THE TWO-BAND MODEL AND THE METAL-NONMETAL TRANSITION IN MAGNETIC SYSTEMS

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Abstract

Using the two band model introduced by Mota and Coutinho-Filho, the metal-nonmetal transition is investigated by taking an approximate model Hamiltonian which takes into accout the hybridization of the two bands, not included in the original model. A Green's function technique is used to obtain the hybrid bands in the Hartree-Fock approximation. Investigating the phenomenon of metal-nonmetal transition, in general, increasing the intra-atomic interaction the tendency of the systems towards nonmetalic behavior increases. But, differently of previous results, for strong hybridization and small intra-atomic interaction, where the Hartree-Fock approximation is valid, the opposite is observed. This may help to understand the difficulty of observing pressure-induced nonmetal-metal transitions in magnetic systems.

Resumo

MODELO DE DUAS BANDAS E TRANSIÇÃO METAL-NÃO METAL EM SISTEMAS MAGNÉTICOS. A transição metal-não metal é investigada usando o modelo de duas bandas apresentado por Mota e Coutinho -Filho utilizando um Hamiltoniano o qual inclui a hibridização de duas bandas não contida no modelo original. A técnica de funções de Green é utilizada para obter as bandas híbridas na aproximação Hartree-Fock. É mostrado que, em geral, com o aumento da interação intra-atômica a tendência do sistema se tornar metálico cresce. Porém, diferentemente de resultados anteriores, para a região de hibridização forte e interação intra-atômica pequena, onde a aproximação Hartree-Fock é válida, o comportamento oposto é observado. Tal comportamento ajuda a entender a difuldade de observar-se transição metal-não metal em sistemas magnéticos.

1 Introduction

Although the two-band model has been under study for decades, much attention has been devoted in the last few years since the discovery of the high-temperature ceramic superconductors. It is also believed that the ability to sinthetiside oxides close to the metal-nonmetal region will always raise the possibility of high-temperature superconductivity[1]. Then, the understanding of the two-band model connected to the metal-nonmetal transition is a very actual subject because this model may contain the correct qualitative properties of low-energy excitations associated with magnetism. Recently, Jellito[2], using a single-band Hubbard model, has tried to elucidate what possible phases to expect as doping and the correlation energy are varied. Other studies[3] have shown that a linearly polarized Hartree-Fock decomposition results in holes staying along boundaries between antiferromagnetic domains. Using more precise two-band model, a domain wall has been found to be stable with one set of parameters[4]. Inui and Littlewood[5] attempted a systematic study of the Hubbard model near half-filling within the Hartree-Fock theory. Nevertheless the Hartree-Fock approximation presents many limitations, this mean-field solution is an appropriate starting point for more sophisticated calculations which incorporate correlation effects more accurately. The richness and complexity of the Hartree-Fock solutions suggest that there is considerably more to be understood, specially associated with the two-band model.

The metal-nonmetal transition in magnetic systems has been under intensive study since Mott[6] proposed a theory predicting a existence of a metal-nonmetal transition under pressure when the lattice passes throught a critical value. Although such a transition has not yet been observed[7], much attention has been devoted to understanding the nature of the electronic localization accompanying this transition in magnetic systems[8].

For many years all the proposed models for the electronic conduction were quite closely related to that of Hubbard[9], normally assuming a single d band. The central idea of Hubbard's paper is that the atomic coulomb repulsion is much larger than the hopping integrals which govern the width of the d band, then the leakage rate from one atom to another is small and the d electrons can be approximately described by their configurations in isolated atoms. As an extension of this model, Kishore and Joshi[10] take accout the hybridization of the s and d

bands. They used this model to investigate the role of the s and d interaction in metal-nonmetal transitions. In this context, Mota and Coutinho-Filho[11] introduced the two-band model for the magnetism of the transition metals and reported results in fairly good agreement with the experimental facts both at low and high temperatures. The main feature of the model is the existence of a degenerate narrow d band, representing "quasi-localized" electrons, and a wide band containing very few quasifree d electrons (itinerant electrons).

In this paper, we assume the two-band model introduced by Mota and Coutinho-Filho and the metal-nonmetal transition is investigated by taking an approximate model Hamiltonian, presented in Sec. 2, which takes into account the hybridization of the two bands, not included in the original model. In our analysis, we use the Green's function method discussed by Zubarev[12]. In Sec. 3, the phenomenon of metal-nonmetal is investigated and the understanding of the difficult to observe pressure-induced metal-nonmetal transition in these materials is discussed.

2 Model Hamiltonian

The model hamiltonian may be written in the form:

$$
\begin{aligned}
H &= \sum_{ij\alpha\sigma} T_{ij}^{\alpha} c_{i\sigma}^{\alpha\dagger} c_{j\sigma}^{\alpha} + \frac{1}{2}\sum_{i\alpha\sigma} U_{\alpha} n_{i\sigma}^{\alpha} n_{i-\sigma}^{\alpha} - 2J_{IL}\sum_{i} \vec{S}_i^{I} \cdot \vec{S}_i^{L} - 2J\sum_{i<j} \vec{S}_i^{L} \cdot \vec{S}_j^{L} \\
&+ \sum_{ik\sigma} (V e^{i\vec{k}\cdot\vec{R}_i} c_{k\sigma}^{I\dagger} c_{i\sigma}^{L} + V^{*} e^{-i\vec{k}\cdot\vec{R}_i} c_{i\sigma}^{L\dagger} c_{k\sigma}^{I})
\end{aligned}
\tag{1}
$$

where $c_{i\sigma}^{\alpha\dagger}$ $c_{i\sigma}^{\alpha}$ is the creation (annihilation) operator for an electron of spin σ at the site i and the band α (L or I), $n_{i\sigma}^{\alpha}$ and J_j^{α} are the occupation number and spin operators of these electrons, respectively. T_{ij}^{α} are the Wannier representation of the electron bands, U_{α} are the intra-atomic intraband Coulomb couplings, J_{IL} is the exchange coupling between itinerant electrons of a wide band I of width Δ (quasi-free-electron states) and "quasi-localized" electrons of a narrow degenerate band L of width ℓ (flat parts of the d bands), J is the inter-atomic exchange coupling between electrons of the narrow band, and V is the hybrid matrix element. In the Hartree-Fock approximation the one-particle Green's functions of the system are given by:

$$G^I_{\vec{k}}(\omega) = \frac{\omega - \epsilon^L_{\vec{k}} - F^L_\sigma}{2\pi\{[\omega - \epsilon^I_{\vec{k}} - F^I_\sigma][\omega - \epsilon^L_{\vec{k}} - F^L_\sigma] - V^2\}}, \tag{2}$$

$$G^L_{\vec{k}}(\omega) = \frac{\omega - \epsilon^I_{\vec{k}} - F^I_\sigma}{2\pi\{[\omega - \epsilon^I_{\vec{k}} - F^I_\sigma][\omega - \epsilon^L_{\vec{k}} - F\sigma^L] - V^2\}}. \tag{3}$$

where $\epsilon^o_{\vec{k}}$ are the noninteracting electron bands. F^I_σ and F^L_σ are given by:

$$F^I_\sigma = U^I < n^I_{-\sigma} > -\frac{J_{IL}}{2}(< n^L_\sigma > - < n^L_{-\sigma} >). \tag{4}$$

$$F^L_\sigma = U^L < n^L_{-\sigma} > -\frac{J_{IL}}{2}(< n^I_\sigma > - < n^I_{-\sigma} >) + \frac{J(0)}{2}(< n^L_\sigma > - < n^L_{-\sigma} >). \tag{5}$$

where $J(\vec{q}) = J\sum_{\vec{\delta}} e^{i\vec{q}.\vec{\delta}}$, with $\vec{\delta}$ being vectors joining first neighbors of a bcc lattice, and $< n >$ are the average number of electrons per atom. We assume, to simplify the calculations, paraboliclike bands and the effective-mass approximation, i.e.,

$$\epsilon^I_{\vec{k}} = \frac{\hbar^2 k^2}{2m^*_I} \tag{6}$$

$$\epsilon^L_{\vec{k}} = T_o - \frac{\ell}{2} + \frac{\hbar^2 k^2}{2m^*_L} \tag{7}$$

where T_o fixes the position of the L band relative to the bottom of the I band. Consequently, $\epsilon^L_{\vec{k}}$ can be represented by the expression:

$$\epsilon^L_{\vec{k}} = \frac{\ell}{\Delta}\epsilon^I_{\vec{k}} + T_o - \frac{\ell}{2} \tag{8}$$

where ℓ and Δ represent the L and I bandwidths, respectively.

3 Metal-Nonmetal Transition

We will restrict ourselves to the particulary simple solution representing paramagnetic state and it will be assumed $U^I = 0$, since it is not a relevant parameter in this analysis. The Equations 2 and 3 have the same poles associated to the one-particle excitations of the electrons and th resulting hybrid bands are given by:

$$\omega^{\pm}_{k\sigma} = \frac{1}{2}\{\epsilon^{I}_{k} + \epsilon^{L}_{k} + U^{L}\frac{< n^{L} >}{2} \pm [(\epsilon^{I}_{k} - \epsilon^{L}_{k} - U^{L}\frac{< n^{L} >}{2})^2 + 4V^2]^{\frac{1}{2}}\} \quad (9)$$

The two original d bands (L and I) are admissed into two new bands with dispersion laws $\omega = \omega^{+}_{k\sigma}$ and $\omega = \omega^{-}_{k\sigma}$. The general form of the hybrid bands is shown in Figure 1. Considering

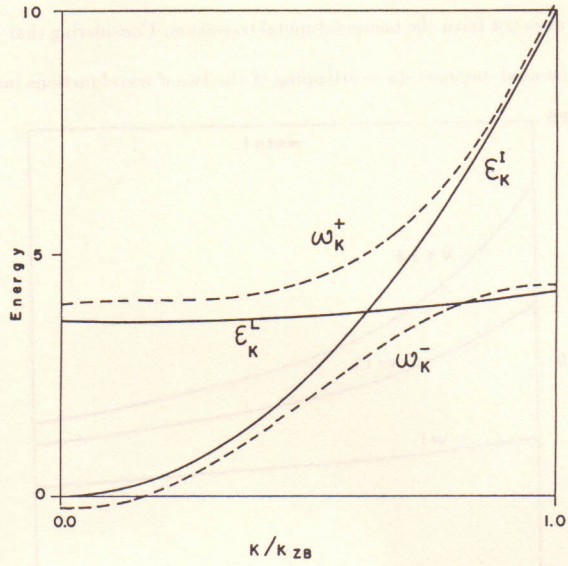

Figure 1 . Hybrid bands in the Hartree-Fock approximation. $\vec{k}_{ZB}$ is the wave vector to the zone boundary.

that the system behaves as a nonmetal provided that there is a gap between the lower and the upper hybrid bands, otherwise it will behave as a metal, a metal-nonmetal transition occurs when the gap vanishes. The gap between the upper and lower hybrid bands can be expressed by:

$$g = \omega^{+}_{k\sigma}(\vec{k} = 0) - \omega^{-}_{k\sigma}(\vec{k} = \vec{k}_{zb}) \quad (10)$$

where $\vec{k}_{zb}$ is the wave vector to the zone boundary. Under the assumption 8 and using Equation 9, we may write g as:

$$\begin{aligned} g \;=\; & \ell^3\Delta + 2\ell^2\Delta^2 - 4\ell^2V^2 + 4\ell\Delta^2T_o - 8\ell\Delta T_o^2 + 4\ell\Delta^2U - 8\ell\Delta V^2 \\ & -8\ell\Delta T_oU - 4\Delta^2V^2 - 4\ell\Delta U^2 \end{aligned} \quad (11)$$

By fixing a particular parameter, one can plot a transition curve for the remaining two parameters. In Figure 2 we have plotted $\Delta - \ell$ curves for different values of V, assuming U fixed. This curve shows that for a particular choice of values of Δ and ℓ we get a critical value of V at which the transition from the nonmelallic to metallic occurs. Figure 2 clearly shows that the increase in V does not favor the nonmetal-metal transition. Considering that V increases as the pressure is increased, because the overlapping of the two d wavefunctions increases due to

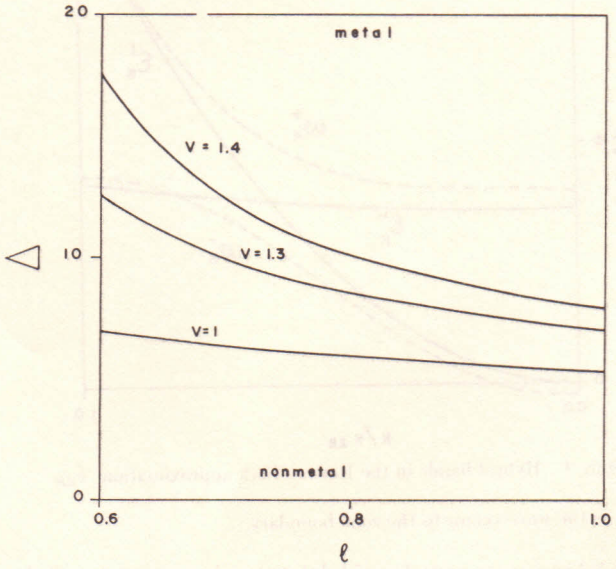

Figure 2 . $\Delta - \ell$ curves for different values of V.

compression of the lattice, thus the $d_{t_{2g}} - d_{t_{2g}}$ hybridization does not favor the nonmetal-metal transition. Then, the considered hybridization opposes the pressure induced nonmetal-metal transition.

Extending the study to include the behavior of the system when U changes, something very peculiar is observed. For $V = 0$, not considering hybridization, by plotting $\Delta - \ell$ transition curves, for different U values, Figure 3 shows that, for any value of U, when U increases the tendency of the system towards nonmetallic behavior increases. Thus we infer that if the hybridization is neglect, the increasing of the intra-atomic interaction opposes the pressure induced nonmetal-metal transition. This result is the same obtained previouly by Kishore and Joshi[13].

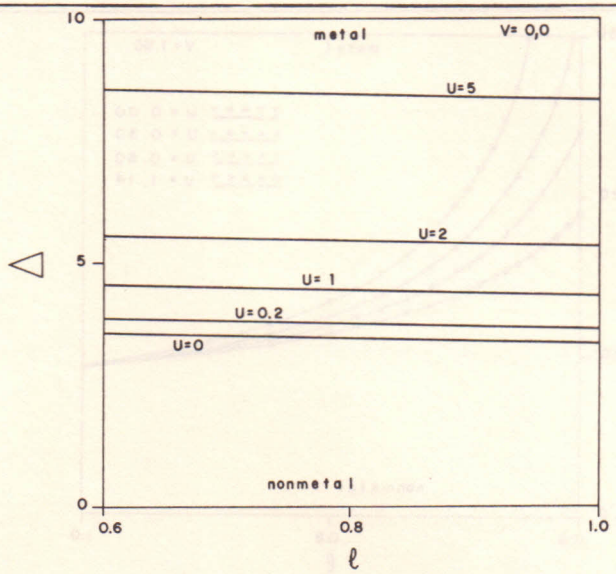

Figure 3 . $\Delta - \ell$ curves for different values of U with $V = 0.0$.

By considering hybridization, the cited strange behavior depends on the U magnitude. For large U the above resuts keep inalterated, but for small U the situation is not so direct. Now, by considering the region of V large and U small, the opposite bevavior is observed. The Figure 4 shows that as we increase the intra-atomic interaction the nonmetallic region decreases, and thus the tendency of a system towards metallic behavior increases. The main point to be elucidated is that considering hybridization we reach to qualitatively different results, depending if we consider large or small values for the intra-atomic interaction. The answer to this puzzle includes to remember that the validity of the Hartree-Fock theory is dubious when the intra-atomic U is large; in this case, the correlation effects must be taken into account. Considering that our results have been obtained using Hartree-Fock approximation, Figure 5 shows cleary that the validity region corresponds to values of U small and V large, and in this region our results are in contradiction with previous one[13].

4 Conclusions

When pressure is applied on a nonmetallic substance, the lattice parameters (the bandwidths ℓ

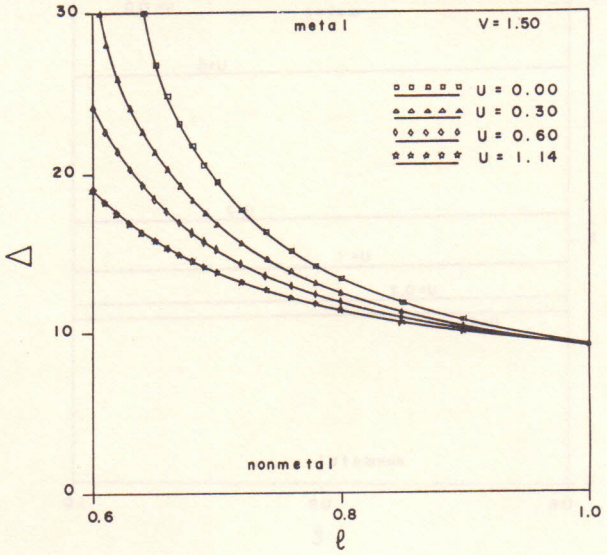

Figure 4 . $\Delta - \ell$ curves for different values of U with $V = 1.5$.

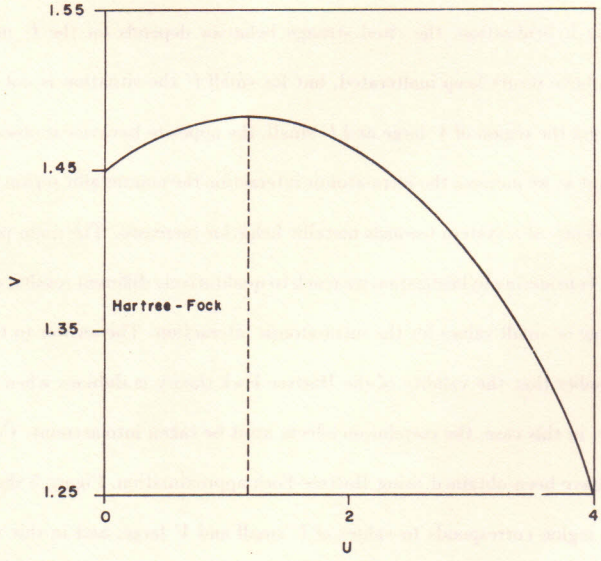

Figure 5 . $V - U$ curve showing the Hartree-Fock region.

and Δ) increase, and a transition from nonmetallic to metallic state should occur at a critica pressure. Otherwise, to explain the difficulty of observing nonmetal-metal transition under

pressure in these materials we need also to consider the role of the interaction parameters. The hybridization parameter V increases as the pressure is increased, because the overlapping of the two wavefunctions and we have shown that the increase in V does not favor the nonmetal-metal transition. The same result are obtained by Kishore and Joshi[10]. Considering that the intra-atomic interaction U decreases when pressure is applied, because ℓ and Δ increase, Figure 4 shows cleary that for small U, exactly the region where the assumed Hartree-Fock approximation is valid, this decreasing in U does not favor the nonmetal-metal transition. Kishore and Joshi[13] investigated how the intra-atomic interaction betweem d electrons affects the nometal-metal transition and the opposite behavior is reported. Our results, in this particular point , are in marked disagreement with the previous one, and seem to be more consistent as the role played by the kinetic parameters (ℓ and Δ) are contrary to the two interaction parameters (V and U) concerning this nonmetal-metal transition when pressure is applied and this kind of approach may explain the difficulty of observing metal-nonmetal transition under pressure in these materials.

Acknowledgments

This work was supported by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul (FAPERGS) (Brazilian Agencies).

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