METAL NONMETAL TRANSITION IN A NEARLY HALF FILLED BAND HUBBARD MODEL FOR HIGH TC SUPERCONDUCTORS

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ABSTRACT

Approximating the quasi-particle self energy of the Hubbard model by a local function, it is found that the electrons near the Fermi energy can be localized above a certain value of U/Δ (U is the intraatomic Coulomb interaction and Δ is the band width of noninteracting electrons). This localization of electrons can give rise to a metal-nonmetal transition in a nealy half filled band as found in the paramagnetic state of high Tc superconductores.

1. Introduction

Recently it has been discovered[1] that in the paramagnetic state the nearly half filled band systems of high Tc superconductors make a transition from a nonmetallic to a metallic state as the number of electrons or holes per lattice site is changed from unity to some critical value. This metal-nonmetal transition cannot be explained from the conventional band models based on either nonintracting[2] or correlated[3] electrons. To understand this phenonmenon here we study the nearly half filled band Hubbard model in paramagnetic state by using a local quasi-particle self energy.

2. Local Quasi Particle Self Energy

Recently the quasi-particle self energy of the Hubbard model has been obtained[4] by using a semi-classical approximation which gives the exact results for the quasi-particle spectrum in both weak and strong correlation regimes which correspond to $U/\Delta << 1$ and $U/\Delta >> 1$ respectively. Here Δ is the band width of nonintracting electrons and

U in the intraatomic Coulomb interaction. However, this semi-classical 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 approximations. For this purpose we approximate the two particlwe correlation functions by using Wick's theorem. Also if we note that Hubbard model neglects all the intraatomic Coulomb interaction, it is reasonable to approximate the nonlocal self energy by a local function. Within these approximations, in case of narrow bands, we get the quasi-particle self energy as

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

This self energy has been postulated earlier by Kishore[5] in order to explain the photoemission experiments in nickel.

It is easy to show that Eq. (1) gives the self energy exactly for both zero band width and zero intra-atomic intration. In the weak correlation regime, it differs from the rigorous results of Kishore[4] but reproduces the Hartree-Fock results. In the strong correlation regime, it gives the Hubbard first approximation[3]. For a Lorentzian form of the bare electron density of states, it gives the Hubbard third approximation[6]. Since the self energy (1) reproduces the known results in appropriate limits, it can be a reasonable starting point for discussing the effects of electron correlations. The main advantage of Eq. (1) is that it is easy to evaluate numerically.

3. Results and Discussions

By using the rectangular form of the bare electron density of states in the self energy expression (1), the density of states in the paramagnetic state has been obtained by Kishore[5]. 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 gape goes to zero with the result that all the bands merge into one. the imaginary part of the self energy is zero in lower and the upper bands. In the middle band, it has a constant value which depends upon U/Δ and makes all the electronics 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 appear. This dip increases as U/Δ increases. The states in this dip are damped which sugests the possibility of the existence of localized states for nearly half filled band. Because of

the damping of states, an electron near the Fermi energy has a finite life time and thereby a finite mean free path which increases with a decreases in U/Δ. For sufficiently 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 localized 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 nonmetallic to a metallic state.

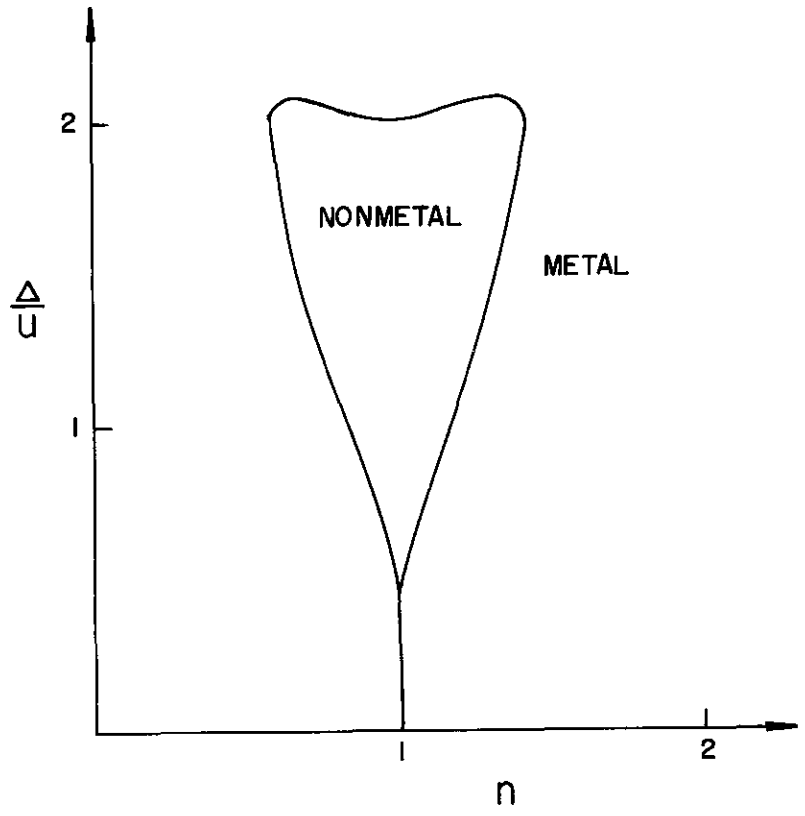

Fig. 1. Phase diagram indicating metal and nonmetal states.

An approximate value of the mean free path at the Fermi energy, λ_f can be obtained from the semi-classical relation $\lambda_f=\tau_f v_f$ where τ_f and v_f are the life time and mean group velocity of electrons at the Fermi energy. The life time τ_f can be obtained from the imaginary part of the self energy but there is no straight forward way to calculate the Fermi velocity v_f. A rough estimate of v_f can be obtained from its semi-classical value for the non intracting electrons. For the rectangular density of states of band width Δ, $v_f=n\Delta/k_f$ where k_f is the Fermi momentum. Since for high Tc superconductors, the basic electronic properties are believed to depend on the nature of electrons or holes of copper-oxygan layers, we consider k for a two dimensional electron gas. In Fig. 1 we have shown the metallic and non-metallic phases in the paramagnetic state. It shows that for a half filled band the system behaves as a non-metal below a certain value of Δ/U. But for nearly half filled band, the non-metallic state occurs between two lower and upper values of Δ/U. This behavior is consistent with the rigorous results 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 exectly one electron par 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 Fig. 1. For large values of Δ/U, according to Hartree-fock results, the system must behave as a metal for all values of n. It should be noted that nonmetallic state for a nearly half filled band occurs because of the localized states which appear due to electron correlations. This localization for nearly half filled band is relevant for the metal-nonmetal transition in high Tc superconducting oxide.

References

1. W.F. Pickett, Rev. Mod. Phys. **61** (1989) 433.
2. A.H. Wilson, Proc. Roy. Soc. (London) **A132**, (1931) 458.
3. J. Hubbard, Proc. Roy Soc. (London) **A276** (1963) 238.
4. R. Kishore, Phys. Rev. **B35** (1987) 6854.
5. R. Kishore, Rev. Bras. Fís. especial volume (1983) 380.
6. J. Hubbard, Proc. Roy. Soc. (London) **A281** (1964) 401.