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Crystallographic Distortion, Electron-Electron Interaction and the Metal-Nonmetal Transition

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Abstract. An analog of Slater's split-band model of antiferromagnetism is described. The analog involves a crystallographic distortion to lower symmetry, the charge distribution of the band electrons adjusting itself selfconsistently to the new ionic charge distribution. The possible importance of Coulomb- and exchange interactions among the band electrons is pointed out.

Recently a great deal of interest has been shown in the so called metal-nonmetal transition and a variety of models have been proposed which predict such a transition. Some of these models have – rather prematurely – been applied to some transition metal compounds, which show apparently a thermal metal-nonmetal transition. However most of the models have remained rather academic, either because they are too idealized or no systems, for which they were invented, have been found in practice. Rather than reviewing the existing literature we refer to a recent article by HYLAND [1] where many of the relevant references are given and to a forthcoming volume in the Solid State Physics series [2]. Instead, our present purpose is to discuss some aspects of a particular kind of metal-nonmetal transition, namely the transition which is caused by a thermal crystallographic distortion. A description of a crystallographic distortion accompanied by an abrupt change in electrical conductivity exists in the literature and was applied there to the lower oxides of vanadium [3]. However, electron-electron interactions were not taken into account explicitly. We wish to remedy this situation and point out qualitatively the possible importance of electron-electron interactions, using the Hartree-Fock approximation.

For simplicity we start with a non-degenerate half filled band with one conduction electron per ion, whereas we assume that the relative positions of the core electrons and the nuclei remain fixed. The periodic crystal potential will be denoted by V_1, the Bloch functions by $|\, \boldsymbol{k}\sigma >$ and the corresponding one-electron energies by $\varepsilon_{\boldsymbol{k}}$. Now, suppose that the crystal is distorted to a lower symmetry, the new periodic potential being V_2. The potential V_2 is characterized by a new wavevector $\boldsymbol{Q}$, which we shall take to be one half of an original reciprocal lattice vector. The new fundamental Brillouin zone is then twice as small as the original zone. The band will now be split into two sub-bands, and if the splitting is large enough – so as to prevent overlap of

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the sub-bands in all directions in k-space – the result will be an insulator. The problem then is to find the gap between the sub-bands selfconsistently. In addition, and more important, one would have to see whether at zero temperature the distorted phase has a lower energy than the undistorted phase. The latter problem is extremely difficult in realistic cases, and we assume that the distorted phase actually is lower in energy.

The hamiltonian of the system will be written as

$$\mathcal{H}_2 = \mathcal{H}_1 - W = \sum_{k,\sigma} \varepsilon_k \, c^+_{k\sigma} \, c_{k\sigma} - \sum_{k,k',\sigma} W_{k,k'} \, c^+_{k\sigma} \, c_{k'\sigma} + \frac{1}{2} \sum_{\substack{k,k',q \\ \sigma,\sigma'}} \langle k+q, k'-q \,|V|\, k', k\rangle \, c^+_{k+q,\sigma} \, c^+_{k'-q,\sigma'} \, c_{k'\sigma'} \, c_{k\sigma} \,, \tag{1}$$

where $W = V_1 - V_2$ and V is the Coulomb interaction among the band electrons. The matrix element $W_{kk'}$ is zero unless $k' = k \pm Q$. We are looking for a selfconsistent Hartree-Fock solution of (1), such that the expectation values of $c^+_{\sigma k} \, c_{k\sigma}$ and $b^+_{k\sigma} = c^+_{k+Q,\sigma} \, c_{k\sigma}$ are finite. These expectation values will be denoted by $n_{k\sigma}$ and $h_{k\sigma}(Q)$, respectively. The required linearized hamiltonian derived from (1) is

$$\tilde{\mathcal{H}} = W_0 + \sum_{k,\tau} \tilde{\varepsilon}_{k\sigma} \, c^+_{k\sigma} \, c_{k\sigma} - \frac{1}{2} \sum_{k,\sigma} (\Delta_{k\sigma} \, b^+_{k\sigma} + \text{C.C.}) \,, \tag{2}$$

where

$$\tilde{\varepsilon}_{k\sigma} = \varepsilon_k + \sum_{k',\sigma'} \langle k, k' \,|V|\, k', k\rangle \, n_{k'\sigma'} - \sum_{k'} \langle k, k' \,|V|\, k, k'\rangle \, n_{k\sigma} \tag{3}$$

and $-W_0$ is a constant equal to one half of the Hartree-Fock interaction energy. The quantity $\Delta_{k\sigma}$ is defined by

$$\Delta_{k\sigma} = W_{k+Q,k} - \sum_{k',\sigma'} [\langle k+Q, k'-Q \,|V|\, k', k\rangle - \delta_{\sigma\sigma'} \langle k+Q, k'-Q \,|V|\, k, k'\rangle] \, h^*_{k'\sigma'}(Q) \tag{4}$$

The hamiltonian (2) can be diagonalized with the help of the transformation

$$\begin{bmatrix} \exp\left(-\frac{i}{2}\gamma_\sigma\right) \cos\theta_{k\sigma} & \exp\left(\frac{i}{2}\gamma_\sigma\right) \sin\theta_{k\sigma} \\ -\exp\left(-\frac{i}{2}\gamma_\sigma\right) \sin\theta_{k\sigma} & \exp\left(\frac{i}{2}\gamma_\sigma\right) \cos\theta_{k\tau} \end{bmatrix}, \tag{5}$$

where k runs over the original Brillouin zone. The parameters $\theta_{k\sigma}$ and γ_σ have to be determined variationally by minimizing the total energy. The gap separating the two sub-bands is given by $2\,|\,\Delta_{k\sigma}\,|$. The second and third term in (4) represent the Coulomb and exchange contribution to the gap, respectively. The average quantities $h_{k\sigma}(Q)$ in Equation (4) can be expressed in terms of $\Delta_{k\sigma}$, and $W_{k+Q,k}$ is also related to $\Delta_{k\tau}$ via the lattice parameters. Consequently, Equation (4) really is an equation from which $\Delta_{k\sigma}$ can in principle be determined, provided the band structure and the matrix elements of the electron-electron interaction are known. The parameter γ_σ is a rather important one. It can easily be verified that for $\gamma_\uparrow = 0$ and $\gamma_\downarrow = \pi$ one has antiferro-

magnetic order and if in addition $W = 0$, one reobtains Slater's split-band model of antiferromagnetism as described by DES CLOIZEAUX [4]. On the other hand, if $\gamma_\uparrow = \gamma_\downarrow = \gamma$, there is no magnetic order and the periodic charge distribution of the band electrons and ionic charge distribution will adjust selfconsistently to one another, leading to at least a partial compensation of the lattice and Coulomb contributions to the gap. For $\gamma = \pi/2$, there will be optimum overlap of the electronic and ionic charge densities. It is obvious that for intermediate values of γ_σ one can achieve states which correspond to mixtures of periodic electronic and spin densities.

In general one needs a gap at least comparable to the band width in order to ensure an insulating ground state. One can obtain large gaps by allowing relatively large crystallographic distortions accompanied by large or small Coulomb- and exchange contributions. However, in order to achieve selfconsistency, both the crystallographic distortion and the Coulomb- and exchange contributions are in general required to be large. This is the point we want to make: in treating crystallographic distortions of the type discussed above, one must not overlook the possible importance of electron-electron interactions. However, detailed numerical calculations on specific systems would be required, in order to decide whether the model has any practical applicability. Of course, ion-ion interactions, which we have neglected so far, would then also have to be taken into account.

Finally, we wish to remark that the model described above is a special case of the charge-density-wave model, recently described by OVERHAUSER [5].

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Ein Analogverfahren zur Berechnung der Eigenschaften von Feldeffekttransistoren

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Shockley hat bereits 1952 eine Theorie des Feldeffekttransistors publiziert, welche die Berechnung der statischen Kennlinien gestattet. Der Gültigkeitsbereich dieser Theorie ist eingeschränkt durch die geometrische Auflage, dass die Länge der Gateelektrode gross gegen die Dicke des Transistors sein muss, und durch die physikali-