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Metallic states in the Hubbard model at half-filling

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Abstract. Using second-order perturbation theory in U for the self-energy, we solve the self-consistent equations for the local Green function of the infinite-dimensional Hubbard model. We consider the cases of Gaussian and semicircular free densities of states (DOS), and calculate the spectral densities $\rho(\omega)$ for various U. In the semicircular case we investigate the existence of a Mott transition at half-filling. Even for large U we obtain a metallic solution. Treating the free DOS as a variable parameter, the method also gives an approximate solution of the finite-dimensional Hubbard model. We consider the case of a (regularized) logarithmic DOS appropriate for the two-dimensional case.

1. Introduction

The theory of systems of correlated fermions on a lattice is greatly simplified in the limit of high dimensions. At least in the weak-coupling limit, essential features such as the correlation energy of systems in three and even lower dimensions are thought to be well described by the results obtained in the infinite-dimensional (d^∞) limit. The d^∞ limit of the Hubbard model was first introduced by Metzner and Vollhardt [1, 2] and developed later by Müller-Hartmann [3, 9].

More recently [4], Georges and Kotliar presented an exact mapping of the Hubbard model in infinite dimensions onto a single-Anderson-impurity (or Wolff) model supplemented by a self-consistency condition. This provides a mean-field picture of strongly correlated systems, which becomes exact as $d \to \infty$.

In this paper, we develop the method from [4] and we use it in the cases of Gaussian, semicircular and logarithmic free densities of states (DOS), calculating the spectral density for various values of U. Three independent groups [5, 8, 9, 10] have found a Mott transition for large enough U for the case of the semicircular free DOS. The Green function Monte Carlo (GFMC) calculations suggest that the system is a Mott insulator at finite temperature [5]. Caffarel and Krauth [6] have developed a method for solving the mean-field equations by mapping them onto an impurity coupled to a finite number of conduction band states and solving the model exactly and self-consistently. They find that the insulating state is stable at $T = 0$ for $U > \sim 4.6$. Rozenberg *et al* [7, 11] find evidence for two critical values of the interaction. For $U < U_{c1}$ there is only a metallic solution to the mean-field equations. For $U_{c1} < U < U_{c2}$ there are both the metallic and insulating self-consistent solutions to the mean-field equations. For $U > U_{c2}$, they found that only the insulating state is stable. They estimate that $U_{c2} \sim 2.8$ [7] partly on the basis of perturbation theory and more recently $U_{c2} \sim 3.37$ [11].

Our work is motivated by the claim that a Mott transition occurs in second-order perturbation theory at $T = 0$. We track the metallic solution of the mean-field equations as

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a function of the interaction U, using second-order perturbation theory. We find that there is a self-consistent metallic solution for larger values of U than in [5, 8], although it is numerically hard to find.

We also suggest a possible reason for the discrepancy between our results and those of [8]. In [8] it was claimed that QMC at a temperature $T = \frac{1}{64}$ should reproduce all the features expected for $T = 0$. The problem is that at large U there is a low-energy scale associated with the width of the central quasiparticle peak in the metallic state which can be smaller than $T = \frac{1}{64}$. The energy scale set by the width of the central peak sets a temperature scale over which the entropy associated with the spin degrees of freedom is quenched. (Because the ground state is assumed homogeneous in spin and space, possible magnetically ordered states have not been considered.)

In the more recent article [11], the authors present an intuitively appealing scaling argument (see also [5]) to suggest that the metallic solution must become unstable once the central peak becomes too narrow. On the basis of this and the numerical solution of the self-consistent equations they estimate $U_{c2} \sim 3.4$. Our results are not consistent with this particular estimate for U_{c2}. We discuss possible origins for this discrepancy.

The method developed for infinite dimensions can be used to devise approximations in the finite-dimensional case and we consider the logarithmic DOS thought by some to be appropriate for the quasi-two-dimensional superconductors.

2. Hubbard model in infinite dimensions

The well known single-band Hubbard model Hamiltonian is given by

$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{HC}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} \tag{1}$$

where t_{ij} is the hopping integral, U is the Coulomb repulsion, $c^{\dagger}_{i\sigma}$, $c_{j\sigma}$ are the creation and annihilation operators, respectively and $n_{i\uparrow}$, $n_{i\downarrow}$ are the occupation numbers.

In the limit $d \to \infty$, the Hamiltonian parameters have to be scaled to keep both the kinetic and potential energy per site finite and the scaling depends on the nature of the lattice.

The self-energy Σ is defined from the interacting single-electron Green function $G(k, \omega)$ by

$$G(k,\omega) = [\omega - \epsilon(k) - \Sigma(\omega) + \epsilon_{\text{F}}]^{-1}. \tag{2}$$

For the Hubbard model at infinite dimensions Σ is independent of momentum (this follows from the irrelevance of momentum conservation at the vertices of skeleton diagrams), and depends only on frequency [1, 9].

In a Fermi liquid the self-energy $\Sigma(\omega)$ as $\omega \to 0$ determines the usual mass renormalization and lifetime effects with

$$\text{Im}\,\Sigma(\omega) = \text{O}(\omega^2) \qquad (\omega \to 0). \tag{3}$$

ϵ_{F} in (2) represents the chemical potential μ and is defined by

$$\epsilon_{\text{F}} = \epsilon^0_{\text{F}} + \Sigma(0) \tag{4}$$

(ϵ^0_{F} is the Fermi energy fixed by the particle density n).

To determine Σ we consider an auxiliary impurity problem (as in [4]) with the single-site action

$$S = U\int_0^{\beta} \text{d}\tau\, n_{\uparrow}(\tau)n_{\downarrow}(\tau) - \int_0^{\beta}\text{d}\tau\int_0^{\beta}\text{d}\tau' \sum_{\sigma} c^{\dagger}_{\sigma}(\tau)G_0^{-1}(\tau-\tau')c_{\sigma}(\tau') \tag{5}$$

where G_0 is the 'bare' Green function of this local dynamics. G_0 does not coincide with the non-interacting site-diagonal Green function of the Hubbard model (except for $U = 0$); in the atomic limit for example, $G_0 = 1/(\omega + \epsilon_F)$.

It is possible to think of S as the action from a model describing a single fermion c_σ hybridized with a conduction band $a_{k\sigma}$ (Anderson model):

$$H_{AM} = \sum_{k\sigma} E_k a^\dagger_{k\sigma} a_{k\sigma} + \epsilon_d \sum_\sigma c^\dagger_\sigma c_\sigma + U n_{c\uparrow} n_{c\downarrow} + \sum_{k\sigma} [V_k a^\dagger_{k\sigma} c_\sigma + \text{HC}]. \quad (6)$$

The dynamics for c_σ is identical to (5) with

$$G_0^{AM}(\omega)^{-1} = \omega - \epsilon_d - \int_{-\infty}^{\infty} d\epsilon \frac{\Delta(\epsilon)}{\omega - \epsilon} \quad (7)$$

where $\Delta(\epsilon) = \sum_k V_k^2 \delta(\epsilon - E_k)$ is a combined measure of the hybridization and of the density of states of the conduction electrons. However, it may be more natural in the present context to view (5) as describing a Wolff model (i.e., a free lattice gas with a local Green function G_0 and U acting on a single site) [10]:

$$H_{WM} = \sum_{k\sigma} E_k c^\dagger_{k\sigma} c_{k\sigma} + U n_{0\uparrow} n_{0\downarrow} \quad (8)$$

then

$$G_0^{WM}(\omega) = \int_{-\infty}^{\infty} d\epsilon \frac{\Delta(\epsilon)}{\omega - \epsilon} \quad (9)$$

where $\Delta(\epsilon) = \sum_k \delta(\epsilon - E_k)$. The second formulation clearly emphasizes the reduction of the infinite-dimensional Hubbard model to a self-consistent single-site Hubbard model. This can be considered as a natural formulation of mean-field theory for lattice fermion models.

The impurity problem has a self-energy $\Sigma_{imp}[G_0, \omega]$ defined from the interacting Green function $G(\omega)$ by

$$G(\omega) = [G_0^{-1} - \Sigma_{imp}]^{-1}. \quad (10)$$

The mean-field equations require that the site diagonal Green function of the Hubbard model (equal to the sum of $G(k, \omega)$ over momenta if the system is homogeneous) actually coincides with (10):

$$G(\omega - i\eta) = \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{\omega + \epsilon_F - \epsilon - \Sigma(\omega - i\eta) - \epsilon_F^0 - i\eta} \quad (11)$$

with $\Sigma = \Sigma_{imp}(\omega)$ and $\epsilon = \epsilon(k) - \epsilon_F^0$. Notice that the nature of the lattice enters into the mean-field equations (5,10,11) via the density of states $D(\epsilon)$ only.

Treating $D(\epsilon)$ as a variable parameter, we will consider the cases of (a) Gaussian DOS; (b) semicircular DOS; (c) logarithmic DOS.

3. Method

We have solved (5), (10) and (11) using second-order perturbation theory at $T = 0$ for the single-site dynamics (5).

It has been shown by Yosida and Yamada [12] that perturbation theory in U is quite well behaved for the Anderson model, provided that the expansion is made around the non-magnetic Hartree–Fock solution. Thus, following the idea from [4], we use the modified 'Hartree–Fock' propagators $G_{HF}^{-1} = G_0^{-1} - Un/2$, to calculate the second-order correction $\Sigma^{(2)}$ and write $\Sigma = Un/2 + \Sigma^{(2)}$.

The imaginary part of $\Sigma^{(2)}$ is given by

$$\sigma(\omega) = \frac{\operatorname{Im}\Sigma^{(2)}(\omega - i\eta)}{\pi} = U^2 \int_0^{\omega} d\mu\, \rho(\mu - \omega) \int_0^{\mu} d\nu\, \rho(\nu)\rho(\mu - \nu) \quad (12)$$

where the spectral density $\rho(\omega)$ is $\rho_{HF} = (\operatorname{Im} G_{HF})/\pi$. The real part of $\Sigma^{(2)}$ is obtained from the Kramers–Kronig relation:

$$\operatorname{Re}\Sigma^{(2)}(\omega) = P \int_{-\infty}^{\infty} d\mu\, \frac{\sigma(\mu)}{\omega - \mu}. \quad (13)$$

Using the technique of Laplace transforms from [3], which makes the numerical solution of the problem more efficient, we define

$$\tilde{\rho_{\pm}}(t) = \int_0^{\infty} \rho(\pm\omega) \exp(-i\omega t)\, d\omega \quad (14)$$

and

$$\tilde{\sigma_{\pm}}(t) = \int_0^{\infty} \sigma(\pm\omega) \exp(-i\omega t)\, d\omega \quad (15)$$

of the particle and hole parts of ρ and σ. Using these, (12) transforms to

$$\tilde{\sigma_{\pm}}(t) = U^2 \tilde{\rho_{+}}(t)\tilde{\rho_{-}}(t)\tilde{\rho_{\pm}}(t) \quad (16)$$

which gives a description of the time evolution of a particle via the creation of a particle–hole pair. Inverting the Laplace transform (15) and using the relation

$$\Sigma^{(2)}(\omega - i\eta) = \int_{-\infty}^{\infty} \frac{\sigma(\mu)}{\omega - \mu - i\eta}\, d\mu \quad (17)$$

we finally get

$$\Sigma^{(2)}(\omega - i\eta) = i \int_0^{\infty} dt\, [\sigma_{+}(-t) + \sigma_{-}(t)] \exp(-i\omega t) \quad (18)$$

that is

$$\Sigma^{(2)}(\omega - i\eta) = \operatorname{Re}\Sigma^{(2)}(\omega) + i \operatorname{Im}\Sigma^{(2)}(\omega). \quad (19)$$

We used (18) to calculate $\Sigma^{(2)}$ and Σ. The integration in (14) and (18) can be reduced to an appropriate finite energy and time interval, respectively.

The self-energy Σ is then used in (11) to find G and define an alternative G_0 from $G_0^{-1} = G^{-1} + \Sigma$ which will establish a new G'_{HF}. We then take a weighted average of the spectral densities corresponding to G_{HF} and G'_{HF}, i.e.

$$\rho''_{HF} = \frac{1}{\pi}(\alpha \operatorname{Im} G_{HF} + \beta \operatorname{Im} G'_{HF}) \quad (20)$$

with $\alpha + \beta = 1$, and use this to recalculate $\Sigma^{(2)}$. The process is then iterated until convergence is reached. There is a tendency to drift from the convergence path. The process described above cured this by choosing β small. During the iteration process the total number of particles remains constant.

4. Results

The three cases considered are explored in the following sections.

4.1. Gaussian DOS

In the case of a hypercubic lattice, the free DOS takes the Gaussian form:

$$D(\epsilon) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(\epsilon + \epsilon_F^0)^2}{2}\right). \tag{21}$$

When U is very small, $\rho(\omega) = D(\omega)$ in (12) and $\sigma(\omega)$ becomes

$$\sigma(\omega) = U^2 \frac{1}{2^{3/2}\pi} \exp\left[-\frac{(\omega + \epsilon_F^0)^2}{6}\right] \times \int_0^\omega d\mu \exp\left(-\left[\frac{\sqrt{3}}{2}(\mu + 2\epsilon_F^0) - \frac{\omega + \epsilon_F^0}{\sqrt{3}}\right]^2\right) \operatorname{erf}\left(\frac{\mu}{2}\right). \tag{22}$$

We find that the real and imaginary parts of the infinitesimal self-energy, $\frac{1}{2}[d^2\Sigma(\omega - i\eta)/dU^2]|_{U=0}$, are in good agreement with the results from [3]. The imaginary part shows the quasi particle property (3) for small energies. The real part contains information about the shift of the Fermi energy (4).

For larger U, the spectral density of states $\rho(\omega)$ is replaced by $\rho_{HF}(\omega)$ in (12) and we use the technique described in the previous section. The results obtained for $\rho(\omega)$ for $U = 2.5\sqrt{2}$, $n = 0.6$ and $U = 2.5\sqrt{2}$, $n = 1$ are in good agreement with the results from [4]. (As pointed out in [4], these results differ considerably from those of [3], in which a single-peaked structure is always found.) We find that $\rho(\omega)$ has the three-peaked structure expected for $n = 1$. The close agreement of our results with the results from [4] suggested that we consider the cases of the semicircular free DOS and logarithmic free DOS where the method has not yet been applied.

4.2. Semicircular DOS

In the case of the Bethe lattice (tree lattice in infinite dimensions), the free DOS has the semicircular form:

$$D(\epsilon) = \frac{2}{D\pi}\sqrt{1 - \left(\frac{\epsilon}{D}\right)^2} \tag{23}$$

where Hubbard's hopping parameter $t = D/2$. We take $D = 1$. The local Green function integral (11) can be solved analytically and we obtain

$$G(\omega - i\eta) = \frac{2}{\omega - i\eta - \Sigma + U/2 + \sqrt{(\omega - i\eta - \Sigma + U/2)^2 - D^2}} \tag{24}$$

for half-filling, where $\epsilon_F = U/2$ and $\eta = 10^{-6}$.

This leads to a simpler computation than for the Gaussian DOS and for half-filling we obtain similar results for the spectral density $\rho(\omega)$. We investigate the existence of a Mott transition at half-filling, but even for large U we obtain a resonant peak in the spectral density $\rho(\omega)$ (narrower for larger U) at $\omega = 0$. We present the results for $U = 3$ at half-filling in figure 1. We have also computed $\rho(\omega)$ for the case $U = 4$. They are different from those in [8] where perturbation theory at finite temperature was used. Using perturbation theory at finite T ($= \frac{1}{64}$) or QMC at the same temperature, everything which occurs on any energy scale smaller than T will not be resolved. This is the case of the central peak for $U > 3.6$. We have calculated Im $\Sigma(0)$ and a few values of Im $\Sigma(\omega)$. We find that Im $\Sigma(\omega)$ is very large close to $\omega = 0$ for large U, but for $\omega = 0$, it is always zero to within computational accuracy, so that we still have a Fermi liquid.

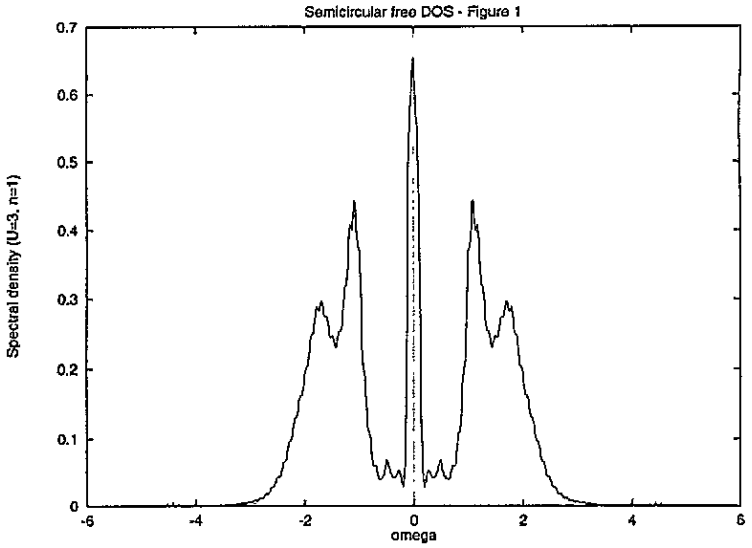

Figure 1. The spectral density $\rho(\omega)$ for $U = 3$ and $n = 1$, for the case of the semicircular free DOS.

Similar results to those shown in figure 1 also appeared in [11] for the case $U = 2.9$. Although the results appear very similar we find more of the 'jagged' structure in the density of states. We find that this fine structure is sensitive to the choice of the parameter η in equation (24). Although it is quite easy to obtain converged solutions for large η ($\sim 10^{-2}$) the full structure only appears when η is chosen very small (we use $\eta \sim 10^{-6}$).

We note that at half-filling, the spectral density at the Fermi energy we obtain, is pinned at its value in the non-interacting system. This is the correct result, if the system is a Fermi liquid (i.e. the imaginary part of the self-energy at $\omega = 0$ becomes zero). This follows after setting $\omega = 0$ in equation (11), which gives:

$$G(0) = P\int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{\epsilon} + i\pi D(\epsilon_F - \mathrm{Re}\,\Sigma(0) - \epsilon_F^0). \tag{25}$$

Replacing the chemical potential ϵ_F defined by equation (4), the spectral density for $\omega = 0$ becomes:

$$\rho(0) = \frac{1}{\pi}\mathrm{Im}\,G(0) = D(0), \tag{26}$$

which does not depend on U. In particular, for the case of the semicircular free DOS, $\rho(0)$ is approximately equal to 0.636, which is precisely the value we obtain after a large iterative calculation. The total number of particles remains constant during the iteration process in all cases.

In figure 2 we show how convergence is obtained for the relatively large value $U = 3$. Convergence is difficult to obtain if $U \geqslant \sim 2.8$, but is possible to obtain using the process described in Section 3, equation (20). However, since we have to choose β small, the number of iterations required is large. For example, in the case $U = 3$, we used $\beta = 0.01$. The iteration process is stable close to the self-consistent solution in the sense that $\epsilon_{\mathrm{It}}(\omega) = |\rho_{\mathrm{HF(It)}}(\omega) - \rho_{\mathrm{HF(It)}}(\omega)|$ vanishes for all ω once the iteration number It is large enough. We always start (It $= -1$) from the non-interacting ($U = 0$) ground state (using ρ_{HF}). In the early stages of the iterative procedure $\epsilon_{\mathrm{It}}(\omega)$ can increase with It for some ω; the procedure leads eventually to convergence (after 800 iterations for $U = 3$). In figure 3,

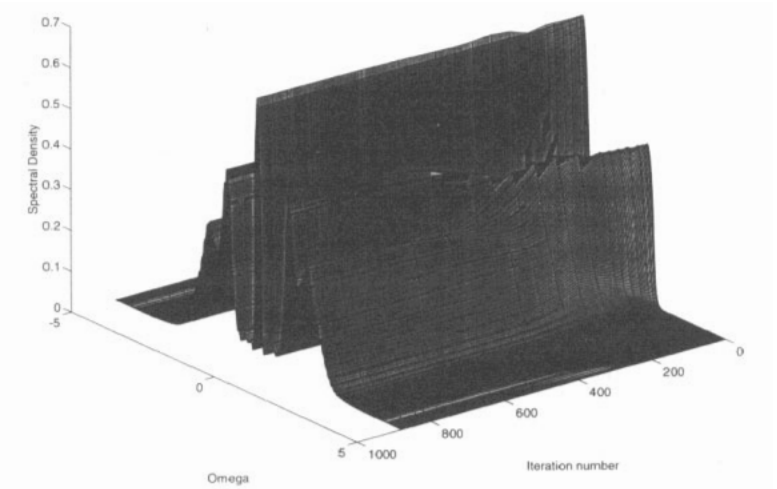

Figure 2. The evolution of the spectral density $\rho(\omega)$ as a function of the iteration number It, for $U = 3$ (semicircular free DOS). We used $\beta = 0.01$ (see equation 20). The lines on the surface which end up parallel to the iteration number axis once convergence has been found show how the value of ρ evolves for any given ω.

we show how convergence is obtained for $U = 6$. Again we start from the non-interacting DOS (at It $= -1$) using $\beta = 0.001$. The change in the form for ρ seen after 700 iterations occurs when we increase β to 0.01.

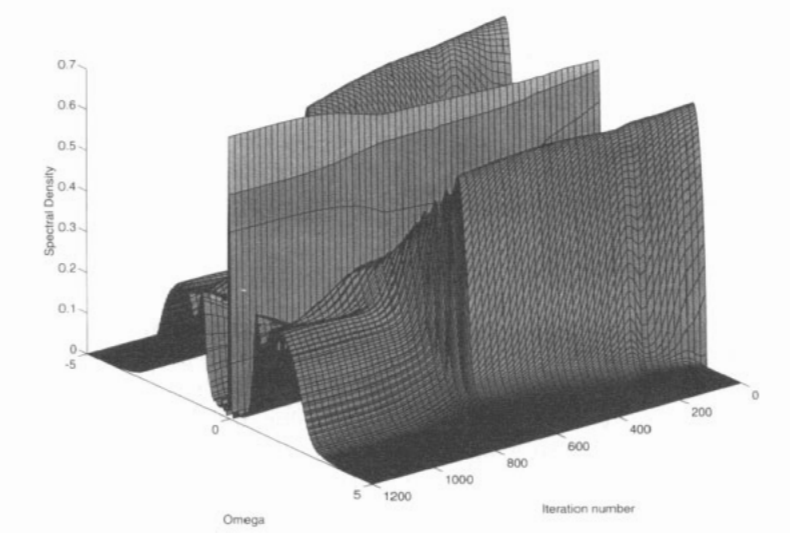

Figure 3. The same as figure 2 with $U = 6$ (semicircular free DOS). The change in the evolution of $\rho(\omega)$ seen at around It $= 700$ occurs when we increase β from 0.001 to 0.01.

In figure 4 we show how the width (FWHM) of the quasiparticle varies with U. We find that even for large U the width will not become zero as was claimed in [8]. For $2.5 < U < 2.75$, there is a plateau, which may explain the suggestion of the critical value $U_{c2} \sim 2.8$.

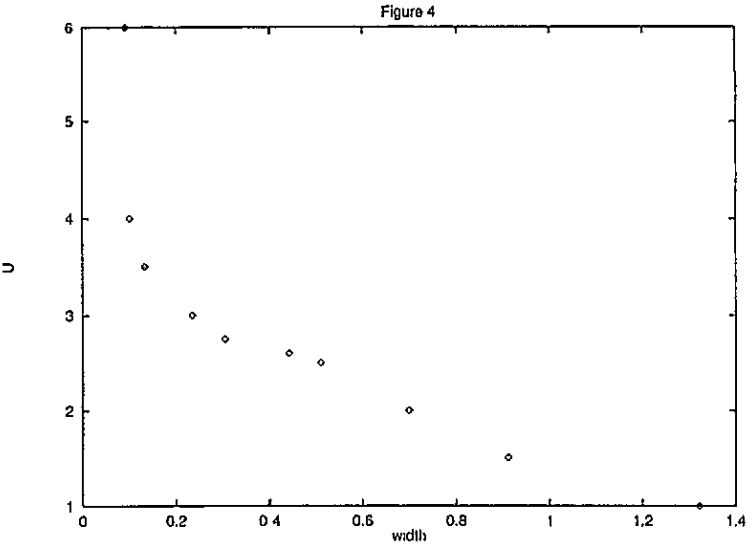

Figure 4. U versus the width (FWHM) of the quasiparticle peak for the semicircular free DOS.

Although the self-consistent solution is hard to pin down, we find that it is there even for large U. As pointed out in [7], the insulating state can also exist as a self-consistent solution for $U > U_{c1} \sim 2.7$ and has an energy very close to that of the metallic solution. This would explain why the metallic solution is numerically hard to find. We believe that it could also explain why different methods [6] find that the insulating solution stabilizes at different values of U.

In [11] it was suggested that in the limit of a very narrow central peak in $\rho(\omega)$, then $G_0(\omega)$ would be dominated by poles at characteristic frequencies $\pm\omega_0$, related to the central peak width of $\rho(\omega)$ and to U. Provided $\omega_0 \gg \Delta$, where Δ $(= (1 - \mathrm{d}\Sigma/\mathrm{d}\omega)^{-1})$ is a measure of the width of the quasiparticle peak, then the Green function can be parametrized using a (universal) function to describe the low-energy scale spectrum and an incoherent part. This parametrization can be used to estimate the critical value U_{c2} at which a metallic solution might collapse. It leads to the estimate $U_{c2} \sim 3.3$, whereas we find a metallic solution for $U > 3.4$. We have looked at our solution to see why this argument might break down. It can be seen in figures 1–3 (and in fact already in figure 2 of [11]) that the spectrum does not completely separate into a low-energy and a high-energy part. There is always spectral weight between the central peak and the incoherent peaks at $\sim U/2$. We can also see this in the spectral weight of the 'mean-field' G_0 or the 'Hartree–Fock' spectral density of states ρ_{HF} (see figure 5). This is (as expected) dominated by a pole at a characteristic frequency ω_0 but there is also a significant peak appearing at lower energies. The simple parametrization of G used in [11] does not account for this second peak in the spectral function for G_0, although we do not have an explanation of why not.

4.3. Logarithmic DOS

The method used in the Gaussian and semicircular cases gives an approximate solution of the finite-dimensional Hubbard model. We consider the case of a (regularized) logarithmic DOS appropriate for the two-dimensional case for parameters which may be relevant to high-T_c superconductors [13, 14].

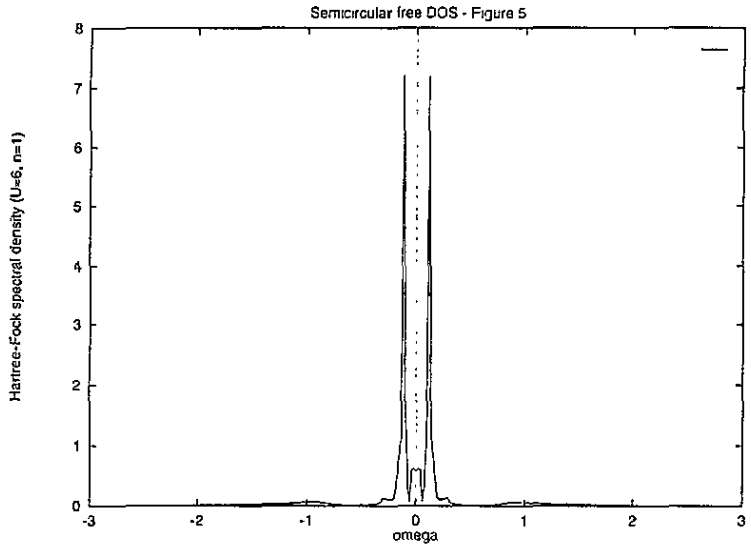

Figure 5. The 'Hartree–Fock' spectral density $\rho_{\mathrm{HF}}(\omega)$ for $U = 6$ and $n = 1$, in the case of the semicircular free DOS. It can be noticed that there is not only one pole at ω_0. There is also a peak appearing at lower energies.

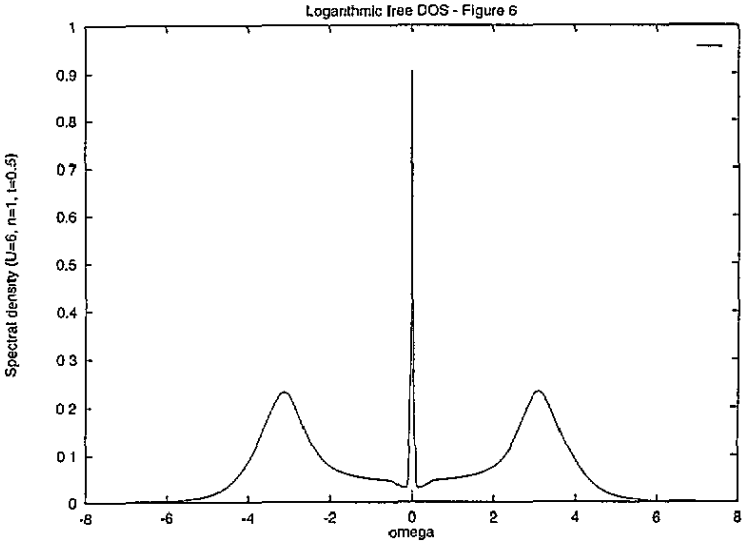

Figure 6. The spectral density $\rho(\omega)$ for $U = 6$, $n = 1$ and $t = 0.5$, in the case of the logarithmic free DOS.

For $n = 1$, around midband, the free density of states ($U = 0$) takes the form [15]

$$\rho_0(\epsilon) = \frac{1}{\pi^2 t}\left[1 - \frac{1}{4}\log\frac{\epsilon^2}{16t^2}\right] \tag{27}$$

per Cu atom and per spin in the case of some cuprates for the tetragonal phase, where

$$\epsilon = -2t(\cos k_x a + \cos k_y b) \tag{28}$$

a, b are lattice parameters and t is the transfer integral in plane.

The van Hove singularity in $\rho_0(\epsilon)$ is broadened in the case of the cuprates because of the transverse coupling between planes and impurity scattering [16]. Around midband the logarithmic term will dominate. We assume for $\rho_0(\epsilon)$

$$\rho_0(\epsilon) = -\frac{2.4674}{4t\pi^2} \log \frac{\epsilon^2 + \Lambda^2}{16t^2} \qquad -4t < \epsilon < 4t. \tag{29}$$

$\rho_0(\epsilon)$ is normalized to conserve the total number of states and $\Lambda \sim 4 \times 10^{-2}t$ [16].

In order to compare the results obtained for the logarithmic DOS with those of the semicircular DOS at any given U we choose t so that the second moments

$$\sigma^2 = \left(\int \rho_0(\epsilon)\epsilon^2 \, \mathrm{d}\epsilon \right) \Big/ \int \rho_0(\epsilon) \, \mathrm{d}\epsilon \tag{30}$$

are the same. For $U = 3$ this gives $t = 0.14$. We find that the spectral density $\rho(\epsilon)$ has a similar three-peaked structure to that shown in figure 1, although the peaks are sharper.

We have also considered the case $t = 0.5$ and $U = 6$ which, it has been claimed, may be appropriate for HTC superconductors [13, 14]. The results are shown in figure 6.

5. Conclusion

The method developed (at $T = 0$) in this paper, which is based on perturbation theory in U, finds similar behaviour for the spectral density for different free DOS.

In the case of the semicircular free DOS within the space of homogeneous (non-magnetically ordered or non-CDW) states, in perturbation theory at $T = 0$, a Mott transition does not occur even for U as large as six.

These results are different from previously published results [5, 8, 11]. We attribute the discrepancy to the fact that these treatments are for systems at finite temperatures and that extrapolation to $T = 0$ of these results was not applicable. We have also analysed the validity of the simple scaling argument given in [11]. We point out that the condition for the validity of this argument do not appear to hold when looking at our numerical results. In particular there is total separation of energy scales.

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