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METAL-NON METAL TRANSITION IN HUBBARD MODEL

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Résumé. — Nous étudions la transition métal-isolant due aux corrélations entre électrons. Nous donnons un critère pour l'apparition de l'état isolant dans une bande à moitié remplie et nous discutons de la relation avec le magnétisme. L'apparition d'un état antiferromagnétique favorise la transition métal-isolant.

Abstract. — We study the metal-non metal transition due to correlations between electrons. We derive a criterion for the appearance of insulating phase in a half filled band. We discuss correlations with magnetism and show that antiferromagnetism favours metal-non metal transition.

In the last years considerable interest has grown up in metal-non metal transition [1] and particularly in transition metal oxides [2]. This is because they prove to be a striking failure for elementary Bloch-Wilson theory. It is a well known result that a material all of whose bands are either completely full or entirely empty is usually an insulator whereas a material with a partially full band must be metallic. Some materials which have full bands can be metallic if there is an overlap of the bands but if a material which must be metallic taking into account all splitting of bands due to crystalline field turns out to be an insulator it is not so simple to find explanation. Such is the case for the vast majority of transition metal oxides. Of course it is always possible to abandon Bloch model admitting that such a narrow band cannot support metallic conductivity. The starting point would be the Heitler-London model which has the immediate advantage to explain the insulating nature of the majority of the transition metal oxides. However, it appears that some of these materials have a conductivity within a factor ten of that of Copper.

Mott was the first to consider transition from Bloch to Heitler-London ground states. He emphasized the importance of correlations between electrons in this problem. In this respect it is strongly connected with magnetism. In this paper we would like to show on a model the transition from Bloch states to Heitler-London states with increasing correlations between electrons in the d band. For small correlations, Block states is a reasonable starting point, for large one Heitler-London states would be better. In the intermediate range one can go from the first to the second one with decreasing temperature.

For our model we will use the two facts : intra-correlation effects only are effective, thus between electrons sitting on the same site and one can define an average effective correlation energy $U$ which gives the average difference of energy between pairs of such electrons. Thus a very convenient starting point is to use the hamiltonian first derived by Hubbard [4]

$$H = \sum_{ij} T_{ij} C_i^+ C_j + \sum_i U n_i n_i.$$  

To obtain equilibrium properties we calculate the partition function. We use a functional integral formalism so $Z$ can be written [5]

$$Z = \int \prod_i d\xi_i \exp\left[-\sum_i \xi_i^2 \right] \text{Tr} T_i \exp[-\beta H_i]$$  

$$H_i = \sum_{ij} T_{ij} C_i^+ C_j + \left(\frac{U}{2} - \mu - \sqrt{\frac{2}{B}} \sigma \xi_i\right) n_{i\sigma}.$$  

In the following we will neglect the s dependence of the scattering potential $\xi_i$. We have shown [6] if $Z(\{\xi_i\})$ is the partition function of our non interacting particles moving in arbitrary scattering potential $\{\xi_i\}$ we have

$$Z = Z_0 \int \prod_i d\xi_i \exp[-F(\{\xi_i\})]$$  

with

$$F(\{\xi_i\}) = \sum_i T \xi_i^2 + \sum_i \frac{1}{\Delta E} \int \frac{d\omega}{1 + e^{\omega/T}} n_{i\sigma}(\omega) - \sqrt{2UT\sigma \xi_i}$$  

$$+ \sum_{\sigma} \left(\frac{U}{2} - \mu - \sqrt{2UT\sigma \xi_i}\right) n_{i\sigma}. \tag{6}$$

We use a saddle point approximation to obtain $Z$ so we determine $\xi_i$ by minimization of $F$

$$F = F_0 - \sum_i T \log \left[1 + e^{-\beta \eta_{i\sigma}}\right] - \frac{1}{\Delta E} \sum_{\sigma} \int \frac{d\omega}{1 + e^{\omega/T}} n_{i\sigma}(\omega) - \sqrt{2UT\sigma \xi_i}$$  

these are the self consistence equations for our problem. $n_{i\sigma}$ is a function of the whole set $\{\xi_i\}$ but in principle we can determine $\xi_i$. If the value of $\xi_i$ we determine is large enough to create a bound state of energy $E_i$ equation (5) can be rewritten:

$$F = F_0 - \sum_i T \log \left[1 + e^{-\beta \eta_{i\sigma}}\right] - \frac{1}{\Delta E} \sum_{\sigma} \int \frac{d\omega}{1 + e^{\omega/T}} n_{i\sigma}(\omega) - \sqrt{2UT\sigma \xi_i}.$$  

For the transition metal oxides. However, it appears that some materials have a conductivity within a factor ten of that of Copper.
The free energy has two contributions. The first one is the free energy of a Heitler-London model and the second one is the free energy of electrons thermally excited in the band. If all sites are equivalent the localised state occurs on each one. At \( T = 0 \) and with one electron per site, all the electrons are in these states and one gets an insulating behavior. The activation energy is the distance between localised states and the band. We want to point out that if there is \( N - 1 \) electrons for \( N \) sites, the hole is expected to hop from sites to sites. Our static approximation will break down because non zero frequencies of order \( h/T_{ij} \) will become important.

Our criterium for an insulating behavior is that the perturbation on the \( i^{th} \) site creates a localised state out of the band of the material without this perturbation on the \( i^{th} \) site. The occurrence of a bound state is related to the shape of the band and in particular to its width. For small binding one gets more easily a bound state. In a tight binding scheme, this width is connected with the extension of the d function in the atomic state and distance between transition metal. This distance being greater in the oxides this favors an insulating behavior. Secondly as you go from the left to the right side of the periodic table the extension of the d atomic functions decreases favorising the metallic behavior. On the contrary one favors the metallic behavior as you go from the first to the third series.

\( \xi_i \) is temperature dependent. In general \( \xi_i \) increases with decreasing temperature. At high temperature \( \xi_i \) can be too small to create a bound state but it can appear below a temperature \( T_M \). So one can go with decreasing temperature from a metallic behavior to an insulating one in the sense that an activation energy appears.

Within this framework the insulating behavior is strongly correlated with magnetism contrary to the usual Block-Wilson insulator. In general there is no relationship between the «Mott temperature» \( T_M \) below which an insulating behavior occurs and the critical temperature of the ordered magnetic phase. But the appearance of an antiferromagnetic phase strongly favors the simultaneous appearance of an insulating behavior because it decreases the width of the band. In that case the Néel temperature equals the Mott temperature \( T_N = T_M \).

There exist other possibilities of relationship with magnetism. In a previous work we introduce a temperature \( T_L \) below which localised moments appear i.e. the value \( \xi_i \) given by eq. (7) is different from zero.

We have shown that \( T_L \) can be equal to \( T_N \) that is there is no localised moment behavior in the high temperature metallic phase. Now we can have \( T_L = T_N = T_M \) i.e. the high temperature phase is a metallic one with Pauli behavior, the low temperature one is an antiferromagnetic insulator. This described a Slater transition.

Up to now we are not able to do a quantitative description of transition metal oxides because good knowledge of the interaction and density of states is needed. But qualitatively this model throws light on the general behavior of these oxides and on the general trends in the three series.

References