Evolution of One–Particle and Double–Occupied Green Functions for the Hubbard Model at Half–Filling With Lifetime Effects Within The Moment Approach.

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(Received March 24, 2022)

We evaluate the one–particle and double–occupied Green functions for the Hubbard model at half–filling using the moment approach of Nolting [1]. Our starting point is a self–energy, \( \Sigma(\vec{k}, \omega) \), which has a single pole, \( \Omega(\vec{k}) \), with spectral weight, \( \alpha(\vec{k}) \), and quasi-particle lifetime, \( \gamma(\vec{k}) \). In our approach, \( \Sigma(\vec{k}, \omega) \) becomes the central feature of the many–body problem and due to three unknown \( \vec{k} \)–parameters we have to satisfy only the first three sum rules instead of four as in the canonical formulation of Nolting [1]. This self–energy choice forces our system to be a non–Fermi liquid for any value of the interaction, since it does not vanish at zero frequency. The one–particle Green function, \( G(\vec{k}, \omega) \), shows the finger–print of a strongly correlated system, i.e., a double peak structure in the one–particle spectral density, \( A(\vec{k}, \omega) \), vs \( \omega \) for intermediate values of the interaction. Close to the Mott Insulator–Transition, \( A(\vec{k}, \omega) \), becomes a wide single peak, signaling the absence of quasi–particles. Similar behavior is observed for the real and imaginary parts of the self–energy, \( \Sigma(\vec{k}, \omega) \).

The double–occupied Green function, \( G_2(\vec{q}, \omega) \), has been obtained from \( G(\vec{k}, \omega) \) by means of the equation of motion. The relation between \( G_2(\vec{q}, \omega) \) and the self–energy, \( \Sigma(\vec{k}, \omega) \), is formally established numerically for the spectral function of \( G_2(\vec{q}, \omega) \), \( \chi^{(2)}(\vec{k}, \omega) \equiv -\frac{1}{\pi} \lim_{\omega \rightarrow 0} \text{Im} \left[ G_2(\vec{k}, \omega) \right] \), are given. Our approach represents the simplest way to include: 1- lifetime effects in the moment approach of Nolting, as shown in the paper; 2- Fermi or/and Marginal Fermi liquid features as we discuss in the conclusions.

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

I. INTRODUCTION

After the discovery of the High-\( T_c \) materials [3], 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 [5,6], since electron correlations are strong, i.e., the on-site electron-electron repulsions \( U \) are much larger than the energies associated to the hybridization of atomic orbitals belonging to different atoms [7]. We consider the study of correlations in the Hubbard model as a rewarding task since it will shed light on still unsolved points of the novel materials. For example, at high temperatures (\( T \sim 30 – 130 \text{ } K \)) these HTSC cuprates, which are poor conductors, become superconductors. This feature is strange indeed because the Coulomb repulsion is strong. 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. [11]. In the present work we explore the effects of having a non–Fermi liquid behavior into the one–particle and double-occupied dynamical properties.

We will use the moment approach (or sum rules) of Nolting [1] for the spectral density, \( A(\vec{k}, \omega) \). It is well known in the literature [10] that the moment approach in the spherical approximation - when the narrowing band factor, \( B(\vec{k}) \), is not \( \vec{k} \)–dependent - always gives a gap in the density of states (\( DOS \)). If the chemical potential happens to be in this gap, then we always have an insulator. It has been argued that the way to cure this unrealistic gap is to have a better approximation for the narrowing band factor, \( B(\vec{k}) \).

We have followed a different path which consists in proposing a single pole structure in the self-energy, \( \Sigma(\vec{k}, \omega) \). Closing the gap for small and intermediate values of \( U/W \) (\( W \) is the bandwidth and \( W = 8t \) in two dimensions), is not the only rationality behind our calculation. It is well documented [11,13] that correlations give rise to lifetime contributions that conspire against the very definition of quasi–particles at the chemical potential. This leads to an
eventual collapse of the Fermi liquid picture of adiabaticity between the electron gas and the electron liquid so well described by the phenomenological treatment of Landau.

This paper is organized as follows. In Section II we present our model Hamiltonian and our self–energy proposal, in which we try to justify our bold choice, as one step forward to understand the physics behind the moment approach of Nolting. This led us to come up with an Ansatz which is not zero at zero frequency, i.e., our system is not a Fermi liquid for any value of the interaction. We could argue that our Ansatz is valid for energy scales not too close to the chemical potential. However, our Ansatz has to become exact in the limit of $U/W \gg 1$. In Section III, we present our results which consist of the real and imaginary parts of the self–energy, and spectral functions of the one- and two–particle Green functions along the diagonal of the Brillouin zone, for different values of the interaction. We have used a system size of $32 \times 32$. In Section IV we present our conclusions and the future trends.

II. MODEL HAMILTONIAN AND SELF-ENERGY ANSATZ

The model we study is the Hubbard Hamiltonian

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

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) are creation (annihilation) electron operators with spin $\sigma$. $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. $U$ 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 (n.n.) $j$ and for spin up and down ($\sigma = \pm 1$). $t_{i,j} = -t$, for n.n. and zero otherwise.

Let us propose for the self–energy, $\Sigma(\vec{k}, \omega)$, the following single pole Ansatz

$$\Sigma(\vec{k}, \omega) = \rho U + \frac{\alpha(\vec{k})}{\omega - \Omega(\vec{k}) - i\gamma(\vec{k})}; \quad \alpha(\vec{k}), \gamma(\vec{k}) \in \mathbb{R} \tag{2}$$

With our choice for $\Sigma(\vec{k}, \omega)$, we have that the real and imaginary parts of the self–energy do satisfy the Kramers–Kronig relations [14], since it is analytic in one of half of the complex plane. In fact, the physical solution to the problem is when $\alpha(\vec{k}) \geq 0$, as it can be checked by finding the roots of $G(\vec{k}, \omega)$ in the complex plane. We postpone the discussion of this point for the conclusions. The Ansatz given in Eq. (2) has some similarity with the Hubbard–I solution [13]. However, we have neglected any frequency dependence in the damping. Our calculations show that $\gamma(\vec{k})$ is $\vec{k}$–independent but strongly $U$–dependent.

The validity of Luttinger theorem [10] has been discussed in Ref. [17]. We argue that most likely the Luttinger theorem is not going to hold because we have a non–Fermi liquid system. Our choice of $\rho U$ in Eq. (2), the Hartree–shift, is very convenient since it redefines an effective chemical potential, $\mu_{eff} = \mu - \rho U$. This effective potential is zero at half–filling, $\rho = 1/2$, since $\mu = U/2$ there. Then, $\omega = 0$ means that we are at the chemical potential. We want to explicitly state that our choice (Eq. (3)) has the advantage of requiring only three sum rules to be satisfied, instead of four as in the now normal procedure of Nolting [1] which starts from the spectral function, $A(\vec{k}, \omega)$, itself. We add that if $\gamma(\vec{k}) = 0$, then we go back to Nolting’s canonical results. In this case [18]

$$\alpha(\vec{k}) = \rho(1 - \rho)U^2; \quad \Omega(\vec{k}) = (1 - \rho)U + B(\vec{k}) \quad , \quad B(\vec{k}) = B + F(\vec{k}) \tag{3}$$

where $B(\vec{k})$ is the narrowing band factor. The $\vec{k}$–independent narrowing band factor, $B$, is calculated in closed form in Ref. [1]. It is a self–consistent quantity, though. The $\vec{k}$–dependent narrowing band factor, $F(\vec{k})$, has been evaluated recently by Herrmann and Nolting [19] using a two–pole ansatz with two poles located at the same energies than the poles of the one–particle Green function. This treatment, beyond the spherical treatment of Nolting [1], can be mapped into the calculations of Kishore and Granato [20] with appropriate identification of our parameters in the paramagnetic phase. Their approach gives a Mott Metal–Insulator transition. All this means that the metal–insulator transition (MMIT) is embedded into the Hubbard model and it does not require of lifetime effects to accomplish this. However, once more, lifetime effects are a natural element of the many–body physics for intermediate and strongly correlated electron systems where the concept of quasi–particle does not apply any longer. We do not pursue anymore here the MMIT, but the interested reader is addressed to references [21,22].

By definition the one–particle Green function, $G(\vec{k}, \omega)$, in terms of $\Sigma(\vec{k}, \omega)$, is given as
\[
G(\vec{k}, \omega) = \frac{1}{\omega - \varepsilon_\vec{k} - \Sigma(\vec{k}, \omega)},
\]

where \(\varepsilon_\vec{k} = -2t(\cos(k_x) + \cos(k_y) - \mu + \rho U)\). Also, we will require the one–particle spectral density, \(A(\vec{k}, \omega)\), which is defined as

\[
A(\vec{k}, \omega) = -\frac{1}{\pi} \lim_{\delta \to 0^+} \text{Im} G(\vec{k}, \omega + i\delta)
\]

Using Eqs. (2 - 3), we arrive to the following expression for the spectral density

\[
A(\vec{k}, \omega) = \frac{\alpha(\vec{k})\gamma(\vec{k})}{\pi \left[(\omega - \varepsilon_\vec{k})(\omega - \Omega_\vec{k}) - \alpha(\vec{k})\right]^2 + \gamma^2(\vec{k})(\omega - \varepsilon_\vec{k})^2}
\]

Using the first three sum rules of Nolting [1] for the the spectral function of Eq. (5) we obtain the following equations

\[
\begin{align*}
\int_{-\infty}^{+\infty} A(\vec{k}, \omega) d\omega & \equiv M_0(\vec{k}) = 1 \\
\int_{-\infty}^{+\infty} \omega A(\vec{k}, \omega) d\omega & \equiv M_1(\vec{k}) = \varepsilon_\vec{k} \\
\int_{-\infty}^{+\infty} \omega^2 A(\vec{k}, \omega) d\omega & \equiv M_2(\vec{k}) = (\varepsilon_\vec{k} - \rho U)^2 + 2\rho U(\varepsilon_\vec{k} - \rho U) + \rho U^2,
\end{align*}
\]

where the \(M_i(\vec{k})\)'s, \(i = 0, 1, 2\), are the first three moments [1]. For example, the first moment \((i = 0)\) is the area below the curve of \(A(\vec{k}, \omega)\) vs \(\omega\), the second moment \((i = 1)\) is the center of gravity of the spectral function and the second order moment (or third moment, \(i = 2\)) is related to the width of the spectral function, \(A(\vec{k}, \omega)\). So, damping effects are controlled by the second order sum rule. We do not use the fourth moment or sum rule because we have three \(\vec{k}\)-dependent unknown parameters (our way of working is different to one of Nolting since in the latter we have to use four moments. The difference lies in the fact that he starts with the one–particle spectral density). We could guess that in order to extend the canonical formalism of Nolting to include lifetime effects, starting from his two pole ansatz, we should have to postulate the following structure for \(G(\vec{k}, \omega)\)

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

from where we see that we would need five moments or sum rules because we have five parameters to determine, i.e., \(\alpha_1(\vec{k}), \omega_1(\vec{k}), \gamma(\vec{k})\), with \(i = 1, 2\). With the proposal (Eq. (2)) we have only three parameters to calculate.

We assume that at \(\rho = 1/2\) the chemical potential, \(\mu = U/2\). The density of states which results of the two pole Ansatz for the one–particle Green function, in the spherical approximation of Nolting [1], always has a gap. This solution (always a gap) is known in the literature as the Hubbard–I solution [23] which has been criticized since many years ago by Laura Roth [24], among others. We call the attention to Ref. [25] where the authors point out to the fact that the \(\vec{k}\)-dependence has to be included in \(B(\vec{k})\). A recent calculation by Kirchhofer [26] is performed at the mean field level for the \(\vec{k}\)-dependence of the band narrowing factor, when the two Hubbard bands are separated. In a more elaborated calculation based on the Mori’s formalism [27] for the one–particle Green function, Kirchhofer et al [28] obtain three peaks in the spectral density, \(A(\vec{k}, \omega)\), which respects particle–hole symmetry. In the end, they get a Mott metal insulator transition, for \(U/t = 5\). Here we are including lifetime effects as a crucial ingredient in the formulation beyond a mean–field treatment. Kirchhofer [28] also considers the presence of antiferromagnetism fluctuations in an empirical way. We could extend Kirchhofer et al’s calculations using the numerical values of the dynamical spin susceptibility, \(\chi(\vec{q}, \omega)\), in the spin–fermin model of superconductivity of Pines, Chubukov and others [29]. The dynamical spin susceptibility has been obtained from nuclear magnetic resonance experiments in the High \(T_c\) cuprates. In Section [11] we present our numerical results and their interpretation.
III. NUMERICAL RESULTS AND THEIR INTERPRETATION

In Figs. 1a, 1b and 1c we present the spectral density, \( A(\vec{k}, \omega) \), vs \( \omega \) along the diagonal of the Brillouin zone \((\vec{k} = 2\pi(n, n)/32)\) for \( U/W = 1/2, 2/3 \) and 1, respectively. We are working with a finite system of periodicity of 32 \times 32. For \( U/W = 1/2 \) we have a double–peaked structure, with visible lifetime effects (the Dirac delta functions of Nolting now have width). This is a feature of correlated electron systems as it has been discussed in the work of Schneider et al [1] for the case of \( U < 0 \). The physics is different but the peak structure is similar. For \( U/W = 2/3 \) we still observe the double peak structure but lifetime effects are stronger. Finally, for \( U/W = 1 \), the double peak structure is practically washed out. As we see, lifetime effects are very much pronounced for the larger values of \( U/W \) presented, i.e., for \( U/W = 1.0 \). The two peaks of \( A(\vec{k}, \omega) \) vs \( \omega \) are separated approximately by a distance of

\[ \sqrt{(\varepsilon_{\vec{k}} - \Omega_{\vec{k}} - \gamma(\vec{k}))^2 + 4\gamma(\vec{k})\varepsilon_{\vec{k}}} \]

In Figs. 2a, 2b and 2c we show the imaginary part of the self–energy, \( -Im[\Sigma(\vec{k}, \omega)] \), vs \( \omega \) along the diagonal of the Brillouin zone for the same values of \( U/W \) of Fig. 1. Again we observe that for increasing values of \( U/W \), damping effects are stronger in the self–energy, as is the case in the one–particle spectral function (see Figs. 1a, 1b and 1c). In addition, we do not observe any Fermi liquid dependence (in frequency) of the imaginary part of the self–energy around \( \omega = 0 \). This is due to our choice of our ansatz (Eq. (2)). We could include Fermi or Marginal Fermi liquid behavior close to the chemical potential as it is suggested in Section IV. However, within the present work, we could say that our approximation is valid for frequencies not too close to the chemical potential. Certainly, for small values of \( U/W \), we should have some Fermi liquid behavior (at least in 2–d), like an imaginary self–energy going to zero as positive power of \( \omega \) at the chemical potential [2].

In Figs. 3a, 3b and 3c we report results for the real part of the self–energy, \( Re[\Sigma(\vec{k}, \omega)] \), vs \( \omega \) along the diagonal of the Brillouin zone for the same values of interaction of Fig. 1. For \( U/W = 1/2, 2/3 \) we see a more o less regular pattern. However, for \( U/W = 1 \), lifetime effects lead to big effects in \( Re[\Sigma(\vec{k}, \omega)] \). For example, the curves are no longer regularly displaced with respect to one another. Also, the frequency range increases appreciably and the heights of the curves decrease. Let us comment that the numerical form of the real part of the self–energy clearly shows that the Kramers–Kronig relations for the self–energy are satisfied, in order to have the roots of the one–particle Green function on the same side of the complex plane. Analytically, it can be proved too. The only requirement coming out of these calculations, with our Ansatz, is that \( \alpha(\vec{k}) \geq 0 \) [3] (see Appendix A). As \( \alpha(\vec{k}) \times \gamma(\vec{k}) \leq 0 \), then \( \gamma(\vec{k}) \leq 0 \). This considerations we have checked in further numerical calculations with lattice sizes of 64 \times 64. Due to these new findings, we correct the results of Ref. [2] since the solutions we found there must satisfy the conditions established here, i.e., \( \alpha(\vec{k}) \geq 0 \) and \( \gamma(\vec{k}) \leq 0 \).

Figs. 4a, 4b and 4c show the imaginary part of the double–occupied Green function, \( -Im[G_2(\vec{k}, \omega)] \), vs \( \omega \) along the diagonal of the Brillouin zone for the same values of interaction as before. Let us recall that \( G_2(\vec{k}, \omega) \) is given by

\[ G_2(\vec{k}, \omega) \equiv \langle T_\tau [\bar{c}_{i,\sigma}(\tau)n_{\bar{\tau},\sigma}(\tau); c_{\bar{\tau},\sigma}^\dagger(0)] \rangle_{\vec{k},\omega} \]  

(9)

where \( \bar{\sigma} = -\sigma \). In Eq. (9), \( \bar{\vec{k}}, \bar{\omega} \) means the Fourier transform of the spatial–temporal correlation function and \( T_\tau \) the usual time ordering of the operators. Using the equation of motion technique for the one–particle Green function, \( G(\vec{k}, \omega) \), we obtain that \( G(\vec{k}, \omega) \) and \( G_2(\vec{k}, \omega) \) are related as follows [2]

\[ (\omega - \varepsilon_{\vec{k}})G(\vec{k}, \omega) = 1 + UG_2(\vec{k}, \omega) \]  

(10)

We observe that there is a big peak in the interval \( \omega \in [-2, -1] \) which is most likely due to the peak in \( A(\vec{k}, \omega) \). However, the right peak at \( (\vec{k}, \omega/W) = (\pi, \pi, \approx 1/3) \) increases with interaction. At the same time, we see that the left frequency peaks \( (\omega < 0) \) start to line up for small momenta but they almost vanish for \( \vec{k} = (3/4, 3/4) \) and \( (1, 1) \).

\[ \chi^{(2)}(\vec{k}, \omega) = -\frac{1}{\pi} \lim_{\delta \to 0^+} Im[G_2(\vec{k}, \omega + i\delta)] \]  

(11)

is the spectral density for the double–occupied Green function. We see from Figs. 4 that there is negative contribution to this spectral density, which is due to the presence of the factor \( \omega - \varepsilon_{\vec{k}} \) in front of the one–particle spectral density, \( A(\vec{k}, \omega) \). In addition, the factor \( \omega - \varepsilon_{\vec{k}} \) is controlling the height of the peaks in \( \chi^{(2)}(\vec{k}, \omega) \). For example, when \( \chi^{(2)}(\vec{k}, \omega) = 0 \) is because this factor is zero. \( \chi^{(2)}(\vec{k}, \omega) \) is given by

\[ U\chi^{(2)}(\vec{k}, \omega) = (\omega - \varepsilon_{\vec{k}}) \times A(\vec{k}, \omega) \]  

(12)
which is identically zero for the non-interacting electron gas, since \( A(\vec{k}, \omega) \) is a Dirac delta function at the same argument of the quantity in front of it. So, any deviation from zero is a signature of an interacting system. Contrary to \( A(\vec{k}, \omega) \), which is always positive, \( \chi^{(2)}(\vec{k}, \omega) \) can be negative. The only requirement is that \[ \int_{-\infty}^{+\infty} \chi^{(2)}(\vec{k}, \omega) d\omega = \rho \ , \] where \( \rho \) is the electron density/spin. This can be easily checked calculating the first moment or moment of zeroth order for the double–occupied Green function. The relation between the self–energy and the double–occupied Green function is the following

\[ UG_2(\vec{k}, \omega) = \frac{\Sigma(\vec{k}, \omega)}{\omega - \varepsilon_\vec{k} - \Sigma(\vec{k}, \omega)} \ . \] (14)

Eq. (14) is an exact relationship and it can be used to keep control of the approximations made in the self–energy and the double–occupied Green functions, as it has been discussed in Ref. [33]. Needless to say that to approximate \( \Sigma(\vec{k}, \omega) \) is equivalent to have an approximation for \( G_2(\vec{k}, \omega) \) and viceversa. In consequence, simple approximations for \( G_2(\vec{k}, \omega) \) are not always equivalent to simple approximations for \( G(\vec{k}, \omega) \) (or \( \Sigma(\vec{k}, \omega) \)) or viceversa. For example, a single pole ansatz (without lifetime effects) in \( G_2(\vec{k}, \omega) \) leads to the Hubbard–I solution as it has been discussed in Ref. [33]. To go beyond the Hubbard–I solution for \( G_2(\vec{k}, \omega) \) we have to use Eqs. (14).

IV. CONCLUSIONS AND FUTURE TRENDS

We have investigated the dynamical quantities, \( A(\vec{k}, \omega) \), \( \text{Re}[\Sigma(\vec{k}, \omega)] \), \( -\text{Im}[\Sigma(\vec{k}, \omega)] \) and \( -\text{Im}[G_2(\vec{k}, \omega)] \), vs \( \omega \) along the diagonal of the Brillouin zone, for three values of the interaction, namely, \( U/W = 1/2, 2/3, 1 \). In all these quantities we observe that the role of correlations and lifetime effects is fundamental. For example, for values of \( U/W \approx 1 \) the one–particle spectral density becomes almost one–peak, while \( -\text{Im}[\Sigma(\vec{k}, \omega)] \) becomes a wider inverted Lorentzian. \( \text{Re}[\Sigma(\vec{k}, \omega)] \), for \( U/W = 1 \) has lost all sign of regularity. \( A(\vec{k}, \omega) \) becomes featureless for large values of \( U/W \). Our treatment of \( G(\vec{k}, \omega) \) and \( G_2(\vec{k}, \omega) \) is not perturbative since we impose sum rules to \( A(\vec{k}, \omega) \) to find \( \Sigma(\vec{k}, \omega) \) and \( G_2(\vec{k}, \omega) \) is found from the equation of motion technique (Eq. (10)).

The choice of self–energy (Eq. (9)) is an attempt to shed some light on Nolting approach to which Eq. (2) reduces when \( \gamma(\vec{k}) = 0 \) [18]. Nolting’s study (when looked upon with our optics, i.e., \( \gamma(\vec{k}) = 0 \), in Ref. [18]) is also a non–Fermi liquid. Our Ansatz for \( \Sigma(\vec{k}, \omega) \) is rather phenomenological, since we have not invoked any microscopic mechanism to postulate it (Eq. (3)). However, we have been guided by the single pole structure of Nolting without lifetime effects. This structure has been fleshed out in a recent paper [18]. Also, we have relied on the calculations of Kishore and Granato [21] which represent a non–Fermi liquid approach for the self–energy. Those interested in a nice interpretation of non–Fermi liquid behavior of the experimental data of High–Temperature Cuprates, please see Ref. [31]. Work is in progress [35] to include Fermi liquid features close to the chemical potential. According to our belief, this type of considerations are much harder to be tackled with the procedure of Nolting, i.e., two poles in the one–particle spectral function, \( A(\vec{k}, \omega) \). For example, the self–energy proposals of Norman et al [36], for the overdoped and underdoped regimes of the cuprate superconductors, can be numerically solved for the attractive Hubbard model [37], for \( d–wave \) superconductivity, where off–diagonal Green function is called for.

A single pole structure in \( \Sigma(\vec{k}, \omega) \) goes beyond the Hubbard–I approximation, since the Hubbard–I approximation is also equivalent to choose a single pole in \( G_2(\vec{k}, \omega) \) (without lifetime effects). This can easily be checked due to the exact relationship given in Eq. (14). However, by comparing the results for the moments without lifetime effects we find that \( \alpha(\vec{k}) \approx \rho(1 - \rho) U^2 \) which proves that our choice for \( \Sigma(\vec{k}, \omega) \) is, at least, a second order expansion in \( U \). This is in agreement with the theoretical findings of Appendix A, since \( \alpha(\vec{k}) \geq 0 \). Thus, \( \alpha(\vec{k}) \) is almost \( \vec{k}–independent \). Similarly, we find that \( \gamma(\vec{k}) \leq 0 \) is independent of \( \vec{k} \), but strongly dependent on \( U \). In consequence, our numerical study proves that our Ansatz is the easiest way to include lifetime effects and to consider Fermi and/or Marginal Fermi liquid behavior in the original proposal of the moment approach of Nolting.

We thank CONICIT–Venezuela (project F-139), the Brazilian Agency CNPq, FAPERGS and the Swiss National Science Foundation for financial support. Interesting discussions with Prof. H. Beck, Prof. M.S. Figueira, Prof. E. Anda and Dr. M.H. Pedersen are fully acknowledged. In particular, Prof. Beck brought to our attention Ref. [26]. Thanks to María Dolores García González for a reading of the manuscript.
With the self-energy ansatz given by Eq. (2), the one-particle Green function becomes
\[
G(\vec{k}, \omega) = \frac{\omega - \Omega(\vec{k}) - i\gamma(\vec{k})}{(\omega - \varepsilon(\vec{k}))(\omega - \Omega(\vec{k})) - \alpha(\vec{k}) - i\gamma(\vec{k})(\omega - \varepsilon(\vec{k}))}
\]  
(15)

From Eq. (15) the poles of the one-particle Green function are given by the roots of the following equation:
\[
z^2 - (\varepsilon(\vec{k}) + \Omega(\vec{k}) + i\gamma(\vec{k}))z - \alpha(\vec{k}) + (\Omega(\vec{k}) + i\gamma(\vec{k}))\varepsilon(\vec{k}) = 0
\]  
(16)

Solving Eq. (16) we get that the two roots are
\[
z_{\pm} = \frac{\varepsilon(\vec{k}) + \Omega(\vec{k}) + i\gamma(\vec{k}) \pm \sqrt{(\varepsilon(\vec{k}) - \Omega(\vec{k}) - i\gamma(\vec{k}))^2 + 4\alpha(\vec{k})}}{2}
\]  
(17)

We have to find the real and imaginary parts of the two roots. For this we follow the standard procedure making
\[
\sqrt{x + iy} = x_1 + iy_1
\]  
(18)

from where we get that
\[
x_1 = \left(\frac{x^2 + y^2 + x}{2}\right)^2; \quad y_1 = \left(\frac{x^2 + y^2 - x}{2}\right)^2
\]  
(19)

Comparing Eqs. (17) and (18) we conclude
\[
x \equiv (\varepsilon(\vec{k}) - \Omega(\vec{k}))^2 + 4\alpha(\vec{k}) - \gamma^2(\vec{k}) \quad ; \quad y \equiv 2\gamma(\vec{k})(\Omega(\vec{k}) - \varepsilon(\vec{k})
\]  
(20)

In consequence, \(z_{\pm}\) are given by
\[
z_{\pm} = \frac{\Omega(\vec{k}) + \varepsilon(\vec{k}) \pm x_1 + i(\gamma(\vec{k}) \pm y_1)}{2}
\]  
(21)

If we require that our roots be on the upper half-complex plane, we must impose that \(\gamma(\vec{k}) \pm y_1 \geq 0\). Carrying out the calculations we arrive to the result that \(\alpha(\vec{k}) \geq 0\), which proves the statement advanced in Section III.
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Figs 1a, 1b and 1c. $A(n, n, \omega) \text{ vs } \omega$ along the diagonal of the Brillouin zone for three different values of interaction, namely, $U/W = 1/2, 2/3$ and $1$. Our system has a periodicity of $32 \times 32$. We are at half-filling, $\rho = 1/2$. As we work in two dimensions, the bandwidth is $W = 8t$. The wave vector along the diagonal is defined as $k = \frac{2\pi}{32}(n, n)$.

Figs. 2a, 2b and 2c. $-\text{Im}\Sigma(n, n, \omega)$ vs $\omega$ along the diagonal of the Brillouin zone. Same parameters of Fig. 1.

Figs 3a, 3b and 3c. $\text{Re}\Sigma(n, n, \omega)$ vs $n$ along the diagonal of the Brillouin zone. Same parameters as previously.

Figs. 4a, 4b and 4c. $-\text{Im}\ G_2(n, n, \omega)$ vs $\omega$ along the diagonal of the Brillouin zone. Same parameters as before.
$U/t = 4.0$  $32\times32$

![Graph showing $A(n,n,\omega)$ vs $\omega/t$ for different $n$ values: $n = 0$, $n = 4$, $n = 8$, $n = 12$, and $n = 16$.](image)
$U/t = 6.0 \quad 32\times32$

![Graph showing $A(n,n,\omega)$ vs $\omega/t$ for different values of $n$.](image-url)
$U/t = 8.0 \ 32\times 32$
$\text{U/t = 4.0  32X32}$

The graph shows the behavior of $-\text{Im}[\Sigma(n,n,\omega)]$ as a function of $\omega/t$ for different values of $n$. The graph includes lines for $n = 0$, $n = 4$, $n = 8$, $n = 12$, and $n = 16$. The y-axis represents the magnitude of the imaginary part of the self-energy, and the x-axis represents $\omega/t$. The graph illustrates how the peak positions and amplitudes change with different $n$ values.
$\omega/t$  

$\Sigma(n,n,\omega)$

$U/t = 6.0$  32X32
$U/t = 8.0 \ 32 \times 32$

The diagram shows the behavior of $\text{Im}[\Sigma(n,n,\omega)]$ for different values of $n$ from 0 to 16. The x-axis represents $\omega/t$, ranging from $-20$ to $20$. The y-axis represents the imaginary part of the self-energy, ranging from 0 to 4.0. The graphs are labeled for $n = 0$, $n = 4$, $n = 8$, $n = 12$, and $n = 16$, each with a specific line style and marker.
$U/t = 4.0 \ 32 \times 32$

The diagram shows the real part of the self-energy $\text{Re}[\Sigma(n,n,\omega)]$ as a function of $\omega/t$ for different values of $n$. The curves are labeled with $n = 0$, $n = 4$, $n = 8$, $n = 12$, and $n = 16$. The x-axis represents $\omega/t$, and the y-axis represents $\text{Re}[\Sigma(n,n,\omega)]$. The plot illustrates the variation of the self-energy with respect to frequency for different momentum states.
$U/t = 8.0 \ 32X32$

Graph showing the real part of the self-energy function $\Sigma(n,n,\omega)$ for different values of $n$: $n = 0$, $n = 4$, $n = 8$, $n = 12$, $n = 16$. The x-axis represents $\omega/t$, ranging from -20 to 20, and the y-axis represents the real part of $\Sigma(n,n,\omega)$, ranging from -5 to 5.
$\omega / t = 4.0$  32X32
$U/t = 8.0$  32X32