian (or the static self energy) reads

$$\mathcal{V}_{rr'}^{(G)} = \delta_{rr'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r} - \mathbf{r}_1|} - \frac{\rho_{rr'}}{|\mathbf{r} - \mathbf{r}'|}, \quad (107)$$

where the integration is taken to run over the three-dimensional coordinate space and to additionally include summation over the spin part. $\rho_r = \rho_{rr}$ denotes the diagonal part of the single-particle density. Of course, the spin part is easily accounted for in the case of a singlet ground state and a purely spatial interaction part remains [38]:

$$\mathcal{V}^{(G)}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \int d\mathbf{r}_1 \frac{\rho(\mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|} - \frac{\rho(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \quad (108)$$

It becomes evident that the static self energy describes the Coulomb repulsion of the projectile electron by the static charge density of the target, the effect of which is diminished by the possibility of exchange of the projectile particle with one of the target particles described by the second term. If the target is approximated by a Slater determinant, the static entity $\underline{\mathcal{R}}^{(G)}$ approximates the projectile-target interaction on the so called **static exchange** level. Taking $\underline{\mathcal{R}}^{(G)}$ with a correlated ground state density instead is known as the **correlated static exchange** approximation [39–41]. Of course, these approximations cannot account for effects due to the response of the target's wavefunction to the incident projectile particle. These effects are called dynamic effects and are described by the dynamic part of the self energy.

2. Feshbach's optical potential

The optical model potential of Feshbach [2] was the first, rigorously derived optical potential. There exist, however, an infinite number of physically equivalent yet mathematically distinct optical potentials. A thorough examination of the mathematical properties of various kinds of single-particle optical potentials has been given by Capuzzi and Mahaux [8]. An equivalent reformulation of the original effective Hamiltonian used by Feshbach including the single-particle kinetic energy and optical potential reads in matrix notation

$$\underline{\underline{h}}^{(F)}(E) = [\underline{\mathcal{R}}^{(F)} + \underline{\mathcal{D}}(E)]\underline{\underline{\sigma}}^{-1}. \quad (109)$$

The connection to the original formulas of Feshbach [2] is established in Ref. [8]. The matrix $\underline{\underline{\sigma}}$ is the difference between the unit matrix and the single-particle ground state density with the matrix elements

$$\begin{aligned} \sigma_{pq} &= \langle \Psi_0^N | a_p a_q^\dagger | \Psi_0^N \rangle \\ &= \delta_{pq} - \rho_{pq}. \end{aligned} \quad (110)$$

Note that the eigenvalues of this matrix are just one minus the natural occupations of the target's ground state. If the target does contain an uncorrelated hard core, the matrix $\underline{\sigma}$ cannot be inverted in the full space of single-particle indices. Rather one has to exclude the hard core explicitly from the accessible space for the projectile's wave function. In the important special case where the target wave function is a Slater determinant, the matrix $\underline{\sigma}$ becomes a projector onto the virtual orbital space.

The matrix $\underline{\mathcal{R}}^{(F)}$ is what we call the static part of the Feshbach Hamiltonian. It is defined by the matrix elements

$$\mathcal{R}_{pq}^{(F)} = \langle \Psi_0^N | a_p [H, a_q^\dagger]_- | \Psi_0^N \rangle. \quad (111)$$

The dynamic part $\underline{D}(E)$, which can be found in the literature [8], possesses poles related to resonances of two-particle-hole and higher excitations and a branch cut above the ionisation threshold. It has an analytic structure similar to the dynamic self energy (42) from the formal point of view. This is not surprising since the projection method for deriving the Feshbach Hamiltonian is formally similar to the derivation of Dyson's equation of Sec. III or in Refs. [26,9]. There, a partitioning was performed yielding a projection to the primary space spanned by the orthonormal Y -states while Feshbach, on the other hand, projected onto the space spanned by the non-orthonormal states $a_r^\dagger | \Psi_0^N \rangle$.

Like we have done for the Green's function optical potential we can also evaluate the static part $\mathcal{R}_{pq}^{(F)}$ of Feshbach's optical Hamiltonian:

$$\mathcal{R}_{pq}^{(F)} = \varepsilon_p \sigma_{pq} + \sum_j v_{pj} \sigma_{jq} + \mathcal{V}_{pq}^{(F)}, \quad (112)$$

with

$$\mathcal{V}_{pq}^{(F)} = \langle \Psi_0^N | [a_p, V]_- a_q^\dagger | \Psi_0^N \rangle. \quad (113)$$

First we note that the $\underline{\sigma}$ matrices cancel with their inverse in Eq. (109), leaving the same single-particle part as for the Green's function optical potential. The interaction part $\mathcal{V}_{pq}^{(F)}$, however, differs from its Green's function analogue $\mathcal{V}_{pq}^{(G)}$ of Eq. (107) by involving the two-particle density

$$\gamma_{ijkl} = \langle \Psi_0^N | a_l^\dagger a_k^\dagger a_i a_j | \Psi_0^N \rangle \quad (114)$$

of the target's ground state. The two-particle density comes into play because the expectation value $\langle \Psi_0^N | [a_p, V]_- a_q^\dagger | \Psi_0^N \rangle$ contains products of three creation and three destruction operators. While one of each is cancelled by the commutator, a two-particle density remains. Considering the fact that the two-particle density of Slater determinants factorise into single-particle densities according to

$$\gamma_{ijkl}^{\text{Sd}} = \rho_{ik}\rho_{jl} - \rho_{il}\rho_{jk}, \quad (115)$$

we may introduce the reminiscent two-particle density

$$\tilde{\gamma}_{ijkl} = \gamma_{ijkl} - \gamma_{ijkl}^{\text{Sd}}. \quad (116)$$

This allows to further simplify $\mathcal{R}_{pq}^{(\text{F})}$ to yield

$$\mathcal{R}_{pq}^{(\text{F})} = \sum_i \mathcal{R}_{pi}^{(\text{G})} \sigma_{iq} + \sum_{jkl} \tilde{\gamma}_{plji} V_{ijlq}. \quad (117)$$

In the case of an uncorrelated (Slater determinantal) target, the static part of the Feshbach Hamiltonian (109) thus reduces to the well-known static exchange approximation. For correlated targets, however, there remains a term due to the non-factorising part of the two-particle density $\tilde{\gamma}_{plji}$ which is not easily interpretable by intuition. We therefore conclude that the Green's function optical potential, which is well defined in the full single-particle space also for hard-core potentials, provides the simpler to compute and more intuitive static part than the Feshbach optical potential. For completeness we would like to mention that the Feshbach approach also has more difficulties with the dynamic part in showing a more complicated energy dependence and nonlocality in studies of nuclear matter, at least at low energy [8,42].

B. Two-particle scattering

We have shown in Ref. [10] that the self energy of the extended particle-particle Green's function $\underline{\mathcal{G}}^{(pp)}(\omega)$ serves as an exact optical potential for elastic scattering of two particle-projectiles by a many-body target. In a situation where both projectile particles are asymptotically free, one may choose the kinetic energy as the zeroth order Hamiltonian H_0 . The effective Hamiltonian in the two-particle space then is given as usual as a sum of the zeroth order part $\underline{H}_{aa}^{(pp)(0)}$, which is now the kinetic energy for the projectile particles, and the self energy $\underline{\mathcal{S}}^{(pp)}(E)$ taking account for the full interaction. Interaction now occurs between the projectile particles, between the projectile and the target particles, within the target and with external fields. The static part of the optical Hamiltonian is given by

$$\mathcal{R}_{rs,r's'}^{(pp)} = \left[\underline{H}_{aa}^{(pp)} \right]_{rs,r's'} = (a_r^\dagger, a_s^\dagger | \hat{H} | a_{r'}^\dagger, a_{s'}^\dagger). \quad (118)$$

Again, the contributions of the single-particle part of the Hamiltonian H may be split off easily due to the linearity $\hat{H} = \hat{H}_0 + \hat{v} + \hat{V}$ of the super-operators:

$$\mathcal{R}_{rs,r's'}^{(pp)} = (\epsilon_r + \epsilon_s)(\delta_{rr'}\delta_{ss'} - \delta_{rs'}\delta_{rs'}) + \mathcal{S}_{rs,r's'}(\infty), \quad (119)$$

with

$$\mathcal{S}_{rs,r's'}^{(pp)}(\infty) = v_{rr'}\delta_{ss'} + \delta_{rr'}v_{ss'} - v_{rs'}\delta_{rs'} - \delta_{rs'}v_{rs'} + \mathcal{V}_{rs,r's'}^{(pp)}. \quad (120)$$

Thus the kinetic energy and the influence of external forces is already described exactly by the static part of the optical Hamiltonian and independent of approximations for the target wavefunction. Note that the possibility for two particles labelled by r and s to exchange can be seen explicitly in the kinetic energy and external field parts of Eqs. (119) and (120) by the terms that antisymmetrise the matrix with respect to interchange of these labels. An expression for the interaction part $\mathcal{V}_{rs,r's'}^{(pp)}$ contained in the static self energy is gained by applying the definitions of Sec. II:

$$\begin{aligned} \mathcal{V}_{rs,r's'}^{(pp)} &= (a_r^\dagger, a_s^\dagger | \hat{V} | a_{r'}^\dagger, a_{s'}^\dagger) \\ &= \langle \Psi_0^N | [a_s a_r, [V, a_{r'}^\dagger a_{s'}^\dagger]_-]_- | \Psi_0^N \rangle + \\ &\quad \left\{ \langle \varphi | [[V, a_{r'}^\dagger]_-, a_r]_+ | \varphi \rangle \langle \Psi_0^N | a_{s'}^\dagger a_s | \Psi_0^N \rangle + \right. \\ &\quad \left. \delta_{ss'} \langle \Psi_0^N | [V, a_{r'}^\dagger]_+ a_r | \Psi_0^N \rangle \right\} - \\ &\quad \left\{ r \leftrightarrow s \right\} - \left\{ r' \leftrightarrow s' \right\} + \left\{ r \leftrightarrow s \ \& \ r' \leftrightarrow s' \right\}, \end{aligned} \quad (121)$$

where the term in braces reappears three more times with interchanged indices as indicated in the last line of Eq. (121). When we again consider the case of Coulomb-interacting electrons and transform Eq. (121) into position space, we get a large number of terms due to the many possibilities of the two electrons to exchange with each other and with the target particles. All terms are written down in App. B. Here we will only motivate some important ones.

Firstly, one certainly expects terms describing the direct repulsion of the two projectile particles as well as the Coulomb interaction of both particles with the static charge density of the target. These terms also arise if the projectile particles are distinguishable from the target, e.g. for positrons. In order to isolate these terms we introduce positronic creation and destruction operators c_r^\dagger and c_r which commute with the electronic operators a_r^\dagger and a_r . Including the Coulomb interactions of the positrons using the interaction operator $V_{\text{composite}}$ for the composite electron-positron system (taken from Ref. [43]), we obtain the following expression for the interaction part of the static self energy of the extended two-positron Green's function:

$$\mathcal{V}_{rs,r's'}^{(\text{positrons})} = (c_r^\dagger, c_s^\dagger | \hat{V}_{\text{composite}} | c_{r'}^\dagger, c_{s'}^\dagger)$$

$$\begin{aligned}
&= (\delta_{rr'}\delta_{ss'} - \delta_{rs'}\delta_{rs'}) \left(\frac{1}{|\mathbf{r} - \mathbf{s}|} \right. \\
&\quad \left. - \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{r}|} - \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{s}|} \right). \quad (122)
\end{aligned}$$

This is a very intuitive result showing that the static particle-particle self energy incorporates the full two-body interaction between both projectile particles as well as the Coulomb interaction with the static charge density of the target. The possibility of exchange between the projectile particles is explicitly present in Eq. (122) through the antisymmetric delta functions.

Returning to the problem of scattering projectile particles that are indistinguishable from the target particles, we can expect additional exchange terms. These terms do indeed occur and a straightforward evaluation of Eq. (121) yields nine different terms:

$$\begin{aligned}
(a_r^\dagger, a_s^\dagger | \hat{V} | a_{r'}^\dagger, a_{s'}^\dagger) &= A + B + C + D + E + F + G + I + J \\
&\quad - (r \leftrightarrow s) - (r' \leftrightarrow s') + (r \leftrightarrow s \& r' \leftrightarrow s'). \quad (123)
\end{aligned}$$

As mentioned before, all terms are written down in App. B. Note that outside of the target, i. e. when the positions r , r' , s , and s' of the projectile particle are such that the target's particle densities vanish, only the terms A and B with their antisymmetric combinations survive. These terms exactly reproduce Eq. (122) except for the obvious change of sign of the projectile-target Coulomb interaction.

Of the remaining terms, $C = -\delta_{ss'} \frac{\rho_{rr'}}{|\mathbf{r} - \mathbf{r}'|}$ is most easily identified as the kind of exchange interaction of a single projectile particle with the target that already appeared in the case of single-particle scattering in Eq. (107). All the other terms have to be attributed either to the possibility of simultaneous projectile-projectile Coulomb interaction with projectile-target exchange ($D - G$) or projectile-target exchange occurring along with the projectile-target Coulomb interaction (I and J). The occurrence of two-particle densities in terms F and I appears quite natural in this context although the intuitive interpretation of these mixed or simultaneous exchange terms remains obscure.

Note that the terms G and J are proportional to the single-particle density $\rho_{ij}^0 = \langle \varphi | a_j^\dagger a_i | \varphi \rangle$ of the secondary reference state $|\varphi\rangle$ that was introduced in the definition (1) of the extended states $|A, B\rangle$. The choice of this reference wavefunction is arbitrary for the algebraic properties of the extended wavefunction and, in particular, for the derivation of the Dyson equation. Here it obviously introduces differences and the freedom of choice can be used to change the static self energy. The only condition that $|\varphi\rangle$ has to comply with in order to have the full formalism at hand, is to be an eigenfunction of the Fock-space Hamiltonian H (c. f. Sec. IIC). The two obvious choices for $|\varphi\rangle$

are the target state $|\Psi_0^N\rangle$ and the Fock-space vacuum $|\text{vac}\rangle$. Choosing the vacuum, the terms G and J vanish because the particle density in the vacuum is zero. This choice was used in Ref. [10]. Choosing instead the target's ground state $|\Psi_0^N\rangle$, the terms G and J look similar to terms F and I , respectively, which involve two-particle densities appearing with a different sign.

Like in the case of single-particle scattering, there are other possibilities of defining optical potentials. Without going into detail we want to mention that an analogous expression to the Feshbach effective Hamiltonian (109) can be derived for two-particle scattering. The static part $\underline{\mathcal{R}}^{(F)}$ has now the matrix elements $\mathcal{R}_{rsr's'}^{(F)} = \langle \Psi_0^N | a_s a_r [H, a_{r'}^\dagger a_{s'}^\dagger]_- | \Psi_0^N \rangle$. For positrons as projectile particles (i. e. distinguishable particles from the target) the same result as Eq. (122) is found. In this special case the static particle-particle self energy and the static part of Feshbach's potential are identical. If all particles are indistinguishable fermions, however, $\underline{\mathcal{R}}^{(F)}$ involves three-particle densities that are cumbersome to evaluate and even more difficult to interpret.

C. Particle-hole scattering

In the preceding section we have discussed the static part of the particle-particle self energy as a scattering potential for two-particle scattering by a correlated many-body target. This point of view is justified by the fact that the particle-particle self energy is in fact an exact optical potential for two-particle scattering [10]. Earlier in this paper we have presented a unified formalism comprising three different types of two-particle Green's functions: the extended particle-particle, particle-hole and hole-hole Green's functions. The strong formal analogy between the three cases already hints towards carrying this analogy to the discussion of scattering potentials. Especially the particle-hole case deserves more attention since we know that in extended electronic systems, particles and holes attract each other and may form bound states known as excitons. The excitons then may act as projectiles and scatter off defects, other kinds of interaction centres, or simply because of the presence of electronic correlation.

Looking at the expression for the static part of the effective particle-hole Hamiltonian [which can be evaluated from Eq. (68)] we notice that the kinetic energy part describes two distinguishable particles with masses of opposite sign:²

²Choosing H_0 to be the kinetic energy operator for electrons, the single particle indices p, q in this equation should be read as the momentum space representation

$$(a_p^\dagger, a_q | \hat{H} | a_{p'}^\dagger, a_{q'}) = \delta_{pp'} \delta_{qq'} (\varepsilon_p - \varepsilon_q) + S_{pp'q'q}^{(ph)}(\infty). \quad (124)$$

The interaction with external (one particle) potentials is contained in the static self energy and also shows different signs like for particles carrying opposite charges:

$$S_{pp'q'q}^{(ph)}(\infty) = v_{pp'} \delta_{qq'} - \delta_{pp'} v_{q'q} + (a_p^\dagger, a_q | \hat{V} | a_{p'}^\dagger, a_{q'}). \quad (125)$$

The interaction potential $(a_p^\dagger, a_q | \hat{V} | a_{p'}^\dagger, a_{q'})$ describes the two-particle interactions and may again be simplified by switching to position-space representation. The full expression, however, is still fairly complicated and can be found in App. C. Note that this interaction part of the static self energy simplifies very much when the projectile particles are outside of the target, i. e. where the particle density has dropped to zero. In this "outer" region we are left with the Coulomb interaction of two oppositely charged particles with the target's charge density:

$$(a_r^\dagger, a_s | \hat{V} | a_{r'}^\dagger, a_{s'}) \Big|_{\text{outer region}} = \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{r}|} - \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{s}|}. \quad (126)$$

In the outer region there is no direct coupling between the particle and the hole. However, there are no formal restrictions that prohibit a hole from being outside the target. In regions of vanishing particle density, holes move with negative mass interacting by opposite charge with external potentials and the target's charge density. Inside the target interactions between the particle and the hole arise. This is best seen when the interaction potential is further simplified by assuming that all two particle densities in Eq. (C1) factorise, which is the case if the target's ground state can be described by a Slater determinant. Choosing further the secondary reference state $|\varphi\rangle$ to be the target's wavefunction we arrive at the following expression:

$$\begin{aligned} (a_r^\dagger, a_s | \hat{V} | a_{r'}^\dagger, a_{s'}) \Big|_{\text{factorised}} &= \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{r}|} - \delta_{ss'} \frac{\rho_{rr'}}{|\mathbf{r} - \mathbf{r}'|} \\ &\quad - \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{s}|} + \delta_{rr'} \frac{\rho_{s's}}{|\mathbf{s} - \mathbf{s}'|} \\ &\quad - \delta_{rr'} \int d\mathbf{r}_1 \frac{\rho_{s'r_1} \rho_{r_1 s}}{|\mathbf{r}_1 - \mathbf{r}|} \end{aligned}$$

where the kinetic energy is diagonal. Later we will again switch to position space representation (with indices r and s) where the local Coulomb force simplifies.

$$\begin{aligned}
& -\delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{rr_1} \rho_{r_1 r'}}{|\mathbf{r}_1 - \mathbf{s}|} \\
& + \rho_{rr'} \rho_{s's} \left(\frac{1}{|\mathbf{r} - \mathbf{s}'|} + \frac{1}{|\mathbf{r}' - \mathbf{s}|} \right) \\
& + \mathcal{V}_{rs, r's'}^A.
\end{aligned} \tag{127}$$

Additionally to the terms of Eq. (126) we now have the usual exchange terms (2nd term on the r.h.s) for the particle and an analogous exchange term (4th term) for the hole. The following two terms (5th and 6th) describe attractive forces between the particle and the hole, mediated through the target. In particular if the one-particle densities are almost diagonal this becomes obvious. The next (7th) term has to be interpreted as an exchange correction to the preceding Coulombic terms. The last term is called the “annihilation potential” $\mathcal{V}_{rs, r's'}^A$ and is given by

$$\mathcal{V}_{rs, r's'}^A = \rho_{rs} \rho_{s'r'} \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|} + \frac{1}{|\mathbf{s} - \mathbf{s}'|} - \frac{1}{|\mathbf{r} - \mathbf{s}'|} - \frac{1}{|\mathbf{r}' - \mathbf{s}|} \right). \tag{128}$$

It plays a special role since the single-particle densities involved mix particle (r, r') and hole (s, s') indices. This term thus originates from the possibility of particle-hole excitations to annihilate. Note also that this term vanishes for a target in a singlet state if the particle-hole pair forms a triplet excitation, e.g., if the spins are opposite [$r = (\uparrow, \uparrow)$, and $s = (\downarrow, \downarrow)$].

VII. CONCLUSIONS

In this paper we have presented a general theory of extended two-particle Green's functions and discussed a number of formal properties as well as the physical interpretation of the corresponding static self energies. We have developed a general formalism and used it to define fermionic extended two-particle Green's functions of three categories: particle-hole, particle-particle, and hole-hole functions. An important property of the treated class of Green's functions is that they obey a Dyson equation in analogy to the well-known single-particle Green's function of traditional many-body theory. Many properties of the extended two-particle Green's functions can be explained by this analogy. Dyson's equation defines well-behaved self energies that are amenable to a perturbation theoretical treatment. A further analogy to the single-particle Green's function lies in the property of the two-particle self energy to serve as an optical potential for elastic scattering of two-particle projectiles by a many-body target.

The fundamental construction principle for fulfilling Dyson's equation is to define the Green's function upon an orthonormal set of primary states. In order to achieve this orthonormality property, the physical two-particle states have to be extended by additional, "unphysical" components. The new components introduce additional poles and branch cuts in the analytic structure of the extended Green's functions. When defining the Green's function for real arguments, however, one can still manipulate the singularities by shifting them off the real axis or choosing principle value singularities. Another consequence of the extensions is the occurrence of zeroth-order degenerate states.

In this contribution we have given particular attention to the two-particle self energies. In the special case of a many-particle system without proper inter-particle forces, where the particles only interact with external potentials or by mean fields, the two-particle self energies take on a particularly simple, energy-independent form. The first order of perturbation theory already solves the full problem in strict analogy to the self energy of the single-particle Green's function.

Also for a truly correlated many-body system it turned out that already the first-order static approximation of the self energy yields a well-behaved approximation as we discussed for the particle-hole case. We have compared the resulting FOSEP approximation for excitation energies and transitions moments with two other well-known first order approximation schemes, the RPA and the TDA. It turned out that the FOSEP approximation is not only consistent in first order but also includes parts of the higher order correlation in a consistent manner without showing the instabilities of the RPA. The RPA, on the contrary, treats higher-order ground state correlation in the excitation energies inconsistently while the TDA fails to yield consistent transition moments. Interestingly both the TDA as well as the RPA can be won as specific approximations to our extended particle-hole self energy. The TDA results by exclusion of the zeroth-order unphysical states and the RPA is gained by inclusion of a class of zeroth-order degenerate states.

The static self energy was also examined from a less formal and more physical perspective by viewing it as a static scattering potential. On the example of Coulomb-interacting fermions we interpreted various terms of the static part of the particle-particle self energy by comparison with the Green's function's and Feshbach's optical potentials for single-particle scattering. We could also draw an analogy to the static self energy of the extended particle-hole Green's function. Apart from describing the static projectile-target interactions, also intra-projectile forces mediated by the target are present. One thinkable application of particle-hole optical potentials is the scattering of excitons in extended systems but room is left for physical imagination.

The development of approximations to the two-particle self energies be-

yond the leading order is certainly a challenging task for the future. In this context, additional insight into the structure and meaning of the dynamic self energy parts is needed. The underlying concepts of the presented formalism, in particular the orthonormal primary set of states, which is invariant under a change of the single-particle basis, form a sound basis for developing powerful approximation schemes. These may go beyond single-determinant based perturbation theory because the choice of the primary reference state $|\Psi_0^N\rangle$ in the definition of the extended Green's functions is not restricted in this way. Multi-configuration, coupled-cluster, or density-functional based approximate wave functions may be employed here. The arbitrariness of the secondary reference state $|\varphi\rangle$, on the other hand, may be used to tailor approximation schemes with particular properties.

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APPENDIX A: FORMAL DEFINITION OF THE HILBERT SPACE \mathcal{Y}

The following formal definition of the space \mathcal{Y} refers to a given choice of reference states $|\psi\rangle$ and $|\varphi\rangle$ [as in Eq. (1)] that are proper eigenstates of a given Fock-space Hamiltonian H . The mathematical concepts used in this formal chapter can be found in common textbooks on functional analysis, e. g. Ref. [22].

Definition Given a set of primary states $\mathcal{P} = \{|A, B\rangle \mid A \in \mathcal{A}, B \in \mathcal{B}\}$ defined by sets of Fock-space operators \mathcal{A} and \mathcal{B} , we define the space \mathcal{Y} as the smallest closed linear space containing \mathcal{P} as a subset $\mathcal{P} \subset \mathcal{Y}$ that is closed under action of the extended operator \check{H} , i. e.

$$|y\rangle \in \mathcal{Y} \quad \Rightarrow \quad \check{H}|y\rangle \in \mathcal{Y}. \quad (\text{A1})$$

Notes

- The “smallest” space satisfying the demanded conditions is defined, like usual, as the intersection of all spaces that fulfil the conditions.
- It should become clear that this definition of a minimal space \mathcal{Y} is appropriate because the extended propagators will be defined by matrix elements of the resolvent of \check{H} between primary states. Thus all states that “couple” to the primary states via \check{H} are relevant.

Proposition Together with the canonical inner product of Sec. II A, the space \mathcal{Y} is a Hilbert space.

This can be shown as follows: An arbitrary element $|p\rangle$ of \mathcal{P} is defined [by definition (1)] by direct sums and products of component states $|\phi_i\rangle$:

$$|p\rangle = |\phi_1\rangle \oplus |\phi_2\rangle \oplus |\phi_3\rangle \otimes |\phi_4\rangle \oplus |\phi_5\rangle \otimes |\phi_6\rangle \oplus |\phi_7\rangle \otimes |\phi_8\rangle \oplus |\phi_9\rangle \otimes |\phi_{10}\rangle. \quad (\text{A2})$$

The component states $|\phi_i\rangle$ are elements of physical Hilbert spaces \mathcal{H}_i with given particle number (if the operator sets \mathcal{A} and \mathcal{B} allow). The extended state $|p\rangle$ is thus an element of a composite space \mathcal{C} , given by the following direct sum of tensor product spaces:

$$\mathcal{C} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3 \otimes \mathcal{H}_4 \oplus \mathcal{H}_5 \otimes \mathcal{H}_6 \oplus \mathcal{H}_7 \otimes \mathcal{H}_8 \oplus \mathcal{H}_9 \otimes \mathcal{H}_{10}. \quad (\text{A3})$$

Due to its definition by direct sums and tensor products, the space \mathcal{C} , with the canonical inner product for sums and products of Hilbert spaces, is a Hilbert space itself. Since the Hamiltonian H is a particle number conserving operator (we only consider non-relativistic systems), the application of H to the component state $|\phi_i\rangle$ will not lead out of the corresponding component space \mathcal{H}_i . It is easily seen that also the application of \check{H} to the extended state $|p\rangle$ then does not lead out of the space \mathcal{C} . Thus the above defined linear space \mathcal{Y} is a subspace of \mathcal{C} . A closed subspace of a Hilbert space, however, is a Hilbert space itself. This concludes the proof of the proposition.

Obviously the given definition of a minimal space \mathcal{Y} is not constructive. For most means, however, it is not really necessary to have the minimal space and the space \mathcal{C} can be taken instead. A basis of \mathcal{C} can be easily constructed from Slater determinantal bases of the component spaces \mathcal{H}_i .

APPENDIX B: STATIC PARTICLE-PARTICLE SELF ENERGY FOR ELECTRONS

Here we present all terms of the static particle-particle self energy for Coulomb-interacting electrons. As usual the static self energy is given by

$$\begin{aligned} \mathcal{S}_{rsr's'}^{(pp)}(\infty) &= (a_r^\dagger, a_s^\dagger | \hat{H}_1 | a_{r'}^\dagger, a_{s'}^\dagger) \\ &= \delta_{rr'} v_{ss'} - \delta_{sr'} v_{rs'} - \delta_{rs'} v_{sr'} + \delta_{ss'} v_{rr'} \\ &\quad + (a_r^\dagger, a_s^\dagger | \hat{V} | a_{r'}^\dagger, a_{s'}^\dagger). \end{aligned} \quad (\text{B1})$$

Evaluating the two-particle interaction part $(a_r^\dagger, a_s^\dagger | \hat{V} | a_{r'}^\dagger, a_{s'}^\dagger)$ from Eq. (121), we arrive at nine different terms:

$$(a_r^\dagger, a_s^\dagger | \hat{V} | a_{r'}^\dagger, a_{s'}^\dagger) = A + B + C + D + E + F + G + I + J \\ - (r \leftrightarrow s) - (r' \leftrightarrow s') + (r \leftrightarrow s \& r' \leftrightarrow s'). \quad (\text{B2})$$

Each of the nine terms also appears with interchanged single-particle indices, which is indicated by the second line of Eq. (B2). The static self energy thereby becomes antisymmetric with respect to interchange within the first or second pair of single particle indices. This antisymmetry is due to the indistinguishable nature of the projectile particles. In the position space notation already used in Sec. VI the nine terms read:

$$A = \frac{\delta_{rr'} \delta_{ss'}}{2|\mathbf{r} - \mathbf{s}|}, \quad (\text{B3})$$

$$B = \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{r}|}, \quad (\text{B4})$$

$$C = -\delta_{ss'} \frac{\rho_{rr'}}{|\mathbf{r} - \mathbf{r}'|}, \quad (\text{B5})$$

$$D = -\delta_{ss'} \frac{\rho_{rr'}}{|\mathbf{r} - \mathbf{s}|}, \quad (\text{B6})$$

$$E = -\delta_{ss'} \frac{\rho_{rr'}}{|\mathbf{r}' - \mathbf{s}|}, \quad (\text{B7})$$

$$F = \frac{\gamma_{rsr's'}}{|\mathbf{r} - \mathbf{r}'|}, \quad (\text{B8})$$

$$G = -\rho_{ss'} \frac{\rho_{rr'}^\varphi}{|\mathbf{r} - \mathbf{r}'|}, \quad (\text{B9})$$

$$I = -\delta_{ss'} \int d\mathbf{r}_1 \frac{\gamma_{rr_1r'r_1}}{|\mathbf{r}_1 - \mathbf{s}|}, \quad (\text{B10})$$

$$J = \delta_{ss'} \rho_{rr'} \int d\mathbf{r}_1 \frac{\rho_{r_1}^\varphi}{|\mathbf{r}_1 - \mathbf{s}|}. \quad (\text{B11})$$

Here, ρ_r and $\rho_{rr'}$ denote the diagonal and full single-particle density with respect to the target's ground state $|\Psi_0^N\rangle$ as usual. The superscript φ indicates that the density $\rho_{rr'}^\varphi = \langle \varphi | a_r^\dagger a_r | \varphi \rangle$ is taken with respect to the secondary reference wavefunction $|\varphi\rangle$ [see also the definition of the extended states (1)]. For the choice $|\varphi\rangle = |\Psi_0^N\rangle$ it is identical to the common single-particle density and for $|\varphi\rangle = |\text{vac}\rangle$ these terms vanish. The latter choice was taken for the extended particle-particle Green's function of Ref. [10]. The two particle density γ_{ijkl} is defined in Eq. (114).

APPENDIX C: STATIC PARTICLE-HOLE SELF ENERGY FOR ELECTRONS

In this appendix we present the interaction part ($a_p^\dagger, a_q | \hat{V} | a_{p'}^\dagger, a_{q'}$) of the static particle-hole self energy discussed in Sec. VIC. We assume Coulomb interacting electrons with the usual position space representation (106) of the two-body interaction V . The expression for the interaction part of the static self particle-hole self energy can then be readily evaluated, either from the definitions of the extended states (1) or from Eq. (68):

$$\begin{aligned}
 (a_r^\dagger, a_s | \hat{V} | a_{r'}^\dagger, a_{s'}) &= \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}^\varphi}{|\mathbf{r}_1 - \mathbf{r}|} - \delta_{ss'} \frac{\rho_{rr'}^\varphi}{|\mathbf{r} - \mathbf{r}'|} \\
 &\quad - \delta_{rr'} \delta_{ss'} \int d\mathbf{r}_1 \frac{\rho_{r_1}}{|\mathbf{r}_1 - \mathbf{s}|} + \delta_{rr'} \frac{\rho_{s's}}{|\mathbf{s} - \mathbf{s}'|} \\
 &\quad + \delta_{ss'} \int d\mathbf{r}_1 \frac{\gamma_{rr_1 r' r_1}}{|\mathbf{r}_1 - \mathbf{s}|} - \delta_{ss'} \rho_{rr'} \int d\mathbf{r}_1 \frac{\rho_{r_1}^\varphi}{|\mathbf{r}_1 - \mathbf{s}|} \\
 &\quad + \delta_{rr'} \int d\mathbf{r}_1 \frac{\gamma_{s' r_1 s r_1}}{|\mathbf{r}_1 - \mathbf{r}|} - \delta_{rr'} \rho_{s's} \int d\mathbf{r}_1 \frac{\rho_{r_1}^\varphi}{|\mathbf{r}_1 - \mathbf{r}|} \\
 &\quad - \frac{\gamma_{rs' r' s}}{|\mathbf{r} - \mathbf{r}'|} + \frac{\rho_{rr'}^\varphi \rho_{s' s}}{|\mathbf{r} - \mathbf{r}'|} \\
 &\quad - \frac{\gamma_{rs' r' s}}{|\mathbf{s} - \mathbf{s}'|} + \frac{\rho_{s' s}^\varphi \rho_{rr'}}{|\mathbf{s} - \mathbf{s}'|} \\
 &\quad + \frac{\gamma_{rs' r' s}}{|\mathbf{r} - \mathbf{s}'|} + \frac{\gamma_{rs' r' s}}{|\mathbf{r}' - \mathbf{s}|}.
 \end{aligned} \tag{C1}$$

The same nomenclature as in App. B and Sec. VI is used.

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