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LETTER TO THE EDITOR

Hubbard model for metal–non-metal transitions in high-T_c superconductors

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Abstract. It is found that in the paramagnetic phase of the Hubbard model, the electrons near the Fermi energy can become localised above a certain value of the ratio between the intra-atomic Coulomb interaction and the bandwidth of the non-interacting electrons. This localisation of electrons can give rise to a metal–non-metal transition in a nearly half-filled band as found in the paramagnetic phase of the high-T_c superconducting oxides.

Metals and non-metals are customarily differentiated in terms of the Wilson model (Wilson 1931) of non-interacting electrons. According to this model, if the valence and conduction bands are separated by an energy gap then the system behaves as a non-metal for the completely filled valence band with two valence electrons per lattice site. If the valence and conduction bands overlap or the number of valence or conduction electrons is different from two, it behaves as a metal. However, this model does not always work as first pointed out by de Boer and Verwey (1937) since nickel oxide, which is non-metal, should be metal according to this model because it has a half-filled valence band with one valence electron per lattice site. Mott (1949, 1969) and Hubbard (1963, 1964) tried to explain this behaviour by introducing the electron correlation into the problem. Hubbard showed that due to electron correlation, the valence band splits into two subbands separated by an energy gap for a large value of electron correlation. For one valence electron per lattice site, the lower band is completely filled and thus the system behaves as a non-metal. A transition from a non-metallic to a metallic state occurs when the band gap goes to zero as the electron correlation is reduced. This non-metallic state due to band splitting is also possible by lattice distortion (Peierls 1955) and by antiferromagnetic ordering (Slater 1951).

Thus it seems that one needs an energy gap in the density of states at the Fermi energy in order to have a non-metallic state. However, it is also possible to have an energy gap in the density of states at the Fermi energy and still have a metallic state as happens in the BCS model (Bardeen *et al* 1957) of superconductivity. Also, strong disorder (Anderson 1958) can lead to a non-metallic state by producing localised states at the Fermi energy instead of creating an energy gap. Wigner (1938) suggested that for a low-density of free electrons in a uniform background of positive charges, electron–electron interactions can produce non-metallic states by localising the electrons into a crystalline lattice.

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Recently it has been discovered (Sleiglet 1988, Pickett 1989) that in the paramagnetic phase the nearly half-filled band systems of high-T_c superconducting oxides make a transition from a non-metallic to a metallic state as the number of electrons or holes per lattice site is changed from unity to some critical value. Since the discovery of these high-T_c superconductors (Bednorz and Müller 1986) there has been a lot of theoretical interest in the nearly half-filled band Hubbard model in order to understand the superconductivity mechanism in these materials (Anderson 1987, Hirsh 1987). The Hubbard model was also used to study the antiferromagnetic ordering (Kaxiras and Manousakis 1988, Krasnitz *et al* 1989) of these materials. The aim of this paper is to study the nearly half-filled band Hubbard model in order to understand the metal–non-metal transition in the paramagnetic phase.

The Hubbard model is described by the Hamiltonian (Hubbard 1963)

$$H = \sum_{ij\sigma} \varepsilon_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{1}$$

where $a_{i\sigma}^{\dagger}$, $a_{i\sigma}$ and $n_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma}$ are respectively the creation and annihilation, and number operators of an electron of spin σ at the lattice site i; ε_{ij} is the transfer integral and U is the intra-atomic Coulomb interaction.

The quasi-particle spectrum of the Hamiltonian (1) can be obtained from the poles of the single-particle Green function

$$G_{\sigma}(k, \omega) = 1/(\omega - \varepsilon_k - M_{\sigma}(k, \omega)) \tag{2}$$

where $M_{\sigma}(k, \omega)$ is the quasi-particle self-energy of the interacting electrons, and the band energy of the bare electrons, ε_k, is given by the Fourier transform of the transfer integral

$$\varepsilon_{ij} = \frac{1}{N} \sum_{k} \varepsilon_k \exp[\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{R}_i - \boldsymbol{R}_j)]. \tag{3}$$

Here, N is the total number of lattice sites.

Recently, the self-energy $M_{\sigma}(k, \omega)$ has been obtained by Kishore (1987) by using a semiclassical approximation which gives the exact results for the quasi-particle spectrum in both weak- and strong-correlation regimes which correspond to $U/\Delta \ll 1$ and $U/\Delta \gg 1$, respectively. Here Δ is the bandwidth of non-interacting electrons. However, this semiclassical self-energy expression is quite complicated to perform any useful calculation. Therefore we try to reduce it to a simple form by making some appropriate approximation. For this purpose, we approximate the two-particle correlation functions, contained in it, by the product of single-particle correlation functions using Wick's theorem (Tyablikov 1967). We obtain a simplified expression

$$M_{\sigma}(k, \omega) = Un_{-\sigma} + \frac{U^2}{N^2} \sum_{k_1, k_2} \frac{n_{k_1-\sigma}(1 - n_{k_2-\sigma}) + (n_{k_2-\sigma} - n_{k_1-\sigma}) n_{k+k_1-k_2\sigma}}{U - U(1 - n_{-\sigma}) + \varepsilon_{k_1} - \varepsilon_{k_2} - \varepsilon_{k+k_1-k_2}} \tag{4}$$

where

$$a_k = \frac{1}{\sqrt{N}} \sum_{i} a_{i\sigma} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_i) \tag{5}$$

$$n_{k\sigma} = \langle a_{k\sigma}^{\dagger} a_{k\sigma} \rangle \tag{6}$$

$$n_\sigma = \frac{1}{N}\sum_k \langle a^\dagger_{k\sigma} a_{k\sigma}\rangle. \tag{7}$$

Here the angle brackets $\langle \ldots \rangle$ denote the thermal average. Although Wick's theorem is valid only for non-interacting electrons, its application may not change the qualitative results because (4) still retains the main features of the original expression. For example, it gives the exact results up to second order in U/Δ in the weak-correlation regime and the zero band width result in the strong-correlation regime. Expression (4) can be further simplified if we note that the Hubbard model neglects all the inter-atomic Coulomb interactions, so it is reasonable to replace the self-energy $M_\sigma(k, \omega)$ by a local function such that

$$M_\sigma(k, \omega) \approx M_\sigma(\omega) = \frac{1}{N}\sum_k M_\sigma(k, \omega).$$

This type of approximation has been made earlier by Treglia *et al* (1980). Also, in the case of narrow bands if we expand ε_{k_1}, ε_{k_2} and $\varepsilon_{k+k_1-k_2}$ about ε_k and keep only the first order term in $\nabla_k \varepsilon_k$, we can replace $\varepsilon_{k_1} - \varepsilon_{k_2} - \varepsilon_{k+k_1-k_2}$ by $-\varepsilon_k$. Thus the self-energy (4) is reduced to

$$M_\sigma(\omega) = Un_{-\sigma} + \frac{U^2 n_{-\sigma}(1 - n_{-\sigma})}{N}\sum_k \frac{1}{\omega - U(1 - n_{-\sigma}) - \varepsilon_k}. \tag{8}$$

It is easy to show that (8) gives the self-energy exactly for both zero band width and zero inter-atomic interaction. In the weak-correlation regime, it differs from the rigorous results of Kishore (1987) but reproduces the Hartree–Fock results. In the strong-correlation regime it gives the Hubbard first-approximation (Hubbard 1963). For a Lorentzian form of the bare electron density of states:

$$\rho_0(\varepsilon_k) = (2\Delta/\pi)[1/4(\varepsilon_k - T_0)^2 + \Delta^2] \tag{9}$$

where

$$T_0 = \frac{1}{N}\sum_k \varepsilon_k$$

is the average band energy and the evaluation of the k-summation on the right hand side of (8) gives the result of the Hubbard third-approximation (Hubbard 1964)

$$M_\sigma(\omega) = Un_{-\sigma} + U^2 n_{-\sigma}(1 - n_{-\sigma})/[\omega - T_0 - U(1 - n_{-\sigma}) + i\Delta/2]. \tag{10}$$

This result was obtained earlier by Acquarone *et al* (1980) by using the Lorentzian form (9) for the bare electron density of states in the self-energy of the Hubbard third-approximation (1964). Thus for this particular bare electron density of states, the approximate self-energy (8) is equivalent to the self-energy of the Hubbard third-approximation. Since the self-energy (8) reproduces the known results within appropriate limits, it can be a reasonable starting point for discussing the effects of electron correlations. The main advantage of (8) is that it is easy to evaluate numerically.

The use of the Lorentzian form for the bare electron density of states can be a good approximation for disordered systems, where tails exist on both low- and high-energy sides of the band. However, for a qualitative understanding of the crystalline narrow

band systems with sharp band edges in the bare electron density of states, we consider a rectangular form

$$\rho_0(\varepsilon_k) = \begin{cases} 1/\Delta & -\Delta/2 < \varepsilon_k - T_0 < \Delta/2 \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

By using (11) in (8), the local single-particle self-energy $M_\sigma(\omega)$ becomes

$$M_\sigma(\omega) = \mathrm{Re}M_\sigma(\omega) + \mathrm{i}\mathrm{Im}\, M_\sigma(\omega) \tag{12}$$

where

$$\mathrm{Re}\, M_\sigma(\omega) = Un_{-\sigma} - \frac{U^2 n_{-\sigma}(1-n_{-\sigma})}{\Delta} \ln \frac{\omega - T_0 - U(1-n_{-\sigma}) - \Delta/2}{\omega - T_0 - U(1-n_{-\sigma}) + \Delta/2} \tag{13}$$

and

$$\mathrm{Im}\, M_\sigma(\omega) = \frac{-\pi U^2 n_{-\sigma}(1-n_{-\sigma})}{\Delta} \Theta[\Delta/2 - |\omega - T_0 - U(1-n_{-\sigma})|] \tag{14}$$

are the real and the imaginary parts of $M_\sigma(\omega)$. The Heaviside step function $\Theta(x)$ is equal to one for $x > 0$ and zero for $x < 0$.

The density of states of the interacting electrons can be obtained from the imaginary part of the Green function. It is given by

$$\rho_\sigma(\omega) = -\frac{1}{\pi N} \sum_k \lim_{\varepsilon \to 0} \mathrm{Im}\, G_0(k, \omega + \mathrm{i}\varepsilon). \tag{15}$$

By substituting the single-particle Green function from (2) in (15), and using the rectangular form for the bare electron density of states (11) and the local single-particle self-energy $M_\sigma(\omega)$ (12) for $M_\sigma(k, \omega)$, the density of states $\rho_0(\omega)$ becomes

$$\begin{aligned} \rho_0(\omega) = (1/\pi\Delta)[&\tan^{-1}[(\omega - T_0 - \mathrm{Re}\, M_\sigma(\omega) + \Delta/2)/|\mathrm{Im}\, M_0(\omega)|] \\ &- \tan^{-1}[(\omega - T_0 - \mathrm{Re}\, M_\sigma(\omega) - \Delta/2)/|\mathrm{Im}\, M_0(\omega)|] \\ &\times \Theta[\Delta/2 - |\omega - T_0 - U(1-n_{-\sigma})|] + (1/\Delta)\{1 - \Theta[\Delta/2 \\ &- |\omega - T_0 - U(1-n_{-\sigma})|]\}\Theta(\Delta/2 - |\omega - T_0 - \mathrm{Re}\, M_\sigma(\omega)|). \end{aligned} \tag{16}$$

We calculated the density of states (16) for a paramagnetic system for which $\rho_0(\omega) = \rho_{-\sigma}(\omega) = \rho(\omega)$, $M_\sigma(\omega) = M_{-\sigma}(\omega) = M(\omega)$, and $n_\sigma = n_{-\sigma} = n/2$. The results of the numerical calculation are shown in figure 1 where $\Delta\rho(\omega)$ are plotted against U/Δ for three values of U/Δ and n. The density of states consists of three bands. The lower and the upper bands are separated from the middle band by an energy gap which decreases with a decrease in the parameter U/Δ. Finally at some value of U/Δ this gap goes to zero with the result that all the bands merge into one. The imaginary part of the local single-particle self-energy is zero in the lower and the upper bands. In the middle band, it has a constant value which depends upon U/Δ and makes all the electronic states in the band damped. The damping of the states increases as U/Δ increases. On the other hand, the number of states in the middle band increases with a decrease in U/Δ. This shows that as U/Δ increases a dip in the middle of the density of states appears. This dip increases as U/Δ increases. The states in this dip are damped and this suggests the possibility of the existence of localised states for the nearly half-filled band. Because of the damping of the states, an electron near the Fermi energy has a finite lifetime and thereby a finite mean free path which increases with a decrease in U/Δ. For a sufficiently

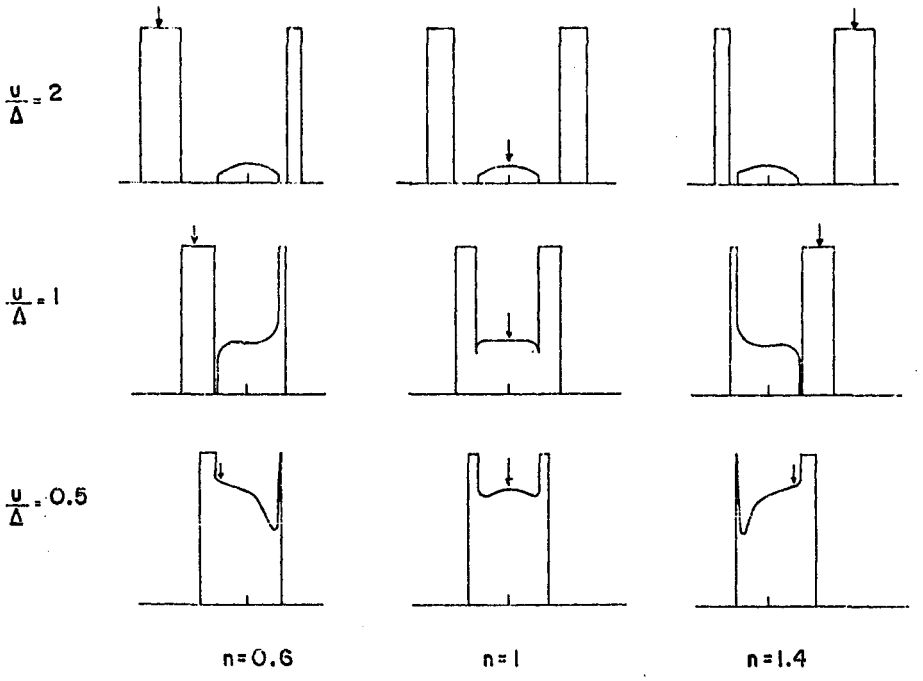

Figure 1. Density of states $\Delta\rho(\omega)$ for various values of U/Δ and n. The position of the Fermi level is indicated by an arrow.

large value of U/Δ the mean free path can be less than the inter-atomic spacing. In this case, all the electrons at the Fermi level are localised at their respective lattice sites and no conduction occurs. By decreasing U/Δ, the mean free path increases, and at some value of U/Δ when it becomes equal or greater than the inter-atomic spacing the system makes a transition from a non-metallic to a metallic state. An approximate value of the mean free path at the Fermi energy, λ_F, can be obtained from the semiclassical relation

$$\lambda_F = \tau_F v_F \tag{17}$$

where τ_F and v_F are the lifetime and mean group velocity of electrons at the Fermi energy. The lifetime τ_F can be obtained from the imaginary part of the self-energy by using the relation

$$\tau_F = -h/2 \operatorname{Im} M(\varepsilon_F) \tag{18}$$

where ε_F is the Fermi energy. But there is no straightforward way to calculate the Fermi velocity v_F. A rough estimate of v_F can be obtained from its semiclassical value for the non-interacting electrons. For non-interacting electrons of band width Δ and rectangular density of states (11) centred at T_0, the Fermi energy ε_F^0 can be related to the Fermi velocity v_F by the relation

$$\varepsilon_F^0 - (T_0 - \Delta/2) = n\Delta/2 = m^* v_F^2/2 \tag{19}$$

where m^* is the effective mass of the electrons. Also since the Fermi momentum k_F is equal to $m^* v_F$, the above relation gives the Fermi velocity as

$$v_F = n\Delta/k_F. \tag{20}$$

To calculate k_F we consider a two-dimensional electron gas which is consistent with

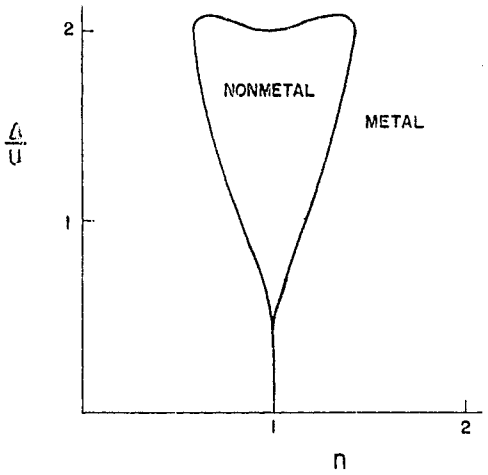

Figure 2. Phase diagram indicating metal and non-metal states.

our assumption of the constant nature of the rectangular density of states. Also, it is an appropriate choice for high-T_c superconductors where the basic electronic properties are believed to depend on the nature of the electrons or holes of the copper–oxygen layers. In this case

$$k_F = (2\pi n)^{1/2}/a \tag{21}$$

where a is the inter-atomic distance and it is assumed that the area of the layer is given by Na^2. Equations (19), (10) and (21) are written for number of electrons $n < 1$. For $n > 1$, we can work with holes by replacing n by $2 - n$. This replacement preserves the electron–hole symmetry of the density of states.

Now, after calculating τ_F from (14) and (18) and v_F from (20) and (21), the condition $\lambda_F > a$ for the transition from a non-metallic to a metallic state becomes

$$(U^2/2\Delta^2)(2-n)(2\pi n)^{1/2}\Theta[\Delta/2 - |\varepsilon_F - T_0 - U(1-n/2)|] < 1 \tag{22}$$

where the Fermi energy ε_F for the interacting electrons can be calculated from the relation

$$n = 2\int_{-\infty}^{\varepsilon_F} \rho(\varepsilon_k)\,\mathrm{d}\varepsilon_k. \tag{23}$$

The condition (22) is plotted in figure 2. It shows that for a half-filled band the system behaves as a non-metal below a certain value of Δ/U. But for a nearly half-filled band, the non-metallic state occurs between two lower and upper values of Δ/U. This behaviour is consistent with the rigorous results (Kishore 1987) of the Hubbard model. According to these results, for small band width, the quasi-particle spectrum of the Hubbard model consists of two separate bands with exactly one electron per lattice site in each band and therefore the system must behave as a non-metal for $n = 1$ and a metal for $n \neq 1$ as shown in figure 2. For large values of Δ/U, according to the Hartree–Fock results, the system must behave as a metal for all values of n. It should be noted that the non-metallic state for a nearly half-filled band occurs because of the localised states which appear due to electron correlations. This localisation for a nearly half-filled band is relevant for the metal–non-metal transition in high-T_c superconducting oxides.

To conclude, a local single-particle self-energy, obtained from the projector operator formalism of the Green function (Kishore 1987), has been used to obtain the density of states of the Hubbard model. It is found that for a nearly half-filled band, the single-particle states near the Fermi level are damped. Because of this damping of states, the electrons near the Fermi level are localised above a certain value of U/Δ. This localisation of electrons provides an explanation of the metal–non-metal transition in the paramagnetic state of high-T_c superconductors.

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