Beyond the Hubbard-I Solution with a One-Pole and a Two-Pole Self-Energy: Moment Approach

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We have postulated a single pole for the self-energy, \( \Sigma(\mathbf{k}, \omega) \), looking for the consequences on the one-particle Green function, \( G(\mathbf{k}, \omega) \) in the Hubbard model. We find that \( G(\mathbf{k}, \omega) \) satisfies the first two sum rules or moments of Nolting (Z. Physik 225, 25 (1972)) for any values of the two unknown \( \mathbf{k} \) parameters of \( \Sigma(\mathbf{k}, \omega) \). In order to find these two parameters we have used the third and four sum rules of Nolting, \( G(\mathbf{k}, \omega) \) turns out to be identical to the one of Nolting (Z. Physik 225, 25 (1972)), which is beyond a Hubbard-I solution. Furthermore, we have also postulated a two-pole Ansatz for \( \Sigma(\mathbf{k}, \omega) \) which is equivalent to a three-pole Ansatz for \( G(\mathbf{k}, \omega) \). In the latter case, we have fixed two of the frequencies. This Green’s function is also beyond the Hubbard-I solution. We present numerical results for the band structure and the spectral weights.

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After the discovery of the high-\( T_c \) materials [1], the study of correlations has gained interested due to the fact that there is the belief [4] that the normal properties of these materials could be explained in the framework of the Hubbard model [3], since electron correlations are strong, i.e., the on-site electron-electron repulsions \( U \) are much larger than the energies associated with the hybridization of atomic orbitals belonging to different atoms [4]. This Hamiltonian is a kind of minimum model [5] which takes into account quantum mechanical motion of electrons in a solid, and nonlinear repulsion between electrons. Even though this model is too simple to describe solids faithfully, serious theoretical studies have revealed that to understand its various properties is a very difficult task, since is the novel materials. For example, at high temperatures \( T > T_c \) these HTSC cuprates, which are poor conductors, become superconductors. This feature is strange indeed because the Coulomb repulsion is strong. Furthermore, the behavior of these materials at \( T > T_c \) is even more puzzling than the superconductivity itself. Contrary to the predictions of the Fermi liquid theory, the resistivity at \( T > T_c \) and optimum doping is linear in temperature, i.e., \( R \approx T \). This suggests a very strong scattering of elementary excitations. A discussion of the possible breakdown of Fermi liquid theory is given in Ref. [3].

In this paper, we will adopt a given pole structure in the self-energy and see its effect on the one-particle Green function. This is done with the idea of reducing the amount of computational effort which is implicit in the moment approach of Nolting which is normally constrained to two poles in \( G(\mathbf{k}, \omega) \). At the same time, without additional effort, we monitor the self-energy which is an important quantity for life-time considerations. We find that by using this approach (one pole in \( \Sigma(\mathbf{k}, \omega) \) and the sum rules for the spectral functions), the one-particle Green function goes beyond the Hubbard-I solution, i.e., it identically satisfies the first two sum rules and its parameters have to be calculated self-consistently. This has motivated us to consider two poles in the self-energy and to see the effects on \( G(\mathbf{k}, \omega) \). The general result that we gain is that \( N \)-poles in \( \Sigma(\mathbf{k}, \omega) \) is equivalent to \( N + 1 \)-poles in \( G(\mathbf{k}, \omega) \). Along the way, we discuss the possibility of obtaining a third peak in \( G(\mathbf{k}, \omega) \) by means of this technique.

The model we study is the Hubbard model [3]

\[
H = t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} n^\dagger_{i\uparrow} n_{i\downarrow} - \mu c^\dagger_{i\sigma} c_{i\sigma},
\]

where \( c^\dagger_{i\sigma} (c_{i\sigma}) \) are creation (annihilation) electron operators with spin \( \sigma \). \( n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} \). \( U \) is the local interaction, \( \mu \) the chemical potential and we work in the grand canonical ensemble. We have adopted Einstein convention for...
repeated indices, i.e., for the \( N_s \) sites \( \vec{i} \), the \( z \) nearest-neighbor sites and for spin up and down \((\sigma = \pm 1)\). \( t_{ij} = -t \), for n.n. and zero otherwise.

The one-particle Green function, \( G(\mathbf{k}, \omega) \), is expressed in terms of the self-energy, \( \Sigma(\mathbf{k}, \omega) \), as

\[
G(\mathbf{k}; \omega) = \frac{1}{\omega - \varepsilon_\mathbf{k} - \Sigma(\mathbf{k}, \omega)} ,
\]

where \( \varepsilon_\mathbf{k} = -2t(\cos(k_x a) + \cos(k_y a)) \), and \( \varepsilon_\mathbf{k} = \varepsilon(\mathbf{k}) - \mu \).

We adopt the following Ansatz for \( \Sigma(\mathbf{k}, \omega) \):

\[
\Sigma(\mathbf{k}, \omega) \equiv \rho U + \frac{\alpha_\mathbf{k}(\omega)}{\omega - \Omega_\mathbf{k}} .
\]

As \( \Sigma(\mathbf{k}, \omega) \) has dimensions of energy, the still unknown parameter \( \alpha_\mathbf{k} \) has dimensions of \((\text{energy})^2\). \( \alpha_\mathbf{k} \) is an energy spectrum of the self-energy. We will calculate \( \alpha_\mathbf{k} \) and \( \Omega_\mathbf{k} \). Along the way, we will give a simple physical interpretation for \( \alpha_\mathbf{k} \).

By using Eq. (3) into Eq. (2), we get that the one-particle Green function has two poles. It can be written as

\[
G(\mathbf{k}, \omega) = \frac{\alpha_1(\mathbf{k})}{\omega - \omega_1(\mathbf{k})} + \frac{\alpha_2(\mathbf{k})}{\omega - \omega_2(\mathbf{k})} ,
\]

where

\[
\omega_1(\mathbf{k}) = \frac{1}{2} \left[ \Omega_\mathbf{k} + \xi_\mathbf{k} + \left( (\Omega_\mathbf{k} - \xi_\mathbf{k})^2 + 4\alpha_\mathbf{k} \right)^{1/2} \right] ,
\]

\[
\omega_2(\mathbf{k}) = \frac{1}{2} \left[ \Omega_\mathbf{k} + \xi_\mathbf{k} - \left( (\Omega_\mathbf{k} - \xi_\mathbf{k})^2 + 4\alpha_\mathbf{k} \right)^{1/2} \right] ,
\]

\[
\alpha_1(\mathbf{k}) = \frac{\omega_1(\mathbf{k}) - \Omega_\mathbf{k}}{\omega_1(\mathbf{k}) - \omega_2(\mathbf{k})} ,
\]

\[
\alpha_2(\mathbf{k}) = \frac{\omega_2(\mathbf{k}) - \Omega_\mathbf{k}}{\omega_2(\mathbf{k}) - \omega_1(\mathbf{k})} .
\]

From Eqs. (3) we immediately see that the following sum rules or moments (4) are identically satisfied:

\[
\alpha_1(\mathbf{k}) + \alpha_2(\mathbf{k}) = 1 ,
\]

\[
\alpha_1(\mathbf{k})\omega_1(\mathbf{k}) + \alpha_2(\mathbf{k})\omega_2(\mathbf{k}) = \xi_\mathbf{k} ,
\]

\[
\xi_\mathbf{k} = \varepsilon(\mathbf{k}) + \rho U .
\]

Eqs. (3) are the first two sum rules for the spectral functions of Nolting (5). In order to evaluate \( \alpha_\mathbf{k} \) and \( \Omega_\mathbf{k} \), we use the next two sum rules of Nolting. This gives:

\[
\omega_1^2(\mathbf{k})\alpha_1(\mathbf{k}) + \omega_2^2(\mathbf{k})\alpha_2(\mathbf{k}) = \xi_\mathbf{k}^2 + \alpha_\mathbf{k} = a_2(\mathbf{k}) ,
\]

\[
\omega_1^2(\mathbf{k})\alpha_1(\mathbf{k}) + \omega_2^2(\mathbf{k})\alpha_2(\mathbf{k}) = \xi_\mathbf{k}^2 + (\Omega_\mathbf{k} + 2\xi_\mathbf{k})\alpha_\mathbf{k} = a_3(\mathbf{k}) ,
\]

where \( a_2(\mathbf{k}) \), \( a_3(\mathbf{k}) \) are given in Ref. (10), (11) as

\[
a_2(\mathbf{k}) = \varepsilon^2(\mathbf{k}) + 2\rho U\varepsilon(\mathbf{k}) + \rho U^2 ,
\]

\[
a_3(\mathbf{k}) = \varepsilon^3(\mathbf{k}) + 3\varepsilon^2(\mathbf{k})(2 + \rho)\rho U^2\varepsilon(\mathbf{k}) + \rho(1 - \rho)UB(\mathbf{k}) + \rho U^3 ,
\]

where \( B(\mathbf{k}) \), in the spherical approximation of Nolting, is given by

\[
\rho(1 - \rho)B(\mathbf{k}) = \sum_{j=1}^{2} \sum_{\mathbf{k}} \left[ \frac{2}{U} (\omega_j(\mathbf{k}) - \varepsilon(\mathbf{k})) - 1 \right] \alpha_j(\mathbf{k})f(\omega_j(\mathbf{k}))\varepsilon(\mathbf{k}) ,
\]

where \( f(x) \) is the Fermi distribution function. By solving Eqs. (7) we find:
\[\alpha(k) = \rho(1 - \rho)U^2,\]
\[\Omega_k = (1 - \rho)U + B(k),\]  \hspace{1cm} (10)

\(B(k)\) is the narrowing band parameter defined by Nolting. This narrowing band parameter has to be calculated self-consistently and in the spherical approximation of Nolting is \(k\) independent. By combining Eqs. (10) we find
\[\omega_1(k) = \frac{1}{2} \left[ H(k) + [K(k)]^{1/2} \right] ; \quad \omega_2(k) = \frac{1}{2} \left[ H(k) - [K(k)]^{1/2} \right],\]  \hspace{1cm} (11)

where
\[H(k) \equiv \epsilon(k)U + B(k),\]
\[K(k) \equiv (\epsilon(k) - U - B(k))^2 + 4\rho U(\epsilon(k) - B(k)).\]  \hspace{1cm} (12)

Eqs. (12) are nothing that the solutions given by Nolting [10] by solving the four unknown \(\alpha_i(k)\) and \(\omega_i(k)\), with \(i = 1, 2\). We have regained Nolting’s solutions in a much easier way, starting from the self-energy, while Nolting does it from the Green function itself. At the same time we have been able to identify the self-energy for the two-pole ansatz (self-energy) into Dyson equation produces immediately the mean-field SDW result. Chubukov and Morr’s analysis [15] is based on the theory of Kamp and Schrieffer [16] where it is assumed that the longitudinal spin susceptibility, \(\chi_s(q, \omega)\) has a \(\delta\)-functional peak at zero frequency and momentum transfer \(Q = (\pi, \pi)\), i.e., \(\chi_s(q, \omega) = \frac{\lambda}{2} \delta(q - Q)\delta(\omega).\) Chubukov and Morr’s paper studies the Fermi surface evolution with interaction. They find that the SDW mean-field solution (valid for large \(U\)) yields a small Fermi surface centered at \((\pi/2, \pi/2)\). Notice, however that they include a term \(t'\) in the free-energy band. Let’s mention that the SDW state has not been observed in FLEX calculations [17] where short-wavelength spin fluctuations are taken into account. By using the Green function given by Eqs. (12),
we can evaluate the dynamical conductance, $\sigma(\omega)$, vs $\omega$, away from half-filling \[14\]. We mention that the two-pole one-particle Green function (Eq. (8) has been used to calculate the static spin susceptibility, $\chi_s(T)$, \[10\]-\[11\] and the results compare rather well with Quantum Monte Carlo simulations \[15\]. Another quantity which can be easily calculated is the specific heat, $c_v$, vs temperature, $T$. \[11\]. See also Ref. \[19\]. We would like to comment on the fact that our two energy branches (second line of Eq. (12)) produce a gap with a value of $U$. This gap is evidently no perturbative contrary to the view of Ref. \[16\].

Now, let us propose a two-pole Ansatz for the self-energy, given by

$$
\Sigma(k, \omega) \equiv \rho U + \frac{\alpha(k)}{(\omega - \Omega_1(k)) - (\omega - \Omega_2(k))}.
$$

The assumption of Eq. (17) is equivalent to have a three-pole structure for the one-particle Green function, i.e.,

$$
G(k, \omega) \equiv \frac{\alpha_1(k)}{\omega - \omega_1(k)} + \frac{\alpha_2(k)}{\omega - \omega_2(k)} + \frac{\alpha_3(k)}{\omega - \omega_3(k)}.
$$

The $\omega_j(k)$'s, $j=1,2,3$, are the roots of the following cubic equation

$$
\omega^3 - A_1(k)\omega^2 + A_2(k)\omega - A_3(k) = 0,
$$

where

$$
A_1(k) \equiv \Omega_1(k) + \Omega_2(k) + \xi_k \quad ; \quad A_2(k) \equiv \xi_k (\Omega_1(k) + \Omega_2(k)) + \Omega_1(k)\Omega_2(k) \quad , \\
A_3(k) \equiv \alpha(k) + \Omega_1(k)\Omega_2(k)\xi_k.
$$

The $\alpha_j(k)$'s, $j=1,2,3$, are given by

$$
\begin{align*}
\alpha_1(k) & \equiv (\omega_1(k) - \Omega_1(k))(\omega_1(k) - \Omega_2(k)) \quad , \\
\alpha_2(k) & \equiv (\omega_2(k) - \Omega_1(k))(\omega_2(k) - \Omega_2(k)) \quad , \\
\alpha_3(k) & \equiv (\omega_3(k) - \Omega_1(k))(\omega_3(k) - \Omega_2(k)) \quad , \\
\end{align*}
$$

Now, as we are after a simple solution to our Eqs. (14-23), we are going to impose the strong condition on the cubic equation (Eq. (19)) that

$$
\omega_3(k) = 0.
$$

Then, Eq. (19) becomes

$$
\begin{align*}
\omega^2 - A_1(k)\omega + A_2(k) & = 0 \quad , \\
\alpha(k) & = -\Omega_1(k)\Omega_2(k)\xi_k.
\end{align*}
$$

If we require that the other two roots are antisymmetric, we get

$$
A_1(k) = \Omega_1(k) + \Omega_2(k) + \xi_k = 0 \quad , \\
\Omega_k^2 = -[\Omega_1(k)\Omega_2(k) + \xi_k (\Omega_1(k) + \Omega_2(k))].
$$

We would like to point out that this condition (the first line of Eq. (24)) is not really necessary. It has been used here to keep the algebra as simple as possible. Otherwise, higher order moments will be needed.

It is easy to express the $\alpha_j(k)$'s as

$$
\begin{align*}
\alpha_1(k) & = \frac{1}{2\Omega_k} (\Omega_k - \Omega_1(k)) (\Omega_k - \Omega_2(k)) \quad , \\
\alpha_2(k) & = \frac{1}{2\Omega_k} (\Omega_k + \Omega_1(k)) (\Omega_k + \Omega_2(k)) \quad , \\
\alpha_3(k) & = -\frac{\Omega_1(k)\Omega_2(k)}{\Omega_k^2}.
\end{align*}
$$
The first two sum rules or moments are satisfied identically since
\[ \alpha_1(k) + \alpha_2(k) + \alpha_3(k) = 1 , \]
\[ \Omega_k (\alpha_1(k) - \alpha_2(k)) = - (\Omega_1(k) + \Omega_2(k)) = \xi_k . \] (26)
The second moment is satisfied due to the fact that \( A_1(k) = 0 \). (See Eq. (24)). Let us point out that the first sum rule is always satisfied, without the requirement that \( \omega_3(k) = 0 \).

The third and four moments are given by
\[ \Omega_k^2 (\alpha_1(k) + \alpha_2(k)) = \Omega_k^2 + \Omega_1(k)\Omega_2(k) = a_2(k) , \]
\[ \Omega_k^2 (\alpha_1(k) - \alpha_2(k)) = - \Omega_k^2 (\Omega_1(k) + \Omega_2(k)) = a_3(k) . \] (27)

Combining Eqs. (26,27) we end with
\[ \Omega_k^2 = \frac{a_3(k)}{a_1(k)} . \] (28)

The other unknowns are easily found. They are:
\[ \Omega_{1,2}(k) = - \xi_k \pm \left[ \xi_k^2 + 4(\Omega_k^2 - a_2(k)) \right]^{1/2} / 2 , \]
\[ \alpha_{1,2}(k) = \frac{\xi_k (a_2(k) \pm [\xi_k a_3(k)]^{1/2})}{2a_3(k)} , \]
\[ \alpha_3(k) = 1 - \frac{\xi_k a_2(k)}{a_3(k)} , \]
\[ \bar{\alpha}(k) = a_3(k) - \xi_k a_2(k) . \] (29)

Now we are in a position to justify the fact that \( \Sigma(k,\omega) \) represents an expansion in powers of \( U \). (See the discussion after Eq. (23)). From the four line of Eq. (29) we can calculate the explicit form of the self-energy weight. We use the expressions for \( a_2(k) \) and \( a_3(k) \). The result is
\[ \bar{\alpha}(k) = \rho(1 - \rho)U^2 [U + 2\epsilon(k) + B(k)] . \] (30)

Then, we see from Eq. (30) that we have an expansion in terms of \( U \). Just imagine the atomic limit!. Let us say that the solutions we have found (Eqs. (18, 22, 28,30)) can also be obtained from the three pole Ansatz for the one-particle Green function, if we require that the first four moments are satisfied together with the conditions of a peak at zero frequency and the other two peaks at antisymmetric frequencies. In Eq. (30) \( B(k) \) is given by
\[ \rho(1 - \rho)B(k) = \sum_{j=1}^{3} \sum_{k} \left[ \frac{2}{U} (\omega_j(k) - \epsilon_k) - 1 \right] \alpha_j(k)f(\omega_j(k))\epsilon(k) . \] (31)

In Fig. 1 we present the energy spectra, i.e., \( \omega_i(\vec{k}) \), \( i = 1, 2, 3 \) vs \( \vec{k} \) along the diagonal of the Brillouin zone, i.e., \( k_x = k_y = k \) for \( T/t = 0.5 \), \( \rho = 0.5 \) and \( \mu = U/2 \), with \( U/t = 7.0 \). In Fig. 2 we show the spectral weights, \( \alpha_i(k) \), \( i = 1, 2, 3 \), for \( k \) along the diagonal of the Brillouin zone for the same parameters as in Fig. 1. In Fig. 3 we plot \( \Omega_i(k) \), \( i = 1, 2 \) along the diagonal of the Brillouin zone for the same parameters as in the first two figures. We observe from all these figures that there are regions of \( k \) which are forbidden, i.e., for which \( \omega_1(k) \) become imaginary. We have neglected these points. However, they could be taken into account if we include lifetime effects. Our choice of a delta function for the spectral function, \( A(k,\omega) \), forbids us to consider imaginary frequencies.

In summary we have proposed a self-energy of \( N \) poles which implies that the Green function is composed of \( N + 1 \) poles. This has been accomplished by the use of Dyson’s equation (Eq. 3). For the case of a one-pole for the self-energy we have reproduced with minor effort the Nolting’s solution (10, 11). The one-pole self-energy leading to Nolting’s solution puts on firm grounds the results found in Refs. (11) where it was argued that the two branches of the one-particle Green function were due to a single branch in the self-energy. For the case of two-pole Ansatz for the self-energy we have worked out the simple case of what we call the Kondo peak. In the later case, we have been able to solve all the unknown parameters. In both cases, the first two sum rules are satisfied identically. In both cases, our Green’s function goes beyond the Hubbard-I solution because we have imposed the condition that the third and
four moments be satisfied. We would like to say that we have found the Green’s function for a strongly correlated system, keeping the full \((k, \omega)\) - dependence. With our rather simple approach we have been able to have a Green’s function with either two poles or three poles. Our approch is somewhat different from the one of the limit of infinite dimensions \([20]\), where only the dynamical properties are taken into account leaving aside the study of the long range behavior. The moment approach is a reliable tool to study strongly correlated electronic systems, in particular, the Hubbard model. A recent calculation by Nolting, Jaya and Rex \([21]\) has applied it to the periodic Anderson model, where the relevant quantity of study is the self-energy.

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Fig. 1. The self-consistent energy spectra, $\omega_i(\vec{k})$, $i = 1, 2, 3$, as function of momentum along the diagonal of the Brillouin zone for $U/t = 7.0$, $\rho = 0.5$, $T/t = 0.5$.

Fig. 2. $\alpha_i(k)$ vs $k$, $i = 1, 2, 3$, with the same parameter of Fig. 1.

Fig. 3. $\Omega_i(k)$ vs $k$, $i = 1, 2$ for the same parameters of Fig. 1.
\[\alpha_1(k)\]

\[\alpha_2(k)\]

\[\alpha_3(k)\]
