Two-particle renormalizations in many-fermion perturbation theory: Importance of the Ward identity

V. Janíš
Institute of Physics, Academy of Sciences of the Czech Republic,
Na Slovance 2, CZ-18221 Praha 8, Czech Republic

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We analyze two-particle renormalizations within many-fermion perturbation expansion. We show that present diagrammatic theories suffer from lack of a direct diagrammatic control over the physical two-particle functions. To rectify this we introduce and prove a Ward identity enabling an explicit construction of the self-energy from a given two-particle irreducible vertex. Approximations constructed in this way are causal, obey conservation laws and offer an explicit diagrammatic control of singularities in dynamical two-particle functions.

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Correlated electrons in metals represent a system with unparalleled features that remain far from being satisfactorily and fully understood. They are unique in that respect that to control their behavior in intermediate and strong coupling regimes we must have at our disposal effective techniques for a reliable description of one- and two-particle characteristics. One-electron functions, such as the spectral function, the self-energy or the density of states carry information about the fermionic character of elementary excitations in metals. They are decisive for the Fermi liquid behavior as well as for deviations from the Landau quasiparticle picture. The two-particle correlation and Green functions control the critical behavior and signal cooperative phenomena and phase transitions via divergences in generalized susceptibilities. In intermediate coupling, where the Coulomb repulsion becomes comparable with the kinetic energy, dynamical fluctuations in the system become strong and may lead to either a phase transition to a new (magnetic) phase or to a breakdown of the Fermi-liquid behavior. In this transition regime we have to treat both single-electron and pair excitations on the same footing and keep the two-particle characteristics. One-electron functions, such as the spectral function, the self-energy or the density of states carry information about the fermionic character of elementary excitations in metals. They are decisive for the Fermi liquid behavior as well as for deviations from the Landau quasiparticle picture. The two-particle correlation and Green functions control the critical behavior and signal cooperative phenomena and phase transitions via divergences in generalized susceptibilities. In intermediate coupling, where the Coulomb repulsion becomes comparable with the kinetic energy, dynamical fluctuations in the system become strong and may lead to either a phase transition to a new (magnetic) phase or to a breakdown of the Fermi-liquid behavior. In this transition regime we have to treat both single-electron and pair excitations on the same footing and keep the two-particle functions directly accessible.

One of the most flexible and physical ways to understand various phenomena of correlated electrons is to use many-body perturbation theory and Feynman diagrams. Except for the single-impurity Anderson and Kondo models, where the Fermi-liquid regime survives to infinite interaction strength, we have to renormalize the perturbation expansion. Baym and Kadanoff were the first who showed how to implement renormalizations into the perturbation theory in a systematic and consistent way. The basic idea of their approach is to express physical quantities, and in particular the self-energy, as a functional of the renormalized one-particle propagator $G$ and the bare interaction $U$, i. e., we construct a self-energy functional $\Sigma(k, \omega_n) = \Sigma[G, U](k, \omega_n)$. Once we find an approximate form of this functional from a diagrammatic expansion free of self-energy insertions, we add the Dyson equation $G^{-1}(k, \omega_n) = G_0^{-1}(k, \omega_n) - \Sigma(k, \omega_n)$ to complete our approximation for the self-energy. We used $G$ to denote the bare one-particle propagator. If we extend our equations to situations with external perturbing potentials, we can derive all necessary thermodynamic functions. Thermodynamic consistence and macroscopic conservation laws are thereby guaranteed.

Although we construct a functional for the self-energy from perturbation theory, the fundamental quantity in the Baym-Kadanoff approach is the generating functional related to the self-energy via a functional differential equation

$$\Sigma[G, U](k, \omega_n) = \frac{\delta \Phi[G, U]}{\delta G(k, \omega_n)}.$$  \hspace{1cm} (1)

When we are able to find the Luttinger-Ward functional $\Phi[G, U]$ explicitly we speak about $\Phi$-derivable approximations.

Higher-order Green functions are derived from the self-energy functional via functional derivatives that may be viewed upon as generalized Ward identities. They connect lower-order with higher-order irreducible (vertex) functions. The identity connecting the two-particle irreducible vertex with the one-particle one (self-energy) reads in the direct space

$$\Lambda^\alpha_{\sigma, \sigma'}(13, 24) = \frac{\delta \Sigma(1, 2)}{\delta G_{\sigma'}(4, 3)} = \frac{\delta^2 \Phi[G, U]}{\delta G(2, 1) \delta G_{\sigma'}(4, 3)}$$  \hspace{1cm} (2)

where we denoted the space-time coordinates $1 = (R_1, \tau_1)$ etc. We also introduced an index $\alpha$ denoting the appropriate two-particle irreducibility channel. We have three topologically nonequivalent two-particle irreducible channels: electron-hole ($\alpha = eh$), electron-electron ($\alpha = ee$), and interaction ($\alpha = U$) channels according to whether we cannot disconnect the diagram by cutting a pair of an electron and a hole, two electron (hole) propagators, or by cutting a polarization bubble, respectively, cf. Ref. Using functional derivatives of the generating functional we derive all two-particle and higher-order Green functions.

The formally exact approach of Baym and Kadanoff uses explicitly only mass renormalization, i. e., the self-energy functional depends explicitly on the renormalized one-electron propagator and the bare interaction. There
is no explicit two-particle renormalization in this formulation. The two-particle functions are passive outputs from functional derivatives of the self-energy functional. We hence cannot assess or directly control the critical behavior via, for example, low-energy scalings or summations of most divergent diagrams. Each change in the two-particle function arises only via an adequate change in the self-energy, which is too cumbersome and sometimes even not viable. This is a severe drawback, in particular in critical regions, where two-particle functions become singular and very sensitive to any small change.

One can improve upon this by an explicit charge renormalization, that means that one replaces the bare Coulomb interaction in the perturbation expansion by appropriate two-particle irreducible vertices $\Lambda^\alpha$. We then obtain a new generating functional in a form $\Phi[G, \Lambda^\alpha]$. The most direct way to do this is to use the so-called parquet approach introduced in the nonrelativistic many-body theory by De Dominicis and Martin. The parquet approach differs from the Baym-Kadanoff construction, as standardly used, in that the parquet scheme takes the two-particle irreducible vertices as primary objects for which one tries to find a functional representation from the diagrammatic theory.

Once we have prescriptions for the two-particle irreducible vertices $\Lambda^\alpha$ we use the Bethe-Salpeter equation from the respective two-particle irreducibility channel to find the full two-particle vertex

$$\Gamma_{\alpha \sigma}(k; q, q') = \Lambda^\alpha_{\sigma \sigma}(k; q, q') - \left(1 + \delta_{\sigma \sigma}\right) [\Lambda^\alpha GG \odot \Gamma]_{\sigma \sigma}(k; q, q'). \quad (3)$$

We introduced four-momenta $k = (\mathbf{k}, i\omega_n), q = (\mathbf{q}, i\nu_m)$ for fermionic and bosonic variables, with Matsubara frequencies $\omega_n = (2n + 1)\pi T$ and $\nu_m = 2m\pi T$ at temperature $T$. Each two-particle scattering channel $\alpha$ is characterized by the way the irreducible vertices are interconnected by pairs of one-particle propagators $GG$, denoted here by the generic symbol $\odot$.

Up to this point the one-particle propagator $G$ and the vertices $\Lambda^\alpha$ have been treated as independent. To find a functional for the self-energy and then also for the generating functional $\Phi$ one uses an exact Schwinger-Dyson equation of motion. Its explicit form depends on the model we choose. Here we use the lattice Hubbard model with completely screened, local Coulomb interaction. The Schwinger-Dyson equation then reads

$$\Sigma_\sigma(k) = U \sum_{k'} G_{-\sigma}(k') - U \sum_{k'q} \Gamma_{-\sigma}(k; q, k' - k) \times G_\sigma(k + q) G_{-\sigma}(k' + q) G_{-\sigma}(k'). \quad (4)$$

We introduced a short-hand notation $\sum_q = N^{-1} \sum_q \beta^{-1} \sum_m$ for $q = (\mathbf{q}, i\nu_m)$ and analogously for $k' = (\mathbf{k}', i\omega')$. The Schwinger-Dyson equation determines the self-energy functional $\Sigma_\sigma[G, \Lambda^\alpha]$ from which we can construct a generating functional $\Phi[G, \Lambda^\alpha]$, which actually has been done for various two-particle approximations of the parquet type. In the parquet approach all physical quantities are represented as functionals of renormalized one-particle propagators $G_\sigma$, representing mass renormalization, and two-particle irreducible vertices $\Lambda^\alpha_{\sigma \sigma}$, standing for charge renormalization. The present way how the parquet-type approximations, or more generally two-particle renormalizations, are applied, however, leads to a scheme effectively equivalent to that of Baym and Kadanoff. An intended direct control over the two-particle functions is lost at the end. We use equation (4) to obtain the self-energy functional in the parquet approach. In conserving theories the physical two-particle functions must be determined via functional derivatives as in Eq. (2). The two-particle vertex constructed via a functional derivative from the self-energy then differs from the vertex we started with. Furthermore, Eq. (4) does no longer play the role of the Schwinger-Dyson equation, since the actual physical two-particle vertex $\Gamma_{\text{phys}}$ differs from $\Gamma$ used in Eq. (3). This discrepancy reflects the general fact that we cannot fulfill both Eq. (2) and Eq. (3) unless we have an exact solution for the two-particle vertex. Hence, Eq. (3) in the parquet construction serves as a generator of the self-energy functional from which all physical quantities are derived via functional differential equations. The two-particle vertices $\Lambda^\alpha, \Gamma$ we use in the parquet approach are only auxiliary functions and not the physical two-particle functions we need.

It is clear that in approximate thermodynamically consistent and conserving schemes in the Baym-Kadanoff form we have to give up the Schwinger-Dyson equation of motion. A question arises whether also with two-particle renormalizations we have to lose the initial meaning and interpretation of the vertex functions. Actually, the two-particle renormalizations in the parquet approach were introduced in the effort to gain a better control over the behavior of two-particle functions in critical regions with singularities in Bethe-Salpeter equations.

To regain the control over the two-particle functions, i.e., to return the meaning of two-particle functions to the diagrammatic representations for the vertices $\Lambda^\alpha$, we have to resolve the Ward identity, Eq. (2), for the self-energy. The self-energy then will no longer be related to the two-particle vertex via Eq. (3) but rather through an integral form of the Ward identity. In this way the two-particle functions will retain their complete diagrammatic representation enabling a direct control of their critical behavior. Using a Ward identity for the determination of the self-energy from a given two-particle vertex guarantees thermodynamic consistency of the theory.

The aim of this paper is to prove the following partially integrated Ward identity between the self-energy and the electron-hole irreducible triplet vertex

$$\Sigma_\sigma(k) - \Sigma_\sigma(k') = \sum_q \Lambda^\alpha_{\sigma \sigma}(k; q, k' - k) \times [G_\sigma(k + q) - G_\sigma(k' + q)] \quad (5)$$
set aside this fundamental fermion trajectory propagating the incoming charge and spin from the rest of the diagram that we denote $X$. Function $X$ contains interaction lines and only closed loops of fermion propagators. It is connected with the fundamental fermion trajectory via interactions as shown in Fig. 2. Each self-energy diagram can be classified according to the length (number of scattering events) of the fundamental fermion trajectory.

We do not need to consider the Hartree term, since it does not contribute to the r.h.s. of Eq. (6). Hence the dynamical self-energy can be represented by an expansion

$$
\Sigma_\sigma(k) = \sum_{n=1}^{\infty} U^{n+1} \times \sum_{q_1, \ldots, q_n} X^{(n)}[G, U](q_1, q_2 - q_1, \ldots, q_n - q_{n-1}, -q_n) \times G_\sigma(k + q_1)G_\sigma(k + q_2)\ldots G_\sigma(k + q_n)
$$

where $n$ denotes the length of the fundamental fermion trajectory ($n = 3$ in Fig. 2). Note that the expansion on the r.h.s. of Eq. (6) is not an expansion in the interaction strength, since the loop function $X$ contains interaction. It is clear that the loop function depends only on the transfer (bosonic) momenta $q_1, \ldots, q_n$ and not on the incoming fermionic momentum $k$.

Only the one-electron propagators contributing to the fundamental fermion trajectory are relevant for the proof of Eq. (6), since only there we can distinguish different external momenta on the l.h.s. of Eq. (6). We utilize the following identity

$$
G_\sigma(k + q_1)\ldots G_\sigma(k + q_n) - G_\sigma(k' + q_1)\ldots G_\sigma(k' + q_n)
$$

$$
= \sum_{i=1}^{n} G_\sigma(k + q_1)\ldots G_\sigma(k + q_{i-1})[G_\sigma(k + q_i) - G_\sigma(k' + q_i)]
$$

and rewrite the expansion for the self-energy to

$$
\Sigma_\sigma(k) - \Sigma_\sigma(k') = \sum_{n=1}^{\infty} U^{n+1} \sum_{i=1}^{n} \sum_{q_1, \ldots, q_n} X^{(n)}(q_1, q_2 - q_1, \ldots, q_n - q_{n-1}, -q_n) \times G_\sigma(k + q_1)\ldots G_\sigma(k + q_{i-1})G_\sigma(k' + q_i)\ldots G_\sigma(k' + q_n) [G_\sigma(k + q_i) - G_\sigma(k' + q_i)]
$$

$$
= \sum_{n=1}^{\infty} U^{n+1} \sum_{i=0}^{n-1} \Lambda^{(i,n-i-1)}_{\sigma \sigma}(k; q, k' - k) [G_\sigma(k + q) - G_\sigma(k' + q)].
$$

We denoted contributions to an electron-hole vertex with $i$ electron and $n-i$ hole propagators from the fundamental fermion lines of the two-particle function as $\Lambda^{(i,n-i-1)}_{\sigma \sigma}$. The vertex $\Lambda$ has the electron-hole structure, since the propagation in momentum $k'$ is in the opposite direction to the propagation of momentum $k$. The vertex $\Lambda$
must be irreducible in the electron-hole channel, since all reducible terms are already incorporated in the renormalized one-electron propagators. On the other hand, each \( eh \)-irreducible two-particle diagram can be uniquely closed to a self-energy via the fundamental fermion trajectory. The expansion in \( n \) and \( i \) hence covers all contributions to the irreducible electron-hole vertex and we can write

\[
\Lambda_{\sigma \rho}^{eh}(k; q, q') = U \sum_{n=0}^{\infty} \sum_{i=0}^{n+1} \Lambda_{\sigma \rho}(i; n, n-i)(k; q, q') \quad (9)
\]

Inserting Eq. (9) into Eq. (8) we reveal identity (6).

Relation (6) has two important consequences. First, continuity equation for two-particle correlation functions can be proved. Second, Eq. (6) can be used to replace Eq. (4) in the determination of the self-energy from a given two-particle vertex \( \Lambda_{\sigma \rho}^{eh} \).

To prove a two-particle continuity equation we use the following relation

\[
G_{\sigma}(k)G_{\sigma}(k + q) = \frac{G_{\sigma}(k) - G_{\sigma}(k + q)}{\nu_m - \epsilon(k + q) + \epsilon(k) - \Sigma(k + q) + \Sigma(k)} \quad (10)
\]

in the Bethe-Salpeter equation for the two-particle function \( L_{\sigma\rho}(k; q, q') = G_{\sigma}(k)G_{\sigma}(k + q')\delta(q) + \Gamma_{\sigma\rho}(k; q, q')G_{\sigma}(k + q)G_{\sigma}(k + q + q') \). The four-momentum delta function for \( q = (q, \nu_m) \) reads \( \delta(q) = N\delta_{q,0}\delta_{\nu_m,0} \).

Function \( L_{\sigma\rho} \) is the two-particle Green function from which the exchange term was removed so that it fulfills a Bethe-Salpeter equation. If we further utilize the symmetry of the two-particle vertex we find another form of the Ward identity \( \sum_{k} \Delta_{k}G_{\sigma}\Lambda_{\sigma \rho}^{eh}(k; k' - k, q) = \Delta_{q}\Sigma_{\sigma}(k') \).

When we multiply the Bethe-Salpeter equation for \( L_{\sigma\rho} \) in the electron-hole channel by the denominator of Eq. (10) and integrate over the incoming and outgoing fermionic momenta we obtain a continuity equation having in the limit of small transfer three-momenta \( q \) the following form

\[
i\nu_m \Xi_{\sigma \rho}(q, i\nu_m) - q \cdot \Xi'_{\sigma \rho}(q, i\nu_m) = 0. \quad (11)
\]

We denoted \( \Xi_{\sigma \rho}(q, i\nu_m) = \sum_{k, q'} L_{\sigma\rho}(k; q', q) \) and \( \Xi'_{\sigma \rho}(q, i\nu_m) = \sum_{k, q'} \nabla_{\epsilon(k)}L_{\sigma\rho}(k; q', q) \).

To use Eq. (11) in the determination of the self-energy, we put \( k' = k \) but let the Matsubara frequencies \( \omega_n \) and \( \omega_{n'} \) independent so that we can analytically continue the self-energy difference to the case with \( \omega + i\eta \) and \( \omega - i\eta \). We then use an analytically continued vertex function \( \Lambda_{\sigma \rho}^{eh}(k, \omega + i\eta; q, \zeta, 0, -2i\eta) \) in the Ward identity (6) to construct the imaginary part of the self-energy \( \Sigma_m(k, \omega + i\eta) \) along the real axis. The intermediate complex frequency \( \zeta \) takes values from an integration contour used to replace the sum over Matsubara frequencies. The shape of the integration contour depends on the analytic structure of the approximated vertex. The real part of the self-energy is calculated from the Kramers-Kronig relation accomplishing thus a causal theory. This construction of the self-energy from the vertex function was already successfully applied in the parquet approach to noninteracting disordered electron systems (6).

To conclude, the principal result of the paper is a partially integrated Ward identity, Eq. (6). It is a consequence of charge and spin conserving particle interaction and was proved by means of a diagrammatic expansion. The primary importance of identity (6) lies in the possibility to regain a direct diagrammatic control over the (critical) behavior of dynamical two-particle functions by defining the self-energy from the triplet vertex function via Eq. (6). The present schemes with two-particle (vertex) renormalizations do not obey the Ward identity (6), except for its infinitesimal limit, and hence are unable to determine the self-energy from the physical two-particle vertices. Utilization of the Ward identity (6) opens new possibilities to study critical behavior of correlated electrons, in particular, when we subject the electrons to a random potential and investigate the effects of electron interactions on the metal-insulator transition.

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* Electronic address: janis@fzu.cz

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