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LETTER TO THE EDITOR

The Mott metal–insulator transition in the two-dimensional Hubbard model at half-filling with lifetime effects within the moment approach

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Abstract. We explore the effect of the self-energy, $\text{Im } \Sigma(\mathbf{k}, \omega)$, having a single pole, $\Omega(\mathbf{k})$, with *spectral* weight $\alpha(\mathbf{k})$ and quasi-particle lifetime $\Gamma(\mathbf{k})$, on the density of states. We obtain the set of parameters $\Omega(\mathbf{k})$, $\alpha(\mathbf{k})$, and $\Gamma(\mathbf{k})$ by means of the moment approach (exact sum rules) of Nolting. Due to our choice of self-energy, the system is not a Fermi liquid for any value of the interaction, a result which also holds in the moment approach of Nolting without lifetime effects. Our self-energy satisfies the Kramers–Kronig relationships since it is analytic in one of the complex half-planes. By increasing the value of the local interaction, U/W , at half-filling ($\rho = 1/2$), there is a transition from a paramagnetic metal to a paramagnetic insulator (a Mott metal–insulator transition) for values of U/W of the order of $U/W \geq 1$ (W is the bandwidth) which is in agreement with numerical results for finite lattices and for an infinite number of dimensions ($D = \infty$). These results expose the main weakness of the spherical approximation of Nolting: a finite gap for any finite value of the interaction, i.e., an insulator for any finite value of U/W . Lifetime effects are absolutely indispensable to making our scheme work better than that based on improving the narrowing band factor, $B(\mathbf{k})$, beyond that obtained from the spherical approximation of Nolting.

Since the discovery of the high- T_c materials [3], the study of correlations has gained interest, due to the fact that there is a 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 repulsion U is much larger than the energy associated with the hybridization of atomic orbitals belonging to different atoms [7]. One strategy, according to Anderson [8], for addressing the problem of the high- T_c superconductivity is to try to find a theory accounting for the normal-state properties of the cuprates, and then find an electron mechanism which destabilizes the normal state towards a superconducting state. The Hubbard Hamiltonian is a kind of minimum model [9] which takes into account quantum mechanical motion of electrons in a solid, and non-linear repulsion between electrons. Even though this model is too simple to describe solids faithfully, in-depth theoretical studies have revealed that achieving an understanding of its various properties is very difficult, as is the simplest many-body Hamiltonian that one can write down which cannot be reduced to a single-particle theory [10]. Its study will prove useful in developing various notions and

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techniques in statistical physics with many degrees of freedom. Besides that in cuprate superconductors, the Hubbard model may also be applicable to describing the metal–insulator transition in materials like $\text{La}_x\text{Sr}_{1-x}\text{TiO}_3$ and V_{2-y}O_3 , for which a paramagnetic metal, an antiferromagnetic insulator, and an antiferromagnetic phase metal can be clearly discerned in the temperature–pressure phase diagram [11]. The fact that the Hubbard model exhibits all of these features shows that it is suitable for reproducing experimental data. Additionally, the study of correlations in the Hubbard model is in itself rewarding, since it sheds light on as-yet unresolved points concerning the novel materials. For example, at high temperatures ($T_c \sim 30\text{--}130$ K) the HTSC cuprates, which are poor conductors, become superconductors. This feature is very strange, because the Coulomb repulsion is strong. Furthermore, the behaviour 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 reference [12]. There is also another approach which consists in studying toy models, i.e., exactly solvable models [13], in order to get some idea of the one-particle properties of highly correlated electron systems. More recently, there have been some studies on Hubbard superlattices [14] carried out in order to monitor the distribution of magnetic order over the different sites.

In this letter, we will use the moment approach (or sum rules) of Nolting [1] for the spectral density, $A(\mathbf{k}, \omega)$. As is well known from the literature [15], one of the drawbacks of the moment approach in the spherical approximation—where $B(\mathbf{k})$, the narrowing band factor, is not k -dependent—is that we *always* find 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 resolve the problem of this unrealistic gap is to find a better approximation for the narrowing band factor, $B(\mathbf{k})$, a task which has previously proven to be difficult [15]. In view of that difficulty, we have followed a different path, which consists in proposing a single-pole structure in the self-energy, $\Sigma(\mathbf{k}, \omega)$.

The model that we study is the Hubbard Hamiltonian

$$H = t_{i,j} c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} n_{i\sigma} n_{i\bar{\sigma}} - \mu c_{i\sigma}^\dagger c_{i\sigma} \quad (1)$$

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

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

$$\Sigma(\mathbf{k}, \omega) = \rho U + \frac{\alpha(\mathbf{k})}{\omega - \Omega(\mathbf{k}) - i\Gamma(\mathbf{k})} \quad \alpha(\mathbf{k}), \Gamma(\mathbf{k}) \in \mathbb{R}. \quad (2)$$

With our choice for $\Sigma(\mathbf{k}, \omega)$, we may introduce some numerical oscillations which are also present in finite lattices. For example, calculating the momentum distribution function $n(\mathbf{k})$, defined by

$$n(\mathbf{k}) \equiv \int_{-\infty}^{+\infty} \frac{A(\mathbf{k}, \omega) d\omega}{\exp(\beta\omega) + 1} \quad (3)$$

where $\beta = (k_B T)^{-1}$, T is a temperature, and k_B is the Boltzmann constant, we find that there are indeed some numerical oscillations [16]. However, for $U/t = 4.0$ we find a well

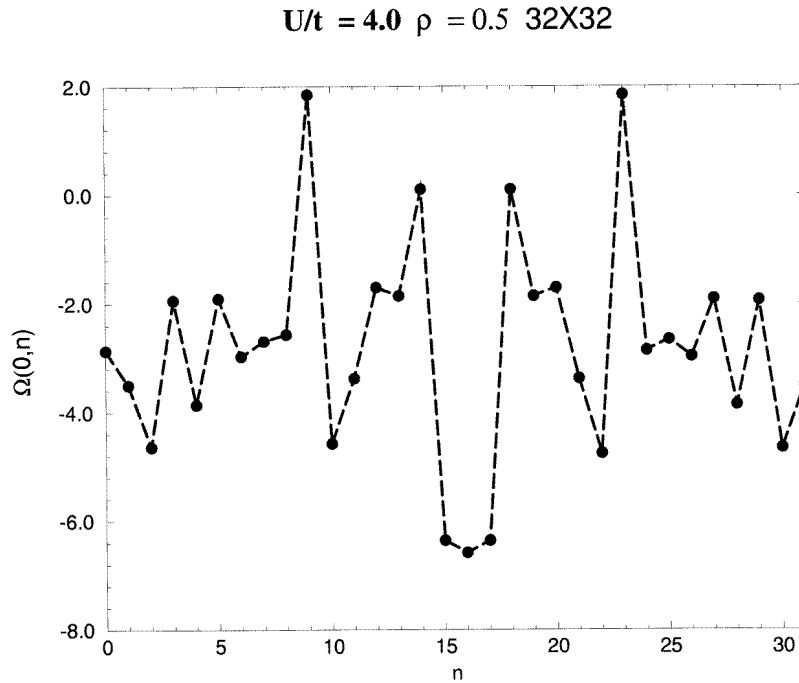


Figure 1. $\Omega_{0,n}$ versus n for $U/t = 4.0$ and $\rho = 0.5$. The k -vector is given by $k = \pi(0, n)/32$. As we work in two dimensions, the bandwidth is $W = 8t$. Compare with the case for $m = 0$ in figure 5, later.

behaved $n(k)$ which allows us to define a Fermi surface. For $U/t \geq 6.0$, the oscillations in $n(k)$ are bigger, which makes it difficult to define a Fermi surface. The spectral function, $A(k, \omega)$, is defined in equation (5).

We stress the fact that in our approach we have set out to generalize that of Nolting (without lifetime effects). Thus, we are working within the framework in which the two-pole structure is assumed to be due to a single-pole structure in the self-energy. However, in the calculation of Sunko and Barisić [17], the authors calculate the self-energy in the one-loop approximation, without vertex corrections. For the imaginary part of the susceptibility, they use a phenomenological expression. They find that their self-energy is not a single pole, especially when $\Gamma = 0$ (see reference [17] for details). Furthermore, the gap in our approach is due to correlations in the paramagnetic (PM) phase which, according to the published literature, happens to occur before the antiferromagnetic (AF) one. We have not studied this here, but it would be worth pursuing it further in order to allow a comparison with the correlation gap obtained from the AF fluctuations, like that carried out by Sunko and Barisić [17].

Even when our self-energy satisfies the Kramers–Kronig relations [18] (it is analytic in one of the complex planes), the self-energy does not have to satisfy the Kramers–Kronig relations [18, 19]. We have not studied the validity of the Luttinger theorem [20], which has been nicely discussed in reference [21]. However, we argue that the Luttinger theorem is not going to hold, because we have a non-Fermi-liquid system [16]. We can also argue that our bold choice of the self-energy (equation (2)) is valid for frequencies that are not too close to the chemical potential. The *ansatz* given as equation (2) is based on the fact

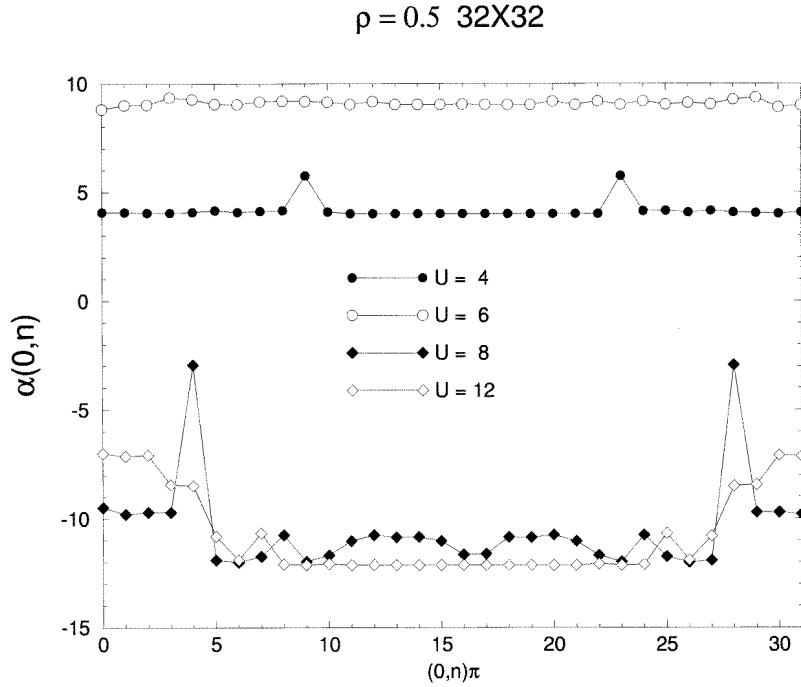


Figure 2. $\alpha(0, n)$ versus n for different values of U/t . The parameters are the same as for figure 1.

that previous authors [22] have proved that, in the absence of lifetime effects, i.e., for $\Gamma(\mathbf{k}) \equiv 0$, the self-energy has the form given by equation (2). In consequence, equation (2) is a generalization. In reference [22], we state that our *ansatz* puts on a firm footing the predictions made in one of our previous papers [15].

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

$$G(\mathbf{k}, \omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)} \quad (4)$$

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

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \lim_{\delta \rightarrow 0^+} \text{Im} G(\mathbf{k}, \omega + i\delta). \quad (5)$$

Using equations (2)–(5), we arrive at the following expression for the spectral density:

$$A(\mathbf{k}, \omega) = \frac{-1}{\pi} \frac{\alpha(\mathbf{k})\Gamma(\mathbf{k})}{((\omega - \varepsilon_{\mathbf{k}})(\omega - \Omega_{\mathbf{k}}) - \alpha(\mathbf{k}))^2 + \Gamma^2(\mathbf{k})(\omega - \varepsilon_{\mathbf{k}})^2}. \quad (6)$$

Using the first three sum rules of Nolting [1] for the spectral function of equation (5),

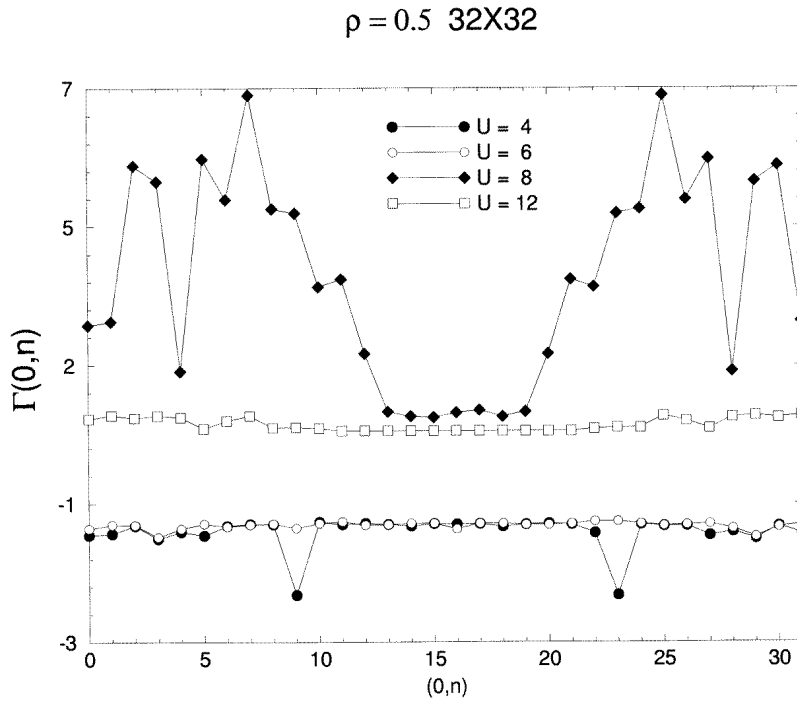


Figure 3. $\Gamma(0, n)$ versus n for different values of U/t . The parameters are the same as for figure 1.

we obtain the following equations:

$$\begin{aligned}
 \int_{-\infty}^{+\infty} A(\mathbf{k}, \omega) \, d\omega &= a_0(\mathbf{k}) \\
 \int_{-\infty}^{+\infty} \omega A(\mathbf{k}, \omega) \, d\omega &= a_1(\mathbf{k}) \\
 \int_{-\infty}^{+\infty} \omega^2 A(\mathbf{k}, \omega) \, d\omega &= a_2(\mathbf{k})
 \end{aligned}
 \tag{7}$$

where the $a_i(\mathbf{k})$, $i = 0, 2$, are given in reference [1] (see also reference [15]). We do not use the fourth moment because we have only three \mathbf{k} -dependent unknown parameters to evaluate. (This is one difference between our approach and that of Nolting, since he starts with the one-particle spectral function, with the result that four parameters have to be evaluated.) Then, we assume that, at $\rho = 1/2$, the chemical potential $\mu = U/2$. This is correct, as we will see from our results. At this point, we would like to reiterate that the drawback of previous calculations (including ours) consists in the density of states which results from the two-pole *ansatz* for the one-particle Green function, in the spherical approximation of Nolting [1], always having a gap. This solution (always a gap) is known in the literature as the Hubbard-I solution [23] which was first criticized many years ago by Roth [24] among others. We call attention to reference [25], where the authors point out the fact that the \mathbf{k} -dependence has to be included in $B(\mathbf{k})$. However, they study the negative Hubbard model in the strong-coupling limit, and in this limit we have a well developed correlation gap, anyway. Oleś and co-workers are advocates of using the two-pole *ansatz*

U/t = 4.0 32X32

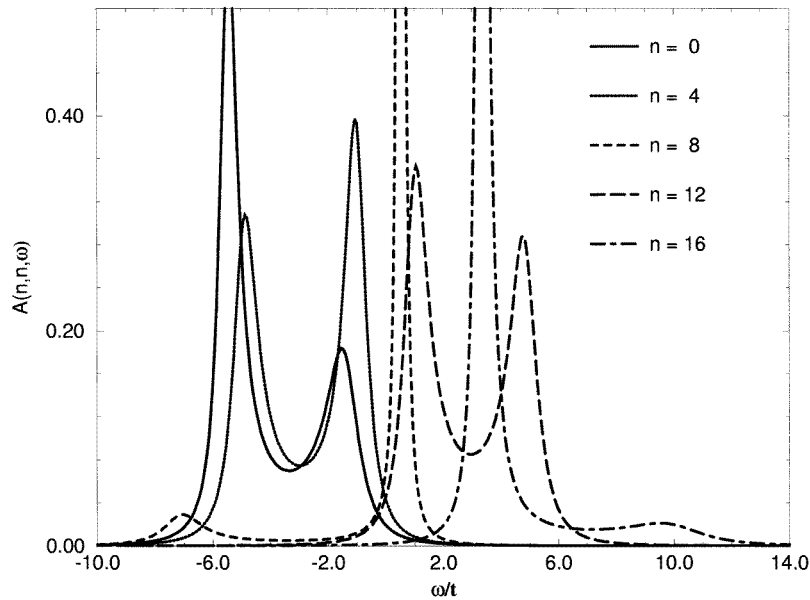


Figure 4. The spectral density, $A(n, n, \omega)$, versus ω for $U/t = 4.0$.

for the one-particle Green function, without lifetime effects. Here, we are including lifetime effects as a crucial ingredient in the formulation. Moreover, our results clearly show that the resolution to the problems inherent in the Hubbard-I solution in the moment approach does not lie in the $B(\mathbf{k})$ -term.

In figure 1 we present the *energy spectrum* of the self-energy for several points in the Brillouin zone, for $U/t = 4$. In figure 2 we show the \mathbf{k} -dependence of $\alpha(\mathbf{k})$ for $U/t = 4, 6, 8, 12$. In figure 3 we present the \mathbf{k} -dependence of $\Gamma(\mathbf{k})$ for several points in the Brillouin zone, for $U/t = 4, 6, 8, 12$. Figure 4 shows the spectral density, $A(\mathbf{k}, \omega)$, versus ω along the diagonal of the Brillouin zone for $U/t = 4.0$. In figure 5 we show the density of states, $N(\omega)$, versus ω . $N(\omega)$ is defined as

$$N(\omega) = \frac{1}{N_s} \sum_{\mathbf{k}} A(\mathbf{k}, \omega). \quad (8)$$

In all of the figures, we have worked with a square lattice with the periodicity of $N_s = 32 \times 32$. We conclude that the *spectral weight*, $\alpha(\mathbf{k})$, and the damping factor, $\Gamma(\mathbf{k})$, do not depend strongly on \mathbf{k} , for small values of U/W . For example, for $U/t = 4.0$, $\Gamma(\mathbf{k})/t \approx 1.5$. However, for larger values of U/W , $\alpha(\mathbf{k})$ has some \mathbf{k} -dependence. In contrast, $\Gamma(\mathbf{k})$ shows a stronger \mathbf{k} -dependence for larger values of U/W . We also note that $\alpha(\mathbf{k})\Gamma(\mathbf{k}) < 0$ if we are to obtain a positive spectral density (see equation (6)), as is shown in figure 4. We see that the spectral density is always positive, and that it has two peaks for every value of the momentum. This is a signature of a strongly correlated system. In contrast, the two-particle spectral function can be negative for certain values of the frequency, a fact known from the literature [26]. Taking a look at the density of states, $N(\omega)$, versus ω , we see that the correlation gap opens up for $U/W \geq 1.0$. This is

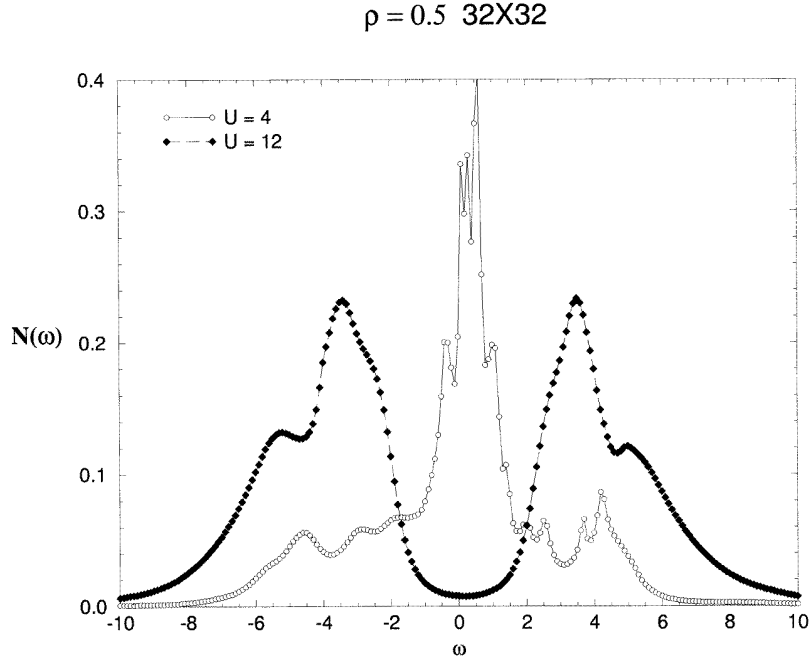


Figure 5. $N(\omega)$ versus ω for $U/t = 4, 12$. We see the opening of the correlation gap for $U/W \geq 1.0$, signalling the Mott metal–insulator transition.

equivalent to the Hubbard-III-like solution [27]. Due to our choice of self-energy, we do not have a Fermi liquid [8, 27]. Edwards and Hertz [28] have studied the breakdown of Fermi-liquid theory in the Hubbard model at $T = 0$. They have drawn a phase boundary between a Fermi liquid and a non-Fermi liquid (ρ versus U in the paramagnetic phase). According to these authors, for small values of U we have a Fermi-liquid behaviour (a metallic Fermi liquid), and for larger values of U we have a non-Fermi-liquid metal. In our approach we have a non-Fermi-liquid behaviour for any strength of the interaction. In order to obtain agreement with reference [28], we have to include an ω^2 -behaviour for frequencies close to the chemical potential in addition to the single-pole structure chosen in the present work. A transition from a metallic Fermi-liquid behaviour to a metallic non-Fermi-liquid behaviour has been obtained by Figueira, Anda and Nogueira [29]. We should mention that the phase diagram of the Hubbard model contains an antiferromagnetic transition [30], which has not been considered here. In our model, even when $-\text{Im}[\Sigma(\mathbf{k}, \omega)] \neq 0$ at the Fermi surface, we have a metal for small values of U/W , since the correlation gap opens up for $U/W \geq 1.0$.

In short, we have postulated a one-pole *ansatz* for the self-energy (equation (2)) in the moment approach of Nolting [1]. Our essential new working idea with respect to the now canonical method of Nolting is that we start from the self-energy while Nolting proposes using a two-pole *ansatz* for the one-particle Green function from the outset. In both approaches, sum rules for the spectral function, $A(\mathbf{k}, \omega)$, are imposed. As a function of the interaction, we see a Mott metal–insulator transition (MMIT) from a metal for weak interaction (no gap at zero frequency) to a well developed gap (an insulator) for large values of the local interaction [2]. Our formulation is not equivalent to the infinite-dimension calculation of Georges *et al* [31], since we have included the \mathbf{k} -dependence of the self-

$U/t = 4.0 \quad \rho = 0.5 \quad 10 \times 10$

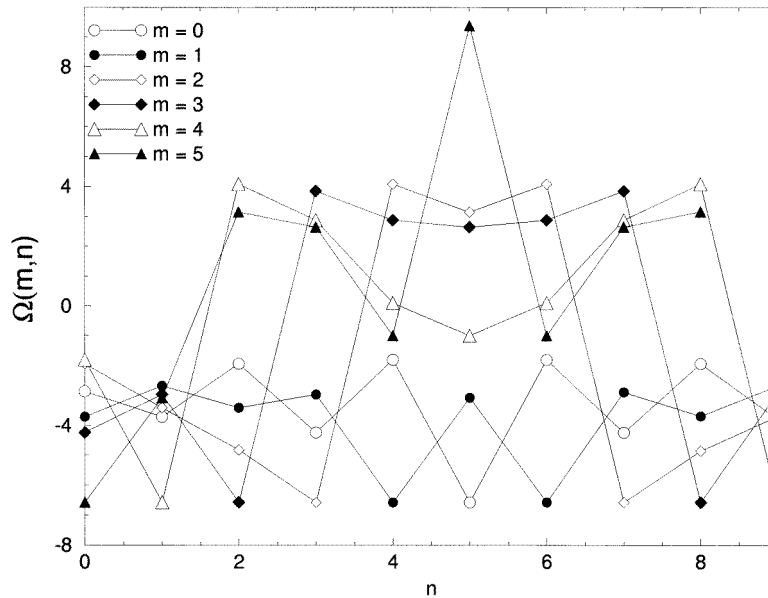


Figure 6. $\Omega(m, n)$ versus n for some fixed values of m . $U/t = 4.0$, $\rho = 0.5$, and our mesh is 10×10 . Compare the case for $m = 0$ with figure 1.

energy (we are working in two dimensions). There is a calculation by Figueira, Anda and Nogueira [29] where the authors have also neglected the \mathbf{k} -dependence of $\Sigma(\mathbf{k}, \omega)$. In particular, the authors of references [29, 31] find a Kondo peak at $\omega = 0$. In our case, with $\rho = 1/2$, the peak-like structure seen at the chemical potential is most probably due to the van Hove logarithmic singularity which always goes away with the opening of the correlation gap. With our precision [32], we cannot reach a conclusion as to whether the Kondo peak is present or not. Nolting himself [33] has also studied the effect of damping on magnetism. We leave for the future a comparison with reference [34], where the authors discuss the use of the moment approach for interpolating $\Sigma(\mathbf{k}, \omega)$ between weak and strong interaction. We include figure 6 to present $\Omega(m, n)$ versus n for fixed values of m , for $U/t = 4.0$ and a 10×10 mesh. It is worth looking at the band structure for $m = 0$. This curve has almost the same structure as the band structure shown in figure 1, for a bigger mesh (32×32). Thus, we can say that finite-size effects are minimal at least as regards the band-structure calculations. (See the discussion in reference [32].) Finally, we would like to say that the non-Fermi-liquid behaviour that we have in our approach (by construction) has nothing to do with any microscopic mechanism. Our arguments rely on general grounds, on a self-energy *ansatz* which is used in the one-particle Green function on which exact sum rules (moments) are imposed. Those interested in the physical mechanisms of non-Fermi-liquid behaviour are encouraged to look at the nice account presented in Anderson's book [35]. We also call attention to the work carried out by Kirchhofer [36], who has used the moment approach of Nolting beyond his spherical approximation, using a mean-field analysis. He finds that there is a metal-insulator transition for the repulsive Hubbard model for nearest- and next-nearest-neighbour hopping integrals.

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