Effect of three-particle correlations
in low dimensional Hubbard models

Theodore C. Hsu(1),(2) and Benoît Douçot(2)∗∗

(1) AECL Research, Chalk River Laboratories, Chalk River, Ontario, Canada K0J 1J0
(2) Centre des Recherches sur les Très Basses Températures,
BP 166, 38042 Grenoble, France
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A simple approximation which captures some non-perturbative aspects of the
one electron Green function of strongly interacting Fermion systems is developed. It
provides a way to go one step beyond the usual dilute limit since particle-particle as
well as particle-hole scattering are treated on the same footing. Intermediate states
are constrained to contain only one particle-hole excitation besides the incoming
particle. The Faddeev equations resulting from an exact treatment of this three-
body problem are investigated. In one dimension the method is able to show spin and
charge decoupling, but does not reproduce the exact nature of power-law singularities.

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I. INTRODUCTION

Since the discovery of high temperature superconductors, much work from both experimental and theoretical sides has suggested that Fermi-liquid theory does not provide a good description of the remarkable normal state properties of these materials. In particular, Anderson [1] has proposed that a better framework is to be found in some two dimensional generalization of the Luttinger liquid, which has been identified by Haldane [2] as a low energy effective theory for many interacting-Fermion systems in one dimension. For example, recent measurements of the temperature dependence of the Hall angle in high \( T_c \) cuprates have been interpreted along this line [3]. However, it has not yet been possible to derive such a picture from a first principles calculation. A suggestive investigation of two-particle scattering in two dimensions in the presence of the Fermi sea has lead Anderson to claim that a finite phase shift and a singular interaction function \( f_{k,k'} \) exist even in the dilute limit [4]. But if the same particle-particle ladder is used in a more conventional many-body calculation, it has been shown by Engelbrecht and Randeria [5] and Fukuyama et al. [6] that the imaginary part of the self-energy is not singular enough in this T-matrix approximation to avoid Fermi-liquid behavior. In fact, the two approaches may not contradict each other. Anderson suggests that an extra particle added to the system induces a shift of all the momenta of the particles already present in a similar way as the deep level in the X-ray edge problem. The present paper is an attempt to connect this physical picture to some microscopic perturbative calculations for the repulsive Hubbard model.

In our approach, we have been guided by the idea already stressed in the work by Abrikosov on the Kondo problem [7], and Nozières et al. on the X-ray edge problem [8], namely that both particle and hole scattering channels with the local impurity lead to similar singularities which may cancel partially. It is then crucial to treat both in an unbiased way. This is for instance a key feature of the parquet summation, which was developed in references [7] and [8]. However, this method is not very easy to implement for many body systems, where the angular dependence of interaction vertices is in general not described by
a small set of relevant parameters (except in one dimension). A simplification occurs if we work in a truncated Hilbert space with only one particle-hole excitation on top of a local potential (X-ray edge problem), a spin (Kondo problem), or an added electron (Hubbard model). This approach is variational in spirit and amounts to treating, exactly, three-particle correlations amongst the particle-hole pair and the analogue of a local scatterer. It has been used in the context of Kondo problems to study various properties [9,10], and for the Hubbard model in the special case of a single overturned spin [11]. It has even been suggested that three-particle correlations between a spin flip and two holes may provide a way to reduce the ground state magnetization away from its maximal value in the infinite-U Hubbard model at any density [12]. Three-body correlations are also investigated as a possible microscopic mechanism leading to a marginal Fermi-liquid [13].

In this paper then, we shall concentrate on the effect of three-particle correlations on the self-energy of an electron. We consider a variational state which consists of one electron plus at most one extra particle-hole pair excitation on top of an otherwise rigid Fermi sea. The scattering in the particle-particle and particle-hole channels are treated on an equal footing. In this sense we attempt to go beyond references [5] and [6] who considered only two-particle scattering. We shall be interested in seeing whether the Fermi-liquid starting point is valid or not. Exact solutions are available for the Luttinger model and the X-ray edge problem and we have decided to compare the electron’s Green function in the three-body approximation to that of the exact solution for these systems. In section 2 we shall discuss the formalism leading to the Faddeev integral equations [14]. We have re-formulated these in order to yield directly the self-energy. Sections 3 and 4 will describe results for the one and two branch Luttinger models respectively and section 5 will describe results for the X-ray problem.

II. FADDEEV EQUATIONS

We begin with the definition of the electron Green function,
\[
G(q, \omega) = \langle N | c_{q\uparrow}[\omega - H + i\delta]^{-1}c_{q\uparrow} + c_{q\uparrow}[\omega + H - i\delta]^{-1}c_{q\uparrow} | N \rangle \tag{2.1}
\]

where the Hamiltonian is
\[
H = \sum_k \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{U}{N_s} \sum_{k,k',p} c_{k+p\uparrow}^\dagger c_{k\uparrow}^\dagger c_{k'\downarrow} c_{k\downarrow} - E_0 . \tag{2.2}
\]

We shall consider a variational state where \( | N \rangle \) is the non-interacting Fermi sea and the Hamiltonian is allowed to create at most one excited particle-hole pair. The corresponding diagrams contributing to the Green function are shown in Fig. \[\] We take \( q > k_F \) and \( E_0 \) is chosen so that \( \langle N | H | N \rangle = 0 \). In this case, defining
\[
\phi \equiv \langle N | c_{q\uparrow}[\omega - H + i\delta]^{-1}c_{q\uparrow} | N \rangle \tag{2.3}
\]
and
\[
\Phi(k, k') \equiv \langle N | c_{q\uparrow}[\omega - H + i\delta]^{-1}c_{k\uparrow}^\dagger c_{k'\downarrow} c_{k+q\downarrow} | N \rangle , \tag{2.4}
\]
the equations of motion of these Green functions truncating terms involving more than three particles are
\[
[\tilde{\omega} - \epsilon_q] \phi - \frac{U}{N_s} \sum_{k,k'} \Phi(k, k') = 1 \tag{2.5}
\]
and
\[
[\tilde{\omega} - \epsilon(k, k')] \Phi(k, k') - \frac{U}{N_s} \phi - \frac{U}{N_s} \sum_{k''} \Phi(k'', k + k' - k'') + \frac{U}{N_s} \sum_{k''} \Phi(k'', k') = 0 \tag{2.6}
\]
where \( \tilde{\omega} = \omega - U(N_1/N_s) \) and \( \epsilon(k, k') = \epsilon_k + \epsilon_{k'} - \epsilon_{k+k'-q} \). The momentum restrictions in the sum are such that the arguments of \( \Phi(k_1, k_2) \) always satisfy \( k_1 \neq q; k_1, k_2 > k_F \) and \( |k_1 + k_2 - q| < k_F \).

We shall find it convenient to define the following functions:
\[
J_1(K) = N_s^{-1} \sum_{k'} \Phi(k', K - k') \tag{2.7}
\]
and
\[ J_2(K) = N_s^{-1} \sum_{k'} \Phi(k', K) \] (2.8)

which correspond roughly to T-matrices for the particle-particle and particle-hole scattering channels respectively. From the equations of motion for \( \phi \) we may see that \( J_1 \) is related to the self-energy by

\[ \Sigma(q, \tilde{\omega}) = U^2 \sum_{K} J_1(K) \] (2.9)

From the equation of motion for \( \Phi \) we see that \( J_1 \) and \( J_2 \) satisfy the coupled integral equations

\[ J_1(K) = N_s^{-1} \frac{F_1(K)}{1 - UF_1(K)} - \frac{U}{N_s} \sum_{k'} \frac{J_2(K - k')}{\tilde{\omega} - \epsilon(k', K - k')} \] (2.10)

and

\[ J_2(K) = N_s^{-1} \frac{F_2(K)}{1 + UF_2(K)} + \frac{U}{N_s} \sum_{k'} \frac{J_1(K + k')}{\tilde{\omega} - \epsilon(k', K)} \] (2.11)

In the summations the same momentum restrictions as the equations of motion Eqs. (2.5) and (2.8) are in effect. \( F_1 \) and \( F_2 \) are defined by

\[ F_1(K) = N_s^{-1} \sum_{k'} \frac{1}{\tilde{\omega} - \epsilon(k', K - k')} \] (2.12)

and

\[ F_2(K) = N_s^{-1} \sum_{k'} \frac{1}{\tilde{\omega} - \epsilon(k', K)} \] (2.13)

The integral equations can be combined into a single one for \( J_1 \) which is the final equation to be solved.

\[ J_1(K) = \frac{1}{N_s^2} \sum_{k'} \frac{1}{(\tilde{\omega} - \epsilon(k', K - k'))(1 + UF_2(K - k'))} \frac{1}{(\tilde{\omega} - \epsilon(k' + k'' - K, K - k''))} \sum_{k''} \frac{J_1(k'' - k', K - k'')}{(\tilde{\omega} - \epsilon(k'' - K, K - k''))(1 + UF_2(K - k''))} \] (2.14)

The technique of truncating the Green function equations of motion at the four point level and finding closed equations for them is not limited to well defined particles and is not new. It has been applied [15] to Green functions for the Hubbard ‘X’ operators [16].
III. ONE–BRANCH LUTTINGER MODEL

In this section we present the exact analytical solution of the integral equation for a one branch Luttinger model (i.e. with right movers only). The total momentum of the three particles is $q > k_F$ and the energy dispersion is defined by $\epsilon_k = v_F (k - k_F)$. The simplification which allows an analytical solution is the fact that

$$\epsilon(k, k') \equiv \epsilon_k + \epsilon_{k'} - \epsilon_{k+k'-q} = v_F(q - k_F).$$

Thus we have

$$F_1(K) = \frac{K - 2k_F}{\omega - v_F(q - k_F)} \quad (3.1)$$

and

$$F_2(K) = \frac{q - K}{\omega - v_F(q - k_F)} \quad (3.2)$$

Defining $\tilde{q} \equiv q - k_F$,

$$j_1(k) \equiv (\tilde{\omega} - v_F \tilde{q})^{-1} J_1(k) \quad (3.3)$$

$$f_1(k) \equiv (\tilde{\omega} - v_F \tilde{q})^{-1} [1 - UF_1(k)]^{-1} \quad (3.4)$$

$$f_2(k - k'') \equiv (\tilde{\omega} - v_F \tilde{q})^{-1} [1 + UF_2(k - k'')]^{-1} \quad (3.5)$$

we absorb a factor of $N_s$ into $J_1$ and go to the continuum obtaining

$$j_1(k) = f_1(k) \int_{k_F}^{k-k_F} dk'' f_2(k - k') \left[ 1 - U^2 \int_{k-k''-k_F}^{q+k_F} dk' j_1(k') \right]. \quad (3.6)$$

There is, in fact, no small parameter in this integral equation, even when $U$ is small. Thus it cannot be solved perturbatively. This can be demonstrated explicitly by defining $j(k) \equiv \tilde{q} U^2 j_1(k)$ and $x \equiv (\tilde{\omega} - v_F \tilde{q})/U \tilde{q}$. Rescaling all momenta with respect to $\tilde{q}$ and setting $k_F = 0$ we have

$$j(k) = \frac{1}{x - k} \int_0^k dk'' \frac{1}{x + 1 - k + k''} \left[ 1 - \int_{k''}^1 dk' j(k') \right]. \quad (3.7)$$

Changing the order of integration allows us to perform one of the nested integrals. Using

$$\int_0^k dk'' \int_{k-k''}^1 dk' = \int_0^k dk' \int_{k-k''}^k dk'' + \int_k^1 dk' \int_0^k dk'' \quad (3.8)$$
we find
\[ j(k) = \frac{1}{x - k} \times \left[ \ln \left( \frac{x+1}{x+1-k} \right) - \int_0^k dk' j(k') \ln \left( \frac{x+1}{x+1-k'} \right) \right] . \] (3.9)

The solution proceeds by conversion into a differential equation. Multiplying by \( x - k \) and differentiating with respect to \( k \) we have
\[ \frac{d}{dk} [(x - k)j(k)] = \frac{1}{x + 1 - k} - \frac{1}{x + 1 - k} \int_k^1 dk' j(k') . \] (3.10)

Multiplying by \( x + 1 - k \) and differentiating,
\[ \frac{d}{dk} [(x + 1 - k)((x - k)j'(k) - j(k))] = j(k) . \] (3.11)

This can be integrated because the integral equation gives us the two boundary conditions
\[ j(0) = 0 \] (3.12)

and
\[ x(x + 1)j'(0) = 1 - \int_0^1 dk j(k) \equiv 1 - (\Sigma(x)/xU\tilde{q}) . \] (3.13)

Integration of Eq. (3.11) results in an equation for \( j(k) \) in terms of \( x, k \), and \( j'(0) \). Integrating over \( k \) from \( k = 0 \) to \( k = 1 \) eliminates \( j(k) \) and \( k \) and results in an equation for the self-energy in terms of \( x \) whose solution is (adding in the imaginary parts now)
\[ \Sigma(x) = xU\tilde{q}\mathcal{A}/(1 + \mathcal{A}) \] (3.14)

where
\[ \mathcal{A} = x^2 \ln \left| \frac{x^2}{1 - x^2} \right| - 1 - i\pi x|x|\theta(x + 1)\theta(1 - x) . \] (3.15)

Substituting back into the electron Green function gives the very simple result
\[ G(x) = x \ln \left| \frac{x^2}{1 - x^2} \right| - i\pi x|x|\theta(x + 1)\theta(1 - x) \] (3.16)
where $\theta(x)$ is the usual step function. Re-inserting the original units,
\[
\text{Im} G(\tilde{\omega}, \tilde{q}) = \pi \left| \frac{\tilde{\omega} - v_F \tilde{q}}{U \tilde{q}} \right|, \quad v_F \tilde{q} - U \tilde{q} < \tilde{\omega} < v_F \tilde{q} + U \tilde{q}
\] (3.17)

The exact Green function is [17]
\[
\text{Im} G(\tilde{\omega}, \tilde{q}) = \left[ (U \tilde{q})^2 - (\tilde{\omega} - v_F \tilde{q})^2 \right]^{-1/2}, \quad v_F \tilde{q} - U \tilde{q} < \tilde{\omega} < v_F \tilde{q} + U \tilde{q}
\] (3.18)

Our result is compared to the exact result in Fig. 2. The spectral weight from the three-body approximation is non-zero over the same energy range as the exact solution and has roughly the same shape. Although the two have maxima in the same place, the three-body approximation is not able to reproduce the square root singularities of the exact solution. Nevertheless spin-charge separation is observed. The charge velocity $v_c = v_F + U$ and the spin velocity $v_s = v_F - U$ agree with the exact result. From the integral equations one can see that the ‘charge’ peak comes from $[1 - UF_1]^{-1}$ and the ‘spin’ peak comes from $[1 + UF_2]^{-1}$.

It should be remarked that the one branch model has the same ground state as non-interacting Fermions. Thus spin-charge separation can co-exist with a Fermi-liquid. The range over which Im $G$ is non-zero is proportional to $q - k_F$ and this goes to zero as $q \to k_F$. Thus the three-body approximation is self-consistent with the assumption of a rigid Fermi surface background. This can be understood by noting that it is impossible to create particle-hole excitations from the ground state and conserve momentum. It is this feature of the one-branch model which renders the three-body approximation tractable. Below, in the two branch model, this phenomenon does not occur.

Finally we would like to emphasize the non-perturbative nature of the integral equation. This feature may help in shedding light on whether or not the two-dimensional Hubbard model has a Fermi-liquid ground state. Initial calculations indicate that $[1 - UF_1]^{-1}$ and $[1 + UF_2]^{-1}$ are less singular in two dimensions and almost certainly will not lead to singular behaviour on their own. We hope to discuss this in detail in a future publication.
IV. TWO BRANCH LUTTINGER MODEL

We consider a spinless Luttinger model for which only the interaction between opposite branches is retained. Again we begin with a particle on the right moving branch but allow the creation of a single particle-hole pair on the left moving branch. In this case the integral equation is (absorbing a factor of $N_s$ into $J_1$),

\[
J_1(K) = \frac{1}{1 - UF_1(K)} \sum_{k''=K+k_F}^{D} \frac{1}{(\tilde{\omega} - \epsilon(k'', K - k'') + U F_2(K - k'')(1 + UF_2(K - k'')))}
\]

\[
- \frac{U^2}{1 - UF_1(K)} \left[ \sum_{k'=q-k_F}^{D} \sum_{k''=K+k_F}^{D} + \sum_{k'=K}^{D-k_F} \sum_{k''=K+k_F}^{D+k-K'} \right]
\]

\[
\times \frac{J_1(k')}{(\tilde{\omega} - \epsilon(k'', K - k''))(1 + UF_2(K - k''))(\tilde{\omega} - \epsilon(k' - K + k'', K - k''))} \tag{4.1}
\]

where the kinetic energy $\epsilon(k', k - k') = (2k' - q - k_F)v_F$ (It doesn’t depend on $k$ because the total momentum must sum to $q$),

\[
F_1(k) = \sum_{k'=k+k_F}^{D} \frac{[\tilde{\omega} - \epsilon(k', k - k')]}{[\tilde{\omega} - \epsilon(k', k - k')]^{-1}} \tag{4.2}
\]

and

\[
F_2(k) = \int_{k'=-k+q}^{D} \frac{[\tilde{\omega} - \epsilon(k', k)]^{-1}}{[\tilde{\omega} - \epsilon(k', k)]^{-1}} . \tag{4.3}
\]

D is a momentum cutoff.

We were not able to solve this analytically, mostly because of the intractability of integrals of the form $\int dz \ln(z)/(z+a)$, and therefore attempted a numerical solution by discretization. In order to control the divergences of the free particle poles we introduced artificial widths. That is, we replaced

\[
\frac{1}{\tilde{\omega} - q} \rightarrow \frac{1}{\tilde{\omega} - q + i\delta} \tag{4.4}
\]

We checked that our results did not depend significantly on the value of $\delta$. The method of numerical solution was checked against the analytical solution, Eq. (3.16) for the one-branch model, to confirm its accuracy.
The exact Green function for this problem is [17]

$$\text{Im} G(\tilde{q}, \tilde{\omega}) = -\frac{\pi}{2D'v_{t}(a)^{2}} \times \left[ \theta(\tilde{\omega} - v\tilde{q})\gamma(a, y_{+})e^{-y_{+}^{a}y_{-}^{-1}} + \theta(-\tilde{\omega} - v\tilde{q})\gamma(a, -y_{+})e^{y_{-}^{a}(-y_{+})^{-1}} \right]$$ (4.5)

where $y_{\pm} = (\tilde{\omega} \pm v\tilde{q})/2D'v$, $v = \sqrt{v_{F}^{2} - U^{2}}$ and 

$$a = \frac{1}{4} \left( \sqrt{\frac{v_{F} - U}{v_{F} + U}} + \sqrt{\frac{v_{F} + U}{v_{F} - U}} - 2 \right) .$$ (4.6)

The parameter $D'$ is a momentum cutoff. In a perturbative expansion of the integral equations of the three-body approximation the parameter $(\tilde{\omega} - v_{F}\tilde{q})/2Dv_{F}$ appears. In order to compare the three-body results to the exact results we need definite values and it seems reasonable to take $D' = D$ for this purpose so that the three-body solution and the exact solution have the same dimensionless parameter $(\tilde{\omega} - v_{F}\tilde{q})/2Dv_{F}$. ImG($\tilde{q}, \tilde{\omega}$) (for the exact and three-body solution) as a function of energy with fixed total momentum are superimposed in Fig. 3. Energies are normalized by $\tilde{q}v_{F}$. We chose a value $U/v_{F} = 0.3$ which is large enough so that the effects of $U$ are apparent but not so large that the integral equations do not converge. The cutoff is $(D - k_{F})/\tilde{q} = 3$ and is not a sensitive parameter.

Some differences are immediately evident. Firstly the exact solution has spectral weight at $\tilde{\omega} < -v\tilde{q}$ (which is not shown in the figure). The three-body approximation misses this. In order to describe this part of the spectrum we would have to include pre-existing particle and hole pair excitations in the $N$-particle ground state whereas the three-body approximation assumes that the background is a rigid Fermi sea. A background of pre-excited particle-hole pairs would require consideration of a minimum of five bodies. The second difference is that the spectral weight of the exact solution is extremely concentrated just above the maximum of the spectral function. That is because, for small $U$, Im $G$ diverges with a negative exponent only slightly greater than $-1$. The exact solution displays an interesting characteristic. For energies $|\tilde{\omega}| < v\tilde{q}$ the spectral weight is exactly zero. We do not know how to explain this in terms of the underlying electrons. This feature is not present in the three-body approximation. Nevertheless the spectral function in that case is asymmetric.
In Fig. 3 the reflection of the spectral function about its maximum is plotted to bring out the asymmetry. We see that the asymmetry is in the right direction. That is, the spectral weight is higher for energies above the maximum. By looking at the numerical solution integral equations it is possible to tell that a pole in \([1 + F_2]^{-1}\) (the particle - hole scattering channel) is the cause of this asymmetry.

Another feature which is reproduced qualitatively is the negative energy shift of the peak position (real part of the self-energy). In the exact solution this manifests itself in a downward renormalization of the Fermi velocity \(v = \sqrt{v_F^2 - U^2}\). In Fig. 4 the shifts in the maxima of \(\text{Im } G\) as a function of \(U\) are plotted. It is interesting to note that the three-body approximation follows the square root behaviour of the exact solution quite accurately except for a factor of two.

To summarize, the three-body approach reproduces qualitatively the real part of the self-energy and the asymmetry of the spectral function. Although it is not shown in Fig. 3, in the three-body approximation the spectral weight of an electron with momentum \(q > k_F\) stretches into negative energy, with a width proportional to \(q - k_F\). However, the integrated spectral weight for negative energies seems to be independent of \(q - k_F\) at small \(q - k_F\) and amounts to a few percent of the total spectral weight (for the given choice of parameters): comparable to that of the exact solution. This flow of spectral weight can be interpreted by saying that the three-body approximation is inducing some correlations which tend to improve the trial ground state. This confirms the idea that correcting the N-particle ground state by coherent particle-hole pair excitations would yield a Green function more like the exact solution.

V. X-RAY PROBLEM

As discussed in the introduction, our goal was to set up an approximation scheme which treats particle-particle and particle-hole interactions on the same footing. Formally, this idea was first discussed in condensed matter physics for the Kondo problem [7], and for the simpler
X-ray edge problem [8]. In this section, we present the results of our simple three-body type of approach for the X-ray edge problem. At this point, it would be helpful to characterize better the expected limitations of our method. The quantity of interest here is the overlap between the wave function of the conduction electron system, after the sudden turning on of a localized potential, and the unperturbed Fermi sea. Going beyond the first calculation by Mahan [18], Nozières and coworkers have shown that the deep level Green’s function defined as above decays as a power-law function of time [19], with an exponent proportional to the square of the phase shift at the Fermi energy due to the local potential. This result has been interpreted in terms of Anderson’s orthogonality catastrophe [20,21], and rederived in the simpler language of Tomonaga bosons [22]. As stressed by many authors, the infrared singularity arises from the excitation of a logarithmically divergent number of Tomonaga bosons. However, the average number of such emitted bosons increases only logarithmically with time, which might enable us to restrict ourselves to the subspace with no more than one excited boson, at least for times shorter than $\frac{1}{W} \exp \left(\frac{W}{2V^2}\right)$, where $W$ is the conduction electron bandwidth and $V$ is the strength of the localized potential.

The Hamiltonian for the X-ray problem is

$$H = \mathcal{E}_0 b^\dagger b + \sum_k \epsilon_k a_k^\dagger a_k - E_0 + b^\dagger \sum_{kk'} V_{kk'} a_{k'}^\dagger a_k . \quad (5.1)$$

$a_k$ is a spinless Fermion annihilation operator and $\mathcal{E}_0$ is the energy of the deep hole. As in the Hamiltonian 2.2, $E_0$ is chosen so that the unperturbed Fermi sea with the deep level occupied is defined to have zero energy. Let $|N\rangle$ be the unperturbed Fermi sea and $|0\rangle \equiv b|N\rangle$ be the unperturbed sea with the deep hole. We shall be interested in the Green function

$$\mathcal{G}(t > 0) = -i\langle N|e^{iHt}b^\dagger e^{-iHt}b|N\rangle = -ie^{-i\mathcal{E}_0 t}\langle 0|e^{-iHt}|0\rangle \quad (5.2)$$

We again set up the three-body approximation using the equation of motion formalism. Defining $|t\rangle \equiv \exp (-iHt)|0\rangle$, we make the approximation

$$|t\rangle \cong \phi(t)|0\rangle + \sum_{k > k_F} \sum_{k' < k_F} \Phi(k, k', t) a_{k'}^\dagger a_k |0\rangle \quad (5.3)$$
with the truncated equations of motion

$$i \frac{\partial \phi}{\partial t}(t) = \mathcal{E}_0 \phi(t) + \sum_{k,k'} V_{k',k} \Phi(k,k',t)$$  \hspace{1cm} (5.4)$$

and

$$i \frac{\partial \Phi}{\partial t}(k,k',t) = (\mathcal{E}_0 + \epsilon_k - \epsilon_{k'}) \Phi(k,k',t) + \sum_{k''} V_{k,k''} \Phi(k'',k',t)$$

$$- \sum_{k''} V_{k,k''} \Phi(k,k'',t) + V_{k,k'} \phi(t) .$$  \hspace{1cm} (5.5)$$

We proceed by expressing $\Phi(k,k',t)$ in the basis of single-particle eigenstates in the presence of scattering $V_{k,k'}$,

$$\Phi(k,k',t) = \sum_{\alpha,\beta} \Phi_{\alpha,\beta}(t) \phi^p_\alpha(k) \phi^h_\beta(k')$$  \hspace{1cm} (5.6)$$
in which case the second equation of motion may be written

$$i \sum_{\alpha,\beta} \phi^p_\alpha(k) \phi^h_\beta(k') \dot{\Phi}_{\alpha,\beta}(t) = \sum_{\alpha,\beta} (\mathcal{E}_0^p + \mathcal{E}_0^h + \mathcal{E}_0) \phi^p_\alpha(k) \phi^h_\beta(k') \Phi_{\alpha,\beta}(t) + V_{k,k'} \phi(t) .$$  \hspace{1cm} (5.7)$$

Using the orthogonality of this basis we have

$$\Phi_{\alpha,\beta}(t) = -i \int_0^t dt' \exp \left[ -i(\mathcal{E}_0^p + \mathcal{E}_0^h + \mathcal{E}_0)(t - t') \right] \phi(t') \sum_{k,k'} \phi^*_{\alpha}(k) \phi^*_\beta(k') V_{k,k'}$$  \hspace{1cm} (5.8)$$

Combining this with the first equation of motion written in the same basis and defining

$$\phi(t) \equiv \exp (-i \mathcal{E}_0 t) \tilde{\phi}(t),$$

$$\tilde{\phi}(t) = 1 + \int_0^t dt' \int_0^t dt'' \sum_{k,k',q,q'} V_{k',k} V_{q,q'} G_{k,q}^p(t' - t'') G_{k',q'}^{h*}(t'' - t''') \tilde{\phi}(t''')$$  \hspace{1cm} (5.9)$$

where

$$G_{k,q}^{p,h}(t) = \sum_{\alpha} e^{-i E_{\alpha}^{p,h}(t)} \phi^p_\alpha(k) \phi^{h*}_{\alpha}(q)$$  \hspace{1cm} (5.10)$$

are the particle and hole Green functions in the presence of the deep hole. Upon Fourier transforming Eq. (5.9) and solving we find that $\tilde{\phi}(\omega) = i/ (\omega - \Sigma(\omega))$ where the self-energy $\Sigma$ is given by

$$\Sigma(\omega) = i \sum_{k,k'} \sum_{q,q'} V_{k',k} V_{q,q'} \int \frac{d \omega'}{2\pi} G_{k,q}^p(\omega') G_{k',q'}^h(\omega - \omega')$$  \hspace{1cm} (5.11)$$
We take the continuum limit and treat the deep hole as a point scatterer thus dropping momentum dependence in $V$. The self-energy becomes

$$\Sigma = iV^2 \int \frac{d\omega'}{2\pi} G^p(\omega')G^h(\omega - \omega')$$

(5.12)

where $G^{p,h}$ are now the on-site Green functions given by

$$G^p(\omega) = \frac{(1/2Dv_F)\ln [(\omega - v_F k_F + i\delta)/(\omega - v_F D + i\delta)]}{1 - (V/2Dv_F)\ln [(\omega - v_F k_F + i\delta)/(\omega - v_F D + i\delta)]}$$

(5.13)

and

$$G^h(\omega) = \frac{(1/2Dv_F)\ln [(\omega + v_F k_F + i\delta)/(\omega - v_F D + i\delta)]}{1 + (V/2Dv_F)\ln [(\omega + v_F k_F + i\delta)/(\omega - v_F D + i\delta)]}.$$  

(5.14)

$D$ is the usual momentum cutoff.

In Fig. 5 we have plotted the imaginary part of the particle and hole Green functions. Note the weak logarithmic singularities which result from single particle bound states. In Fig. 6 is plotted the resulting real and imaginary parts of the self-energy. The critical features in the latter plot are the sharpness of the cusp in $\text{Im}\Sigma(\omega)$, and the steepness of the inflection point of $\text{Re}\Sigma(\omega)$ near $\omega \sim 0$. As this numerical calculation shows, the weak logarithmic divergences of the single particle spectral density do not have a great effect on the self-energy.

In view of this, we proceed with an analytical calculation of the quasiparticle residue which replaces the spectral functions plotted in Fig. 5 by the constant $-(2Dv_F)^{-1}$ multiplied by appropriate step functions. For small $\omega$,

$$\text{Re}\Sigma(\omega) \cong (V/2Dv_F)^2 \left[ v_F(D - k_F)\ln \left(\frac{D - k_F}{2D}\right) + v_F(D + k_F)\ln \left(\frac{D + k_F}{2D}\right) \right.$$

$$+\omega\ln \left(\frac{|\omega|2Dv_F}{v_F(D-k_F)v_F(D+k_F)}\right)$$

$$\left. \right] .$$

(5.15)

The pole in the deep hole Green function occurs at $\omega_p = \text{Re}\Sigma(\omega_p)$ which is

$$\omega_p = -\frac{V^2}{2Dv_F} \left(\ln 2 + \mathcal{O}(k_F/D)^2\right)$$

(5.16)

in the $k_F << D$ limit. The residue of the deep level pole is
\[ Z_p \equiv \left[ 1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma(\omega) \right]_{\omega_p}^{-1} \approx 1 - (V/2Dv_F)^2 \ln \left( \frac{v_F^2 D^2}{V^2 \ln^2} \right). \quad (5.17) \]

These expressions have been quantitatively checked with a numerical calculation.

This calculation shows that the simple three-body approach does not reproduce the power-law singularity of the deep level Green’s function at low energy. Instead of a power-law decay at long times, we obtain a long-lived level, with a residue close to unity at small coupling. This result is by itself not too surprising. It simply confirms the intuitive idea that the possibility of exciting many particle-hole pairs should be retained, in order to describe the power-law singularities. In fact, this feature is present in the parquet diagram approach used by Abrikosov and Nozières and coworkers [7,8]. The similarity between a parquet calculation and our simple three-body approach arises because in the former the three-particle vertex function involves only successive two-particle interactions. However, since the same parquet diagram corresponds to several time orderings for the interaction events, the actual number of particle-hole pairs is not fixed to unity. Unfortunately, our simplified approach does not seem to provide a way to bypass the cumbersome parquet algebra. The main complication encountered upon going from the Faddeev approach, with fixed particle number, to the parquet algebra in the full Hilbert space, is reflected by the need to keep frequencies as additional integration variables in the internal lines of the graphs. For the X-ray edge problem with a separable potential, momentum integrations are straightforward and we recover a one-dimensional problem (in the time direction). For more realistic systems, such as the two-dimensional Hubbard model, such a simplification is not so obvious. This is why our simpler method may still be useful there, since it may for instance be able to indicate the presence of spin and charge decoupling. We hope to be able to address this issue in a forthcoming investigation.
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* Present Address: AECL Research, Chalk River Laboratories, Chalk River, Ontario, Canada, K0J 1J0. E-mail: hsut@cu26.crl.aecl.ca

** E-mail: doucot@crtbt.polycnrs-gre.fr

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FIGURES

FIG. 1. Diagrams in the one-electron self-energy accounted for in the Faddeev Equations. As opposed to the usual convention the vertices are time ordered from left to right. This prevents a violation of the variational assumption of the presence of at most three excitations at one time. The middle line is the spin up electron and the outer lines are the spin down particle-hole pair.

FIG. 2. One branch Luttinger model: comparison of Im G for the exact solution (dashed line) and the exact solution of the three-body approximation (solid line) as a function of normalized energy $x = (\tilde{\omega} - v_F \tilde{q})/U \tilde{q}$ for fixed total momentum $q$.

FIG. 3. Two branch Luttinger model: Im G as a function of normalized energy $\tilde{\omega}/v_F \tilde{q}$. Solid line: three-body approximation; Short dashed line: exact solution; Long dashed line: three-body approximation reflected about its maximum. The non-zero part of Im G at negative energies is not shown.

FIG. 4. Two branch Luttinger model: Real part of the self-energy defined as the energy shift (relative to and normalized by the non-interacting quasi-particle energy $v_F \tilde{q}$) of the peak of Im G as a function of the interaction strength $U/v_F$. Dashed line: exact solution; Diamonds: three-body approximation.

FIG. 5. Spectral density of the on-site particle (solid line) and hole (dashed line) Green functions in the presence of the deep hole. The values $k_F/D = 0.1$ and $V/Dv_F = 0.2$ have been used.

FIG. 6. Self energy of the deep level as a function of frequency using the same parameters as in Fig. 5. Real part: solid line, Imaginary part: dashed line.