Evolution of one-particle and double-occupied Green functions for the Hubbard model, with interaction, at half-filling with lifetime effects within the moment approach

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We evaluate the one-particle and double-occupied Green functions for the Hubbard model at half-filling using the moment approach of Nolting [Z. Phys. **255**, 25 (1972); *Grund Kurs: Theoretische Physik. 7 Viel-Teilchen-Theorie* (Verlag Zimmermann-Neufang, Ulmen, 1992)]. 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 quasiparticle lifetime, $\gamma(\vec{k})$ [J. J. Rodríguez-Núñez and S. Schafroth, J. Phys. Condens. Matter **10**, L391 (1998); J. J. Rodríguez-Núñez, S. Schafroth, and H. Beck, Physica B (to be published); (unpublished)]. 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 [Z. Phys. **255**, 25 (1972); *Grund Kurs: Theoretische Physik. 7 Viel-Teilchen-Theorie* (Verlag Zimmermann-Neufang, Ulmen, 1992)]. 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 fingerprint of a strongly correlated system, i.e., a double peak structure in the one-particle spectral density, $A(\vec{k},\omega)$, vs ω 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 quasiparticles. 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 and numerical results for the spectral function of $G_2(\vec{k},\omega)$, $\chi^{(2)}(\vec{k},\omega)\equiv-(1/\pi)\lim_{\delta\to 0^+}\mathrm{Im}[G_2(\vec{k},\omega)]$, are given. Our approach represents the simplest way to include (1) lifetime effects in the moment approach of Nolting, as shown in the paper, and (2) Fermi or/and marginal Fermi liquid features as we discuss in the conclusions. [S0163-1829(99)03528-6]

I. INTRODUCTION

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,[3,4] 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.[5] 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_c 30−130 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., $R\approx T$.[6] This suggests a very strong scattering of elementary excitations. A discussion of the possible breakdown of Fermi liquid theory is given in Ref. 7. In the present work we explore the effects of having a non-Fermi liquid behavior into the one-particle Green function and double-occupied Green function.

We will use the moment approach (or sum rules) of Nolting[8] for the spectral density, $A(\vec{k},\omega)$. It is well known in the literature[9] that the moment approach in the spherical approximation—when the narrowing band factor, $B(\vec{k})$, is not 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[10–12] that correlations give rise to lifetime contributions that conspire against the very definition of quasiparticles at the chemical potential. For a discussion of this point we refer the reader to Fig. 2 where $-\mathrm{Im}[\Sigma(\vec{k},\omega)]$ vs ω is always finite for $\omega/t=0$ for wave vectors along the diagonal of the Brillouin zone. By construction [Eq. (2)], we are working with a non-Fermi liquid picture for low energies.

For a discussion of this point we refer the reader to Fig. 2 where $-\mathrm{Im}[\Sigma(\vec{k},\omega)]$ vs ω is always finite for $\omega/t=0$ for all the wave vectors along the diagonal of the Brillouin zone. By

construction, we are working with a non-Fermi liquid picture at low energies.

This paper is organized as follows. In Sec. 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 Sec. III, we present our results which consist of the real and imaginary parts of the self-energy, and spectral functions of the one-particle and double-occupied Green functions along the diagonal of the Brillouin zone, for different values of the interaction. We have used a system size of 32×32. In Sec. IV we present our conclusions and the future trends.

II. MODEL HAMILTONIAN AND SELF-ENERGY ANSATZ

The model we study is the Hubbard Hamiltonian

$$H = t_{\vec{i},\vec{j}} c^{\dagger}_{\vec{i}\sigma} c_{\vec{j}\sigma} + \frac{U}{2} n_{\vec{i}\sigma} n_{\vec{i}\bar{\sigma}} - \mu c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}\sigma}, \tag{1}$$

where $c^{\dagger}_{\vec{i}\sigma}$ ($c_{\vec{i}\sigma}$) are creation (annihilation) electron operators with spin σ. $n_{\vec{i}\sigma} \equiv c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}\sigma}$. U is the local interaction, μ 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 (NN) $\vec{j}$ and for spin up and down ($\sigma = -\bar{\sigma} = \pm 1$). $t_{\vec{i},\vec{j}} = -t$, for NN and zero otherwise.

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

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

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,[13] 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.[14] 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[15] has been discussed in Ref.16. We argue that most likely the Luttinger theorem is not going to hold because we have a non-Fermi liquid system. Our choice of ρU in Eq. (2), the Hartree shift, is very convenient since it redefines an effective chemical potential, $\mu_{\mathrm{eff}} = \mu - \rho U$. 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. (2)] has the advantage of requiring only three sum rules to be satisfied, instead of four as in the now normal procedure of Nolting[8] 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[17]

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

$$B(\vec{k}) = B + F(\vec{k}), \tag{3}$$

where $B(\vec{k})$ is the narrowing band factor. The $\vec{k}$-independent narrowing band factor, B, is calculated in closed form in Ref. 8. 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[18] using a two-pole ansatz with the two poles located at the same energies than the poles of the one-particle Green function. This treatment, beyond the spherical treatment of Nolting,[8] can be mapped into the calculations of Kishore and Granato[19] with appropiate 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 quasiparticle does not apply any longer. The interested reader is addressed to Refs. 7 and 20–22.

However, we have a metal for $U \leq U_c = W$, since a metal is defined by $N(\omega = 0) \neq 0$ [see Eq. (231) of Ref. 23]. In a previous paper,[20] we have shown that the density of states at $\omega/t = 0$ is different from zero for $U \leq U_c$. This type of metal we call a *strange metal*. Furthermore, we have said in the Introduction of our paper that our approach is valid for energy not too close to the chemical potential. Work is in progress to consider Fermi and marginal Fermi liquid behavior close to the chemical potential, i.e.,

$$\Sigma(\vec{k},\omega) = \frac{\alpha(\vec{k})}{\omega - \Omega(\vec{k}) - i\gamma(\vec{k})\omega^n}, \tag{4}$$

with $n = 0,1$.[24]

By definition the one-particle Green function, $G(\vec{k},\omega)$, in terms of $\Sigma(\vec{k},\omega)$, is given as

$$G(\vec{k},\omega) = \frac{1}{\omega - \varepsilon_{\vec{k}} - \Sigma(\vec{k},\omega)}, \tag{5}$$

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

$$A(\vec{k},\omega) = -\frac{1}{\pi} \lim_{\delta \to 0^+} \mathrm{Im}\, G(\vec{k},\omega + i\delta). \tag{6}$$

Using Eqs. (2)–(6), we arrive to the following expression for the spectral density:

$$A(\vec{k},\omega)=\frac{-1}{\pi}\frac{\alpha(\vec{k})\gamma(\vec{k})}{((\omega-\varepsilon_{\vec{k}})(\omega-\Omega_{\vec{k}})-\alpha(\vec{k}))^2+\gamma^2(\vec{k})(\omega-\varepsilon_{\vec{k}})^2}. \quad (7)$$

Using the first three sum rules of Nolting[8] for the the spectral function of Eq. (6) we obtain the following equations:

$$\int_{-\infty}^{+\infty}A(\vec{k},\omega)d\omega\equiv M_0(\vec{k})=1,$$

$$\int_{-\infty}^{+\infty}\omega A(\vec{k},\omega)d\omega\equiv M_1(\vec{k})=\varepsilon_{\vec{k}},$$

$$\int_{-\infty}^{+\infty}\omega^2 A(\vec{k},\omega)d\omega\equiv M_2(\vec{k})=\varepsilon_{\vec{k}}^2+2\rho U\varepsilon_{\vec{k}}^2+\rho U^2, \quad (8)$$

where the $M_i(\vec{k})$'s, $i=0,1,2$, are the first three moments.[8] For example, the first moment ($i=0$) is the area below the curve of $A(\vec{k},\omega)$ vs ω, 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 the 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 $G(\vec{k},\omega)$:

$$G(\vec{k},\omega)=\frac{\alpha_1(\vec{k})}{\omega-\omega_1(\vec{k})+i\gamma(\vec{k})}+\frac{\alpha_2(\vec{k})}{\omega-\omega_2(\vec{k})+i\gamma(\vec{k})}, \quad (9)$$

from where we see that we would need five moments or sum rules because we have five parameters to determine, i.e., $\alpha_i(\vec{k})$, $\omega_i(\vec{k})$, $\gamma(\vec{k})$, 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,[8] always has a gap. This solution (always a gap) is known in the literature as the Hubbard-I solution[25] which has been critized since many years ago by Laura Roth,[26] among others. We call the attention to Ref. 27 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[28] 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[29] for the one-particle Green function, Kirchhoffer *et al.*[28,30] 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[28,30] also considers the presence of antiferromagnetism fluctuations in an empirical way. We could extend Kirchhoffer *et al.*'s calculations using the numerical values of the dynamical spin susceptibility, $\chi(\vec{q},\omega)$, in the spin-fermion model of superconductivity of Pines, Chubukov and others.[31] The dynamical spin susceptibility has been obtained from nuclear magnetic resonance experiments in the high-T_c cuprates. In Sec. III, we present our numerical results and their interpretation.

III. NUMERICAL RESULTS AND THEIR INTERPRETATION

In Figs. 1(a), 1(b), and 1(c) we present the *spectral density*, $A(\vec{k},\omega)$, vs ω 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 32×32. 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.*[9] 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 ω are separated approximately by a distance of $\sqrt{[\varepsilon_{\vec{k}}-\Omega_{\vec{k}}-\gamma(\vec{k})]^2+4\gamma(\vec{k})\varepsilon_{\vec{k}}}$.

We would like to compare the results of our approach with the ones of Ref. 28. The work of Kirchhofer is based on a different approach, i.e., Mori's continuous fraction. We recall that the Mori's continuous fraction for $G(\vec{k},\omega)$ is based on a cumulant expansion with as many poles as we keep terms. This cumulant expansion is approximated by Kirchhofer[28] by the one-particle Green's function itself. Closing the continuous fraction with $G(\vec{k},\omega)$ itself is equivalent to group together the poles. As a result we get branch cuts, rather than isolated poles, ending up with a square root expression for $G(\vec{k},\omega)$.

From these considerations it is easy to obtain three structures in $A(\vec{k},\omega)$. The central one, close to the chemical potencial, is a delta function, i.e., $\alpha_o(\vec{k})\delta(\omega-\varepsilon_{\vec{k}})$, with a weight which depends of U. Kirchhofer[28] has calculated U_c as that value of U for which $\alpha_o(\vec{k})=0$. When constructing the correlated density of states, $N(\omega)=-(1/\pi)\lim_{\delta\to O^+}\Sigma_{\vec{k}}\mathrm{Im}[G(\vec{k},\omega+i\delta)]$, this shows the lowering of the van Hove singularity with increasing U in a 2D discrete Hubbard Hamiltonian.

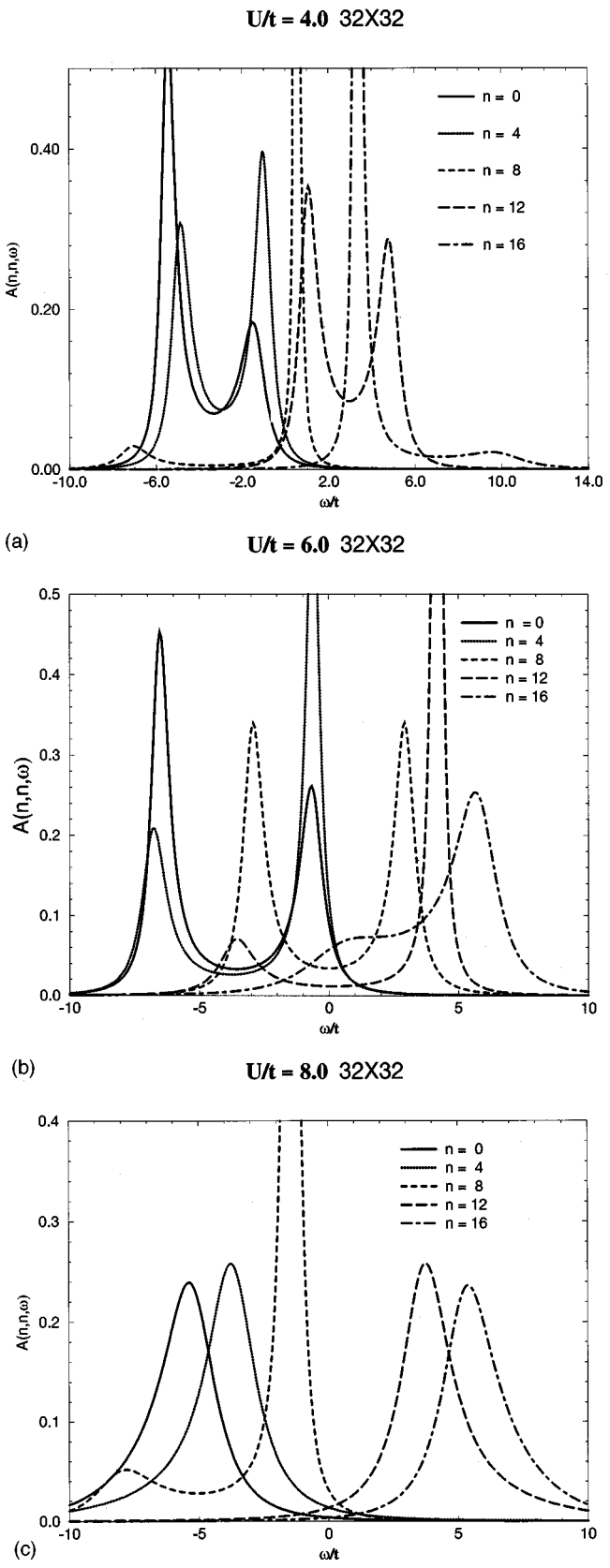

FIG. 1. (a)–(c) $A(n,n,\omega)$ vs ω along the diagonal of the Brillouin zone for three different values of interaction, namely, $U/W=1/2$, 2/3, and 1. Our system has a periodicity of 32×32. We are at half-filling, $\rho=1/2$. As we work in two dimensions, the bandwidth is $W=8t$. The wave vector along the diagonal is defined as $\vec{k}\equiv(2\pi/32)(n,n)$.

From these considerations we cannot conclude that a third peak in $A(\vec{k},\omega)$ $[\alpha_o(\vec{k})\neq0]$ is equivalent to a third peak in the correlated density of states. In fact, if we adopt a flat free density of states ($U=0$), we can interpret the results of our papers and the one of Kirchhofer[28] as the superposition of two bands, each of weight 1/2, for $U=0$, around the chemical potential ($\omega=\mu$). With interaction ($U\neq0$) these two symmetric bands start to displace in opposite directions in frequencies, giving origin to the lower and the upper Hubbard bands (for $U\geqslant U_c$). In consequence, three peaks in $A(\vec{k},\omega)$[28] basically produces our density of states, and the ones of the so-called Hubbard-III like approximation of Refs. 32 and 19.

In Figs. 2(a), 2(b), and 2(c) we show the imaginary part of the self-energy, $-\mathrm{Im}[\Sigma(\vec{k},\omega)]$, vs ω 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. 1(a), 1(b), and 1(c)]. 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 Sec. 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 2D), like an imaginary self-energy going to zero as positive power of ω at the chemical potential.[33]

There are dynamical mean-field theory[23] numerical results which suggest the presence of a third peak around the chemical potential in the correlated density of states. However, the results on this so-called *collective single-band Kondo effect* is not a well established fact as it will be shown below. This third peak is located in between the so-called lower and upper Hubbard bands.[23] According to our knowledge, the calculations of Ref. 23 do not show the spectral functions which are the central issue of the present paper. From the point of view developed in our paper, i.e., one single-pole structure for the self-energy, we are lead to two pole-structure for the spectral function, $A(\vec{k},\omega)$. As we have just said, the dynamical function discussed by Georges *et al.*[23] is the density of states, $N(\omega)$, and this shows well defined structures, with a central peak which defines the Kondo effect. Another study of the dynamical mean-field approximation has been performed by Pruschke *et al.*[34] for various dopings. These authors do not get the collective single-band Kondo effect at half-filling ($\rho=1/2$) but for other dopings. Naturally there is a contradiction between the results of Ref. 23 and the ones of Ref. 34. In consequence, the appearance of the Kondo peak is not a fully established fact in the published literature. In addition, a recent paper by Fisher[35] performs a critical study of the Mott metal-insulator transition in infinity dimensions ($d\equiv\infty$) concluding that it is absent. His conclusions are reached after discussing the very premises of the $d\equiv\infty$ theory. In particular, we mention two relevant points.

(1) If the limit of infinity dimensions is taken on a Bravais lattice, the free one-particle density of states has an infinity

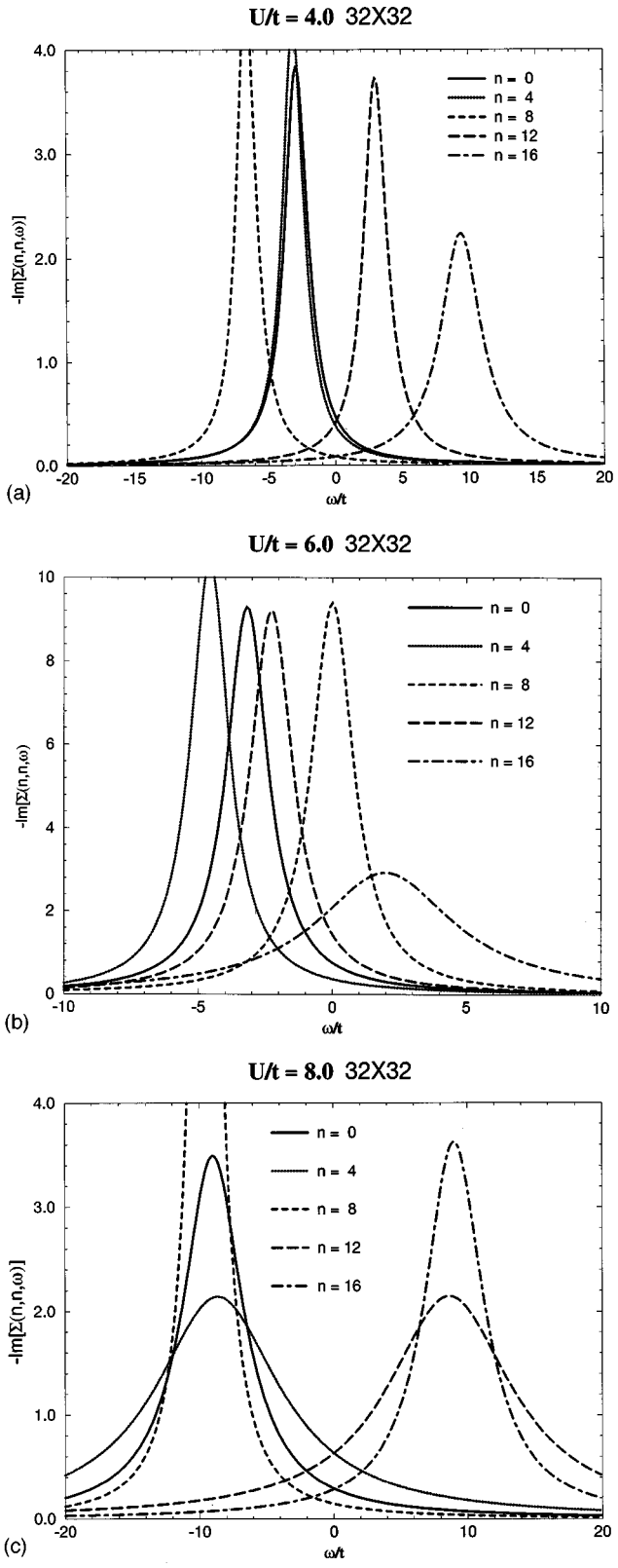

FIG. 2. (a)–(c) $-\mathrm{Im}\,\Sigma(n,n,\omega)]$ vs ω along the diagonal of the Brillouin zone. Same parameters of Fig. 1.

width. As a consequence of that, it does have a Mott metal-insulator transition.[36]

(2) The $d\equiv\infty$ relies on a free semicircular density of states, which is realized for a lattice where the hopping matrix elements are distant *independent*, Gaussian distributed random variables, to fully frustate antiferromagnetic ordering. Then, as he proves, the Bethe and the fully frustated lattice, have no well defined thermodynamical limit, and hence no well defined one-particle density of states.[37,38]

To close this point, we can affirmatively state that our approach is definitively different from the one of Georges, Kotliar, Krause, and Rozenberg[23] (more about this later). We could argue that one missing element in our approach could be that we are not considering the presence of antiferromagnetic (AF) fluctuations. This could give rise to an additional depletion of the density of states in between the two Hubbard bands.[39] In any case, as we can conclude from our previous discussion, the *collective single-band Kondo effect* is a controversial issue and we cannot perform a definitive comparison with the $d\equiv\infty$ approximation.

The fact that we have a two peak structure in $A(\vec{k},\omega)$ does not lead necessarily to a central peak in $N(\omega)$, separated from the other two structures. For example, from Fig. 31 of Georges *et al.*[23] we cannot conclude the presence of a third peak in the spectral function since their self-energy is featureless. From our one-peak self-energy we can surely answer that the one-particle spectral density has a two-pole structure. We can definitively say that our correlated $A(\vec{k},\omega)$ and $N(\omega)$ are similar to a Hubbard-III like solution, as it has been shown by Ikeda, Larsen, and Mattuck[32] and Kishore-Granato.[19] The only difference with the results of this papers is that we have included lifetime effects in the moment approach of Nolting.[20] Just recently, Rodríguez-Núñez *et al.*[40] have rederived the Hubbard-III like approximation of Refs. 32 and 19 and explicitly shown the Mott metal-insulator transition, for a flat density of states. The MIT occurs for $U=W\equiv 8t$. On spite of our differences with the results of Ref. 23, we agree with the results of Ref. 34. Their Fig. 6(a)[34] shows the spectral function, $N(\vec{k},\omega)$ or $A(\vec{k},\omega)$, for $U=4$ and $\rho=n/2=1/2$. Our results agree quite well with the ones presented by Pruschke *et al.*:[34] two peaks along the diagonal of the Brillouin zone, with different weights.

In Figs. 3(a), 3(b), and 3(c) we report results for the real part of the self-energy, $\mathrm{Re}[\Sigma(\vec{k},\omega)]$, vs ω 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 or less regular pattern. However, for $U/W=1$, lifetime effects lead to big effects in $\mathrm{Re}[\Sigma(\vec{k},\omega)]$. 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 $\alpha(\vec{k})\geqslant 0$ (Ref. 41) (see the Appendix). As $\alpha(\vec{k})\times\gamma(\vec{k})\leqslant 0$, then $\gamma(\vec{k})\leqslant 0$. This consideration we have checked in further numerical calculations with lattice sizes of 64×64. Due to these new findings, we correct the results of Ref. 20 since the solutions we found there must satisfy the conditions established here, i.e., $\alpha(\vec{k})\geqslant 0$ and $\gamma(\vec{k})\leqslant 0$.

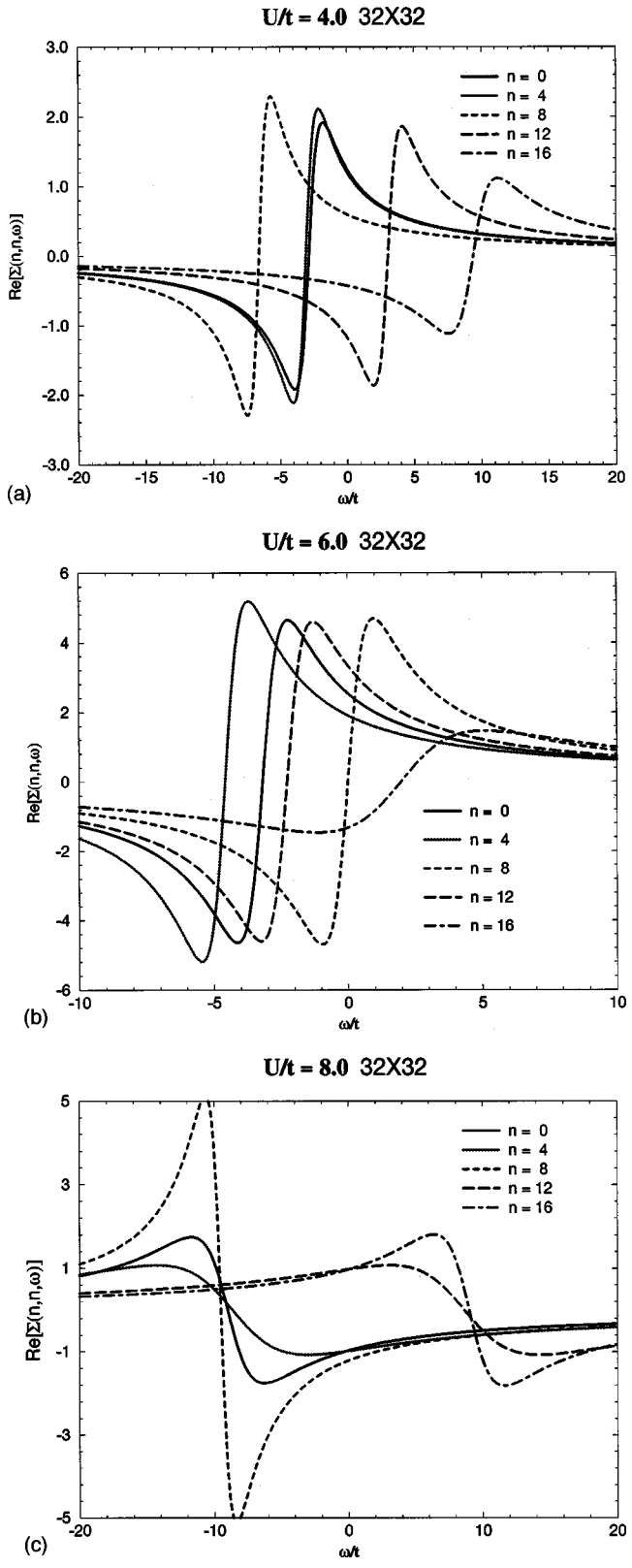

FIG. 3. (a)–(c) $\mathrm{Re}[\Sigma(n,n,\omega)]$ vs n along the diagonal of the Brillouin zone. Same parameters as previously.

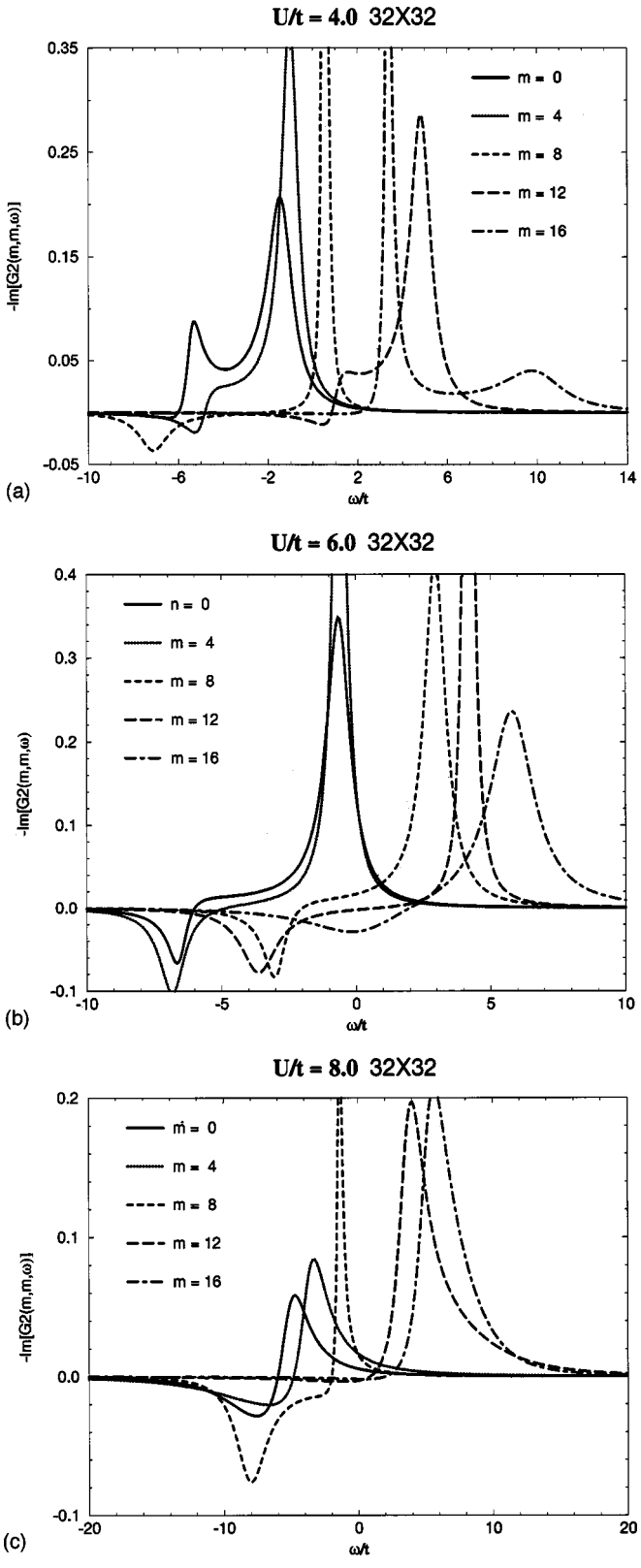

FIG. 4. (a)–(c) $-\mathrm{Im}[G_2(n,n,\omega)]$ vs ω along the diagonal of the Brillouin zone. Same parameters as before.

Figures 4(a), 4(b), and 4(c) show the imaginary part of the double-occupied Green function, $-\mathrm{Im}[G_2(\vec{k},\omega)]$, vs ω 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

$$G_2(\vec{k},\omega)\equiv\langle T_\tau[c_{\vec{i},\sigma}(\tau)n_{\vec{i},\bar{\sigma}}(\tau);c^\dagger_{\vec{j},\sigma}(0)]\rangle_{(\vec{k},\omega)}, \qquad (10)$$

where $\bar{\sigma}=-\sigma$. In Eq. (10) $(\vec{k},\omega)$ means the Fourier transform of the spatial-temporal correlation function and T_τ 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:[42]

$$(\omega-\varepsilon_{\vec{k}})G(\vec{k},\omega)=1+UG_2(\vec{k},\omega). \tag{11}$$

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 $\vec{k}=\pi(3/4,3/4)$ and $\pi(1,1)$:

$$\chi^{(2)}(\vec{k},\omega)\equiv-\frac{1}{\pi}\lim_{\delta\to 0^+}\mathrm{Im}[G_2(\vec{k},\omega+i\delta)] \tag{12}$$

is the spectral density for the double-occupied Green function. We see from Fig. 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

$$U\chi^{(2)}(\vec{k},\omega)=(\omega-\varepsilon_{\vec{k}})\times A(\vec{k},\omega), \tag{13}$$

which is identically zero for the noninteracting 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[42]

$$\int_{-\infty}^{+\infty}\chi^{(2)}(\vec{k},\omega)d\omega=\rho, \tag{14}$$

where ρ 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:

$$UG_2(\vec{k},\omega)=\frac{\Sigma(\vec{k},\omega)}{(\omega-\varepsilon_{\vec{k}}-\Sigma(\vec{k},\omega))}. \tag{15}$$

Equation (15) 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. 40. Needless to say that to approximate $\Sigma(\vec{k},\omega)$ is equivalent to have an approximation for $G_2(\vec{k},\omega)$ and vice versa. 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 vice versa. 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. 40. To go beyond the Hubbard-I solution for $G_2(\vec{k},\omega)$ we have to use Eqs. (5) and (15).

IV. CONCLUSIONS AND FUTURE TRENDS

We have investigated the dynamical quantities, $A(\vec{k},\omega)$, $\mathrm{Re}[\Sigma(\vec{k},\omega)]$, $-\mathrm{Im}[\Sigma(\vec{k},\omega)]$ and $-\mathrm{Im}[G_2(\vec{k},\omega)]$, vs ω 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 $-\mathrm{Im}[\Sigma(\vec{k},\omega)]$ becomes a wider inverted Lorentzian. $\mathrm{Re}[\Sigma(\vec{k},\omega)]$, 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. (11)].

The choice of self-energy [Eq. (2)] is an attempt to shed some light on Nolting's approach to which Eq. (2) reduces when $\gamma(\vec{k})=0$.[17] Nolting's study (when looked upon with our optics, i.e., $\gamma(\vec{k})=0$, in Ref. 17) 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. (2)]. 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.[17] Also, we have relied on the calculations of Kishore and Granato[19] 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. 43. Work is in progress[24] to include Fermi liquid features close to the chemical potential. According to our belief, these types 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.*,[44] for the overdoped and underdoped regimes of the cuprate superconductors, can be numerically solved for the attractive Hubbard model,[24] for *d*-wave superconductivity, where off-diagonal Green functions are called for.

Now, we will compare our numerical results with the ones of Ulmke, Scalettar, Nazarenko, and Dagotto.[45] Their results are performed for the 3D single band Hubbard model, though. For example, their QMC results (Fig. 4) show a clear gap for $U/t=12$, $\rho=1/2$, and $T=0.25$ for a $4\times4\times4$ lattice. In addition, their quasiparticle dispersion (Fig. 5)[45] for the same parameters as previously shows two well defined brances, $E_1(\vec{k})$ and $E_2(\vec{k})$, which are equivalent to our two branches. We have presented our results (Fig. 1) along the diagonal of the Brillouin zone, from $\vec{k}=(0,0)$ (Γ point) to $\vec{k}=(\pi,\pi)$ (M point). We get qualitative agreement with the ones of QMC/ME results of Ref. 45. We have already said thar our results compare reasonably well with the spectral function of Ref. 34 [see their Fig. 6(a)] which is a calculation performed in infinity dimensions.

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. (15). 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 the Appendix, since $\alpha(\vec{k}) \geqslant 0$. Thus, $\alpha(\vec{k})$ is almost $\vec{k}$-independent. Similarly, we find that $\gamma(\vec{k}) \leqslant 0$ 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.

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APPENDIX: POLES OF THE ONE-PARTICLE GREEN FUNCTION

With the self-energy ansatz given by Eq. (2), the one-particle Green function becomes

$$G(\vec{k},\omega) = \frac{\omega - \Omega(\vec{k}) - i\gamma(\vec{k})}{(\omega-\varepsilon_{\vec{k}})(\omega-\Omega(\vec{k})) - \alpha(\vec{k}) - i\gamma(\vec{k})(\omega-\varepsilon_{\vec{k}})}. \tag{A1}$$

From Eq. (A1) the poles of the one-particle Green function are given by the roots of the following equation:

$$z^2 - (\varepsilon_{\vec{k}} + \Omega(\vec{k}) + i\gamma(\vec{k}))z - \alpha(\vec{k}) + (\Omega(\vec{k}) + i\gamma(\vec{k}))\varepsilon_{\vec{k}} = 0. \tag{A2}$$

Solving Eq. (A2) we get that the two roots are

$$z_{\pm} = \frac{\varepsilon_{\vec{k}} + \Omega(\vec{k}) + i\gamma(\vec{k}) \pm \sqrt{(\varepsilon_{\vec{k}} - \Omega(\vec{k}) - i\gamma(\vec{k}))^2 + 4\alpha(\vec{k})}}{2}. \tag{A3}$$

We have to find the real and imaginary parts of the two roots. For this we follow the standard procedure making

$$\sqrt{x+iy} = x_1 + iy_1, \tag{A4}$$

from where we get that

$$x_1 = \left(\frac{\sqrt{x^2+y^2}+x}{2}\right)^2; \quad y_1 = \left(\frac{\sqrt{x^2+y^2}-x}{2}\right)^2. \tag{A5}$$

Comparing Eqs. (A3) and (A4) we conclude

$$x \equiv (\varepsilon_{\vec{k}} - \Omega(\vec{k}))^2 + 4\alpha(\vec{k}) - \gamma^2(\vec{k}); \quad y \equiv 2\gamma(\vec{k})(\Omega(\vec{k}) - \varepsilon_{\vec{k}}). \tag{A6}$$

In consequence, $z_{\pm}$ are given by

$$z_{\pm} = \frac{\Omega(\vec{k}) + \varepsilon_{\vec{k}} \pm x_1 + i(\gamma(\vec{k}) \pm y_1)}{2}. \tag{A7}$$

If we require that our roots be on the upper half-complex plane, we must impose that $\gamma(\vec{k}) \pm y_1 \geqslant 0$. Carrying out the calculations we arrive to the result that $\alpha(\vec{k}) \geqslant 0$, which proves the statement advanced in Sec. III.

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