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LETTER TO THE EDITOR

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

V Janiš

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

E-mail: janis@fzu.cz

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Abstract

We analyse two-particle renormalizations within the many-fermion perturbation expansion. We show that present diagrammatic theories suffer from a lack of 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 explicit diagrammatic control of singularities in dynamical two-particle functions.

Correlated electrons in metals represent a system with unparalleled features that remain far from being satisfactorily and fully understood. To control their behaviour 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, and the density of states, carry information about the fermionic character of elementary excitations in metals. They are decisive for the Fermi liquid behaviour as well as for deviations from the Landau quasiparticle picture. The two-particle correlation and Green functions control the critical behaviour and signal cooperative phenomena and phase transitions via divergences in generalized susceptibilities. For 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 behaviour. In this transition regime we have to treat 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 [1, 2], we have to renormalize the perturbation expansion. Baym and Kadanoff were the first to show how to implement renormalizations into the perturbation theory in a systematic and consistent way [3]. 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 $\Sigma_\sigma(\boldsymbol{k}, \mathrm{i}\omega_n) = \Sigma_\sigma[G, U](\boldsymbol{k}, \mathrm{i}\omega_n)$. Once we find an approximate form of this functional from a diagrammatic expansion free of self-energy insertions, we add the Dyson equation $G_\sigma^{-1}(\boldsymbol{k}, \mathrm{i}\omega_n) = \mathcal{G}_\sigma^{-1}(\boldsymbol{k}, \mathrm{i}\omega_n) - \Sigma_\sigma(\boldsymbol{k}, \mathrm{i}\omega_n)$ to complete our approximation for the self-energy. We used $\mathcal{G}$ 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 [4]. Thermodynamic consistency 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

$$\Sigma_\sigma[G, U](\boldsymbol{k}, \mathrm{i}\omega_n) = \frac{\delta\Phi[G, U]}{\delta G_\sigma(\boldsymbol{k}, \mathrm{i}\omega_n)}. \tag{1}$$

When we are able to find the Luttinger–Ward functional $\Phi[G, U]$ explicitly, we speak of Φ-derivable approximations[1] [5]

Higher-order Green functions are derived from the self-energy functional via functional derivatives that may be viewed 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 self-energy reads in direct space

$$\Lambda^\alpha_{\sigma\sigma'}(13, 24) = \frac{\delta\Sigma_\sigma(1, 2)}{\delta_\alpha G_{\sigma'}(4, 3)} = \frac{\delta^2\Phi[G, U]}{\delta_\alpha G_\sigma(2, 1)\, \delta_\alpha G_{\sigma'}(4, 3)} \tag{2}$$

where we have denoted the space-time coordinates as $1 = (\boldsymbol{R}_1, \tau_1)$ etc. We also introduced an index α denoting the appropriate two-particle irreducibility channel. We have three topologically nonequivalent two-particle irreducibility channels: electron–hole ($\alpha = \mathrm{eh}$), electron–electron ($\alpha = \mathrm{ee}$), and interaction ($\alpha = U$) channels, according to whether we cannot disconnect the diagram by cutting a pair of an electron propagator and a hole propagator, by cutting a pair of two electron (hole) propagators, or by cutting a polarization bubble, respectively (cf [5]). 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 behaviour 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.

[1] Most of the weak-coupling approximations are Φ-derivable, but mean-field-type approximations based on the atomic solution of the Hubbard model, such as the complete dynamical mean-field functional and the Falicov–Kimball mean-field functional, do not fall into this category. In these cases it is necessary to use explicitly the self-energy to write a generating functional in closed form. See also the discussion in [5].

One can improve upon this by an explicit charge renormalization, which means that one replaces the bare Coulomb interaction in the perturbation expansion by appropriate two-particle irreducible vertices Λ^α. 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 [6]. The parquet approach differs from the Baym–Kadanoff construction, as normally 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 Λ^α we use the Bethe–Salpeter equation from the respective two-particle irreducibility channel to find the full two-particle vertex

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

We have introduced four-momenta $k = (\boldsymbol{k}, \mathrm{i}\omega_n), q = (\boldsymbol{q}, \mathrm{i}\nu_m)$ 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 α is characterized by the way in which the irreducible vertices are interconnected by pairs of one-particle propagators GG, denoted here by the generic symbol $\odot$ (cf [4]). The full vertex is then related to the full two-particle Green function as

$$\begin{aligned} G^{(2)}_{\sigma\sigma'}(k; q_h, q_v) &= G_\sigma(k)G_{\sigma'}(k + q_v)[\delta(q_h) + \Gamma_{\sigma\sigma'}(k; q_h, q_v)G_\sigma(k + q_h)G_{\sigma'}(k + q_h + q_v)] \\ &\quad - \delta_{\sigma\sigma'}\delta(q_v)G_\sigma(k)G_{\sigma'}(k + q_h) \end{aligned} \tag{4}$$

from which the two-particle correlation function can be deduced. The four-momentum delta function is defined for $q = (\boldsymbol{q}, \mathrm{i}\nu_m)$ as $\delta(q) = N\delta_{\boldsymbol{q},\boldsymbol{0}}\beta\delta_{m,0}$.

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

$$\Sigma_\sigma(k) = U\sum_{k'} G_{-\sigma}(k')\left[1 - \sum_q \Gamma_{\sigma-\sigma}(k; q, k' - k)G_\sigma(k + q)G_{-\sigma}(k' + q)\right]. \tag{5}$$

We have introduced the shorthand notation $\sum_q = N^{-1}\sum_{\boldsymbol{q}}\beta^{-1}\sum_m$ for $q = (\boldsymbol{q}, \mathrm{i}\nu_m)$ and an analogous form for $k' = (\boldsymbol{k}', \mathrm{i}\omega_{n'})$. 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 [4, 7].

In the parquet approach all physical quantities are represented as functionals of renormalized one-particle propagators G_σ, representing mass renormalization, and two-particle irreducible vertices $\Lambda^\alpha_{\sigma\sigma'}$, standing for charge renormalization. Parquet-type approximations use equation (5) to obtain the self-energy functional from the two-particle vertex. However, in conserving theories the physical two-particle functions must be consistent with the functional derivatives from equation (2). The two-particle vertex constructed via a functional derivative from the self-energy derived from equation (5) then differs from the vertex that we started with. Hence, equation (5) no longer plays the role of the Schwinger–Dyson equation. This discrepancy reflects the general fact that we cannot fulfil both equations (2) and (5) in approximate solutions for the two-particle vertex. Equation (5) serves only as a generator of the self-energy functional from which all physical quantities are derived via functional differential equations. The two-particle vertices Λ^α, Γ that we use in the present formulation of the parquet approach are only auxiliary functions and not the physical two-particle functions that we need.

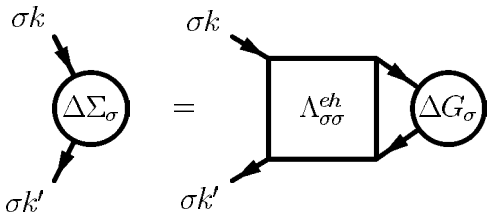

Figure 1. The Ward identity connecting the self-energy and the triplet irreducible vertex. The interaction acts vertically between the upper line and the lower line in two-particle functions.

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 Λ^{α}, we have to resolve the Ward identity, equation (2), for the self-energy. The self-energy will then no longer be related to the two-particle vertex via equation (5) but rather through an integral form of the Ward identity. In this way the two-particle functions will retain their complete diagrammatic representation, enabling direct control of their critical behaviour. 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 letter is to prove the following partially integrated Ward identity between the self-energy and the electron–hole irreducible triplet vertex:

$$\Sigma_\sigma(k) - \Sigma_\sigma(k') = \sum_q \Lambda^{\mathrm{eh}}_{\sigma\sigma}(k; q, k'-k)[G_\sigma(k+q) - G_\sigma(k'+q)]. \tag{6}$$

Its diagrammatic representation is given in figure 1. Equation (6) holds for arbitrary four-momenta k and k'. It is a generalization of a Ward identity for noninteracting electrons in a random potential proved by Vollhardt and Wölfle [8].

We stress that the Ward identity (6) can be proved only for the triplet irreducible vertex $\Lambda_{\sigma\sigma}$. This is important in particular for the Hubbard model where the local Coulomb interaction acts only between particles with opposite spins and singlet vertex functions $\Lambda^{\alpha}_{\sigma-\sigma}$ are preferentially used.

We use diagrammatic arguments similar to those applied to noninteracting disordered systems to prove the identity (6). Due to spin and charge conservation in the vertices of the perturbation theory, each diagram for the self-energy contains just a single electron trajectory connecting the incoming with the outgoing external electron line. We set aside this fundamental fermion trajectory propagating the incoming charge and spin from the rest of the diagram, which 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 figure 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 rhs of equation (6). Hence the dynamical self-energy can be represented by an expansion

$$\Sigma_\sigma(k) = \sum_{n=1}^{\infty} U^{n+1} \sum_{q_1,\ldots,q_n} X^{(n)}[G,U](q_1, q_2-q_1, \ldots, q_n - q_{n-1}, -q_n) \times G_\sigma(k+q_1)G_\sigma(k+q_2)\cdots G_\sigma(k+q_n) \tag{7}$$

where n denotes the length of the fundamental fermion trajectory ($n = 3$ in figure 2). Note that the expansion on the rhs of equation (7) is not an expansion in the interaction strength, since the loop function X contains interaction lines. It is clear that the loop function

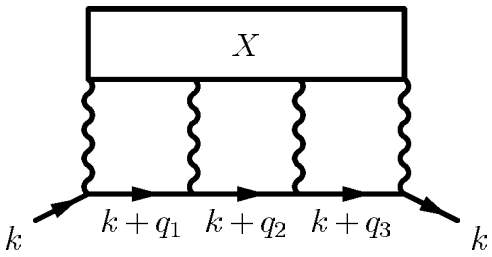

Figure 2. A typical self-energy diagram with internal loops (X) connected with the propagating electron only via the interaction (wavy) lines.

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 equation (6), since only there can we distinguish different external momenta on the lhs of equation (6). We utilize the following identity:

$$\begin{aligned} &G_\sigma(k+q_1)\cdots G_\sigma(k+q_n) - G_\sigma(k'+q_1)\cdots G_\sigma(k'+q_n) \\ &\quad = \sum_{i=1}^{n} G_\sigma(k+q_1)\cdots G_\sigma(k+q_{i-1})[G_\sigma(k+q_i) \\ &\quad\quad - G_\sigma(k'+q_i)]G_\sigma(k'+q_{i+1})\cdots G_\sigma(k'+q_n) \end{aligned} \tag{8}$$

and rewrite the expansion for the self-energy as

$$\begin{aligned} \Sigma_\sigma(k) - \Sigma_\sigma(k') &= \sum_{n=1}^{\infty} U^{n+1} \sum_{i=1}^{n} \sum_{q_1,\ldots,q_n} X^{(n)}(q_1, q_2-q_1, \ldots, q_n - q_{n-1}, -q_n) \\ &\quad \times G_\sigma(k+q_1)\cdots G_\sigma(k+q_{i-1})G_\sigma(k'+q_{i+1})\cdots G_\sigma(k'+q_n) \\ &\quad \times [G_\sigma(k+q_i) - G_\sigma(k'+q_i)] \\ &= \sum_{n=1}^{\infty} U^{n+1} \sum_{i=0}^{n-1} \Lambda_{\sigma\sigma}^{(i,n-i-1)}(k; q, k'-k)[G_\sigma(k+q) - G_\sigma(k'+q)]. \end{aligned} \tag{9}$$

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 $\Lambda_{\sigma\sigma}^{(i,n-i)}$. The vertex Λ has the electron–hole structure, since the propagation of momentum k' is in the opposite direction to the propagation of momentum k. The vertex Λ 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 electron–hole 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[2]

$$\Lambda_{\sigma\sigma}^{\mathrm{eh}}(k; q, q') = U \sum_{n=0}^{\infty} U^{n+1} \sum_{i=0}^{n} \Lambda_{\sigma\sigma}^{(i,n-i)}(k; q, q'). \tag{10}$$

Inserting equation (10) into (9), we reveal identity (6).

Relation (6) has two important consequences. First, the continuity equation for the two-particle correlation function can be proved. Second, equation (6) can be used to replace

[2] Note that the electron–hole irreducible vertex is generated by cutting only the fundamental fermion line in the self-energy. Cutting the fermion lines in the loop function X generates contributions to the electron–electron and interaction irreducible functions.

equation (5) in the determination of the dynamical self-energy (beyond the static Hartree term) from a class of Feynman diagrams contributing to the triplet electron–hole irreducible vertex function $\Lambda^{\mathrm{eh}}_{\sigma\sigma}$.

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

$$G_\sigma(k)G_\sigma(k+q) = \frac{G_\sigma(k) - G_\sigma(k+q)}{\mathrm{i}\nu_m - \epsilon(\boldsymbol{k}+\boldsymbol{q}) + \epsilon(\boldsymbol{k}) - \Sigma_\sigma(k+q) + \Sigma_\sigma(k)} \tag{11}$$

in the Bethe–Salpeter equation for the two-particle function $L_{\sigma\sigma}(k;q,q') = G^{(2)}_{\sigma\sigma}(k;q,q') + \delta(q')G_\sigma(k)G_\sigma(k+q)$, which is the two-particle Green function from which the exchange term was removed. It is then the function L, not $G^{(2)}$, that fulfils a Bethe–Salpeter equation. If we further utilize the symmetry of the two-particle vertex we find another form of the Ward identity, $\sum_k \Delta_q G_\sigma \Lambda^{\mathrm{eh}}_{\sigma\sigma}(k;k'-k,q) = \Delta_q \Sigma_\sigma(k')$. When we now multiply the Bethe–Salpeter equation in the electron–hole channel by the denominator of equation (11) and integrate over the incoming and outgoing fermionic momenta, we obtain a continuity equation having in the limit of small transfer three-momenta $\boldsymbol{q}$ the following form:

$$\mathrm{i}\nu_m \Xi_{\sigma\sigma}(\boldsymbol{q},\mathrm{i}\nu_m) - \boldsymbol{q}\cdot\boldsymbol{\Xi}^{v}_{\sigma\sigma}(\boldsymbol{q},\mathrm{i}\nu_m) = 0. \tag{12}$$

We used the notation

$$\Xi_{\sigma\sigma}(\boldsymbol{q},\mathrm{i}\nu_m) = \sum_{k,q'} L_{\sigma\sigma}(k;q',q), \qquad \boldsymbol{\Xi}^{v}_{\sigma\sigma}(\boldsymbol{q},\mathrm{i}\nu_m) = \sum_{k,q'} \boldsymbol{\nabla}\epsilon(\boldsymbol{k}) L_{\sigma\sigma}(k;q',q).$$

Equation (12) holds for arbitrary Matsubara frequency ν_m. For larger momenta $\boldsymbol{q}$, we must replace the term $\boldsymbol{q}\cdot\boldsymbol{v}(\boldsymbol{k})$ in the continuity equation by an energy difference $\epsilon(\boldsymbol{k}+\boldsymbol{q}) - \epsilon(\boldsymbol{k})$.

To determine the dynamical self-energy from the two-particle vertex we put $\boldsymbol{k}' = \boldsymbol{k}$ but let the Matsubara frequencies $\mathrm{i}\omega_n$ and $\mathrm{i}\omega_{n'}$ be independent in equation (6) so that we can analytically continue the self-energy difference to the case with $\omega + \mathrm{i}\eta$ and $\omega - \mathrm{i}\eta$. We then use an analytically continued vertex function $\Lambda^{\mathrm{eh}}_{\sigma\sigma}(\boldsymbol{k},\omega+\mathrm{i}\eta;\boldsymbol{q},\zeta,\boldsymbol{0},-2\mathrm{i}\eta)$ in the Ward identity (6) to construct the imaginary part of the self-energy $\Sigma_\sigma(\boldsymbol{k},\omega+\mathrm{i}\eta)$ along the real axis. To exemplify the construction of the self-energy, we use the simplest nontrivial approximation for the irreducible electron–hole vertex, which is a sum of polarization bubbles, i.e., multiple electron–hole scatterings in the interaction channel. The resulting vertex depends only on a single transfer momentum and frequency. The analytic continuation of the Ward identity to real frequencies can be performed explicitly and we obtain for the imaginary part of the self-energy

$$\begin{aligned}\operatorname{Im}\Sigma_\sigma(\boldsymbol{k},\omega_+) = \frac{1}{N}\sum_{\boldsymbol{k}'}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\,[&b(\omega')\operatorname{Im}\Lambda^{\mathrm{eh}}_{\sigma\sigma}(\boldsymbol{k}'-\boldsymbol{k},\omega'_+)\operatorname{Im}G_\sigma(\boldsymbol{k}',\omega'_+ + \omega)\\ &+ f(\omega')\operatorname{Im}\Lambda^{\mathrm{eh}}_{\sigma\sigma}(\boldsymbol{k}'-\boldsymbol{k},\omega'_+ - \omega)\operatorname{Im}G_\sigma(\boldsymbol{k}',\omega'_+)]\end{aligned} \tag{13}$$

where $b(\omega)$, $f(\omega)$ are Bose and Fermi functions and $\omega_+ = \omega + \mathrm{i}0^+$. The vertex function reads $\Lambda^{\mathrm{eh}}_{\sigma\sigma}(q) = -U^2 X_{-\sigma-\sigma}(q)/[1 - U^2 X_{\sigma\sigma}(q)X_{-\sigma-\sigma}(q)]$, where $X_{\sigma\sigma}(q) = \sum_k G_\sigma(k)G_\sigma(k+q)$ is the polarization bubble in the four-momentum representation.

There is no equation relating the real part of the self-energy to the vertex function. To complete the determination of the one-particle self-energy we use its analyticity and determine the real part from a Kramers–Kronig relation:

$$\operatorname{Re}\Sigma_\sigma(\boldsymbol{k},\omega_+) = P\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\,\frac{\operatorname{Im}\Sigma_\sigma(\boldsymbol{k},\omega'_+)}{\omega'-\omega}. \tag{14}$$

Thereby, causality of the approximation is guaranteed. Unlike in the standard approach with equation (5), the irreducible vertex $\Lambda^{\mathrm{eh}}_{\sigma\sigma}$ used in equation (13) is the same as that entering the Bethe–Salpeter equation (3) determining the full vertex Γ. The maximal negative eigenvalue

of the integral kernel $\Lambda^{\mathrm{eh}}_{\sigma\sigma}(k'-k)G_\sigma(k')G_\sigma(k'+q)$ in active variables k, k' from equation (3) decides whether singularities arise in the dynamical two-particle Green and correlation functions. Further on, the self-energy determined from the irreducible vertex via equation (6) allows a direct incorporation of impurity scatterings. The effects of interactions and disorder can then be consistently approximated within a unified diagrammatic theory via contributions to the two-particle irreducible electron–hole vertex with consequent determination of the self-energy by means of the derived Ward identity equally valid for interacting and disordered electrons [9][3].

To conclude, the principal result of this letter is a partially integrated Ward identity (equation (6)). It is a consequence of the charge- and spin-conserving character of the particle interaction and was proved by means of a diagrammatic expansion. The primary importance of identity (6) lies in the possibility of regaining direct diagrammatic control over the (critical) behaviour of dynamical two-particle functions by defining the self-energy from the triplet vertex function via equation (6). The present schemes with two-particle (vertex) renormalizations and equation (5) do not obey the Ward identity (6), except in its infinitesimal limit. Utilization of the Ward identity (6) for the determination of the self-energy from the irreducible vertex opens up new possibilities for studying critical behaviour of correlated electrons, in particular when subjected to a random potential, and investigating the effects of electron interactions on electron diffusion and the metal–insulator transition [10].

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[3] Note that there is no Schwinger–Dyson equation for noninteracting electron systems.