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# Green functions in the renormalized many-body perturbation theory for correlated and disordered electrons

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The ways of introducing and handling renormalizations in the many-body perturbation theory are reviewed. We stress the indispensable role the technique of Green functions plays in extrapolating the weak-coupling perturbative approaches to intermediate and strong couplings. We separately discuss mass and charge renormalizations. The former is incorporated in a self-consistent equation for the self-energy derived explicitly from generating Feynman diagrams within the Baym and Kadanoff approach. The latter amounts to self-consistent equations for two-particle irreducible vertices. We analyze the charge renormalization initiated by De Dominicis and Martin and demonstrate that its realization via the parquet approach may become a powerful and viable way of using the many-body diagrammatic approach reliably in non-perturbative regimes with cooperative phenomena induced by either strong interaction or strong static randomness.

**Key words:** *electron correlations, random potential, Green functions and many-body perturbation theory, mass and charge renormalization, parquet equations, high spatial dimensions*

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## 1. Introduction

Electric and magnetic properties of solids are determined by the behavior of valence electrons weakly bound to the atoms forming the crystalline lattice. The behavior of the gas of valence electrons in solids is most profound in metals with an open Fermi surface. Conduction electrons in metals can be described in a number of situations and for various purposes quite accurately by Bloch waves, eigenstates of the Fermi-gas Hamiltonian. We know, however, that electrons even in metals are not a noninteracting gas. They are generally exposed to forces driving them out of the equilibrium state of the Fermi gas. Firstly, no metal is a pure crystal and hence the electrons do not move freely in space. They are scattered on randomly distributed impurities and lattice defects. Secondly, the electrons are neither free and their mutual repulsion cannot be neglected particularly for transition and heavy metals. It is the most important and long standing task of condensed-matter theorists to comprehend and qualitatively capture the deviations in the behavior of electrons in real metals from their idealized representation via Bloch waves.

The problem with quantification of the behavior of electrons beyond the almost free-electron picture is in paucity of available tools for accomplishing this task. Even if we can reduce the description of the electron gas in metals to rather simple and generic models, we are unable to solve them exactly, except for a few limiting cases that mostly do not correspond to situations of physical interest. With the increasing power of modern computers the role of numerical solutions and numerical "brute force" approaches has increased. Numerical solutions are usually unbiased and can reach a rather high level of quantitative precision. In some aspects they substitute the missing exact analytic solutions. Numerical solutions are suitable and even indispensable in showing and displaying the trends and some global features of the models studied. They, however, fail in critical regions of phase transitions in the vicinity of singularities in correlation functions. In these

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situations analytic methods, even approximate, are superior to numerical approaches. We need an analytic description of singularities in physical quantities so that we could decide about the way the critical point is reached and which symmetry-breaking order parameters emerge in the ordered phase. That is why developing and improving approximate analytic treatments of cooperative phenomena leading to a critical behavior is still very actual.

Most systems of interacting particles can be described by the generic Hamiltonian

$$\widehat{H} = \widehat{H}_0 + \widehat{H}_I \tag{1.1}$$

with the noninteracting part $\widehat{H}_0$ and an interaction $\widehat{H}_I$. The former term is a kinetic energy having Bloch waves as exact eigenstates labeled by momenta and spin. The force driving the system out from stationary Bloch waves is the interaction $\widehat{H}_I$. Usually the two components of the total Hamiltonian do not commute and we are unable to find the eigenstates of the full Hamiltonian. Even if we were able to find some of the exact eigenstates of the full Hamiltonian, they would be coherent states composed of (infinite)many Bloch waves. We could not easily match these complicated coherent states with experiment. Experimentally we observe only asymptotic states described by renormalized Bloch waves. Hence, the problem we are facing is not to find stationary many-body eigenstates of the full Hamiltonian but rather to solve a problem of scattering of asymptotic Bloch waves induced by the interacting term $\widehat{H}_I$. The most natural way to treat such a problem is to use the time-dependent perturbation expansion and Green functions. The latter offers a means to gain non-perturbative results from the perturbation expansion. But what is more important is that they are one of the few available analytic means of treating the singularities and the way how to go around poles in physical quantities. The strength of Green functions lies in that they involve boundary conditions and enable us to formulate and solve the problem off the mass shell, that is for complex energies. Moreover, we can keep consistency of approximate solutions by satisfying the demanded analytic properties of Green functions. Thereby we significantly improve upon reliability of otherwise hard controllable approximations having no small expansion parameter.

In this paper we discuss a way of efficiently using the Green functions in deriving non-perturbative approximations by means of the many-body perturbation theory in systems with interacting and disordered electrons. The advantage of the many-body perturbation theory is its universality when represented via Feynman diagrams. The diagrammatic representation of the scattering events of asymptotic particles gives us a physically motivated clue to selecting the relevant processes to be included when constructing a suitable approximation for various physical phenomena. Here we concentrate on the application of the many-body perturbation theory in critical regions of singularities caused either by a strong electron-electron interaction or a strong random potential. We show the possibility of introducing effectively of renormalizations of one-particle and two-particle Green functions and developing the mean-field-type non-perturbative approximations for quantum critical phenomena.

The paper is organized as follows. In section 2 we introduce the model and many-body Green functions. In section 3 we discuss important exact equations of motion needed for a correct handling of renormalizations. Mass renormalization within the scheme of Baym and Kadanoff is discussed in section 4 and charge renormalization provided by the parquet approach in Sec 5. An example of a successful application of the parquet approach to a nontrivial problem – Anderson localization – is presented in section 6. We summarize in section 7.

## 2. Generic model and Green functions

We use a generic tight-binding model for the description of the electron gas in metals, namely the one-band Hubbard model with a fully screened electron-electron interaction characterized by a Hamiltonian

$$\widehat{H}_{\mathrm{H}} = \sum_{\mathbf{k}\sigma} \left(\epsilon(\mathbf{k}) - \sigma B\right) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{i}\sigma} V_{\mathbf{i}} \widehat{n}_{\mathbf{i}\sigma} + U \sum_{\mathbf{i}} \widehat{n}_{\mathbf{i}\uparrow} \widehat{n}_{\mathbf{i}\downarrow} \ . \tag{2.1}$$

We used the standard notation for the kinetic energy $\epsilon(\mathbf{k})$, external magnetic field $B$ and the Hubbard interaction $U$. We also added local atomic potentials $V_{\mathbf{i}}$ that may either represent impurities or different atoms forming an alloy. We generally assume that these potentials are statically randomly distributed and cause elastic scatterings of Bloch waves. The Bloch state with momentum $\mathbf{k}$ and spin projection $\sigma$ is created in the Fock space by the creation operator $c^\dagger_{\mathbf{k}\sigma}$ and destructed by the annihilation operator $c_{\mathbf{k}\sigma}$. The operator of the local density is $\widehat{n}_{\mathbf{i}\sigma} = N^{-2}\sum_{\mathbf{qk}} \exp\{\mathrm{i}\mathbf{q}\cdot\mathbf{R}_{\mathbf{i}}\} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}$.

Our first task in statistical mechanics is to find a thermodynamic potential that for quantum systems in the many-body perturbation theory is the grand potential with a chemical potential $\mu$

$$\Omega = -k_{\mathrm{B}}T\left\langle \ln \mathrm{Tr} \exp\left\{-\beta\left(\widehat{H} - \mu\widehat{N}\right)\right\}\right\rangle_{\mathrm{av}} . \tag{2.2a}$$

The trace Tr is taken over the whole Fock space and the angular brackets $\langle\rangle_{\mathrm{av}}$ denote static (quenched) averaging over the given distribution of the random potential $V_{\mathbf{i}}$.

Knowledge of the grand potential does not contain the complete information of the equilibrium thermodynamic state. That is, the information about the distribution of the eigenenergies and the corresponding eigenvectors of the underlying Hamiltonian. For a full reconstruction of the equilibrium macroscopic state we also need to add all moments of the density-matrix operator to the grand potential. The moments quite generally are

$$\begin{aligned}\Xi^{(n,m)}&(\mathbf{k}_1\sigma_1,\ldots\mathbf{k}_n\sigma_n,\mathbf{k}_{\bar m}\sigma_{\bar m},\ldots,\mathbf{k}_{\bar 1}\sigma_{\bar 1}) = \\ &= \left\langle \frac{1}{\mathcal{Z}}\mathrm{Tr}\left[c_{\mathbf{k}_1\sigma_1}\ldots c_{\mathbf{k}_n\sigma_n} c^\dagger_{\mathbf{k}_{\bar m}\sigma_{\bar m}}\ldots c^\dagger_{\mathbf{k}_{\bar 1}\sigma_{\bar 1}} \exp\left\{-\beta\left(\widehat{H}-\mu\widehat{N}\right)\right\}\right]\right\rangle_{\mathrm{av}} .\end{aligned} \tag{2.2b}$$

So far we have introduced only static, equilibrium quantities defined on the energy (mass) shell where the dispersion relation between energy and momentum is obeyed. Since we are unable to find the spectrum of the full Hamiltonian we have to go off the mass shell and introduce time-dependent functions or states where the energy is detached from momentum. We introduce an imaginary time $\tau \in (0,\beta)$ and let propagate the creation and annihilation operators with the free-electron Hamiltonian $\widehat{H}_0 = \sum_{\mathbf{k}\sigma}(\epsilon(\mathbf{k}) - \sigma B)\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$. We define $c_{\mathbf{k}\sigma}(\tau) = \exp\{\tau\widehat{H}_0\} c_{\mathbf{k}\sigma} \exp\{-\tau\widehat{H}_0\}$ and analogously the time-dependent creation operator. Moving the creation and annihilation operators off the mass shell we can introduce Green functions as time-ordered moments of the density-matrix operator

$$G^{(n,m)}(1,\ldots,n,\bar m,\ldots,\bar 1) = \left\langle \frac{1}{\mathcal{Z}}\mathrm{Tr}_0\mathcal{T}\left[c\ (1)\ldots c\ (n), c^\dagger(\bar m)\ldots c^\dagger(\bar 1)\exp\left\{-\int_0^\beta \mathrm{d}\tau \widehat{H}_I(\tau)\right\}\right]\right\rangle_{\mathrm{av}}, \tag{2.2c}$$

where we denoted $\mathrm{Tr}_0\widehat{X} = \mathrm{Tr}\left[\widehat{X}\exp\{-\beta(\widehat{H}_0 - \mu\widehat{N}\}\right]$ and $\mathcal{Z} = \mathrm{Tr}_0\mathcal{T}\exp\left\{-\int_0^\beta \mathrm{d}\tau\widehat{H}_I(\tau)\right\}$. We introduced a short-hand labeling of the space-time and spin variables $l = (\mathbf{R}_l, \tau_l, \sigma_l)$. Only when we know the full time-dependent off-shell moments of the density-matrix operator or Green functions we can properly handle singularities in physical quantities and go around poles in approximate treatments.

Instead of separately treating the thermodynamic potential and time-dependent moments of the density-matrix operator we can use generalized external potentials and define a generating functional from which we can derive all moments via functional derivatives. To do so we have to use the time-dependent creation and annihilation operators introduced above. We perturb the equilibrium state with a general non-equilibrium external potential interacting with arbitrary density-type particle operators. For physical interpretation it is more convenient to treat the spin independently of the space-time variables. We write the most general non-equilibrium Hamiltonian for the external potential as a sum of several terms

$$\begin{aligned}\widehat{H}_{\mathrm{ext}} = \sum_{\mathbf{R}_1\mathbf{R}_2}\int_0^\beta \mathrm{d}\tau_1\mathrm{d}\tau_2\Bigg\{ &\sum_\sigma \left[\eta^{||}_\sigma(1,2)c^\dagger_\sigma(1)c_\sigma(2) + \bar\xi^{||}_\sigma(1,2)c_\sigma(1)c_\sigma(2) + \xi^{||}_\sigma(1,2)c^\dagger_\sigma(1)c^\dagger_\sigma(2)\right] \\ &+ \left[\eta^\perp(1,2)c^\dagger_\uparrow(1)c_\downarrow(2) + \bar\eta^\perp(1,2)c^\dagger_\downarrow(2)c_\uparrow(1)\right] + \left[\bar\xi^\perp(1,2)c_\uparrow(1)c_\downarrow(2) + \xi^\perp(1,2)c^\dagger_\downarrow(2)c^\dagger_\uparrow(1)\right]\Bigg\}.\end{aligned} \tag{2.3}$$

the meaning of which can be explained in physical terms [1]. The diagonal elements of the real fields $\eta_\sigma^{||}$ invoke changes of the equilibrium state conserving charge as well as spin. They stand for the physical external fields like magnetic or electric ones. The others are nonconserving external sources, being complex numbers, that either add or remove charge, spin or both from the equilibrium many-particle state. The field $\eta^\perp$ conserves charge but increases spin of the equilibrium state by two elementary units. The fields $\xi^\perp$ increase charge while $\xi_\sigma^{||}$ increase both charge and the appropriate spin projection. The complex conjugate fields lower the respective quantities. The complex non-equilibrium fields are convenient when the equilibrium system may undergo transitions either to a magnetic order in the transverse plane to the easy quantization axis or to a superconducting state.

The generating functional with the time-dependent external perturbation driving the system out of thermal equilibrium can then be represented as

$$\Omega[\mathcal{J}] = -k_\mathrm{B}T\left\langle \ln \mathrm{Tr}_0 \mathcal{T} \exp\left\{-\int_0^\beta \mathrm{d}\tau \widehat{H}_I(\tau) - \widehat{H}_\mathrm{ext}\right\}\right\rangle_\mathrm{av} . \tag{2.4}$$

We are not interested in the full non-equilibrium potential $\Omega[\mathcal{J}]$ but rather only in small deviations from the equilibrium so that we could generate the Green functions of interest. It is clear that $\Omega[0]$ coincides with the equilibrium grand potential. Beyond this we shall be interested only in one- and two-particle Green functions. If $\mathcal{J}_\alpha$ denotes a chosen external source perturbing the equilibrium system, i. e. it stands generically for $\eta^{||}$, $\eta^\perp$, $\xi^{||}$, and $\xi^\perp$, we can write for the one-particle equilibrium Green function

$$G^\alpha(12) = \left.\frac{\delta\beta\Omega[\mathcal{J}]}{\delta\mathcal{J}_{\bar{\alpha}}(2,1)}\right|_{\mathcal{J}=0} , \tag{2.5a}$$

where the index $\alpha$ denotes a "channel" or type of the one-particle propagator. It need not generally be a normal propagator conserving charge and spin, but may be any combination of creation and annihilation operators required by the physics of the problem, that is, by the structure of the equilibrium state. Analogously we can define two-particle equilibrium Green functions

$$G^{(2)\alpha}(13,24) = \left.\frac{\delta^2\beta\Omega[\mathcal{J}]}{\delta\mathcal{J}_\alpha(4,3)\delta\mathcal{J}_{\bar{\alpha}}(2,1)}\right|_{\mathcal{J}=0} . \tag{2.5b}$$

We can see that the more derivatives w.r.t. the external fields the more different types of higher-order Green function we can generate. In this paper we shall deal only with normal Green functions conserving charge and spin. That is, at the one-particle level we use only the real field $\eta^{||}$, and hence we drop the index $\alpha$ at this level. But at the two-particle level we have more options to generate a Green function conserving the total spin and charge and we keep the "channel" index $\alpha$ there. Hereinafter we use different types of external perturbations in distinguishing different types of two-particle irreducible Green functions.

## 3. Renormalized many-body perturbation expansion and exact equations of motion

The basic idea of the many-body perturbation theory is to expand the non-equilibrium grand potential from equation (2.4) in powers of the interacting and external time-dependent Hamiltonians $\widehat{H}_I$ and $\widehat{H}_\mathrm{ext}$. It is a standard procedure to develop a diagrammatic representation for this expansion and to define the rules for the construction of Feynman diagrams. However, a simple perturbative summation of diagrams up to a fixed finite power of the interaction Hamiltonian is not the way in which we could successfully describe a critical behavior of interacting and disordered many-electron systems. We have to introduce renormalizations into the perturbation expansion, that is, we have to reorganize the perturbation expansion in that we sum up classes of specific diagrams to infinite order of the interaction strength. The way of choosing the diagrams to be summed to infinite order depends on the physical situation at which we want to apply the many-body perturbation expansion.

The fundamental step in the formulation of a renormalized many-body perturbation theory was made by Baym and Kadanoff [2,3]. They proposed a construction that is capable of keeping renormalizations, i. e., summations of infinite-many diagrams under control. Their idea was to reformulate the expansion containing the bare interaction strength $U$ and the bare one-electron propagators $G^{(0)}$ in terms of the renormalized one-electron propagator $G$. Moreover in this formulation we do not sum the diagrams for the grand potential but rather for the one-particle vertex, being the self-energy $\Sigma$. The self-energy is defined via the Dyson equation that in energy-momentum representation reads

$$\Sigma_\sigma(k) = G_\sigma^{-1}(k) - G_\sigma^{(0)-1}(k) \ . \tag{3.1}$$

We used a four-vector notation $k = (\mathrm{i}\omega_n, \mathbf{k})$ with Matsubara frequency $\omega_n = (2n+1)\pi k_{\mathrm{B}} T$ to which we shall keep throughout this paper.

In the diagrammatic language the self-energy is a sum of all one-particle irreducible diagrams (1PI). In the renormalized theory we then try to construct a functional $\Sigma[G, U]$ depending only on the renormalized propagator related to the bare one by the Dyson equation (3.1). It means that this functional does not contain diagrams with self-energy insertions in the one-electron propagators. If we know the self-energy functional $\Sigma[G, U]$ we can in principle construct a genearting functional leading to the given self-energy. We denote this functional $\Phi[G, U]$. It is related to the self-energy via a functional derivative

$$\Sigma(1,2) = \frac{\delta\Phi[G,U]}{\delta G(2,1)} \ . \tag{3.2}$$

To find the generating functional $\Phi[G, U]$ from the above equation is generally not straightforward and we show the way of doing it for simple approximations. For more elaborate approximations, however, this potential need not always be explicitly attainable. Approximations with the $\Phi$ functional in closed form are called $\Phi$-derivable. We show in the next section that the dynamical mean-field theory or atomic limit are not $\Phi$-derivable theories.

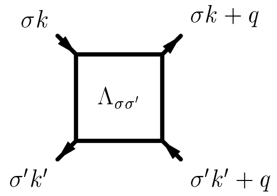


**Figure 1.** Generic two-particle function with three independent four-momenta and two spins with a defined order of incoming and outgoing fermions used in this paper.

The self-energy contains essentially the entire information about the equilibrium state. The only things we have to enter by hand are symmetry-breaking order parameters for long-range orders that may emerge at low temperatures. The order parameters can either have a form of an anomalous self-energy as in the case of superconductivity or can be built up of a combination of self-energies vanishing in the high-temperature phase. To recognize which symmetry of the high-temperature phase has to be broken we have to analyze two-particle functions. The normal two-particle function conserving the total charge and spin is defined from the generating non-equilibrium functional $\Omega[\mathcal{J}]$ in equation (2.5b) with the real fields $\eta_\sigma^{||}$. Instead of working with the full two-particle Green function $G^{(2)}$ we come over to the vertex function $\Gamma$ defined from an equation in four-momentum representation

$$\begin{aligned} G^{(2)}_{\sigma\sigma'}(k,k';q) \quad &= \quad G_\sigma(k)G_{\sigma'}(k')\left[\delta(q) - \Gamma_{\sigma\sigma'}(k,k';q)G_\sigma(k+q)G_{\sigma'}(k''+q)\right] \\ &\quad - \delta_{\sigma,\sigma'}\delta(k-k')G_\sigma(k)G_\sigma(k+q), \end{aligned} \tag{3.3}$$

where the four-momentum $\delta$-function is defined for $q = (\mathrm{i}\omega_n, \mathbf{q})$ as $\delta(q) = \beta\delta_{m,0}\delta(\mathbf{q})$. We use the attribution of four-momenta to two-particle function as in figure 1.

Analogously to the Dyson equation for one-particle functions there is a similar equation of motion for the two-particle vertex $\Gamma$. It is called Bethe-Salpeter equation and can generically be written as

$$\Gamma(k,k';q) = \Lambda^\alpha(k,k';q) - \left[\Lambda^\alpha GG \odot \Gamma\right](k,k';q), \tag{3.4}$$

where $\odot$ denotes an appropriate integration over intermediate momenta. Unlike the Dyson equation the generic Bethe-Salpeter equation is no longer an algebraic equation but rather a convolutive integral equation. Moreover, the Bethe-Salpeter equation is not uniquely defined which we marked with a label $\alpha$. As we can see from equation (3.4) it is only the vertex $\Lambda^\alpha$ and the sum over intermediate momenta which are ambiguous. The full two-particle vertex $\Gamma$ must not depend on the choice of the vertex $\Lambda^\alpha$. This vertex is called two-particle irreducible (2PI) and is related to the one-particle irreducible vertex, self-energy, via a functional derivative either in direct representation

$$\Lambda^\alpha(13,24) = \frac{\delta\Sigma^\alpha(1,2)}{\delta G^\alpha(4,3)}\ , \tag{3.5a}$$

or in four-momentum representation

$$\Lambda^\alpha_{\sigma\sigma'}(k,k';q) = \frac{\delta\Sigma^\alpha_\sigma(k,k+q)}{\delta G^\alpha_{\sigma'}(-k',-k'-q)}\ . \tag{3.5b}$$

Although the equilibrium self-energy does not depend on the index $\alpha$ we have to use the non-equilibrium self-energy in the presence of an external perturbation to derive the two-particle vertex. The non-equilibrium self-energy depends on the index $\alpha$ if appropriate terms appear in the external perturbation. Different contributions in the external perturbation $\widehat{H}_{\mathrm{ext}}$ from equation (2.3) generate different two-particle Bethe-Salpeter equations. Different Bethe-Salpeter equations correspond to different types of two-particle reducibility of diagrams, i. e., the way to disconnect a diagram by cutting a pair of one-particle propagators. The field $\eta^{||}$ leads to reducible functions in the interaction ($U$) channel where diagrams can be disconnected by cutting a virtual electron-hole pair, internal loop propagators. This type of perturbation invokes normal density responses and susceptibilities. The field $\eta^\perp$ leads to the electron-hole ($eh$) reducibility (diagram can be disconnected by cutting an electron and a hole line of asymptotic incoming and outgoing particles). Finally, the field $\xi^\perp$ leads to the electron-electron ($ee$) reducibility where diagrams can be disconnected by cutting two electron (hole) propagators of asymptotic particles. Second derivatives w.r.t. $\xi^{||}$ vanish in equilibrium without anomalous functions. Thus, we can attach external perturbations to generators of different two-particle irreducible vertices $\Lambda^\alpha$ and their respective Bethe-Salpeter equations.

Different Bethe-Salpeter equations are distinguished by the selection of the 2PI vertex $\Lambda^\alpha$ and simultaneously by the summation over intermediate states denoted generically by symbol $\odot$. This summation must correspond to the way we derived the irreducible vertex $\Lambda^\alpha$. This summation depends on the way we interconnect the left and the right two-particle functions with a pair of one-particle propagators. For the three irreducible vertices we have in the electron-hole ($\alpha = eh$), electron-electron ($\alpha = ee$), and interaction ($\alpha = U$) channels, respectively

$$\left[\widehat{X}GG\bullet\widehat{Y}\right]_{\sigma\sigma'}(k,k';q) = \frac{1}{\beta\mathcal{N}}\sum_{q''} X_{\sigma\sigma'}(k,k';q'')G_\sigma(k+q'')G_{\sigma'}(k'+q'') \times Y_{\sigma\sigma'}(k+q'',k'+q'';q-q'')\ , \tag{3.6a}$$

$$\left[\widehat{X}GG\circ\widehat{Y}\right]_{\sigma\sigma'}(k,k';q) = \frac{1}{\beta\mathcal{N}}\sum_{q''} X_{\sigma\sigma'}(k,k'+q'';q-q'')G_\sigma(k+q-q'')G_{\sigma'}(k'+q'') \times Y_{\sigma\sigma'}(k+q-q'',k';q'')\ , \tag{3.6b}$$

$$\left[\widehat{X}GG\star\widehat{Y}\right]_{\sigma\sigma'}(k,k';q) = \frac{1}{\beta\mathcal{N}}\sum_{\sigma''k''} X_{\sigma\sigma''}(k,k'';q)G_{\sigma''}(k'')G_{\sigma''}(k''+q) \times Y_{\sigma''\sigma'}(k'',k';q)\ . \tag{3.6c}$$

For convenience we used separate symbols for each multiplication scheme. Note that only the interaction (vertical) channel mixes the spin singlet ($\uparrow\downarrow$) and triplet ($\sigma\sigma$) functions. The three types of convolutions in the Bethe-Salpeter equations can be at best visualized via Feynman diagrams. The Bethe-Salpeter equation in the electron-hole channel is plotted in figure 2, the electron-electron is shown in figure 3 and finally the vertical $U$-channel is shown in figure 4. We took into account all the possibilities of interconnecting electron lines in the vertical channel with triplet two-particle propagators.

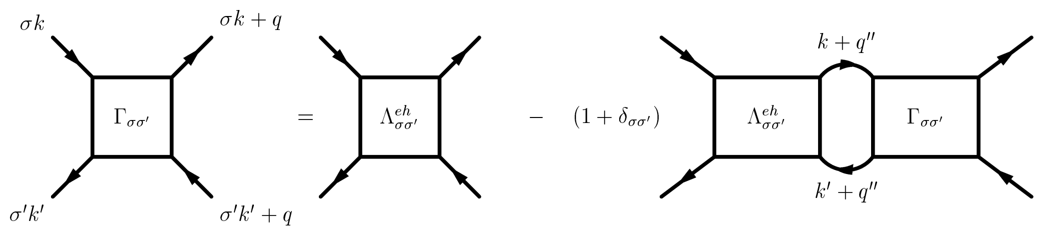


**Figure 2.** Diagrammatic representation of the the Bethe-Salpeter equation in the electron-hole scattering channel.

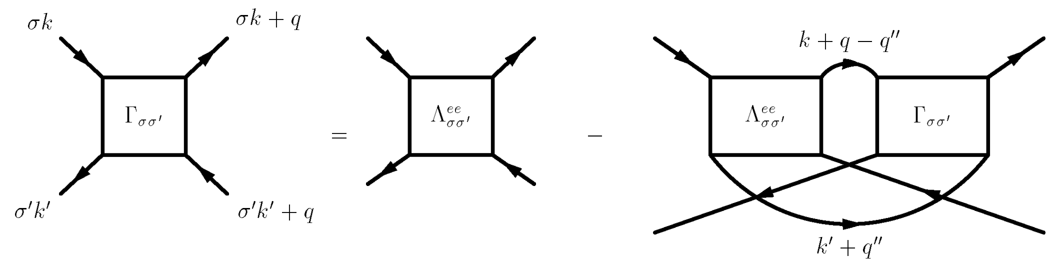


**Figure 3.** Diagrammatic representation of the the Bethe-Salpeter equation in the electron-electron scattering channel.

Having the Bethe-Salpeter equations fully defined we can improve upon our construction of a renormalized perturbation theory. Instead of diagrammatically representing the one-particle self-energy $\Sigma$ we can choose a two-particle vertex $\Lambda^{\alpha}$ as a generator of our approximation. We then use equation (3.5) to determine the self-energy from $\Lambda^{\alpha}$ and further equation (3.2) to determine the thermodynamic potential $\Phi$. Such a construction is mostly viable only for simple approximations, since it is not easy to invert functional differential equations. For more involved approximations for 2PI vertices we need not be able to find the corresponding diagrammatic representation for the self-energy, even if we can construct it in a closed analytic form.

We need not use equation (3.5) to determine the self-energy from a known two-particle irreducible vertex. A better and more explicit way of doing so is to use an integral form of the functional derivative (3.5) playing the role of a global Ward identity proved in [4]. It reads

$$\Sigma_{\sigma}(k) - \Sigma_{\sigma}(k') = \sum_{q} \Lambda^{eh}_{\sigma\sigma}(k;k';q) \left[G_{\sigma}(k+q) - G_{\sigma}(k'+q)\right] \ . \tag{3.7}$$

We can use special matrix elements of this Ward identity to determine the imaginary part of the self-energy and then use the Kramers-Kronig relation to determine its appropriate real part so that the necessary analytic properties are fulfilled [4].

The most widely used method of deriving the self-energy from the two-particle vertex, however, is to use the dynamical equation of motion, that is, Schrödinger equation projected to Green functions. This is the Schwinger equation. We use its form called Schwinger-Dyson equation. There

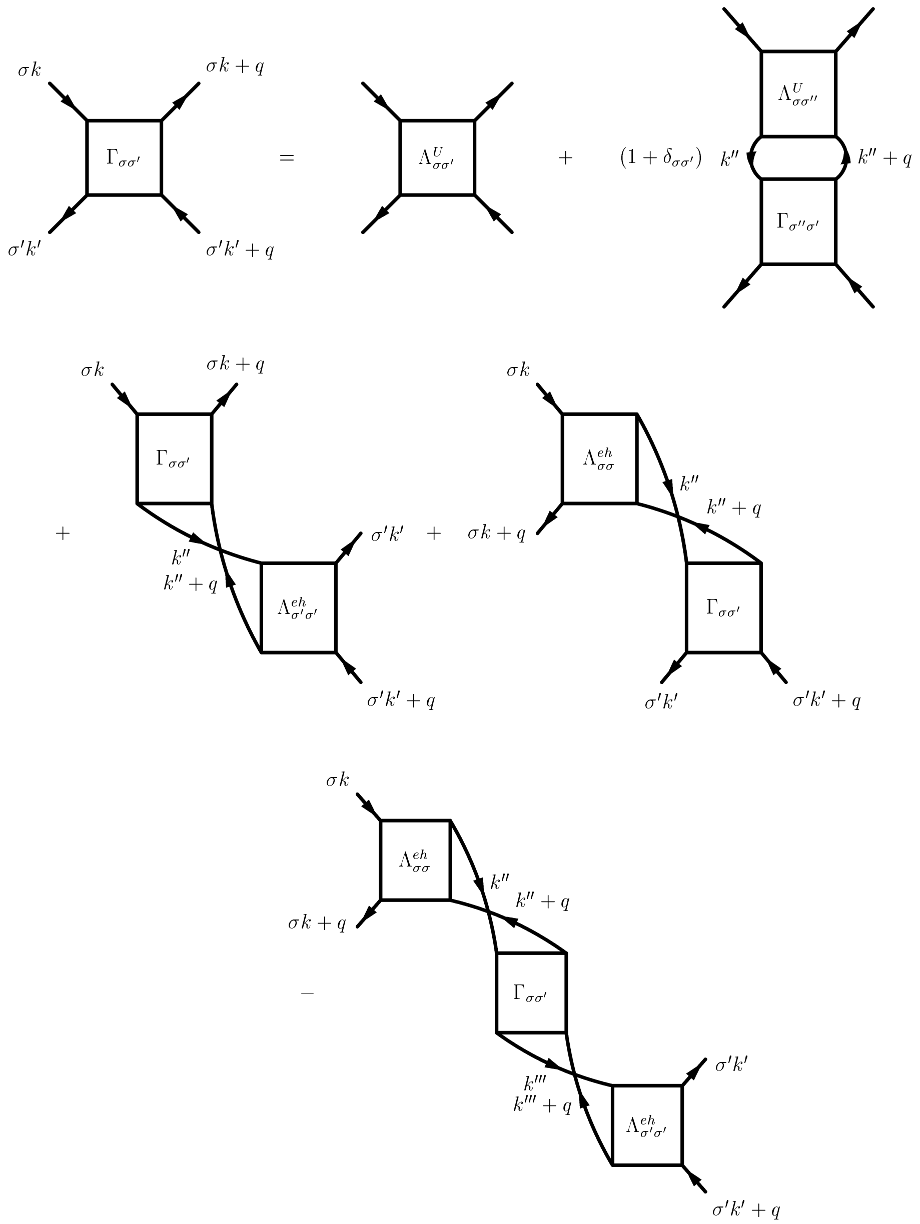


**Figure 4.** Diagrammatic representation of the the Bethe-Salpeter equation in the vertical channel with all ways one-electron propagators can be interconnected in vertices. Note that in the diagrams with crossed lines, the irreducible vertex must originate from the electron-hole channel. The last term is a correction removing the doubly counted diagrams.

the one-electron self-energy is directly related to the full vertex $\Gamma$. It reads

$$\Sigma_\sigma(k) = \frac{U}{\beta N}\sum_{k'} G_{-\sigma}(k') - \frac{U}{\beta^2 N^2}\sum_{k'q}\Gamma_{\sigma-\sigma}(k,k';q)G_\sigma(k+q)G_{-\sigma}(k'+q)G_{-\sigma}(k'). \tag{3.8}$$

The first term on the right-hand side is the static Hartree self-energy and the latter contains second and higher-order, dynamical corrections. We can use the Schwinger-Dyson equation to determine the self-energy from the vertex function $\Lambda^\alpha$ which enters the full two-particle vertex $\Gamma$ via the Bethe-Salpeter equation (3.4). We thereby get a closed functional $\Sigma[G]$.

The advantage of the above general formulation with equations of motion is that we treat the one- and two-particle functions consistently on the same footing within one renormalization scheme. This is essential for identifying the possible instabilities that may emerge at low temperatures. For this purpose we rewrite the summation over intermediate states in the Bethe-Salpeter equations as a matrix multiplication. We thereby manifestly distinguish active and inactive (conserved) variables (parameters) in each equation. We introduce new notations in which only the active four-momenta are used as variables. We define the following symbols

$$[XGG]^{eh}_{\sigma\sigma'}[q](k,k') = X_{\sigma\sigma'}(k,k+q,k'-k)G_\sigma(k')G_{\sigma'}(k'+q), \tag{3.9a}$$

$$[XGG]^{ee}_{\sigma\sigma'}[q](k,k') = X_{\sigma\sigma'}(k,k';q-k-k')G_\sigma(k')G_{\sigma'}(q-k') \ , \tag{3.9b}$$

$$[XGG]^{U}[q](\sigma k,\sigma' k') = X_{\sigma\sigma'}(k,k';q)G_{\sigma'}(k')G_{\sigma'}(k'+q) \ . \tag{3.9c}$$

The bosonic variable $q$ is in each channel inactive in the above matrix representation, or conserved during the scatterings within the chosen two-particle channel. Each channel, however, has a different conserving variable. To decide about the instability of a solution means to find a singularity in one of the Bethe-Salpeter equations.

We can, in principle, formulate an exact criterion on the existence/nonexistence of singularities in the Bethe-Salpeter equations. We formally find eigenvalues and eigenvectors for the matrices $[\Lambda^\alpha GG]^\alpha$, kernels of the Bethe-Salpeter equations (3.4), and denote them $Q^\alpha$. They are complex bosonic four-vectors. Only real four-vectors, i. e. for zero Matsubara frequency, both the conserved four-momenta $q^\alpha$ as well as the eigenvectors $Q^\alpha$ are important in determining the stability conditions of equilibrium states, i. e., nonexistence of singularities in the Bethe-Salpeter equations. They may formally be written as

$$\min\,[\Lambda^\alpha GG]^\alpha\,[\mathbf{q}^\alpha,0](\mathbf{Q}^\alpha,0) \geqslant -1. \tag{3.10}$$

We have just set up a framework for renormalizing the many-body perturbation expansion. We have two types of irreducible vertices, the one-particle vertex, the self-energy $\Sigma_\sigma(k)$ and the two-particle vertices $\Lambda^\alpha_{\sigma\sigma'}(k,k';q)$ and a set of exact equations of motion from which we are able to reconstruct the salient features of the equilibrium state if we know either of these irreducible functionals. It means that we can choose whether to use the diagrammatic input for the one-particle self-energy or for a two-particle irreducible vertex. The former corresponds to explicit mass renormalization, i. e., renormalization of the kinetic energy. The latter then reflects charge renormalization, that is, renormalization of the inter-particle interaction.

## 4. Mass renormalization, self-energy, and generating functionals

The standard way of introducing the renormalizations into the many-body perturbation theory is to use the Dyson equation (3.1) and to find a diagrammatic representation for the self-energy as a functional of the full renormalized propagator and the bare interaction $\Sigma[G,U]$ as dictated by the Baym and Kadanoff construction. In this way we automatically include all self-energy insertions, that is, one-particle reducible diagrams and subdiagrams. From the self-energy we then try to find the corresponding generating functional $\Phi[G,U]$ from equation (3.5) and higher-order irreducible vertices via functional derivatives as in equation (3.5). We usually make the selection of generating diagrams contributing to the self-energy by “educated guesses”. Control and in particular systematics of renormalizations in the many-body expansion go lost when a small expansion parameter is missing. Recently, a new systematics to mass renormalizations in many-body theories was brought by the dynamical mean-field theory (DMFT) [5,6]. This theory introduces inverse spatial dimension $d^{-1}$ as a small parameter and represents thereby a systematic way of classifying the local approximations with suppressed spatial fluctuations. It is important that quantum fluctuations should not go lost in this construction and we can separate quantum dynamical fluctuations from classical spatial ones.

There are several ways of deriving DMFT for lattice models. Here we present a construction of the DMFT generating functional introduced in [7]. We assume that the partition function can be represented via a functional integral with a set of internal degrees of freedom that we do not explicitly specify in order to keep the reasoning simple. We can write

$$\begin{aligned}\Omega\left\{G^{(0)-1},U;\mathcal{J}\right\} &= -\beta^{-1}\ln\left[\mathsf{Z}\left\{G^{(0)-1},U;\mathcal{J}\right\}\right]\\ &= -\beta^{-1}\ln\int\mathcal{D}\varphi\mathcal{D}\varphi^{*}\exp\left\{\varphi^{*}\left[G^{(0)-1}-\mathcal{J}\right]\varphi+U\left[\varphi^{*},\varphi\right]\right\}, \qquad (4.1)\end{aligned}$$

where again $\mathcal{J}$ is an (non-equilibrium) external potential. We introduce renormalizations into functional $\Omega\left\{G^{(0)-1},U;\mathcal{J}\right\}$ as in the Baym and Kadanoff formalism via the Dyson equation (3.1). We replace the bare propagator with $G^{-1}+\Sigma$, that is by a sum of two unknown "self-consistent" parameters. We incorporate the defining equations for these parameters into the generating functional via stationarity conditions. That is, we extend functional $\Omega\left\{G^{-1}+\Sigma,U;\mathcal{J}\right\}$ to a functional $\Psi[G,\Sigma]$ so that its variations w.r.t. $G$ and $\Sigma$ vanish. We have

$$\frac{\delta\beta\Psi}{\delta\Sigma}=\frac{\delta\beta\Omega}{\delta G^{(0)-1}}+\left[G^{(0)-1}-\Sigma\right]^{-1}, \qquad (4.2a)$$

$$\frac{\delta\beta\Psi}{\delta G}=\frac{1}{G^{2}}\frac{\delta\beta\Omega}{\delta G^{(0)-1}}-G^{-1}. \qquad (4.2b)$$

It is now a straightforward way of writing down the new functional

$$\Psi\left[G,\Sigma,U;\mathcal{J}\right]=\Omega\left\{G^{-1}+\Sigma,U\right\}-\beta^{-1}\mathrm{tr}\ln G-\beta^{-1}\mathrm{tr}\ln\left[G^{(0)-1}-\Sigma-\mathcal{J}\right]\ . \qquad (4.3)$$

We moved in this functional the external potential from functional $\Omega$ to the last term describing the electron gas in an effective medium $\Sigma$ and an external potential $\mathcal{J}$. It is easy to verify the validity of stationarity equations

$$\frac{\delta\Psi\left[G,\Sigma\right]}{\delta\Sigma}=0\ , \qquad (4.4a)$$

$$\frac{\delta\Psi\left[G,\Sigma\right]}{\delta G}=0\ , \qquad (4.4b)$$

where the former condition is the Dyson equation and the latter is an equation for the effective medium (self-energy) $\Sigma$.

In the above formal replacement we excluded the bare propagator $G^{(0)}$ from the many-body perturbation expansion, i e., expansion of functional $\Omega$. We have not yet introduced any reduction or simplification of the perturbation expansion. The self-energy can be anything and hence we do not know yet how to simplify the evaluation of functional $\Omega$. The aim of the above construction is not to reduce the number of diagrams contributing to the functional $\Omega$ but rather to offer a method for simplifying the evaluation of a renormalized perturbation theory. Such a simplification is offered by the limit to infinite spatial dimensions. This limit leads to suppression of nonlocal spatial fluctuations in order to keep the energy linearly proportional to the volume as required by thermodynamic consistency. To take advantage of this simplification one must have the perturbation expansion reformulated in terms of the renormalized propagators $G$ and the self-energy $\Sigma$. And this is just representation (4.3). One can easily show [7] that the asymptotic behavior of these two functions for interacting and disordered electrons reads

$$G=G^{\mathrm{diag}}\left[d^{0}\right]+G^{\mathrm{off}}\left[d^{-1/2}\right], \qquad (4.5a)$$

$$\Sigma=\Sigma^{\mathrm{diag}}\left[d^{0}\right]+\Sigma^{\mathrm{off}}\left[d^{-3/2}\right], \qquad (4.5b)$$

where $G^{\mathrm{diag}}$ and $\Sigma^{\mathrm{diag}}$ are the diagonal elements in the direct (lattice) space. Taking the limit $d\to\infty$ in equation (4.3) with the asymptotics (4.5) we obtain directly the generating functional of the dynamical mean-field theory of disordered and correlated electrons

$$\Psi\left[G,\Sigma\right]=\Omega\left\{G^{\mathrm{diag}\ -1}+\Sigma^{\mathrm{diag}}\right\}-\beta^{-1}\mathrm{tr}\ln G^{\mathrm{diag}}-\beta^{-1}\mathrm{tr}\ln\left[G^{(0)-1}-\Sigma^{\mathrm{diag}}-J\right]\ . \qquad (4.6)$$

Mean-field functional (4.6) is a non-perturbative representation for mass renormalization represented by the self-energy $\Sigma$. It does not suppress any physical process (Feynman diagram), but rather simplifies the evaluation of sums over intermediate states. This simplification lies in the relaxation of momentum conservation that does not hold in individual vertices [8]. Only the total momentum in each diagram remains conserved so that translational invariance of the equilibrium state is guaranteed. This is, on the one hand, an advantage, since quantum-dynamical fluctuations are not affected by this simplification. On the other hand, we are unable to find exact expressions for the self-energy in most interacting models. This makes us use approximations within the DMFT to reach quantitative results (i. e., to find an impurity solver). There is another restriction to the application of the mean-field functional (4.6). It uniquely determines only local quantities being irreducible vertex functions, either one- or more-particle ones. It is due to the fact that only local one-particle quantities appear in this functional. Once we want to define nonlocal two-particle functions we do not have a unique definition of the full two-particle propagator [7]. In particular we cannot represent the full two-particle vertex in the limit of high spatial dimensions as a solution of a single Bethe-Salpeter equation. We have to choose its appropriate representation via a Bethe-Salpeter equation with a local ($d = \infty$) irreducible vertex according to the physical quantity we are interested in so that only leading-order terms are kept. In any case, due to summations over intermediate scattering processes, we have to keep terms of the order $O(d^{-1})$ in non-local two-particle functions. Since spatial coherence of two-particle functions is generally important for stability of equilibrium states and for the existence of phase transitions, we have to go beyond the strictly local representation and turn to two-particle functions and their renormalizations.

The means via which we can introduce renormalizations into two-particle Green functions are the Bethe-Salpeter equations. They introduce two-particle irreducible vertices and the way the full vertex is to be constructed from them. If we further use the Schwinger-Dyson equation (3.8) we can replace an approximate diagrammatic representation of the self-energy by a diagrammatic representation of 2PI vertices $\Lambda^\alpha$. And if the approximation on a 2PI vertex is sufficiently simple we can even construct the generating functional $\Phi$. To demonstrate this way of renormalizing the many-body perturbation theory we choose the simplest approximations with the bare interaction such as the 2PI vertex (Hartree approximation at the two-particle level). In this way we obtain three approximations commonly called fluctuation-exchange ($FLEX$) [9]. If $\Lambda^{eh} = U$ then the Bethe-Salpeter equation yields the full vertex

$$\Gamma_{\sigma\sigma'}(k,k';q) = \frac{U}{1 + UX_{\sigma\sigma'}(q)} \ , \tag{4.7}$$

where we denoted the electron-hole bubble

$$X_{\sigma\sigma'}(q) = \frac{1}{\beta\mathcal{N}} \sum_{k''} G_\sigma(k'')G_{\sigma'}(k''+q) \ . \tag{4.8}$$

It is a great simplification of this simplest two-particle approximation that the full vertex $\Gamma$ depends only on a single transfer four-momentum that remains conserved during the multiple electron-hole scatterings introduced by the Bethe-Salpeter equation.

Using the Schwinger-Dyson equation (3.8) we obtain a dynamical correction to the Hartree self-energy

$$\Delta\Sigma_\sigma(k) = -\frac{U}{\beta N} \sum_q G_{-\sigma}(k+q) \ \frac{X_{\sigma-\sigma}(q)}{1 + UX_{\sigma-\sigma}(q)} \ . \tag{4.9}$$

This equation closes the approximation and all physical quantities can be determined explicitly, including the generating thermodynamic potential. That is, we can integrate back equation (3.2) and we obtain an explicit generating functional for this approximation

$$\Phi^{RPA}[U,G] = -\frac{1}{\beta\mathcal{N}} \sum_{\mathbf{q}m} \mathrm{e}^{\mathrm{i}\nu_m 0^+} \left\{ UX_{\uparrow\downarrow}(\mathbf{q},\mathrm{i}\nu_m) - \ln[1 + UX_{\uparrow\downarrow}(\mathbf{q},\mathrm{i}\nu_m)] \right\} \ . \tag{4.10}$$

This renormalized RPA is one of a few approximations the generating functional of which we know explicitly in analytic form.

The same also holds for a renormalized $T$-matrix approximation (TMA) summing electron-electron multiple scatterings, the generating functional of which reads

$$\Phi^{TMA}[U,G] = -\frac{1}{\beta\mathcal{N}}\sum_{\mathbf{q}m} \mathrm{e}^{\mathrm{i}\nu_m 0^+}\left\{UY_{\uparrow\downarrow}(\mathbf{q},\mathrm{i}\nu_m) - \ln[1+UY_{\uparrow\downarrow}(\mathbf{q},\mathrm{i}\nu_m)]\right\}, \qquad (4.11)$$

where we denoted the particle-particle bubble

$$Y_{\sigma\sigma'}(q) = \frac{1}{\beta\mathcal{N}}\sum_{k''} G_\sigma(k'')G_{\sigma'}(q-k") \ . \qquad (4.12)$$

The third approximation with multiple pair scatterings the analytic form of which we know explicitly is the bubble-chain approximation summing all the ring diagrams. Its generating functional for the Hubbard model reads

$$\Phi^{Ring}[U,G](\mathbf{q},\mathrm{i}\nu_m) = \frac{1}{2\beta\mathcal{N}}\sum_{\mathbf{q}m} \mathrm{e}^{\mathrm{i}\nu_m 0^+}\ln\left[1 - U^2 X_{\uparrow\uparrow}(\mathbf{q},\mathrm{i}\nu_m)X_{\downarrow\downarrow}(\mathbf{q},\mathrm{i}\nu_m)\right] \ . \qquad (4.13)$$

It is needless to say that we obtain the TMA if $\Lambda^{ee}_{\uparrow\downarrow} = U$ and the ring approximation if $\Lambda^{U}_{\uparrow\downarrow} = U$ in the appropriate Bethe-Salpeter equations.

Although the FLEX-type approximations just discussed start with a Bethe-Salpeter equation for the two-particle vertex and the generating diagrams for these approximations are chosen at the level of two-particle irreducible vertices, we did not go beyond the simplest approximation with the bare interaction. It is kind of a two-particle version of the Hartree approximation and due to the ambiguity in two-particle irreducibility we have three simplest two-particle approximations. These simplest approximations do not contain vertex corrections and no charge renormalization has been achieved. To do so we have to go to a more intricate (dynamical) approximations for two-particle irreducible vertices.

## 5. Charge renormalization and parquet equations

To reach a qualitative improvement upon the FLEX-type approximations from the preceding section we have to achieve a self-consistency at the two-particle level. That is, we have to introduce nonlinear equations for the two-particle irreducible vertices. A systematic renormalization of the many-body perturbation theory including vertex corrections was proposed by De Dominicis and Martin [10] who reformulated the perturbation expansion in such a way that not only the bare one-particle propagators are replaced by their renormalized versions but also the bare interaction is simultaneously replaced by renormalized two-particle vertices. Their construction was a bold extension of the very first attempt to self-consistently mix the electron-electron and electron-hole scatterings from [11]. The two-particle self-consistency achieved by a nonlinear mixing of different scattering channels is now called the parquet approach. Since its introduction to non-relativistic many-body theories by De Dominicis and Martin the parquet construction has been used to a number of problems in condensed matter [12–17]. Here we show how to use the parquet scheme in practice in order to derive a manageable approximation with a charge renormalization applicable at intermediate and strong-coupling regimes.

The basic idea of the parquet approach is to take advantage of the fact that two-particle functions reducible in one scattering channel are generally irreducible in the other channels. This feature is a consequence of topological nonequivalence of different two-particle channels. If we denote by $\mathcal{K}^\alpha$ the sum of all vertex diagrams reducible in the channel $\alpha$, then we know that the full vertex

$$\Gamma = \Lambda^\alpha + \mathcal{K}^\alpha \qquad (5.1)$$

does not depend on the channel index $\alpha$. We denote $I$ the vertex irreducible simultaneously in all two-particle channels. The irreducible vertex in the channel $\alpha$ then can be represented as a sum of the completely irreducible vertex $I$ and reducible functions from the other channels. Thus, the fundamental parquet equation can be written using equation (5.1) as

$$\Lambda^{\alpha}_{\sigma\sigma'} = I_{\sigma\sigma'} + \sum_{\alpha'\neq\alpha}\left[\Gamma_{\sigma\sigma'} - \Lambda^{\alpha'}_{\sigma\sigma'}\right]. \tag{5.2}$$

It is not a closed equation. We exclude the full vertex $\Gamma$ from the parquet equation by using the Bethe-Salpeter equations (3.4) to obtain a set of equations for the two-particle irreducible vertices $\Lambda^{\alpha}$

$$\Lambda^{\alpha} = I + \sum_{\alpha'\neq\alpha}\left\{1 - \left[\Lambda^{\alpha'}GG\right]\odot\right\}^{-1}\left[\Lambda^{\alpha'}GG\right]\odot\Lambda^{\alpha'} \tag{5.3}$$

that are now fully determined by the completely irreducible vertex $I_{\sigma\sigma'}$ and the one-particle propagators $G_{\sigma}$. Note that there is no direct relation to the self-energy and the one-particle propagators can be either fully renormalized or bare. That is, the parquet equations define a two-particle self-consistency independently of the one-particle one. The solution of these equations are two-particle irreducible vertices as functionals of the completely irreducible vertex and the one-particle propagators

$$\Lambda^{\alpha} = L^{\alpha}\left[I[U;G,\Lambda];\Lambda,G\right]. \tag{5.4}$$

The parquet approximation is the simplest approximation in the parquet equations where we replace the completely irreducible vertex $I$ by the bare interaction $U$.

Even the simplest approximation in the parquet scheme does not allow for exact solutions. The problem is that the parquet equations (5.3) are nonlinear integral equations for functions with three variables that are mixed when different channels are mixed. Hence, there is no apparent way of solving these equations either numerically or analytically. A numerical solution can be reached only in the regions where the differences between the parquet and FLEX solutions are insignificant. Since the effort with solving parquet equations pays off, one has to apply them in critical regions close to poles in the Bethe-Salpeter equations. We cannot avoid approximations there.

First, the number of channels explicitly taken into account is reduced to two. Experience shows that the best results are obtained if we equally treat the electron-electron and the electron-hole multiple scatterings. Hence, we take into consideration only the $ee$ and $eh$ channels. Since the Hubbard interaction acts only between opposite spins we obtain a two-channel parquet approximation for singlet vertices

$$\begin{aligned}\Lambda^{ee}_{\sigma-\sigma}(k,k';q) = U - \frac{1}{\beta\mathcal{N}}\sum_{q'}\Lambda^{eh}_{\sigma-\sigma}(k,k';q')G_{\sigma}(k+q')G_{-\sigma}(k'+q')\\ \times\left[\Lambda^{eh}_{\sigma-\sigma}(k+q',k'+q';q-q') - U + \Lambda^{ee}_{\sigma-\sigma}(k+q',k'+q';q-q')\right]\ ,\end{aligned} \tag{5.5a}$$

$$\begin{aligned}\Lambda^{eh}_{\sigma-\sigma}(k,k';q) = U - \frac{1}{\beta\mathcal{N}}\sum_{q'}\Lambda^{ee}_{\sigma-\sigma}(k,k'+q-q';q')G_{\sigma}(k+q')G_{-\sigma}(k'+q-q')\\ \times\left[\Lambda^{ee}_{\sigma-\sigma}(k+q',k';q-q') - U + \Lambda^{eh}_{\sigma-\sigma}(k+q',k';q-q')\right]\ .\end{aligned} \tag{5.5b}$$

Neither these equations are solvable and a numerical solution would demand a tremendous effort. To achieve quantitative results one has to simplify these equations. We have to reduce the number of relevant degrees of freedom of the vertices $\Lambda^{eh}$ and $\Lambda^{ee}$. One gets a rigorous simplification in high spatial dimensions where momentum convolutions reduce to Gaussian integrations [18]. This simplification, however, does not affect frequency convolutions. In infinite spatial dimensions we reduce the problem to a single impurity or to the DMFT where only frequencies do appear. Even this situation is not solvable. To gain an impression of the behavior of solutions of the parquet equations one has to introduce further simplifications without a firm mathematical justification. The simplest or mean-field-like approximation would be a static approximation to the vertex functions. The vertex functions then become positive numbers and the parquet equations can be satisfied only at a single transfer frequency in two-particle bubbles $X_{\uparrow\downarrow}(q)$ and $Y_{\uparrow\downarrow}(k+k'+q)$ We choose their zero values and denote them $X_0$ and $Y_0$, respectively. With this static approximation we turn the integral equations algebraic. We can easily solve them explicitly with the result

$$\Lambda_{eh} = U - \frac{[U(1+\Lambda_{eh}X_0) - \Lambda_{eh}^2 X_0]^2 Y_0}{(1+\Lambda_{eh}X_0)[(1+\Lambda_{eh}X_0)(1+UY_0) - \Lambda_{eh}^2 X_0 Y_0]} \tag{5.6a}$$

and

$$\Lambda_{ee} = U - \frac{[U(1+\Lambda_{ee}Y_0) - \Lambda_{ee}^2 Y_0]^2 X_0}{(1+\Lambda_{ee}Y_0)[(1+\Lambda_{ee}Y_0)(1+UX_0) - \Lambda_{ee}^2 X_0 Y_0]} \ . \tag{5.6b}$$

The only input to these equations are the bare interaction and the static values of the electron-hole and electron-electron bubbles. At half-filling we have $0 < Y_0 = -X_0$. We can see that the bare interaction is screened by the electron-electron scatterings and enhanced by the electron-hole scatterings, see figure 5.

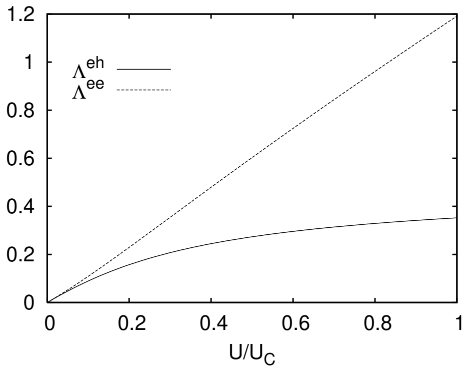


**Figure 5.** Static effective interactions calculated from the parquet equations with two channels. We choose half-filling and denoted the RPA critical interaction $U_c = 1/Y_0 = -1/X_0$.

The strong-coupling asymptotics of the irreducible vertices is $\Lambda_{eh} \to 1/2Y_0$ and $\Lambda_{ee} \to U+1/2Y_0$ and the full two-particle vertex does not approach a pole even for $U \to \infty$. This is a significant change with respect to the single-channel RPA approach where a pole in this asymptotics causes the approximation to break down for rather small interaction strengths $U \sim U_c = -1/X_0$. Hence, we can see that the parquet-type charge renormalization, even in its simplest static approximation qualitatively changes the behavior of the FLEX approximations. Now we can use the calculated irreducible vertices in the Bethe-Salpeter equations to determine the full two-particle vertex. Since we have taken into account two-channels we build up the two-particle vertex as a sum of both vertices from which we subtract the bare interaction. The correction to the Hartree self-energy then reads

$$\Delta\Sigma_\sigma(k) = -\frac{U}{\beta N}\sum_q \left[\frac{G_{-\sigma}(k+q)\Lambda_{eh}X_{\sigma-\sigma}(q)}{1+\Lambda_{eh}X_{\sigma-\sigma}(q)} + \frac{G_{-\sigma}(q-k)\Lambda_{ee}Y_{\sigma-\sigma}(q)}{1+\Lambda_{ee}Y_{\sigma-\sigma}(q)} - UG_{-\sigma}(k+q)X_{\sigma-\sigma}(q)\right] \tag{5.7}$$

and remains numerically stable up to infinite interaction strength. Hence, the static parquet approximation for the irreducible vertex can replace the bare $U$ in the FLEX-type approximations and extend the validity of the approximation defined by equation (5.6) and equation (5.7) from weak to intermediate interaction strengths.

We cannot, however, rely on the static parquet approximation up to the strong-coupling regime where we expect the Kondo behavior. The Kondo asymptotics is a hallmark for the genuine strong-coupling limit of correlated electrons with enhanced electron-hole scatterings (half-filling). The Kondo asymptotics is neither reproduced by the FLEX nor by the static parquets. To improve toward the Kondo behavior one has to allow for dynamical vertex corrections. There is no systematic or rigorously controlled way of introducing a frequency-dependent charge renormalization but one can try to do this by keeping only the relevant bosonic transfer frequencies in the irreducible vertices [19]. Although the way of simplifying the parquet equations to a manageable and stable approximation is ambiguous, we developed a few physically motivated reductions in the frequency dependence of the irreducible vertex functions that seem to qualitatively correctly reproduce the Kondo asymptotics of the single-impurity Anderson model [20].

## 6. Disordered electrons in high spatial dimensions

Usefulness and strength of the parquet approach to reach qualitatively new results beyond the mean-field or static approximations can be demonstrated more rigorously in a simplified situation with noninteracting electrons elastically scattered on static impurities provided by the Anderson model of disordered electrons. The self-energy correcting the propagation of the Bloch waves due to scatterings on randomly distributed impurities is a function of the Fermi energy only. The vertex functions then are the functions of two energies that are not dynamical variables. Then the parquet equations for the vertex functions contain only convolutions of momenta and these convolutions can be rigorously simplified in high spatial dimensions. Thereby we obtain a controlled simplification of the parquet equations allowing for an (exact) analytic solution of the two-channel approximation in the asymptotic limit to high spatial dimensions. The solution of the parquet equations in this limit provides a mean-field theory for the Anderson localization transition nonexistent before [18,21]

The Anderson model of noninteracting electrons scattered on random atomic potentials is defined by a Hamiltonian

$$\widehat{H}_A = \sum_{\langle ij\rangle} t_{ij}\widehat{c}_i^\dagger \widehat{c}_j + \sum_i V_i \widehat{c}_i^\dagger \widehat{c}_i \ , \tag{6.1}$$

where the atomic potentials $V_i$ are uncorrelated random variables. The solution to this model, that is the self-energy comprising the effects of scatterings of Bloch waves on the random potential cannot be found exactly except for the mean-field limit, the solution in infinite spatial dimensions. There, the exact solution is the well-known Coherent Potential Approximation (CPA) [22,23]. This solution is generally considered to be a mean-field approximation for noninteracting disordered electrons. It proved successful not only for model systems but also in realistic and first-principles calculations [24,25]. Although very powerful for one-particle quantities, the CPA is not capable of producing vertex corrections to the electrical conductivity [26] The transport properties of the CPA are essentially determined by a single-particle (Boltzmann) term. In this approximation we are unable to see any hints of electron localization due to vanishing of diffusion predicted by Anderson [27]. To derive a quantitative mean-field-like approximation for this phenomenon is more complicated and one has to go beyond the strict $d = \infty$ limit.

In [18,21] we developed a mean-field-like theory of the Anderson localization transition in that we used a renormalized expansion around the CPA solution. The small parameter in this expansion is a difference of the renormalized one-electron propagator $G(\mathbf{k}, z)$ and the local CPA propagator $G^{\mathrm{loc}}(z)$: $\bar{G}(\mathbf{k}, z) = G(\mathbf{k}, z) - G^{\mathrm{loc}}(z)$. In the perturbation expansion around the local CPA we can use the parquet construction for nontrivial renormalizations of two-particle irreducible vertex functions. Notice that the parquet approach is not applicable in static local theories such as CPA, since different two-particle scattering channels do not in fact exist. Even if we formally construct the scatterings with electrons and holes, the result is the same and these channels are mathematically identical. We have no tool for distinguishing an electron from a hole with local static diagrams only. We must introduce either time or spatial distance to be able to discern the forward and the backward propagation.

We generally mark with a bar the Green functions obtained from the expansion around the CPA. Thus we can write the fundamental two-channel parquet equation

$$\Gamma_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \bar{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) + \bar{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) - \gamma(z_+, z_-) \ . \tag{6.2}$$

The dynamical variables are only momenta $\mathbf{k}$, $\mathbf{k}'$. The bosonic momentum $\mathbf{q}$ and energies $z_+, z_-$

are external variables. We denoted the full local two-particle CPA vertex as

$$\gamma(z_1, z_2) = \frac{\lambda(z_1, z_2)}{1 - \lambda(z_1, z_2) G(z_1) G(z_2)} , \tag{6.3}$$

where the irreducible vertex $\lambda$ obeys a CPA equation

$$\lambda(z_1, z_2) = \frac{1}{G(z_1)G(z_2)} \left[ 1 - \left\langle \frac{1}{1 + [\Sigma(z_1) - V_i]\, G(z_1)} \frac{1}{1 + [\Sigma(z_2) - V_i]\, G(z_2)} \right\rangle_{\text{av}}^{-1} \right] . \tag{6.4}$$

We remind that the local propagator $G(z) = \int_{-\infty}^{\infty} d\epsilon \rho(\epsilon) [z - \epsilon - \Sigma(z)]^{-1}$ and the self-energy $\Sigma(z)$ obey a Soven equation

$$1 = \left\langle \frac{1}{1 + G(z)[\Sigma(z) - V_i]} \right\rangle_{\text{av}} . \tag{6.5}$$

Now we have to determine the irreducible vertices $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$ from parquet equations that are constructed in the same manner as those for the interacting systems. The convolutions are taken only over three-momenta and the completely irreducible vertex is the CPA vertex $\gamma$. We evaluate momentum convolutions in the leading $1/d$ order, that is in the asymptotic limit to high spatial dimensions. We choose $z_+ = E_F + \omega + \mathrm{i}0^+, z_- = E_F - i0^+$ and denote $G_\pm(\mathbf{k}) = G(\mathbf{k}, z_\pm)$. If the electron-hole and the electron-electron bubbles are

$$\chi^{\pm}(z_1, z_2; \mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} G(\mathbf{k}, z_1) G(\mathbf{q} \pm \mathbf{k}, z_2) , \tag{6.6}$$

respectively and $\bar{\chi}(\mathbf{q}) = \chi(\mathbf{q}) - G_+ G_-$, we can prove that in the leading asymptotic order $d \to \infty$ the following relations hold

$$\frac{1}{N} \sum_{\mathbf{q}'} \bar{\chi}(\mathbf{q}' + \mathbf{q}) \bar{G}_\pm(\mathbf{q}' + \mathbf{k}) \doteq \frac{Z}{4d} \bar{G}_\pm(\mathbf{q} - \mathbf{k}) , \tag{6.7a}$$

$$\frac{1}{N} \sum_{\mathbf{q}} \bar{\chi}(\mathbf{q} + \mathbf{q}_1) \bar{\chi}(\mathbf{q} + \mathbf{q}_2) \doteq \frac{Z}{4d} \bar{\chi}(\mathbf{q}_1 - \mathbf{q}_2) . \tag{6.7b}$$

We used abbreviations $Z = t^2 \langle G_+^2 \rangle \langle G_-^2 \rangle$ with $\langle G_\pm^2 \rangle = N^{-1} \sum_{\mathbf{k}} G_\pm(\mathbf{k})^2$. The functions $\bar{G}_\pm(\mathbf{k})$ and $\bar{\chi}(\mathbf{q})$ form a closed algebra of Gaussian random variables with respect to momentum convolutions. We can use equations (6.7) to simplify the parquet equations for the irreducible vertices $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$. Before we do this we use the electron-hole symmetry

$$\bar{G}(\mathbf{k}, z) = \bar{G}(-\mathbf{k}, z) , \tag{6.8a}$$

$$\Gamma_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \Gamma_{\mathbf{k}\mathbf{k}'}(z_+, z_-; -\mathbf{Q}) = \Gamma_{-\mathbf{k}'-\mathbf{k}}(z_+, z_-; \mathbf{Q}). \tag{6.8b}$$

that acts on the irreducible vertices as follows

$$\bar{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; \mathbf{q}) = \bar{\Lambda}^{eh}_{\mathbf{k}\mathbf{k}'}(z_+, z_-; -\mathbf{Q}) = \bar{\Lambda}^{eh}_{-\mathbf{k}'-\mathbf{k}}(z_+, z_-; \mathbf{Q}) . \tag{6.8c}$$

Using this simplification in the parquet equations with the electron-hole and the electron-electron channels we obtain a single equation for a vertex $\bar{\Lambda}^{ee}_{\mathbf{k}\mathbf{k}'}(E_F + \omega + \mathrm{i}0^+, E_F - \mathrm{i}0^+; \mathbf{q}) \equiv \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$

$$\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \frac{1}{N} \sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}\mathbf{k}''}(-\mathbf{q} - \mathbf{k} - \mathbf{k}'') \bar{G}_+(\mathbf{k}'') \bar{G}_-(\mathbf{q} + \mathbf{k}'') \left[ \bar{\Lambda}_{\mathbf{k}''\mathbf{k}'}(-\mathbf{q} - \mathbf{k}' - \mathbf{k}'') + \bar{\Lambda}_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}) - \gamma \right] . \tag{6.9}$$

We apply the Gaussian rules (6.7) for the evaluation of momentum convolutions and reduce the integral equation (6.9) to an algebraic one for an averaged vertex

$$\bar{\Lambda}(\mathbf{q}) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) . \tag{6.10}$$

The asymptotic solution of the parquet equation (6.9) in high spatial dimensions reads

$$\bar{\Lambda}(\mathbf{q}) = \gamma + \bar{\Lambda}_0 \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q})} \ , \tag{6.11}$$

where we denoted $\bar{\Lambda}_0 = N^{-1} \sum_{\mathbf{q}} \bar{\Lambda}(\mathbf{q})$. The only parameter to be determined self-consistently is the superlocal vertex $\bar{\Lambda}_0$. Summing both sides of equation (6.11) over momenta we obtain a mean-field self-consistent equation for this vertex

$$\bar{\Lambda}_0 = \gamma + \bar{\Lambda}_0^2 \frac{1}{N} \sum_{\mathbf{q}} \frac{\bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q})} \ . \tag{6.12}$$

If we denote the standard irreducible vertex by $\Lambda_0 = \bar{\Lambda}_0/(1 + \bar{\Lambda}_0 G_+ G_-)$, we can represent the high-dimensional asymptotic form of the full two-particle vertex as a sum of three contributions

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \Lambda_0 \left[ \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \Lambda_0 \chi(\mathbf{q})} + \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{k} + \mathbf{k}' + \mathbf{q})}{1 - \Lambda_0 \chi(\mathbf{k} + \mathbf{k}' + \mathbf{q})} \right] \ . \tag{6.13}$$

The first term on the r.h.s. is the local CPA ($d = \infty$) vertex, the second term is the nonlocal part of the full CPA vertex [26] and the third one is a term missing in earlier calculations based on the CPA or high-dimensional constructions. This term is required for the two-particle electron-hole symmetry and is responsible for the so-called weak electron localization [28]. It is obtained only if the electron-hole and electron-electron scatterings are treated on the same footing as done in the parquet approach.

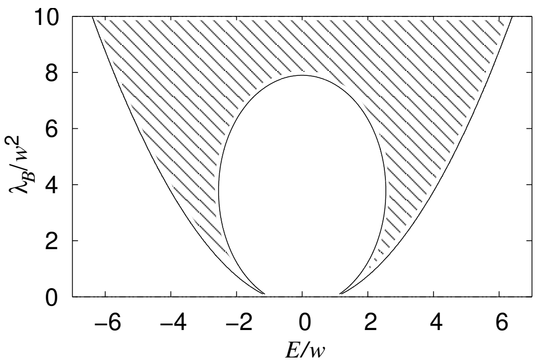


**Figure 6.** Phase diagram for Anderson localization for $\Lambda_{\mathrm{B}} = cV^2$, $c$ is the concentration of impurities with the atomic potential $V$ and $w$ is the energy half bandwidth. The hatched area denotes localized states. From [21].

The parquet approach does not only correctly include the weak localization but due to its self-consistency in the determination of the two-particle irreducible vertex it is capable of describing the vanishing of diffusion due to strong scatterings of electrons on random impurities. To demonstrate this we evaluate the density-density correlation function

$$\Phi_{\mathrm{E}}^{RA}(\mathbf{q}, \omega) = \frac{1}{N^2} \sum_{\mathbf{k}\mathbf{k}'} G^{(2)}_{\mathbf{k}\mathbf{k}'}(E + \omega + \mathrm{i}0^+, E - \mathrm{i}0^+; \mathbf{q}) \ . \tag{6.14}$$

in the parquet approximation in high spatial dimensions. Then, in the limit of small frequency and momentum transfer, we obtain:

$$\Phi_{\mathrm{E}}^{RA}(\mathbf{q}, \omega) \approx \frac{2\pi n_{\mathrm{E}}/A_{\mathrm{E}}}{-\mathrm{i}\omega + D^0_{\mathrm{E}}(\omega)/A_{\mathrm{E}} \mathbf{q}^2} \ , \tag{6.15}$$

where $n_{\mathrm{E}}$ is the density of states at the Fermi energy $E$. In this expression $n_{\mathrm{E}}/A_{\mathrm{E}}$ is the number of extended states at the Fermi energy and $D^0_{\mathrm{E}}(\omega)/A_{\mathrm{E}}$ is the diffusion constant for these extended states. With the disorder strength increasing, the constant $A_{\mathrm{E}} \to \infty$ if $\lambda \to \lambda_{\mathrm{c}}$. The critical disorder strength $\lambda_{\mathrm{c}}$ determines the Anderson localization transition at which the diffusion in the random system vanishes and the metal goes over to an insulator. A typical phase diagram calculated from the parquet approximation with the Born approximation for the self-energy (coherent potential) is plotted in figure 6.

## 7. Conclusions

In this paper we discussed the role that the Green functions play in renormalizations of the many-body perturbation theory. In most situations of physical interest we are unable to exactly solve the microscopic models and we have to resort to approximations. The most straightforward way of reaching the quantitative results in interacting and disordered electron systems is the many-body perturbation expansion. A mere perturbation expansion in a small parameter is of little significance for cooperative phenomena that we are mostly interested in. The only way of capturing at least the qualitative features of collective critical phenomena is to introduce renormalizations into the perturbation expansion. In order to treat the critical points and singularities emerging there one must leave the mass shell and formulate the perturbation expansion with non-equilibrium perturbations and use Green functions with complex energies. At present there is no alternative to Green functions in critical regions of phase transitions of correlated and disordered electrons. To combine exact equations of motion for Green functions with a diagrammatic input embodied in a renormalized theory is actually the modern way of using the many-body perturbation theory with Feynman diagrams

In this paper we reviewed the ways of achieving various stages of renormalizations of the many-body perturbation expansion. We argued that there are two fundamental concepts of renormalization connected with two contributions to the microscopic Hamiltonian: kinetic energy and interaction. The standard way of treating the renormalizations was introduced by Baym and Kadanoff and amounts to finding the one-particle self-energy as a functional of the renormalized one-particle propagator and the bare interaction. In this approach the Feynman diagrams are explicitly taken into play at the one-particle level. In this way we achieve an explicit renormalization of the dispersion relation and the kinetic energy. We then speak about mass renormalization. Although the Baym and Kadanoff construction is formally exact it is very difficult to find approximations for the self-energy that would accurately describe a critical behavior of Bethe-Salpeter equations for two-particle Green functions. The mass renormalization scheme does not presently provide a suitable framework for a reliable extrapolation of the many-body perturbation theory from the weak to the strong-coupling regimes. Mass renormalization alone is insufficient in the strong-coupling regime and is unable to explain or reproduce the Kondo strong-coupling asymptotics in the impurity models. We can conclude that renormalizations introduced only at the level of the one-particle self-energy are suitable for weak and moderate coupling.

If we want to reliably extrapolate the many-body perturbation theory to the strong-coupling regime, we have to introduce explicit charge renormalizations. That is, we have to replace not only one-particle irreducible diagrams within the self-energy, but also to replace two-particle irreducible diagrams with two-particle irreducible vertices in the perturbation expansion. The diagrammatic input into approximations with charge renormalization lies at the two-particle level. One could directly approximate the 2PI vertices diagrammatically. Hovewer, this approach is not very effective, since we cannot easily introduce non-perturbative vertex corrections to the bare interaction. There is, however, an elegant way of introducing a two-particle self-consistency. It is offered by the parquet approach introduced into the non-relativistic many-body theory by De Dominicis and Martin. The parquet approach utilizes topological nonequivalence of different two-particle irreducibility channels and assumes the diagrammatic input to a completely irreducible two-particle vertex. The vertices irreducible in individual channels are then determined by parquet equations. The full two-particle vertex is defined via a Bethe-Salpeter equation and the self-energy is defined from the Schwinger-Dyson equation. Such an advanced method of renormalization of the perturbation theory may become very efficient if an appropriate simplification of the parquet equations is found. It is presently the major obstacle to a wider application of the parquet approach in many-body theories that we do not have a systematic and mathematically controlled way of reducing the parquet equations to a manageable form with an explicit solution.

In spite of lacking the systematic ways of reducing the complexity of the parquet equations in many-body theories we substantiated the potential prospects of the parquet approach. Already the simplest static approximation on the irreducible vertices in two-channel parquet equations led to significant improvements upon the single-channel FLEX approximations in intermediate coupling. We also reported the first evidence that simplest dynamical irreducible vertices in the parquet approach with the electron-hole and the electron-electron channels may qualitatively correctly reproduce the Kondo strong-coupling asymptotics.Research in this direction is under way.

Last but not least, the parquet approach and non-perturbative charge renormalization become invaluable in the description of Anderson localization in disordered noninteracting electrons. The parquet approach in this model with only elastic scatterings can be used only if nonlocal fluctuations are included, hence beyond the mean-field approximation. Unlike the case of interacting electrons, disordered electrons allow for a systematic and controlled simplification of the parquet equations. This simplification is offered by the limit to high spatial dimensions where momentum convolutions reduce to Gaussian integrations. The parquet equations with the electron-hole and the electron-electron scatterings can be solved in high spatial dimensions asymptotically exactly. Their solution is capable of describing vanishing of diffusion induced by strong randomness and appears to be a mean-field theory of Anderson localization.

To conclude, the many-body perturbation theory when accompanied by nontrivial mass and charge renormalizations involved in one- and two-particle Green functions can become a very powerful means of quantitatively describing and qualitatively understanding the physical phenomena driven by strong electron-electron interaction or randomness beyond the limits of the adiabatic Fermi-liquid theory.

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# Функції Гріна в перенормованій теорії збурень багатьох тіл для скорельованих та невпорядкованих електронів

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Зроблено огляд способів введення перенормування в теорії збурень багатьох тіл. Підкреслено важливу роль техніки функцій Гріна при екстраполяції пертурбативних підходів слабкого зв'язку на випадок проміжного та сильного зв'язку. Окремо обговорено масове та зарядове перенормування. Перше має місце при розгляді самоузгодженого рівняння для власної енергії, що отримується з діаграм Фейнмана в межах підходу Бейма та Каданова. Друге має місце при розгляді самоузгоджених рівнянь для двочастинкових незвідних вершин. Проаналізовано зарядове перенормування, запропоноване Де Домініцісом та Мартіном, та показано, що його реалізація за допомогою паркетного підходу може стати потужним способом використання діаграмного підходу теорії багатьох тіл у непертурбативних режимах із кооперативними явищами, що ведуть до далекосяжних зв'язків та критичної поведінки з сингулярностями двочастинкових функцій Гріна, спричиненими сильною взаємодією чи сильним статичним безладом.

**Ключові слова:** *електронні кореляції, випадковий потенціал, функції Гріна і багаточастинкова теорія збурень, ренормалізація маси і заряду, паркетні рівняння, велика розмірність простору*

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