STRONGLY CORRELATED ELECTRONS:
DYNAMICAL VERTEX RENORMALIZATION

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Abstract

Single-band Hubbard model at criticality of the metal-insulator transition is studied using approximations derived from parquet theory. It is argued that only the electron-hole and interaction two-particle channels in the parquet algebra are relevant. A scheme is proposed how to reduce the parquet equations to a manageable form the complexity of which is comparable with single-channel approximations such as the renormalized RPA. The newly derived approximation, however, contains dynamical vertex corrections, remains self-consistent at the two-particle level and allows only for integrable singularities. A qualitatively new approach for studying two-particle singularities at zero temperature is obtained.

1 INTRODUCTION

Strongly correlated electrons and heavy fermions display a number of phenomena not understandable within simple Fermi-liquid theory of metals. These unusual effects include dynamical formation of magnetic local moments and magnetic orders, mixed-valence fluctuations, Kondo and heavy-fermion behavior, non-Fermi-liquid phases and metal-semiconductor transitions. At present there are two principal approaches for treating electron correlations. Ab-initio investigation within the density-functional theory and the local-density approximation takes explicitly into account the Coulomb repulsion to equilibrium states within elementary cells (muffin-tin sphere) spread over a few interatomic distances. Short-range effects of the electron correlations in the ground state are quite well captured. Much less reliable are the results of the local-density approximations for long-range effects and low-energy excitations above the ground state. This failure can be attributed to the underestimation of the Pauli exclusion principle and long-range
fluctuations spreading over thousands of lattice constants. The other approach to the treatment of the electron correlations is based on tight-binding model calculations. The microscopic structure of the electron lattice gas is significantly simplified by taking into account only a few atomic (Wannier) orbitals. On the other hand, large-scale effects and low-energy excitations are well described. Presently the two approaches are more or less complementary.

A realistic description of the electron correlations has to join the two existing approaches to enable a sufficiently accurate treatment of both short as well as long distances. However, to succeed in a more reliable description of the electron correlations on small and large scales, it is mandatory to pick up and maintain the relevant aspects of each of the construction. The former supply us with realistic static properties of the ground-state. The latter offers qualitatively accurate estimates of dynamical fluctuations and collective responses to low-energy excitations of strongly correlated systems.

It appears that most of the physics of strongly correlated electrons is covered by the archetypal Anderson impurity and Hubbard lattice models with only a local electron interaction. The weak-coupling regime is governed by a Hartree-Fock mean field and Fermi-liquid theories. Extended systems at low temperatures are Pauli paramagnets with smeared out local magnetic moments. For bipartite lattices antiferromagnetic long-range order sets in at half filling at arbitrarily small interaction. In the strong-coupling regime the Hubbard model at half filling maps onto a Heisenberg antiferromagnet with pronounced local magnetic moments and the Curie-Weiss law for the staggered magnetic susceptibility. The spectral structure is dominated by separated lower and upper Hubbard bands and the strongly correlated system seems insulating even in the paramagnetic phase. The most difficult task of the model calculations is to address the transition region between the weak and strong coupling limits.

We present in this paper a theoretical approach based on many-body perturbation theory with sophisticated renormalizations of one as well as two-particle Green functions (propagators). In particular we show how the complicated algebra of two-particle multiple scatterings can be simplified to a manageable form. The presented single-band theory can be extended to the multi-band case and can hence be used for a more realistic electron-structure calculations.

2 TRANSITION FROM WEAK TO STRONG COUPLING IN THE HUBBARD MODEL

We have at our disposal relatively reliable techniques to describe the two extreme limits of weak and strong couplings of the Hubbard model. We can use perturbation expansions in each of the limits. In the former case it is the expansion in the interaction strength while in the latter in the kinetic energy (hopping matrix). The problem is that the two expansions do not match each other and break down before the transition regime is reached. The effective Coulomb repulsion becomes comparable with the kinetic energy in the transition region and there is no apparent small parameter at intermediate coupling.

Dynamical fluctuations control the low-temperature physics of interacting electrons at intermediate coupling and neither weak-coupling nor atomic-like perturbation theories are adequate. Weak and strong-coupling perturbation expansions with the bare interac-
tion can no longer reflect the relevant physics with creation and annihilation of long-living electron-hole pairs. The electron-hole pairs start to condense and lead to metal-insulator and magnetic transitions generating poles in appropriate two-particle Green functions.

The failure of the existing analytic-numerical methods to describe properly the transition between weak and strong coupling lies in an inadequate treatment of the two-particle criticality. While the one-particle functions are usually renormalized due to a self-consistency in the self-energy, the coupling constant and two-particle vertices remain unrenormalized. However, the two-particle criticality demands a theory with a dynamical renormalization of the relevant two-particle Green functions.

To succeed in a quantitative description of this complex situation, it is necessary to reformulate perturbation theory in such a way that the bare interaction be systematically replaced with fully renormalized two-particle functions determined from multiple two-particle scattering processes. It means that we have to use a perturbation theory at the level of two-particle Green functions including dynamical vertex renormalizations.

3 PARQUET DIAGRAMS

The most advanced approximation for two-particle functions are the so-called parquet diagrams. Parquet diagrams were introduced to describe interaction of mesons more effectively. Since then a number of attempts have been made to utilize the nontrivial renormalization scheme of the parquet algebra in condensed matter. Kondo effect, x-ray edge problem, formation of the local magnetic moment are among the most well known applications. Inability to solve the parquet equations effectively has impeded broader application of the method.

Parquet diagrams represent a systematic way of a summation and renormalization of Feynman graphs for two-particle Green functions. Instead of concentrating on the one-particle irreducible diagrams and the Dyson equation, the parquet approach sums two-particle diagrams contributing to vertex functions for which Bethe-Salpeter equations are constructed. The resulting algebra is much more complicated than that of the one-particle approximations. There are namely three topologically inequivalent definitions of a two-particle irreducibility. It may be defined according to cutting an electron-hole or electron-electron pair propagation, or according to cutting a polarization bubble shielding the electron-electron interaction. Each possibility defines a two-particle channel of multiple pair scatterings characterized by a different binding of independent variables in the vertex functions.

A general two-particle quantity will be denoted in this paper as in Fig. 1. Each two-particle function carries three independent four-momenta and two spin indices. We generally denote the fermionic four-momenta \( k = (k, i\omega_n) \) and the transferred bosonic ones as \( q = (q, i\nu_m) \), where \( \omega_n = (2n + 1)\pi T \) and \( \nu_m = 2m\pi T \) are the respective Matsubara frequencies at temperature \( T = \beta^{-1} \).

It is convenient to introduce a matrix notation in the spin indices to distinguish different two-particle channels in the parquet diagrams. We define a \( 2 \times 2 \) matrix for the generic two-particle function \( X_{\sigma\sigma'} \):

\[
\hat{X} = \begin{pmatrix}
X_{\uparrow\uparrow} & X_{\uparrow\downarrow} \\
X_{\downarrow\uparrow} & X_{\downarrow\downarrow}
\end{pmatrix}.
\]
Figure 1: Generic two-particle function with three independent four-momenta and a defined order of incoming and outgoing fermions.

We speak about singlet and triplet contributions to a two-particle function if the spins of the involved fermions are antiparallel or parallel, respectively.

We define three matrix multiplication schemes for the two-particle quantities

$$\begin{align*}
\left[ \hat{X} \cdot \hat{Y} \right]_{\sigma\sigma'}(k, k'; q) &= \frac{1}{\beta N} \sum_{q''} X_{\sigma\sigma'}(k, k'; q'') Y_{\sigma\sigma'}(k + q'', k' + q''; q - q''), \\
\left[ \hat{X} \circ \hat{Y} \right]_{\sigma\sigma'}(k, k'; q) &= \frac{1}{\beta N} \sum_{q''} X_{\sigma\sigma'}(k, k' + q''; q - q'') Y_{\sigma\sigma'}(k + q - q'', k'; q''), \\
\left[ \hat{X} \star \hat{Y} \right]_{\sigma\sigma'}(k, k'; q) &= \frac{1}{\beta N} \sum_{\sigma'' k''} X_{\sigma\sigma''}(k, k''; q) Y_{\sigma''\sigma'}(k'', k'; q)
\end{align*}$$

representing summations over the intermediate states in the three inequivalent two-particle channels, electron-hole, (eh), electron-electron, (ee), and interaction, (U), respectively. We see that the variables of the two-particle functions are convoluted differently in inequivalent channels. Note that only the interaction channel mixes the singlet and triplet contributions.

We decompose the full two-particle Green function into a sum of always reducible and irreducible projections onto each inequivalent channel

$$K_{\sigma\sigma'}(k, k'; q) = K^{\alpha}_{\sigma\sigma'}(k, k'; q) + \Gamma^{\alpha}_{\sigma\sigma'}(k, k'; q)$$

where $\alpha = eh, ee, U$ refers to a two-particle channel.

The parquet diagrams can at best be represented graphically. Having in mind the above introduced notation and a general convention that double primed variables are summed over, we can write

$$\begin{align*}
K^{eh}_{\sigma\sigma'} &= - \Lambda^{eh}_{\sigma\sigma'} + \kappa_{\sigma\sigma'}
\end{align*}$$
Equations (4) are the Bethe-Salpeter equations and represent one set of the full parquet approximation. To complete it we must add relations connecting the two-particle reducible, $K^\alpha$, and irreducible, $\Lambda^\alpha$, functions. For this purpose we introduced two-particle bubbles for each channel

\[ G^{(2)ch}_{\sigma\sigma'}(k, k'; q) = G_{\sigma}(k + q)G_{\sigma'}(k' + q), \quad G^{(2)ee}_{\sigma\sigma'}(k, k'; q) = G_{\sigma}(k + q)G_{\sigma'}(k') , \quad (5a) \]

\[ G^{(2)U}_{\sigma\sigma'}(k, k'; q) = G_{\sigma'}(k')G_{\sigma}(k' + q). \quad (5b) \]

The functions $\Lambda^\alpha$ are then defined as

\[ \Lambda^\alpha_{\sigma\sigma'}(k, k'; q) = I^\alpha_{\sigma\sigma'}(k, k'; q)G^{(2)\alpha}_{\sigma\sigma'}(k, k'; q) \]

\[ = \left[ U \delta_{\sigma', -\sigma} + \Delta I_{\sigma\sigma'}(k, k'; q) + \sum_{\alpha'' \neq \alpha} K^{\alpha''}_{\sigma\sigma'}(k, k'; q) \right] G^{(2)\alpha}_{\sigma\sigma'}(k, k'; q) \quad (6) \]

where $\Delta I_{\sigma\sigma'}$ is a sum of all Feynman diagrams simultaneously irreducible in each two-particle channel. The sum contains only higher-order diagrams where three and more particles are multiply interconnected. In the usual treatment with only two-particle multiple scatterings this irreducible part is neglected. We hence put $\Delta I_{\sigma\sigma'} = 0$.

Parquet equations (4) define the two-particle functions as a functional of the renormalized one-particle propagators containing the self-energy. The self-energy is a functional of the full two-particle function $K$ from the parquet equations. Hence to complete the parquet approximation we have to add formulas determining the dependence of the one-particle propagator on the self-energy (Dyson equation) and the self-energy on the full
two-particle function. The consistency between one and two-particle quantities demands

\[ G_\sigma(k, i\omega_n) = \left[i\omega_n + \mu_\sigma - \epsilon(k) - Un_{-\sigma} - \Sigma_\sigma(k, i\omega_n)\right]^{-1}, \]  

(7)

\[ \Sigma_\sigma(k) = -\frac{U}{\beta^2N^2} \sum_{\sigma'}\sum_{k,q} G_\sigma(k+q)K_{\sigma\sigma'}(k+q, k'; -q)G_{\sigma'}(k')G_{\sigma'}(k'+q) \]  

(8)

where \( n_\sigma \) is the particle density, \( \mu_\sigma = \mu + \sigma B \), and \( \mu \) is the chemical potential and \( B \) an external magnetic field.

Equations (3)-(8) constitute the parquet approximation. In this approximation only fully renormalized one and two-particle functions appear. It means that not only all one-particle propagators are fully renormalized with the self-energy insertions but also the bare electron-electron interaction in the two-particle scatterings is replaced by corresponding irreducible two-particle (vertex) functions. What is missing in the parquet diagrams are three-particle and higher-order cumulant functions. They are, however, not expected to be relevant for the static Coulomb interaction. They contribute via dipole and higher-order multi-pole interactions and are weak in the Hubbard model.

4 SIMPLIFIED PARQUET ALGEBRAS

Parquet diagrams differ significantly from simpler, single-channel approximations using multiple two-particle scatterings such as RPA, GWA or T-matrix (TMA). The difference manifest itself in the effective interaction in the two-particle scattering processes. The bare interaction in the two-particle scattering events remains unrenormalized in the single-channel approximations. In the parquet equations it is replaced by renormalized vertex functions representing a dynamically screened interparticle potential. A qualitative difference between a solution to the full parquet equations and to the single-channel approximations becomes evident at the two-particle criticality. The vertex functions from one or more channels get critical and sharply peaked around the Fermi energy. The exchange between the scattered particles becomes strongly energy dependent and cannot be approximated by a static effective interaction. Moreover, the singularity at the critical point in the parquet approximation must be integrable, while the single-channel approximations usually display logarithmic divergences in the integrated quantities (e. g. self-energy).

On the other hand the nonlinear integral equations represented by the parquet diagrams are extremely complicated with an intricate analytic structure of the solution. Each two-particle function entering the parquet equations contains three independent (complex) variables. Neither of them can simply be neglected, since the variables are mutually interconnected due to the scatterings in different inequivalent channels. Consequently, a nonperturbative solution to the parquet equations has not yet been found. That is also why the parquet diagrams are relatively little used in condensed matter although being in existence more than thirty years.

The only hope that the parquet approximation may become useful for quantitative calculations of the effects of the electron correlations is that one succeeds in simplifying

\[ \text{The self-energy } \Sigma \text{ in our notation measures corrections to the static Hartree approximation contained in the particle densities } n_\sigma \text{ determined from a sum rule } n_\sigma = (\beta N)^{-1} \sum_k G_\sigma(k). \]
the full parquet algebra to a manageable form. To this purpose we have to decide where we want the parquet approximation to be reliable. As discussed in the Introduction it is the intermediate coupling with critical two-particle functions where we need to improve upon easy-minded approximations. We hence demand asymptotic reliability of the parquet diagrams at the two-particle critical points and in particular at the metal-insulator transition. We retain only the diagrams making the effective mass of the electrons divergent at the metal-insulator transition.

4.1 Two-Variable Two-Particle Functions

It was recently argued that at least at half filling only two of the three inequivalent channels are relevant in the critical region of the metal-insulator transition \[5\]. Only multiple scatterings in the electron-hole and interaction channels contribute to divergent diagrams at the critical point. This simplification, called dipole approximation, however, does not reduce the number of the variables in the two-particle functions. It only simplifies the algebra of the parquet approximation. To lower the number of the relevant variables we utilize the fact that the singularities in the two-particle functions in the parquet approximation must be integrable. It means that when integrating over the variable in which the singularity arises we obtain a finite result. Our approximation consists in neglecting all finite (nondiverging) contributions at the critical point and keeping only the divergent ones. This must be done at the level of the diverging two-particle functions.

There is always one relevant bosonic variable in each two-particle channel. It is the variable remaining untouched in the scattering processes. It can easily be seen from multiplication rule (2) that it is \(k - k', k + k' + q\), and \(q\) for the electron-hole, electron-electron, and interaction channels, respectively. Divergences in the reducible functions appear in the respective conserved variables. For the metal-insulator transition only \(k - k'\) and \(q\) are relevant.

In the first step we reduce the number of the relevant variables in the two-particle functions to two. This is achieved when we neglect mixing of the reducible functions from different channels. We replace the full two-particle function \(K\) on the right-hand side of (4) by \(U + K^\alpha\), i.e. by the sum of the completely irreducible vertex and the reducible function in the \(\alpha\)-channel. Such a replacement does not change the (universal) critical behavior of the resultant reducible function \(K^\alpha\). The bare interaction is a constant and consequently the solution does not depend on the outgoing variables. Further on, the triplet functions can be eliminated from this approximation, since \(I_{\sigma,\bar{\sigma}}\) gets irrelevant. If we denote \(I^v_{\sigma,-\sigma} = U + K_{\sigma,-\sigma}^{eh}\) and \(I^h_{\sigma,-\sigma} = U + K_{\sigma,-\sigma}^U\), the parquet equations reduce to

\[
I^v_{\sigma,-\sigma}(k; q) = U - \frac{1}{\beta N} \sum_{q'} I^h_{\sigma,-\sigma}(k; q')G_{\sigma}(k + q')G_{-\sigma}(k + q + q')I^v_{\sigma,-\sigma}(k + q'; q) ,
\]

(9)

\[
I^h_{\sigma,-\sigma}(k; q) = U + \frac{1}{\beta^2 N^2} \sum_{q',q''} I^v_{\sigma,-\sigma}(k; q')G_{-\sigma}(k + q + q')G_{-\sigma}(k + q + q + q'')
\]

\[
\times I^v_{\sigma,-\sigma}(k + q'; q'' - q')G_{\sigma}(k + q'' + q)G_{\sigma}(k + q'' + q)I^h_{\sigma,-\sigma}(k + q''; q) .
\]

(10)
The bosonic variable $q$ has different meaning in the functions $I^h$ and $I^v$. It is the horizontal, vertical transfer momentum for the former and the latter, respectively.

Because of breaking of the symmetry between the incoming and outgoing variables in the two-particle functions we must be careful in deriving the equation for the self-energy. To be consistent we use a symmetrized formula with the bare interaction at the incoming and outgoing momentum. We obtain

$$
\Sigma_\sigma(k) = -\frac{U}{2\beta^2 N^2} \sum_{k',q} G_\sigma(k + q) G_{-\sigma}(k') G_{-\sigma}(k' + q) \left[ I^h_{\sigma,\sigma}(k + q; -q) 
+ I^h_{-\sigma,\sigma}(k'; q) + I^v_{\sigma,\sigma}(k + q; k' - k) + I^v_{-\sigma,\sigma}(k'; k - k') - 2U \right].
$$

The reduced two-channel parquet approximation with two-variable two-particle functions has the critical behavior of the full parquet approximation. The universal quantities derived from the divergent functions of the parquet equations (4) are reproduced in equations (9)-(11). Only nonuniversal quantities such as the critical interaction do not come out in this simplification as in the full parquet approximation.

We achieved a simplification of the full parquet algebra without loosing leading critical behavior of the solution, but the resulting equations have nonlinear convolutive character. We have to find a nonperturbative solution to these equations when addressing the metal-insulator transition. This is, however, still beyond the reach of our analytic-numerical tools. We must find a further reduction of complexity of the parquet equations to make them useful for a quantitative analysis.

### 4.2 One-Variable Two-Particle Functions

It is the bosonic variable $q$ in the two-particle functions $I^h, I^v$ that is relevant at the critical point and in which the singularity arises. The fermionic variable $k$ in both functions labels the eigenvalues of the integral kernel in equations (9), (10). The maximal eigenvalue governs the critical behavior. If we are interested only in the critical asymptotic behavior we can approximate the actual maximal eigenvalue by a value at the lowest-lying fermionic four-momentum. By such an approximation we neglect mixing of the fermionic four-momenta in the equations and replace $k$-dependence in the two-particle functions by a constant, their value at $k = 0$. This approach corresponds to a low-energy expansion used by Hamann [6] by assessing the strong-coupling limit of the renormalized RPA of Suhl in the single-impurity problem.

The suggested simplification is possible only at zero temperature, where the difference between the fermionic and bosonic Matsubara frequencies vanishes. We hence put $T = 0$, which is the most interesting case for the metal-insulator transition. Using the above ansatz, neglecting $k$-dependence in $I^h, I^v$, and putting $k = 0$ in the one-electron propagators we reduce the parquet equations to a manageable form. We introduce new functions

$$
\Gamma_\sigma(q) = \frac{1}{\beta N} \sum_{q'} I^h_{\sigma,\sigma}(q' \sigma) G_\sigma(q') G_{-\sigma}(q' + q),
$$

$$
\mathcal{K}_\sigma(q) = \frac{1}{\beta N} \sum_{q'} I^v_{-\sigma,\sigma}(q' \sigma) G_\sigma(q') G_{\sigma}(q' + q),
$$

(12)

(13)
with the aid of which we obtain for the two-particle functions

\[ I^v_{\sigma,-\sigma}(q) = \frac{U}{1 + \Gamma_\sigma(q)}, \quad \text{(14)} \]

\[ I^h_{\sigma,-\sigma}(q) = \frac{U}{1 - K_{-\sigma}(q)K_\sigma(q)}. \quad \text{(15)} \]

The above equations have the complexity of the single-channel approximations, but contain the full vertex renormalization in the two-particle scatterings. It is always the renormalized vertex function that enters the denominator of equations (14), (15) via the functions \( \Gamma \) and \( K \). The single channel approximations replace the two-particle vertex functions \( I^h, I^v \) in (12), (13) by the bare interaction \( U \).

It is easy to derive the corresponding equation for the self-energy. It reads

\[ \Sigma_\sigma(k) = -\frac{U}{2\beta N} \sum_q \left[ G_\sigma(k + q)X_{\sigma,-\sigma}(q) \left( I^h_{\sigma,-\sigma}(q) + I^h_{-\sigma,-\sigma}(-q) - U \right) + G_{-\sigma}(k + q)X_{\sigma,-\sigma}(q) \left( I^v_{\sigma,-\sigma}(q) + I^v_{-\sigma,-\sigma}(-q) - U \right) \right] \quad \text{(16)} \]

where we introduced a single bubble

\[ X_{\sigma,\sigma'}(q) = \frac{1}{\beta N} \sum_{k'} G_\sigma(k')G_{\sigma'}(k' + q). \quad \text{(17)} \]

Equations (12)-(17) replace the original parquet approximation. They fully determine the generating two- and one-particle functions. All thermodynamic and spectral quantities can be calculated from them. Since we used a number of approximate steps in the derivation of the reduced parquet algebra, any new quantity must first be formulated within the full parquet approximation. The simplifications are then introduced via the generating one- and two-particle functions. In this way a consistent theory is built up, since the parquet approximation can be viewed upon as a conserving approximation derived from a generating functional.

### 4.3 Electron-Hole Symmetry

An exact solution as well as the full parquet approximation fulfill a number of identities and symmetries. One of the most important features of the exact solution is the electron-hole symmetry. It means, that the physics must not depend on whether we use the particle or the hole picture. The electron-hole symmetry is obeyed by the complete parquet approximation. It is not clear whether we have not lost some of the required symmetries in course of simplifying the parquet algebra.

We lost the symmetry between the incoming and outgoing variables in our approximate equations. Further on we also lost the electron-hole symmetry in only one particle

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2There is a different way how to reduce the parquet approximation to single-variable equations. The other reduction is based on the so-called leading logarithmic divergences in single-loop diagrams. This approach is inappropriate in the strong-coupling limit, where such divergences cannot survive because of the integrability of the singularities in the parquet equations.
of the pair in the two-particle scatterings. The former was lost during the reduction to two-variable two-particle functions and the latter due to the suppression of the electron-electron channel. These losses are not so serious if we are in the critical region of the metal-insulator transition. The one-sided electron-hole transformation changes the sign of the effective interaction and hence breaks the bound electron-hole pair.

The full electron-hole symmetry in all variables must hold for any approximate theory, otherwise we were unable to guarantee the Fermi liquid properties at weak coupling. The electron-hole transformation may be defined in the parameter space of the Hubbard model as

\[ \mu \to \bar{\mu} = U - \mu, \quad B \to \bar{B} = -B, \quad \epsilon_k \to \bar{\epsilon}_k = -\epsilon_{-k} \]  

where the bar denotes a hole representation. It is easy to check by inspection that a solution to the reduced parquet equations (12)-(17) fulfill the following symmetry relations

\[
G_{\sigma}(k) = -\bar{G}_{\sigma}(-k), \quad \Sigma_{\sigma}(k) = -\bar{\Sigma}_{\sigma}(-k), \quad n_{\sigma} = 1 - \bar{n}_{\sigma}
\]

\[
\Gamma_{\sigma}(q) = -\bar{\Gamma}_{\sigma}(-q), \quad K_{\sigma}(q) = \bar{K}_{\sigma}(-q).
\]

This electron-hole symmetry together with the analyticity of the one- and two-electron functions is used to prove Fermi-liquid properties of solutions to (12)-(17) for sufficiently weak interaction, i.e. before poles in the vertex functions \( I^v, I^h \) appear.

## 5 EFFECTIVE IMPURITY MODEL

Up to know we have worked with a very general formulation of the parquet approximation applicable in any spatial dimension. However, recent studies indicate that most of the effects of strong electron correlations can qualitatively be understood already within a dynamical mean-field theory or impurity models [8]. It is sufficient in many situations to reduce the effects of strong correlations to a dynamical mean-field where the self-energy and vertex functions are local, but frequency-dependent. Such an approach significantly reduces the numerical complexity but keeps much of the interesting physics of strongly correlated electrons.

We apply the simplified parquet approximation to a single impurity or a dynamical mean field model. The fluctuations in space do not contribute to the dynamics and the four-momenta from the general formulation of the parquet approximation collapse to frequencies. This simplification enables one to perform explicitly analytic continuation from the Matsubara to the real frequencies using contour integrals. Realizing that the reduced equations hold for \( T = 0 \) and introducing \( \zeta, z \) for the bosonic, fermionic complex frequencies, respectively, we can write for the two-particle functions

\[
\mathcal{K}_{\sigma}(\zeta) = -U \int_{-\infty}^{0} \frac{d\omega}{\pi} \left[ G_{\sigma}(\omega + \zeta) \text{Im} \frac{G_{\sigma}(\omega_+)}{1 + \Gamma_{-\sigma}(\omega_+)} + \frac{G_{\sigma}(\omega - \zeta)}{1 + \Gamma_{-\sigma}(\omega - \zeta)} \text{Im} G_{\sigma}(\omega_+) \right],
\]

\[
\Gamma_{\sigma}(\zeta) = -U \int_{-\infty}^{0} \frac{d\omega}{\pi} \left[ G_{-\sigma}(\omega + \zeta) \text{Im} \frac{G_{\sigma}(\omega_+)}{1 - \mathcal{K}_{\sigma}(\omega_+) \mathcal{K}_{-\sigma}(\omega_+)} + \frac{G_{\sigma}(\omega - \zeta)}{1 - \mathcal{K}_{\sigma}(\omega - \zeta) \mathcal{K}_{-\sigma}(\omega - \zeta)} \text{Im} G_{-\sigma}(\omega_+) \right]
\]
and analogously for the one-particle self-energy

\[
\Sigma_\sigma(z) = U \int_{-\infty}^{0} \frac{d\omega}{\pi} \left\{ G_\sigma(\omega + z) \text{Im} \left[ X_{-\sigma,-\sigma}(\omega_+) \left( I_{h,-\sigma,-\sigma}^h(\omega_+) - U \right) \right] + X_{-\sigma,-\sigma}(\omega - z) \left( I_{-\sigma,-\sigma}^h(\omega_+) - U \right) \text{Im} G_\sigma(\omega_+) + G_\sigma(\omega + z) \text{Im} \left[ X_{\sigma,-\sigma}(\omega_+) \left( I_{\sigma,-\sigma}^\nu(\omega_+) \right) \right] + X_{\sigma,-\sigma}(\omega - z) \left( I_{\sigma,-\sigma}^\nu(\omega_+) \right) \text{Im} G_\sigma(\omega_+) \right\}
\] (23)

where \( \omega_+ = \omega + i0^+ \). The local propagator is for the mean field

\[
G_\sigma(z) = \int_{-\infty}^{\infty} d\epsilon \rho(\epsilon) \frac{1}{z + E_\sigma - \Sigma_\sigma(z) - \epsilon}
\] (24)

and for the impurity model

\[
G_\sigma(z) = \left[ z + E_\sigma - V^2 g(z + \sigma B) - \Sigma_\sigma(z) \right]^{-1}
\] (25)

where \( E_\sigma = \mu + \sigma B - Un_{-\sigma} \) for the mean-field and \( E_\sigma = \mu + \sigma B - \varepsilon \) for the impurity model. In the former \( \rho(\epsilon) \) is the density of states and in the latter, the parameter \( \varepsilon \) is the energy of the impurity orbital, \( V \) hybridization to the conduction electrons, and \( g(z) \) the one-electron local Green function of the conduction electrons. Note that there is no difference at the two-particle level between the impurity and mean-field equations.

### 5.1 Intermediate Coupling

We use the local formulation of the simplified parquet approximation to demonstrate that intermediate coupling is dominated by a two-particle criticality. We confine ourselves only to half filling and the spin symmetric case (paramagnet) where the singularity indicates a metal-insulator transition. We further assume a bipartite lattice, i.e. \( \rho(\epsilon) = \rho(-\epsilon) \).

A solution to equations (21)-(23) has at weak coupling the required Fermi-liquid properties. The two-particle functions \( X, \Gamma, K \) are real at the Fermi energy. Iterations starting with \( U = 0 \) converge to a unique solution. Such a procedure becomes numerically unstable if we increase the interaction beyond \( U_c \) defined as

\[
U_c = - \left[ X_0(0) \right]^{-1}, \quad X_0(0) = - \int_{-\infty}^{0} \frac{d\omega}{\pi} \text{Im} \left[ G^{(0)}(\omega_+)^2 \right]
\] (26)

where \( G^{(0)} \) is a noninteracting one-particle propagator. The value \( U_c \) corresponds to the critical interaction determined from the RPA pole in the electron-hole susceptibility. Explicitly, \( U_c = V^2 \pi^2 \rho(0) \) for a mean-field (\( d = \infty \)) model with a Lorentzian DOS (infinite bandwidth) and \( U_c = 3\pi w/4 \) for a Bethe \( d = \infty \) lattice (finite bandwidth). This interaction need not necessarily represent a critical point. It only indicates that we cannot start iterations from an unperturbed solution and that weak-coupling perturbation theories get numerically unstable. We can say that the weak-coupling regime goes over at \( U_c \) to an intermediate one. The transition is, however, smooth for effective impurity models.

At intermediate coupling the functions \( I^\nu \) and \( I^h \) approach a pole at the Fermi energy \( \zeta = 0 \). It means that \( 1 + \Gamma(0) \) as well as \( 1 - K(0)^2 \) approach zero. A new small
(dimensionless) scale $\Delta = 1 + \Gamma(0) \approx 1 - K(0)^2$ arises. This scale cannot be derived from the one-electron model parameters. It is a consequence of a two-particle criticality. In the single-impurity case it is related to the Kondo scale. The scale vanishes at the metal-insulator transition if it is of second order.

The vanishing scale $\Delta$ causes nonanalyticities in the two-particle functions $\Gamma(\omega)$ and $K(\omega)$, and in the one-electron self-energy $\Sigma(\omega)$. Since the singularity in the vertex functions $I^v(\omega), I^h(\omega)$ must be integrable, the functions $\Gamma, K, \Sigma$ remain bounded (continuous). Only their derivatives show divergences at the Fermi energy at the critical point. It is straightforward to show that leading-order divergences in (21) - (23) are

$$\text{Im } K'(0) \doteq -\frac{U}{\pi} \frac{[\text{Im } G(0)]^2}{1 + \Gamma(0)}, \quad \text{Im } \Gamma'(0) \doteq -\frac{U}{\pi} \frac{[\text{Im } G(0)]^2}{1 - K(0)^2}, \quad (27)$$

$$\text{Re } \Sigma'(0) \doteq -\frac{U}{\pi} U X(0) \text{ Im } G(0) \left[ \frac{1}{1 + \Gamma(0)} + \frac{1}{1 - K(0)^2} \right] \quad (28)$$

where the prime denotes the derivative w.r.t. the frequency variable. We utilized the symmetry of the half-filled case, $\text{Re } G(0) = 0$ in the derivation of (27), (28).

The Mott-Hubbard metal-insulator transition is defined by divergence of the effective mass $\Delta$. Since $m^*/m \propto |\Sigma'(0)|$ we have proved that the singularity in the two-particle vertex functions $I^v, I^h$ causes divergence of the effective electron mass and hence the Mott-Hubbard metal-insulator transition. The way the effective electron mass diverges is essentially determined by vanishing of the Kondo scale $\Delta$. It means that the Kondo scale sets an interval around the Fermi energy within which the Landau quasiparticle picture holds not only for the one-electron but also for the two-electron functions. The narrow quasiparticle Kondo-Suhl peak is then a consequence of sharply peaked two-particle vertex functions. No effective static interaction can describe the Kondo strong-coupling asymptotics and the Mott-Hubbard metal-insulator transition with (27), (28) reliably.

The simplified parquet approximation describes qualitatively well the weak-coupling Fermi-liquid regime. It also correctly binds divergence of the effective mass with the Kondo scale arising from a singularity in two-particle functions. The derived approximate theory does well on the metallic side of the metal-insulator transition. Whether the approximation can correctly capture the physics up to the transition point must be decided from the dependence of the Kondo scale $\Delta$ onto the interaction strength $U$ or better on the parameter $1 - U/U_c$. The correct behavior must reproduce the exponential law $\Delta \propto \exp{-U \rho(0)}$ for the single-impurity model. We need a deeper analysis of equations (21) - (23) to decide whether this really is the case. It will be done in a separate paper.

Next we have to address the strong-coupling regime for $U > U_c$. Fermi-liquid theory no longer holds and it is unclear how to iterate towards a stable solution. The problem is to choose the value of the self-energy at the Fermi level. It vanishes in the Fermi-liquid, metallic phase but diverges in the atomic, insulating solution. What value the self-energy acquires in a self-consistent insulating solution to (21) - (23) needs to be investigated in more details. One can, however, easily check that the simplified parquet approximation allows for a consistent $U \rightarrow \infty$ limit. After an appropriate scaling of the variables one recovers an atomic solution at zero temperature. Dynamical fluctuations then enter as perturbations in $w/U$, where $w$ is an effective bandwidth of the conduction electrons. A
perturbation expansion in $w/U$ can be a good starting point for iterations to the full solution of equations (21)-(23) in the strong-coupling, insulating phase.

6 CONCLUSIONS

We demonstrated in this paper that a successful description of intermediate and strong coupling regimes in correlated electron systems demands sophisticated approximations with a dynamical renormalization of two-particle vertex functions. A transition regime between the weak and strong coupling limits is governed by the formation and condensation of long-living electron-hole pairs resulting in poles in two-particle Green functions. These dynamical effects cannot properly be rendered by theories with only effective static interactions. The well-known single-channel two-particle approximations such as RPA, TMA, or GWA are inadequate at intermediate coupling, since the interaction in the multiple scatterings remains unrenormalized. Only the full parquet approximation with all two-particle irreducible diagrams can be expected to capture the relevant physics at the two-particle criticality of intermediate coupling.

The parquet diagrams lead to a qualitatively different critical behavior than that obtained from the simple-minded single-channel approximations. The only singularities that can appear in the parquet approximation are integrable ones, i.e. convolutions of singular and regular functions must be finite. This feature distinguishes the parquet theory from the other existing approximations in correlated electron systems.

The parquet algebra is too intricate to allow for a nonperturbative solution. Only an appropriate reduction in the complexity of the parquet approximation can lead to a successful application of the method. We proposed in this paper a scheme how to reduce the nonlinear convolutive integral parquet equations to a system of quasi-algebraic equations not more complicated than the single-channel approximations. The only difference is that the effective interaction in the scattering events in one channel is dynamically renormalized by scatterings from other channels.

The reduction of the parquet algebra is enabled by taking into account only leading-order divergences at the metal-insulator transition and a low-energy expansion around the maximal eigenvalue of the parquet equations. The resulting equations allow only for integrable singularities and lead to sharply peaked two-particle vertex functions in the vicinity of the critical metal-insulator transition. They correctly bind divergence of the effective one-electron mass with the Kondo scale stemming from a two-particle singularity. What still remains to do is to show how well the simplified parquet approximation reproduces the strong-coupling asymptotics of the Kondo scale in the single-impurity problem known from an exact solution. Only then we can be sure we have a reliable interpolation between the weak and strong-coupling regimes of Hubbard-like models.

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