Beyond the Hubbard-I Solution with a One-Pole Self-Energy at Half-Filling within the Moment Approach: Non-Linear Effects.

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(March 24, 2022)

We have postulated a single pole for the self-energy, $\Sigma(\vec{k}, \omega)$, looking for the consequences on the one-particle Green function, $G(\vec{k}, \omega)$ in the Hubbard model. We find that $G(\vec{k}, \omega)$ satisfies the first two sum rules or moments of Nolting (Z. Physik 255, 25 (1972)) for any values of the two unknown $\vec{k}$ parameters of $\Sigma(\vec{k}, \omega)$. In order to find these two parameters we have used the third and four sum rules of Nolting. $G(\vec{k}, \omega)$ turns out to be identical to the one of Nolting (Z. Physik 225, 25 (1972)), which is beyond a Hubbard-I solution since satisfies four sum rules. With our proposal we have been able to obtain an expansion in powers of $U$ for the self-energy (here to second order in $U$). We present numerical results at half-filling for 1- the static spin susceptibility, $\chi(T)$ vs $T/t$ and 2- the band narrowing parameter, $B(T)$ vs $T/t$. The two-pole Ansatz of Nolting for the one-particle Green function is equivalent to a single pole Ansatz for the self-energy which remains the fundamental quantity for more elaborated calculations when, for example, lifetime effects are included.

Pacs numbers: 74.20.-Fg, 74.10.-z, 74.60.-w, 74.72.-h

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 [2] 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].

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 fleshing out the basic elements implicit in the moment approach of Nolting.

The model we study is the Hubbard model [3]

$$H = t_{ij} \sum_{\sigma, \sigma'} c_{i\sigma}^{\dagger} c_{j\sigma'} + \frac{U}{2} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{\sigma, \sigma'} c_{i\sigma}^{\dagger} c_{i\sigma},$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) are creation (annihilation) electron operators with spin $\sigma$. $n_{i\sigma} \equiv c_{i\sigma}^{\dagger} c_{i\sigma}$. $U$ 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 $i$, 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, $G(\vec{k}, \omega)$, is expressed in terms of the self-energy, $\Sigma(\vec{k}, \omega)$, as

$$G(\vec{k}, \omega) = \frac{1}{\omega - \epsilon(\vec{k}) - \Sigma(\vec{k}, \omega)},$$

where $\epsilon(\vec{k}) = -2t(\cos(k_x a) + \cos(k_y a))$, and $\epsilon(\vec{k}) = \epsilon(\vec{k}) - \mu$.

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

$$\Sigma(\vec{k}, \omega) \equiv \rho U + \frac{\alpha(\vec{k})}{\omega - \Omega_{\vec{k}}},$$

As $\Sigma(\vec{k}, \omega)$ has dimensions of energy, the still unknown parameter $\alpha(\vec{k})$ has dimensions of $(\text{energy})^2$. $\alpha(\vec{k})$ is kind of a spectral weight and $\Omega_{\vec{k}}$ is the energy spectrum of the self-energy. We will calculate $\alpha(\vec{k})$ and $\Omega_{\vec{k}}$. We have included...
the Hartree shift directly in the self-energy (the first term of Eq. 3). In Eq. 3, ρ is the carrier concentration per spin orientation, i.e., ρ = n/2. We are assuming that we are in the paramagnetic phase 3. The physical reason of having chosen a single pole in the self-energy is due to the fact that, for intermediate to strong coupling, the self-energy gives rise to two energy branches in the one-particle and ultimately to the two Hubbard bands.

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

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

where

\[ \omega_1(\vec{k}) = \frac{1}{2} \left[ \Omega_\vec{k} + \xi_\vec{k} + \left( (\Omega_\vec{k} - \xi_\vec{k})^2 + 4\alpha(\vec{k}) \right)^{1/2} \right], \quad \omega_2(\vec{k}) = \frac{1}{2} \left[ \Omega_\vec{k} + \xi_\vec{k} - \left( (\Omega_\vec{k} - \xi_\vec{k})^2 + 4\alpha(\vec{k}) \right)^{1/2} \right], \]

\[ \alpha_1(\vec{k}) = \frac{\omega_1(\vec{k}) - \Omega_\vec{k}}{\omega_1(\vec{k}) - \omega_2(\vec{k})}, \quad \alpha_2(\vec{k}) = \frac{\omega_2(\vec{k}) - \Omega_\vec{k}}{\omega_2(\vec{k}) - \omega_1(\vec{k})}. \] (5)

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

\[ \alpha_1(\vec{k}) + \alpha_2(\vec{k}) = 1, \quad \alpha_1(\vec{k}) \omega_1(\vec{k}) + \alpha_2(\vec{k}) \omega_2(\vec{k}) = \xi_\vec{k}, \quad \xi_\vec{k} = \epsilon(\vec{k}) + \rho U. \] (6)

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

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

\[ \omega_1^3(\vec{k}) \alpha_1(\vec{k}) + \omega_2^3(\vec{k}) \alpha_2(\vec{k}) = \xi_\vec{k}^3 + (\Omega_\vec{k} + 2\xi_\vec{k}) \alpha(\vec{k}) = a_3(\vec{k}), \] (7)

where a_2(\vec{k}), a_3(\vec{k}) are given in Ref. 3-6 as

\[ a_2(\vec{k}) = c^2(\vec{k}) + 2\rho U \epsilon(\vec{k}) + \rho U^2, \]

\[ a_3(\vec{k}) = c^3(\vec{k}) + 3U \epsilon^2(\vec{k})(2 + \rho) \rho U^2 \epsilon(\vec{k}) + \rho (1 - \rho) U B(\vec{k}) + \rho U^3. \] (8)

Temperature enters due to the presence of the B-term. Solving Eqs. 3 we find:

\[ \alpha(\vec{k}) = \rho (1 - \rho) U^2, \quad \Omega_\vec{k} = (1 - \rho) U + B(\vec{k}). \] (9)

The narrowing band parameter has to be calculated self-consistently and is \vec{k}-independent in the spherical approximation (See Ref. 3)). Combining Eqs. 3 we find

\[ \omega_1(\vec{k}) = \frac{1}{2} \left[ H(\vec{k}) + [K(\vec{k})]^{1/2} \right]; \quad \omega_2(\vec{k}) = \frac{1}{2} \left[ H(\vec{k}) - [K(\vec{k})]^{1/2} \right], \]

where

\[ H(\vec{k}) \equiv \epsilon(\vec{k}) U + B(\vec{k}), \quad K(\vec{k}) \equiv \left( \epsilon(\vec{k}) - U - B(\vec{k}) \right)^2 + 4\rho U \left( \epsilon(\vec{k}) - B(\vec{k}) \right). \] (10)

Eqs. 3 are nothing else that the solutions given by Nolting 3 by solving the four unknown \alpha_i(\vec{k}) and \omega_i(\vec{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. The self-energy has the meaning of being an expansion in powers of U. In our case, due to the choice of a single pole for the self-energy, α(\vec{k}) is of second order in U, since the first order is the Hartree shift, ρU.

As our solutions given by Eqs. 3 satisfy the first four sum rules or moments, our Green function is beyond the Hubbard-I solution 3 and as a consequence we have an improved solution 3. The drawback of the Hubbard-I solution, i.e., a gap for any value of the interaction, was pointed out by Laura Roth 3 many years ago. This gap also exists, for all values of U, in the spherical approximation of Nolting 3,4,5. The B-term gives rise to magnetism, a feature which is not present in the Hubbard-I solution.

In Fig. 1 we present the spin susceptibility, \( \chi(T) \) vs \( T/t \) for the two-pole Ansatz for the one-particle Green function, or the one-pole Ansatz for the self-energy (See Eq. 3), for \( U/t = 4.0 \) at half-filling. We see that the spin susceptibility
looks Curie-like at large temperatures and it has a bending towards zero at low temperatures. This type of behavior is similar to the results found for the attractive Hubbard model at half-filling. Let us remember that the attractive and repulsive Hubbard model become identical at half-filling. In Fig. 2 we show the band-narrow parameter, $B(T)$ vs $T/t$ for the same parameters of Fig. 1. We comment here that the band-narrowing factor, $B(T)$, in general, is $\vec{k}$-dependent. This dependence has been explicitly been shown recently to be important by Eskes and Oleś [11].

In summary we have proposed a self-energy of one pole which implies that the Green function is composed of two poles. This has been accomplished by the use of Dyson’s equation (Eq. (2)). We have reproduced with minor effort the Nolting’s solution [6]. [7]. The one-pole self-energy leading to Nolting’s solution puts on firm grounds the results found in Refs. [7] where it was argued that the two branches of the one-particle Green function were due to a single pole in the self-energy. With a single pole-ansatz for the self-energy, we recuperate known results in the literature with less analytical effort, at the same time shedding light on the structure of the self-energy itself. Our Green’s function goes beyond the Hubbard-I solution because we have imposed the condition that the third and four moments be satisfied. For us, Hubbard-I means that the first two moments are satisfied. We add that besides these features we have justified that, for the particular pole structure for our self-energy, this one represents an expansion in powers of $U$. The first order is represented by the Hartree shift, or $\rho U$. (See Eq. (3)). With our rather simple approach we have been able to have a Green’s function with two poles. Our approach is different from the one of the limit of infinite dimensions [12] 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 [13] has applied it to the periodic Anderson model, where the relevant quantity of study is the self-energy.

Acknowledgments

We would like to thank the CNPq (project No.300705/95-6) and also from CONICIT (project F-139). We thank María Dolores García for reading the manuscript. Fruitful discussions with Prof. M.A. Continentino, Prof. E. Anda, Prof. M.S. Figueira, Dr. M.H. Pedersen and Prof. H. Beck are fully appreciated.

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Fig. 1. The static spin susceptibility, $\chi(T)$, vs $T/t$ for the one-pole Ansatz for the self-energy. Here $U/t = 4.0$ and half-filling. The expression for $\chi(T)$ has been borrowed from Ref. [7].

Fig. 2. The narrowing band parameter, $B(T)$ vs $T/t$, for the same parameters of Fig. 1.