

# MAGNETIC, ORBITAL AND CHARGE ORDERED STATES IN A TWO-BAND EXTENDED HUBBARD MODEL

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A two-band model of transition metal compound is discussed. Within the Hartree-Fock approximation magnetic, orbital and charge orderings are considered for the case of two electrons per atom. The insulator-metal transition temperatures are given and the ground state stability of the ordered phases is determined.

## 1. Introduction

Magnetic and charge orderings in an extended Hubbard model with intra and interatomic interactions between the electrons have been studied by various authors [1-6]. The possibility of insulator-metal transitions in that model has also been discussed [4-6]. The papers cited above are restricted to the case of a narrow nondegenerate band. This is an essential limitation of the theory. In transition metals and their compounds, orbital degeneracy and interorbital electron interactions necessarily play a very important role [7-9].

Owing to the presence of five  $d$  orbitals per atom, the  $3d$  band is strongly degenerated. Although the crystal field can lower the degree of degeneracy, it does not remove the latter completely.

During recent years, the problem of orbital degeneracy has been dealt with repeatedly [10-12]. Those considerations bore on the simplest model including degeneracy i.e. the two-band Hubbard model, and the authors studied the stability of the ferromagnetic state for the case of very strong intraatomic correlations.

The possibility of a very interesting effect of interorbital interactions, consisting in orbital ordering, was predicted on the basis of the two-band Hubbard model by Roth [13, 14] for the case of one electron per atom. This is two-sublattice ordering. In either sublattice, the electron occupy predominantly one of the orbitals. Simultaneously with orbital ordering, the system exhibits for  $T = 0$ , ferromagnetic ordering as well [13-16]. From the analysis of the model  $T > 0$  performed in the Molecular Field Approximation, it results that the orbital ordering disappears at a temperature higher than the Curie

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temperature [16]. As we shall show further on, in the case of two electrons per atom situation is entirely different: magnetic ordering and orbital ordering exclude mutually.

In this paper, we consider a simplified two-band model of transition metal compound taking into account intra- and interatomic interactions between the electrons.

We shall deal primarily with the case of  $N$  atoms and  $2N$  electrons:  $n = 2$  ( $n$  — the average number of electrons per site), as being of essential interest to us with regard to the possibility of insulator-metal transitions.

We carry out the analysis of our model employing the standard technique of Zubarev's double-time temperature dependent Green functions [17] and decoupling the two-particle Green propagators in the Hartree-Fock scheme [4]. We shall be considering ferromagnetic, antiferromagnetic, charge and orbital orderings in the model. We shall moreover determine the stability of the ground state of the system by performing a comparison of the ground state energies of the various ordered phases.

## 2. Hamiltonian, and general formulation

The Hamiltonian for the model is given as

$$\begin{aligned} \hat{H} = & \sum_{ij\sigma\gamma} T_{ij}^{\gamma} c_{i\sigma\gamma}^{+} c_{j\sigma\gamma} + \frac{1}{2} \sum_{\substack{ij\gamma\gamma' \\ \sigma\sigma'}} U_{ij}^{\gamma\gamma'} n_{i\sigma}^{\gamma} n_{j\sigma'}^{\gamma'} \\ & + \frac{1}{2} \sum_{\substack{ij\gamma\gamma' \\ \sigma\sigma'}} K_{ij}^{\gamma\gamma'} c_{i\sigma\gamma}^{+} c_{j\sigma'\gamma'}^{+} c_{i\sigma'\gamma} c_{j\sigma\gamma} - \mu \sum_{i\gamma\sigma} n_{i\sigma}^{\gamma} \end{aligned} \quad (1)$$

with

$$\begin{aligned} U_{ij}^{\gamma\gamma'} &= (U_{\gamma} \delta_{\sigma, -\sigma'} \delta_{\gamma, \gamma'} + U' \delta_{\gamma, -\gamma'}) \delta_{ij} + W_{\gamma\gamma'} f_{ij}, \\ K_{ij}^{\gamma\gamma'} &= K \delta_{\gamma, -\gamma'} \delta_{ij} + J_{\gamma\gamma'} f_{ij}; \end{aligned} \quad (2)$$

$\gamma = \pm 1$  — orbital index,  $\sigma$  — spin index,  $T_{ij}^{\gamma}$  — hopping integrals between the same orbital states of nearest neighbours,  $U$ ,  $U'$  and  $W_{\gamma\gamma'}$  — intra- and interatomic Coulomb interactions, respectively,  $K$  — intraatomic exchange interaction,  $J_{\gamma\gamma'}$  — interatomic exchange interactions,  $\mu$  — chemical potential,  $f_{ij} = 1$  if  $i, j$  are nearest neighbours and  $f_{ij} = 0$  otherwise. Here, for simplicity, we neglect the hopping integrals  $T_{ij}^{\gamma-\gamma}$  connecting electrons in different orbital states. We assume moreover that the crystal field integrals are independent of  $\gamma$ , i. e.  $T_{ii}^{\gamma\gamma} = T_{ii}^{-\gamma-\gamma} = 0$ .<sup>1</sup>

The equation of motion for the Green function  $G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega) = \langle\langle C_{i\sigma\gamma}; C_{j\sigma'\gamma'}^{+} \rangle\rangle_{\omega}$  for the system described by the Hamiltonian (1) is of the form

$$\begin{aligned} (\omega + \mu) G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega) &= \frac{\delta_{ij} \delta_{\sigma\sigma'} \delta_{\gamma\gamma'}}{2\pi} + \sum_i T_{ii}^{\gamma} G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega) \\ &+ \sum_{\sigma_1\gamma_1} (U_{\gamma} \delta_{\gamma, \gamma_1} \delta_{-\sigma, \sigma_1} + U' \delta_{\gamma, -\gamma_1}) \langle\langle n_{i\sigma_1}^{\gamma_1} c_{i\sigma\gamma}; c_{j\sigma'\gamma'}^{+} \rangle\rangle \end{aligned}$$

<sup>1</sup> Preliminary analysis of this model for the case  $J = 0$ ,  $U = U'$ , has been published by the author [18].

$$\begin{aligned}
& + \sum_{l\sigma_1\gamma_1} W_{\gamma\gamma_1} \langle n_{l\sigma_1}^{\gamma_1} c_{l\sigma\gamma}; c_{j\sigma'\gamma'}^+ \rangle + \sum_{\sigma_1} K \langle c_{i\sigma_1-\gamma}^+ c_{i\sigma_1\gamma} c_{i\sigma-\gamma}; c_{j\sigma'\gamma'}^+ \rangle \\
& + \sum_{l\sigma_1\gamma_1} J_{\gamma\gamma_1} \langle c_{l\sigma_1\gamma_1}^+ c_{l\sigma_1\gamma} c_{l\sigma\gamma_1}; c_{j\sigma'\gamma'}^+ \rangle. \quad (3)
\end{aligned}$$

This equation contains higher order Green functions, to which we apply the following decoupling (which corresponds to the Hartree-Fock approximation):

$$\langle n_{i-\sigma}^{\gamma} c_{i\sigma\gamma}; c_{j\sigma'\gamma'}^+ \rangle = \langle n_{i-\sigma}^{\gamma} \rangle G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega) - \langle c_{i-\sigma\gamma}^+ c_{i\sigma\gamma} \rangle G_{ij\gamma\gamma'}^{-\sigma\sigma'}(\omega), \quad (4a)$$

$$\langle n_{i\sigma_1}^{-\gamma} c_{i\sigma\gamma}; c_{j\sigma'\gamma'}^+ \rangle = \langle n_{i\sigma_1}^{-\gamma} \rangle G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega), \quad (4b)$$

$$\langle n_{i\sigma_1}^{\gamma_1} c_{i\sigma\gamma}; c_{j\sigma'\gamma'}^+ \rangle = \langle n_{i\sigma_1}^{\gamma_1} \rangle G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega), \quad (4c)$$

$$\langle c_{l\sigma_1\gamma_1}^+ c_{i\sigma_1\gamma} c_{l\sigma\gamma_1}; c_{j\sigma'\gamma'}^+ \rangle = -\langle c_{i\sigma_1\gamma_1}^+ c_{l\sigma\gamma_1} \rangle G_{ij\gamma\gamma'}^{\sigma_1\sigma'}(\omega). \quad (4d)$$

Furthermore, we assume that the system is magnetized in the  $x$ -direction rather than in that of the conventional  $z$ -axis. In this case

$$\langle \sigma_{iy}^z \rangle = \langle \sigma_{iy}^x \rangle = 0, \quad (5)$$

where  $\sigma_{iy}^z$  are the components of the electron spin operator  $\sigma_{iy}$

$$\sigma_{iy}^x = \frac{1}{2} \sum_{\sigma} c_{i\sigma\gamma}^+ c_{i-\sigma\gamma}, \quad \sigma_{iy}^y = -\frac{1}{2} i \sum_{\sigma} \sigma c_{i\sigma\gamma}^+ c_{i-\sigma\gamma}, \quad \sigma_{iy}^z = \frac{1}{2} \sum_{\sigma} \sigma c_{i\sigma\gamma}^+ c_{i\sigma\gamma}. \quad (6)$$

With regard to (5), we have

$$\langle c_{i\sigma\gamma}^+ c_{i-\sigma\gamma} \rangle = \langle c_{i-\sigma\gamma}^+ c_{i\sigma\gamma} \rangle, \quad \langle c_{i\sigma\gamma}^+ c_{i\sigma\gamma} \rangle = \langle c_{i-\sigma\gamma}^+ c_{i-\sigma\gamma} \rangle. \quad (7)$$

On applying Eqs (4), (7), and on performing the Fourier transformation

$$\begin{aligned}
c_{i\sigma\gamma} &= N^{-1/2} \sum_{\mathbf{k}} c_{\mathbf{k}\sigma\gamma} \exp(i\mathbf{k} \cdot \mathbf{R}_i), \\
G_{ij\gamma\gamma'}^{\sigma\sigma'}(\omega) &= N^{-1} \sum_{\mathbf{k}_1\mathbf{k}_2} G_{\mathbf{k}_1\mathbf{k}_2\gamma\gamma'}^{\sigma\sigma'}(\omega) \exp(i\mathbf{k}_1 \cdot \mathbf{R}_i - i\mathbf{k}_2 \cdot \mathbf{R}_j), \quad (8)
\end{aligned}$$

where  $N$  is the total number of lattice sites, Eq. (3) takes the form

$$\begin{aligned}
(\omega + \mu - E_k^{\gamma}) G_{kk'\gamma\gamma'}^{\sigma\sigma'}(\omega) &= \frac{\delta_{kk'} \delta_{\sigma\sigma'} \delta_{\gamma\gamma'}}{2\pi} + \frac{1}{N} \sum_{k_1 k_2} U_{\gamma} \langle c_{k_1\sigma\gamma}^+ c_{k_2\sigma\gamma} \rangle \\
& + (2U' - K) \langle c_{k_1\sigma-\gamma}^+ c_{k_2\sigma-\gamma} \rangle \{ G_{k+k_1-k_2\gamma\gamma'}^{\sigma\sigma'}(\omega) \\
& + \frac{1}{N} \sum_{k_1 k_2 \gamma_1} \{ 2W_{k_1}^{\gamma\gamma_1} \langle c_{k_2\sigma\gamma_1}^+ c_{k_1+k_2\sigma\gamma_1} \rangle - J_{k_1}^{\gamma\gamma_1} \langle c_{k_2\sigma\gamma_1}^+ c_{k_1+k_2\sigma\gamma_1} \rangle \} G_{k-k_1, k'\gamma\gamma'}^{\sigma\sigma'}(\omega) \\
& - \frac{1}{N} \sum_{k_1 k_2} \{ U_{\gamma} \langle c_{k_1-\sigma\gamma}^+ c_{k_2\sigma\gamma} \rangle + K \langle c_{k_1-\sigma-\gamma}^+ c_{k_2\sigma-\gamma} \rangle \} G_{k+k_1-k_2, k'\gamma\gamma'}^{-\sigma\sigma'}(\omega) \\
& - \frac{1}{N} \sum_{k_1 k_2 \gamma_1} J_{k_1}^{\gamma\gamma_1} \langle c_{k_2-\sigma\gamma_1}^+ c_{k_1+k_2\sigma\gamma_1} \rangle G_{k-k_1, k'\gamma\gamma'}^{-\sigma\sigma'}(\omega), \quad (9)
\end{aligned}$$

here  $E_k^{\gamma}$ ,  $W_k^{\gamma\gamma'}$ ,  $J_k^{\gamma\gamma'}$  denote, respectively, the Fourier transforms of  $T_{ij}^{\gamma}$ ,  $W_{ij}^{\gamma\gamma'}$ ,  $J_{ij}^{\gamma\gamma'}$ .

For the correlation functions  $\langle C_{k_1\sigma\gamma}^+ C_{k_2\sigma'\gamma} \rangle$  we assume, after Kishore and Joshi [4], that

$$\langle C_{k_1\sigma\gamma}^+ C_{k_2\sigma'\gamma} \rangle = \langle C_{k_1\sigma\gamma}^+ C_{k_1\sigma'\gamma} \rangle \delta_{k_1 k_2} + \langle C_{k_1\sigma\gamma}^+ C_{k_1+Q\sigma'\gamma} \rangle \delta_{k_2, k_1+Q}, \quad (10)$$

where  $Q$  is half the smallest reciprocal lattice vector. This approximation amounts to considering only charge and spin density waves with wave-vectors  $q = 0$  and  $q = Q$ .

We introduce the following definitions:

$$n_\gamma = \frac{1}{N} \sum_{i\sigma} \langle c_{i\sigma\gamma}^+ c_{i\sigma\gamma} \rangle = \frac{1}{N} \sum_{k\sigma} \langle c_{k\sigma\gamma}^+ c_{k\sigma\gamma} \rangle, \quad (11)$$

$$\Delta n_\gamma = \frac{1}{N} \sum_{i\sigma} \langle c_{i\sigma\gamma}^+ c_{i\sigma\gamma} \rangle \exp(iQ \cdot R_i) = \frac{1}{N} \sum_{k\sigma} \langle c_{k+Q\sigma\gamma}^+ c_{k\sigma\gamma} \rangle, \quad (12)$$

$$m_q^\gamma = \frac{2}{N} \sum_i \langle \sigma_{i\gamma}^x \rangle \exp(iq \cdot R_i) = \frac{1}{N} \sum_{k\sigma} \langle c_{k+q\sigma\gamma}^+ c_{k-\sigma\gamma} \rangle, \quad (13)$$

$n_\gamma$  denotes the average number of electrons per orbital  $\gamma$ ;  $\Delta n_\gamma$  is the charge order parameter; and  $m_q^\gamma$  is the magnetic order parameter for these orbitals ( $q = 0$  corresponding to ferromagnetic and  $q = Q$  to antiferromagnetic order).

With regard to Eqs (10) and (11)–(13), Eq. (9) becomes

$$\begin{aligned} & (\omega + \mu - E_k^\gamma - A_0^\gamma) G_{kk'\gamma\gamma}^{\sigma\sigma'}(\omega) + B_0^\gamma G_{kk'\gamma\gamma}^{-\sigma\sigma'}(\omega) \\ & - A_Q^\gamma G_{k+Q, k'\gamma\gamma}^{\sigma\sigma'}(\omega) + B_Q^\gamma G_{k+Q, k'\gamma\gamma}^{-\sigma\sigma'}(\omega) = \frac{\delta_{kk'} \delta_{\sigma\sigma'} \delta_{\gamma\gamma'}}{2\pi}, \end{aligned} \quad (14)$$

where we have used the notation

$$A_0^\gamma = \frac{1}{2} [(U_\gamma + 2zW^{\gamma\gamma} - zJ^{\gamma\gamma})n_\gamma + (2U' - K + 2zW^{\gamma-\gamma} - zJ^{\gamma-\gamma})n_{-\gamma}], \quad (15)$$

$$A_Q^\gamma = \frac{1}{2} [(U_\gamma - 2zW^{\gamma\gamma} + zJ^{\gamma\gamma})\Delta n_\gamma + (2U' - K - 2zW^{\gamma-\gamma} + zJ^{\gamma-\gamma})\Delta n_{-\gamma}], \quad (16)$$

$$B_0^\gamma = \frac{1}{2} [(U_\gamma + zJ^{\gamma\gamma})m_0^\gamma + (K + zJ^{\gamma-\gamma})m_0^{-\gamma}], \quad (17)$$

$$B_Q^\gamma = \frac{1}{2} [(U_\gamma - zJ^{\gamma\gamma})m_Q^\gamma + (K - zJ^{\gamma-\gamma})m_Q^{-\gamma}], \quad (18)$$

$z$  is the number of nearest neighbours.

### 3. Selfconsistent equations and the density of states

#### A. Charge or orbital ordered states

In these states  $m_0 = m_Q = 0$ . Since  $G_{k+2Q, k'\gamma\gamma}^{\sigma\sigma'} = G_{kk'\gamma\gamma}^{\sigma\sigma'}$ , we derive from Eq. (14) the following form of the Green function  $G_{kk'\gamma\gamma}^{\sigma\sigma'}(\omega)$ :

$$G_{kk'\gamma\gamma}^{\sigma\sigma'}(\omega) = \frac{\delta_{\sigma\sigma'}}{2\pi} \frac{(\omega + \mu - E_{k+Q}^\gamma - A_0^\gamma) \delta_{kk'} + A_Q^\gamma \delta_{k+Q, k'}}{(\omega - \omega_{k\gamma}^-) (\omega - \omega_{k\gamma}^+)}, \quad (19)$$

where

$$\omega_{k\gamma}^{\pm} = -\mu + A_0^{\gamma} + \frac{1}{2} (E_k^{\gamma} + E_{k+Q}^{\gamma}) \pm A_{k\gamma}, \quad (20)$$

$$A_{k\gamma} = [\frac{1}{4} (E_k^{\gamma} - E_{k+Q}^{\gamma})^2 + (A_Q^{\gamma})^2]^{1/2}. \quad (21)$$

Henceforth we shall consider but those bands for which

$$E_{k+Q}^{\gamma} = -E_k^{\gamma}. \quad (22)$$

Once the Green function (19) is known, we can calculate the correlation function  $\langle c_{k'\sigma\gamma}^{\dagger} c_{k\sigma\gamma} \rangle$  required to determine the number of electrons per atom and charge order parameters  $\Delta n_{\gamma}$

$$\begin{aligned} \langle c_{k'\sigma\gamma}^{\dagger} c_{k\sigma\gamma} \rangle &= \frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega f(\omega) \left\{ \delta_{kk'} [\delta(\omega - \omega_{k\gamma}^-) + \delta(\omega - \omega_{k\gamma}^+)] \right. \\ &\quad \left. + \delta_{k+Q,k'} \frac{A_Q^{\gamma}}{\sqrt{E_k^{\gamma} + (A_Q^{\gamma})^2}} [\delta(\omega - \omega_{k\gamma}^-) - \delta(\omega - \omega_{k\gamma}^+)] \right\}, \quad (23) \end{aligned}$$

where

$$f(\omega) = [\exp(\beta\omega) + 1]^{-1}, \quad \beta = (k_B T)^{-1}.$$

By having recourse to Eqs (11)–(12) and (23), we obtain equations for  $n$  and  $\Delta n_{\gamma}$

$$n = n_1 + n_{-1} = \frac{2}{N} \sum_{k\gamma} [f(\omega_{k\gamma}^-) + f(\omega_{k\gamma}^+)], \quad (24)$$

$$\Delta n_{\gamma} = -\frac{2A_Q^{\gamma}}{N} \sum_k \frac{f(\omega_{k\gamma}^-) - f(\omega_{k\gamma}^+)}{A_{k\gamma}}. \quad (25)$$

## B. Ferromagnetic state

In the ferromagnetic state  $m_Q^{\gamma} = \Delta n_{\gamma} = 0$ . On solving Eq. (14) for  $G_{kk'\gamma\gamma}^{\sigma\sigma'}(\omega)$ , we obtain

$$G_{kk'\gamma\gamma}^{\sigma\sigma'}(\omega) = \frac{\delta_{kk'} (\omega + \mu - E_k^{\gamma} - A_0^{\gamma}) \delta_{\sigma\sigma'} - B_0^{\gamma} \delta_{-\sigma\sigma'}}{2\pi (\omega - \omega_{k\gamma}^-) (\omega - \omega_{k\gamma}^+)}, \quad (26)$$

where

$$\omega_{k\gamma}^{\pm} = -\mu + E_k^{\gamma} + A_0^{\gamma} \pm B_0^{\gamma}. \quad (27)$$

Hence the correlation function is

$$\begin{aligned} \langle c_{k'\sigma'\gamma}^{\dagger} c_{k\sigma\gamma} \rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \{ [\delta(\omega - \omega_{k\gamma}^-) + \delta(\omega - \omega_{k\gamma}^+)] \delta_{\sigma\sigma'} \\ &\quad - [\delta(\omega - \omega_{k\gamma}^-) - \delta(\omega - \omega_{k\gamma}^+)] \delta_{-\sigma\sigma'} \} \delta_{kk'}. \end{aligned}$$

By this equation and Eqs (11), (12), we obtain the equations for  $n$  and  $m_0^y$

$$n = \frac{2}{N} \sum_{k\gamma} [f(\omega_{k\gamma}^-) + f(\omega_{k\gamma}^+)], \quad (28)$$

$$m_0^y = \frac{2}{N} \sum_k [f(\omega_{k\gamma}^-) - f(\omega_{k\gamma}^+)]. \quad (29)$$

### C. Antiferromagnetic state

In this state  $\Delta n_\gamma = m_0^y = 0$ , and from Eq. (14) we have

$$G_{kk'\gamma\gamma}^{\sigma\sigma'}(\omega) = \frac{1}{2\pi} \frac{(\omega + \mu + E_k^\gamma - A_0^\gamma) \delta_{kk'} \delta_{\sigma\sigma'} - B_Q^\gamma \delta_{k+Q, k'} \delta_{-\sigma\sigma'}}{(\omega + \mu - E_k^\gamma - A_0^\gamma)(\omega + \mu + E_k^\gamma - A_0^\gamma) - (B_Q^\gamma)^2}. \quad (30)$$

The poles  $G_{kk'\gamma\gamma}^{\sigma\sigma'}$  are given by

$$\omega_{k\gamma}^\pm = -\mu + A_0^\gamma \pm \sqrt{(E_k^\gamma)^2 + (B_Q^\gamma)^2}. \quad (31)$$

The equations for  $n$  and  $m_Q^y$  are given by

$$n = \frac{2}{N} \sum_{k\gamma} [f(\omega_{k\gamma}^-) + f(\omega_{k\gamma}^+)], \quad (32)$$

$$m_Q^y = \frac{2B_Q^\gamma}{N} \sum_k \frac{f(\omega_{k\gamma}^-) - f(\omega_{k\gamma}^+)}{\omega_{k\gamma}^+ - \omega_{k\gamma}^-}. \quad (33)$$

The density of states per atom for all types of order have the form

$$\rho(\omega) = \frac{1}{N} \sum_{k\gamma} [\delta(\omega - \omega_{k\gamma}^+) + \delta(\omega - \omega_{k\gamma}^-)] \quad (34)$$

with  $\omega_{k\gamma}^\pm$  given by (20), (27) and (31), respectively. Eq. (34) shows that the number of states per atom in each band is equal to one. If  $E_{k+Q}^\gamma = -E_k^\gamma$  the bands  $\omega_{k\gamma}^-$  and  $\omega_{k\gamma}^+$  are separated by the energy gaps

$$E_{g\gamma}^C = 2A_0^\gamma, \quad (35)$$

$$E_{g\gamma}^F = 2B_0^\gamma - D_\gamma, \quad (36)$$

$$E_{g\gamma}^{AF} = 2B_Q^\gamma, \quad (37)$$

where  $D_\gamma$  is a bandwidth of  $E_k^\gamma$  band. The difference in centre of gravity of the bands  $\omega_{k(1)}$  and  $\omega_{k(-1)}$

$$E_{1,-1}^0 = A_0^{(1)} - A_0^{(-1)}.$$

Henceforth, we shall restrict our considerations to the case for which  
(i) the interelectronic interactions are independent of the band index  $\gamma$ ,

$$(ii) \quad n_1 + n_{-1} = 2, \quad (38)$$

$$(iii) \quad J^{\prime\prime\prime} = 0$$

The case of two electrons per atom is of essential interest with regard to the possibility of insulator-metal transitions, whereas the assumption (iii) was introduced by us in order to restrict the number of parameters.

We denote

$$U_\gamma = U, \quad zW^{\prime\prime} = W, \quad zW^{\prime\prime\prime} = W', \quad zJ^{\prime\prime} = J. \quad (39)$$

For  $n$  given by (24), (28) or (32), we can easily obtain the solutions of Eq. (38). With regard to (39), we get

$$n_\gamma = n_{-\gamma} = 1, \quad \mu = A_0, \quad (40)$$

with

$$A_0 = A_0^\gamma = A_0^{-\gamma} = \frac{1}{2}(U + 2U' + 2W + 2W' - K - J).$$

Now Eqs (25), (29), (33) for the order parameters take the form

1. charge or orbital ordered state

$$\Delta n_\gamma = -\frac{A_0^\gamma}{N} \sum_k \frac{\text{th} [\frac{1}{2} \beta \sqrt{(E_k^\gamma)^2 + (A_0^\gamma)^2}]}{\sqrt{(E_k^\gamma)^2 + (A_0^\gamma)^2}}, \quad (41)$$

2. ferromagnetic state

$$m_0^\gamma = \frac{1}{N} \sum_k \text{th} [\frac{1}{2} \beta (E_k^\gamma + B_0^\gamma)], \quad (42)$$

3. antiferromagnetic state

$$m_Q^\gamma = \frac{B_Q^\gamma}{N} \sum_k \frac{\text{th} [\frac{1}{2} \beta \sqrt{(E_k^\gamma)^2 + (B_Q^\gamma)^2}]}{\sqrt{(E_k^\gamma)^2 + (B_Q^\gamma)^2}}, \quad (43)$$

where

$$A_Q^\gamma = \frac{1}{2} [(U + J - 2W)\Delta n_\gamma + (2U' - 2W' - K)\Delta n_{-\gamma}], \quad (44)$$

$$B_0^\gamma = \frac{1}{2} [(U + J)m_0^\gamma + Km_0^{-\gamma}], \quad (45)$$

$$B_Q^\gamma = \frac{1}{2} [(U - J)m_Q^\gamma + Km_Q^{-\gamma}]. \quad (46)$$

If Eq. (40) is fulfilled, then obviously  $E_{1-1}^0 = 0$ , and for  $E_{g(1)} > 0$ ,  $E_{g(-1)} > 0$  the system behaves like an insulator. The lower subbands  $\omega_{k\gamma}^-$  are then completely occupied, whereas the upper subbands  $\omega_{k\gamma}^+$  are empty. If one of the gaps  $E_{g(1)}$  or  $E_{g(-1)}$  or both

simultaneously decrease to zero, an insulator-metal transition takes place. As it follows from Eqs (35), (37), the insulator-metal transition temperature  $T_M$  for the charge and antiferromagnetic ordered states is equal to the long range ordering temperature. For the ferromagnetic state,  $T_M$  is determined by  $2B_0^y = D_y$  and obviously is always lower than the Curie temperature  $T_c$ .

#### 4. Discussion of the solutions for two electrons per atom

We now proceed to consider two particular cases

- A. identical bands ( $E_k^{(1)} = E_k^{(-1)} = E_k$ , for all  $k$ ),  
 B. zero width of one of the bands ( $E_k^{(-1)} = 0$ ,  $E_k^{(1)} = E_k$ ).

##### 4.1. The case of identical bands

##### 4.1.1. Charge or orbital ordering

Here, the selfconsistent equations (41) for the order parameters take the form

$$\Delta n_y = - \frac{A_1 \Delta n_y + A_2 \Delta n_{-y}}{N} \sum_k \frac{\text{th} \left\{ \frac{1}{2} \beta \sqrt{(E_k^y)^2 + (A_1 \Delta n_y + A_2 \Delta n_{-y})^2} \right\}}{\sqrt{(E_k^y)^2 + (A_1 \Delta n_y + A_2 \Delta n_{-y})^2}}, \quad (47')$$

where

$$A_1 = \frac{1}{2}(U + J - 2W), \quad A_2 = \frac{1}{2}(2U' - K - 2W'). \quad (48)$$

At sufficiently low temperatures Eqs (47) can have other non-zero solutions besides  $\Delta n_y = 0$ , thus

$$(i) \Delta n_y, \Delta n_{-y} > 0; \quad (ii) \Delta n_y > 0, \quad \Delta n_{-y} < 0.$$

The first pair corresponds to the charge ordered state and the other pair to the orbital ordered state.

Let us consider these solutions for  $T = 0$ .

(i)  $\Delta n_y = \Delta n_{-y}$ ; in this case we obtain from (47)

$$1 = - \frac{A_1 + A_2}{N} \sum_k \frac{1}{\sqrt{(E_k)^2 + (A_1 + A_2)^2 (\Delta n_y^0)^2}}, \quad (49)$$

whence, for the square density of states for the bands  $E_k$

$$P(E) = \frac{1}{D}, \quad \text{if } -\frac{1}{2}D < E < \frac{1}{2}D, \quad (50)$$

$$= 0 \quad \text{otherwise,}$$

we have

$$\Delta n_y^0 = - \frac{D}{2(A_1 + A_2)} \left[ \text{sh} \frac{D}{-2(A_1 + A_2)} \right]^{-1}, \quad \text{if } A_1 + A_2 < 0, \quad (49a)$$

$$\Delta n_y^0 = 0, \quad \text{in the other case.}$$



(ii)  $\Delta n_\gamma = -\Delta n_{-\gamma}$ ;

$$\Delta n_\gamma^0 = -\frac{D}{2(A_1 - A_2)} \left[ \operatorname{sh} \frac{D}{2(A_2 - A_1)} \right]^{-1}, \quad \text{if } A_1 - A_2 < 0, \quad (51)$$

$$\Delta n_\gamma^0 = 0, \quad \text{in the other case.}$$

In the case (i) the average occupancy number of both orbitals in one sublattice is higher than in the other sublattice (charge ordering). The case (ii) corresponds to alternate

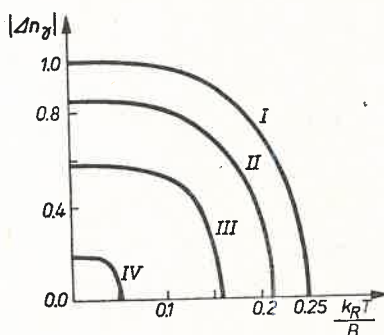


Fig. 1. The charge ordering parameters  $|\Delta n_\gamma|$  as functions of the temperature  $T$ , for  $\frac{D}{B} = 0$  (I); 1.5 (II); 3.0 (III); 6.0 (IV);  $B = -2(A_1 + A_2)$  in the charge ordered state and  $B = 2(A_2 - A_1)$  in the orbital ordered state

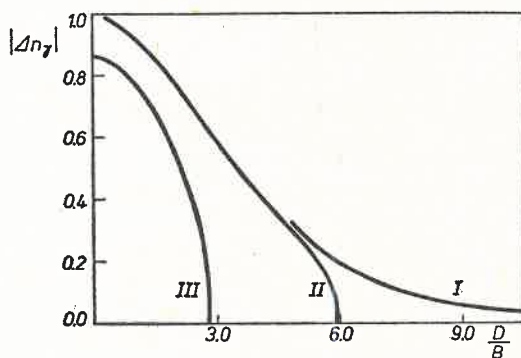


Fig. 2. The charge ordering parameters  $|\Delta n_\gamma|$  as functions of the bandwidth  $D$ , for  $\frac{2k_B T}{B} = 0$  (I); 0.10 (II); 0.33 (III)

orbital occupancy: in one sublattice the electrons occupy predominantly the  $\gamma$  orbital and in the other sublattice the  $(-\gamma)$  orbital (orbital ordering).

As the temperature rises the parameters  $\Delta n_\gamma$  gradually decrease. At a critical temperature (which is identical for both subsystems  $\gamma$ ) a phase transition occurs from charge or orbital ordered insulator to metal. This temperature, for the charge ordered state, is

given by

$$T_{co} = \frac{0.57}{k_B} \exp \left[ \frac{D}{2(A_1 + A_2)} \right], \quad (52)$$

and for the orbital ordered state by

$$T_{oo} = \frac{0.57}{k_B} \exp \left[ \frac{D}{2(A_1 - A_2)} \right]. \quad (53)$$

For the case considered above, in the orbital ordered state the number of electrons per atom in both sublattices is the same, since  $\Delta n_\gamma = \Delta n_{-\gamma}$ . The situation is different for bands of different widths (see § 4.2). In Fig. 1 we show the variation of the charge ordering parameters  $|\Delta n_\gamma|$  as functions of  $T$  for various fixed values of the bandwidth  $D$ , and in Fig. 2 — the variations  $|\Delta n_\gamma|$  as functions of  $D$  for various fixed  $T$ .

#### 4.1.2. Ferro and antiferromagnetic states

For  $E_k^\gamma = E_k^{-\gamma} = E_k$ , Eqs (42) and (43) have the form

(i) ferromagnetic state

$$m_0^\gamma = \frac{1}{N} \sum_k \text{th} \left\{ \frac{1}{2} \beta [E_k + (U+J)m_0^\gamma + Km_0^{-\gamma}] \right\}, \quad (54)$$

(ii) antiferromagnetic state

$$m_Q^\gamma = \frac{(U-J)m_Q^\gamma + Km_Q^{-\gamma}}{2N} \sum_k \frac{\text{th} \left\{ \frac{1}{2} \beta \sqrt{(E_k)^2 + \frac{1}{4} [(U-J)m_Q^\gamma + Km_Q^{-\gamma}]^2} \right\}}{\sqrt{(E_k)^2 + \frac{1}{4} [(U-J)m_Q^\gamma + Km_Q^{-\gamma}]^2}}. \quad (55)$$

These equations likewise to Eqs (41), can have nonzero solutions  $m^\gamma = \pm m^{-\gamma} \neq 0$ . Ferromagnetic coupling  $K > 0$  causes that the solutions  $m^\gamma = -m^{-\gamma}$  are always unstable with respect to the solutions  $m^\gamma = m^{-\gamma}$ . We therefore consider only the case  $m^\gamma = m^{-\gamma}$ . At  $T = 0$ , for (5), we have

$$(i) \quad m_0^\gamma = 1, \quad \text{if } U+J+K > D, \\ m_0^\gamma = 0, \quad \text{in the other cases.} \quad (56)$$

$$(ii) \quad m_Q^\gamma = \frac{D}{U-J+K} \left[ \text{sh} \frac{D}{U-J+K} \right]^{-1}. \quad (57)$$

From (56) it follows that at  $T = 0$  in the ferromagnetic state the discontinuous ferromagnetic insulator — paramagnetic metal transition takes place for  $D = U+K+J$ . In the antiferromagnetic state, the situation is different. Here, the ordering parameters  $m_Q^\gamma$  vary continuously from 1 to 0 as the band-width  $D$  grows from 0 to  $\infty$ . Hence at  $T = 0$  in this state no insulator-metal transition can occur. From (54) and (55) we obtain equa-

tions for the critical temperatures  $T_c$  and  $T_N$

$$(i) \quad \frac{4}{U+J+K} = \frac{1}{N} \sum_k \frac{\beta_c}{\cos^2 h(\frac{1}{2} \beta_c E_k)}, \quad (58)$$

$$(ii) \quad 1 = \frac{U-J+K}{2N} \sum_k \frac{\text{th}(\frac{1}{2} \beta_N E_k)}{E_k}. \quad (59)$$

These equations, for square density of states (50), give

$$(i) \quad T_c = \frac{D}{4k_B} \text{arth}\left(\frac{D}{U+J+K}\right), \quad (60)$$

$$(ii) \quad T_N = \frac{0.57D}{k_B} \exp\left(\frac{-D}{U-J+K}\right). \quad (61)$$

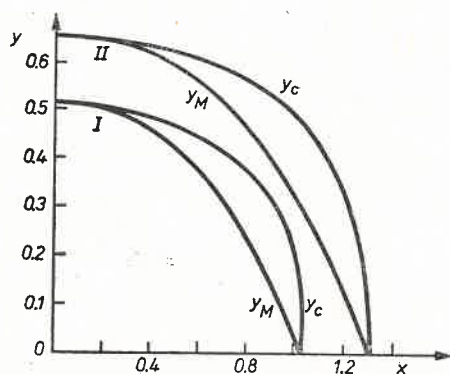


Fig. 3. Variation of the Curie temperature  $\left(y_c = \frac{2k_B T_c}{U+K}\right)$  and the insulator — metal temperature  $\left(y_M = \frac{2k_B T_M}{U+K}\right)$  as a function of the bandwidth  $\left(x = \frac{D}{U+K}\right)$ , for  $\frac{J}{U+K} = 0.03$  (I); 0.3 (II)

Eq. (61) has been obtained on the assumption  $\frac{U-J+K}{D} \ll 1$ . In the ferromagnetic state, the insulator-metal transition temperature  $T_M$  is given, for a square density of states, by

$$\frac{D\beta_M}{2} = \frac{U+J+K}{D} \ln \cosh \frac{D\beta_M}{4}. \quad (62)$$

Hence, for  $D < U+J+K$ , the ferromagnetic insulator first goes over into an ferromagnetic metal at  $T_M$  and then into a paramagnetic metal at  $T_c$ . The variations of the Curie temperature  $T_c$  and the insulator-metal temperature  $T_M$  as functions of the bandwidth, for two fixed values  $\frac{J}{U+K}$  are shown in Fig. 3.

## 4.2. Zero width of one of the bands

### 4.2.1. Charge or orbital ordered states

If one of the bands is very narrow, we obtain from Eqs (41) that for  $T = 0$  in the charge ordered state

$$\Delta n_{(-1)}^0 = 1, \\ \Delta n_{(1)}^0 = -\frac{A_1 \Delta n_{(1)}^0 + A_2}{N} \sum_k \frac{1}{\sqrt{(E_k)^2 + (A_1 \Delta n_{(1)}^0 + A_2)^2}}, \quad \text{if } -A_2 \Delta n_{(1)}^0 > A_1, \quad (63)$$

whereas in the orbital ordered state

$$\Delta n_{(-1)}^0 = -1, \\ \Delta n_{(1)}^0 = \frac{-(A_1 \Delta n_{(1)}^0 - A_2)}{N} \sum_k \frac{1}{\sqrt{(E_k)^2 + (A_1 \Delta n_{(1)}^0 - A_2)^2}}, \quad \text{if } A_2 \Delta n_{(1)}^0 > A_1. \quad (64)$$

Transitions to the nonordered metallic state occur in the temperatures  $T_{co}$  and  $T_{oo}$ , respectively, which are given by

$$\frac{\beta_{co} A_1 + 4}{-A_1(\beta_{co} A_1 + 4) + A_2^2 \beta_{co}} = \frac{1}{2N} \sum_k \frac{\text{th}(\frac{1}{2} \beta_{co} E_k)}{E_k}, \quad (65)$$

$$\frac{\beta_{oo} A_1 - 4}{A_1(\beta_{oo} A_1 - 4) - A_2^2 \beta_{oo}} = \frac{1}{2N} \sum_k \frac{\text{th}(\frac{1}{2} \beta_{oo} E_k)}{E_k}. \quad (66)$$

As it results from (64), in the orbital ordered state too the average number of electrons per atom in the one sublattice ( $2 + \Delta n_{\gamma} + \Delta n_{-\gamma}$ ) differs from that in the other ( $2 - \Delta n_{\gamma} - \Delta n_{-\gamma}$ ). However, the difference in average electron occupancy of the atoms in different sublattices is smaller than in the charge ordered state.

### 4.2.2. Ferromagnetic state

At  $T = 0$ , in addition to the solutions  $m_0 = 0$  there exist yet other pairs of solutions. For a square density of states (50), one has

$$m_0^{(-1)} = 1, \\ m_0^{(1)} = 1, \quad \text{for } U + J + K > D \quad (67)$$

and

$$m_0^{(-1)} = 1, \\ m_0^{(1)} = \frac{K}{D - U - J}, \quad \text{for } U + J + K < D. \quad (68)$$

Contrary to the situation of case § 4.1. here ferromagnetism is possible, for  $T = 0$ , even if  $D > U + J + K$ . In this case  $E_g^{(1)} = 0$  and the system is metallic. For  $D = U + J + K$ ,

at  $T = 0$  a ferromagnetic insulator-ferromagnetic metal transition takes place. Moreover, by (68) the wide band subsystem exhibits but incomplete ferromagnetic order ( $m_0^{(1)} < 1$ ).

The Curie temperature  $T_c$  is determined as

$$\frac{\beta_c(U+J)-4}{(U+J)[\beta_c(U+J)-4]-K^2\beta_c} = \frac{\beta_c}{4N} \sum_k \frac{1}{\cos^2 h(\frac{1}{2}\beta_c E_k)}, \quad (69)$$

whereas  $T_M$  — by Eqs (42) (in which we get  $E_k^{(-1)} = 0$ ) and the equation  $(U+J)m_0^{(1)} + Km_0^{(-1)} = D$ .

#### 4.2.3. Antiferromagnetic state

At  $T = 0$  the nonzero solutions for  $m_Q$  have the form  $m_Q^{(-1)} = 1$

$$m_Q^{(1)} = \frac{(U-J)m_Q^{(1)} + K}{2N} \sum_k \frac{1}{\sqrt{E_k^2 + \frac{1}{4} [(U-J)m_Q^{(1)} + K]^2}}, \quad (70)$$

whereas the Neel temperature is given by

$$\frac{\beta_N(U-J)-4}{(U-J)[\beta_N(U-J)-4]-K^2\beta_N} = \frac{1}{2N} \sum_k \frac{\text{th}(\frac{1}{2}\beta_N E_k)}{E_k}. \quad (71)$$

For this type of order we obtain no new qualitative conclusions in comparison with the case of identical bands.

### 5. Internal energy of the system and stability the ordered phases

The internal energy per atom of the system described by the Hamiltonian (1) can be expressed by the one-particle Green function [4, 17]

$$E = \frac{\langle \hat{H} \rangle}{N} = \frac{i}{2N} \lim_{\epsilon \rightarrow 0+} \sum_{k\alpha\gamma} \int_{-\infty}^{\infty} (\omega + \mu + E_k^{\alpha}) [G_{kk\gamma\gamma}^{\sigma\sigma}(\omega + i\epsilon) - G_{kk\gamma\gamma}^{\sigma\sigma}(\omega - i\epsilon)] f(\omega) d\omega. \quad (72)$$

By insertion of the corresponding Green functions into this equation we evaluate, as in the one-band model [4, 5], the internal energy of the system for paramagnetic, ferromagnetic, antiferromagnetic, charge and orbital ordered states in the case of two electrons per atom.

#### 1. Paramagnetic state

$$E_p = A_0 - \frac{1}{2N} \sum_{k\gamma} E_k^{\gamma} f(E_k^{\gamma}), \quad (73)$$

#### 2, 3. Charge or orbital ordered states

$$E_{c,o} = A_0 - \frac{1}{2N} \sum_{k\gamma} \frac{2(E_k^{\gamma})^2 + (A_Q^{\gamma})^2}{\sqrt{(E_k^{\gamma})^2 + (A_Q^{\gamma})^2}} \text{th} [\frac{1}{2}\beta \sqrt{(E_k^{\gamma})^2 + (A_Q^{\gamma})^2}], \quad (74)$$

## 4. Ferromagnetic state

$$E_F = A_0 - \frac{1}{2} \sum_{\gamma} B_0^{\gamma} m_0^{\gamma} - \frac{1}{N} \sum_{k\gamma} E_k^{\gamma} [f(E_k^{\gamma} + B_0^{\gamma}) + f(E_k^{\gamma} - B_0^{\gamma})], \quad (75)$$

## 5. Antiferromagnetic state

$$E_{AF} = A_0 - \frac{1}{2N} \sum_{k\gamma} \frac{2(E_k^{\gamma})^2 + (B_0^{\gamma})^2}{\sqrt{(E_k^{\gamma})^2 + (B_0^{\gamma})^2}} \operatorname{th} \left[ \frac{1}{2} \beta \sqrt{(E_k^{\gamma})^2 + (B_0^{\gamma})^2} \right]. \quad (76)$$

When deriving  $E$ , we had recourse to Eqs (19), (26), (30) as well as to the selfconsistent equations for the order parameters, and the equality  $E_{k+Q}^{\gamma} = -E_k^{\gamma}$ .

Eqs (73)–(76) in the case  $T = 0$  define the ground state energy per atom  $E^0$ , for the states analysed.

We have

$$1. \quad E_p^0 = A_0 + \frac{2}{N} \sum_{k\gamma(E_k^{\gamma} < 0)} E_k^{\gamma}, \quad (77)$$

$$2,3. \quad E_{c,o}^0 = A_0 - \frac{1}{2N} \sum_{k\gamma} \frac{2(E_k^{\gamma})^2 + (A_1 \Delta n_{\gamma} + A_2 \Delta n_{-\gamma})^2}{\sqrt{(E_k^{\gamma})^2 + (A_1 \Delta n_{\gamma} + A_2 \Delta n_{-\gamma})^2}}, \quad (78)$$

$$4. \quad E_F^0 = A_0 - \frac{1}{2} \sum_{\gamma} [(U+J)m_0^{\gamma} + Km_0^{(-\gamma)}] m_0^{\gamma}, \quad (79)$$

$$5. \quad E_{AF}^0 = A_0 - \frac{1}{2N} \sum_{k\gamma} \frac{2(E_k^{\gamma})^2 + [(U-J)m_0^{\gamma} + Km_0^{(-\gamma)}]^2}{\sqrt{(E_k^{\gamma})^2 + [(U-J)m_0^{\gamma} + Km_0^{(-\gamma)}]^2}}. \quad (80)$$

Hence, for the square density of states (50) and on the assumption of  $D_{(1)} = D_{(-1)} = D$ , we obtain

$$1. \quad E_p^0 = A_0 - \frac{D}{2}, \quad (81)$$

$$2. \quad E_c^0 = A_0 - \frac{D}{2} \operatorname{cth} \left[ \frac{D}{-2(A_1 + A_2)} \right], \quad (82)$$

$$3. \quad E_o^0 = A_0 - \frac{D}{2} \operatorname{cth} \left[ \frac{D}{2(A_2 - A_1)} \right], \quad (83)$$

$$4. \quad E_F^0 = A_0 - \frac{1}{2} (U+J+K), \quad \text{for } D < U+J+K, \\ = E_p^0, \quad \text{for } D > U+J+K, \quad (84)$$

$$5. \quad E_{AF}^0 = A_0 - \frac{D}{2} \operatorname{cth} \left( \frac{D}{U-J+K} \right). \quad (85)$$

Comparing  $E^0$  for these five cases we are able to say which of them has the lowest energy for given values of the parameters and thus to decide what type of order the system as a whole will exhibit.

In the particular case of zero interatomic interactions, we obtain that the ground state of the system is always antiferromagnetic, whereas in the case  $J = 0$  the paramagnetic and ferromagnetic states are always unstable in relation to the other types of ordering.

In general,

- (i) if  $-2(A_1 + |A_2|) < U + K + J$  the ground state is charge-ordered for  $A_2 < 0$  and orbital-ordered for  $A_2 > 0$ ,
- (ii) for  $-2(A_1 + |A_2|) < U + K + J$  the regions of stability of the ordered phases are shown in Fig. 4.

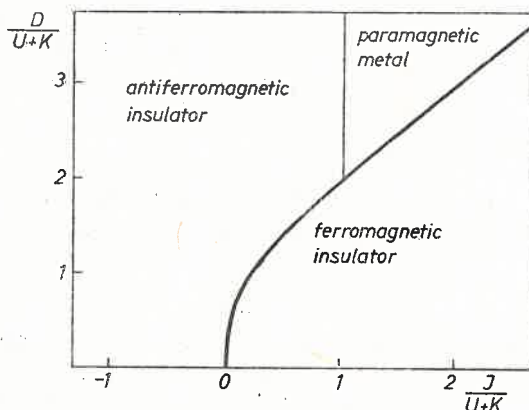


Fig.4. The phase boundaries between ordered states for  $-2(A_1 + |A_2|) < U + K + J$

For  $U = U'$ ,  $K = J = 0$ , these criteria simplify considerably; in this situation, the ground state is antiferromagnetic for  $U < W, W'$ , charge ordered for  $W, W' > U$ , and orbital ordered for  $W > U > W'$ .

### 5. Final remarks

In this work we considered a two-band extended Hubbard model taking into account intra- and interatomic interaction between electrons. We investigated primarily the case of half-filled bands ( $n = 2$ ).

In a two-band Hubbard model only antiferromagnetic ordering is possible for this case. Here we obtained that the system can exhibit ferromagnetic, antiferromagnetic, charge or orbital ordering, according to the values the interaction parameters. Both charge and orbital ordering is due to interatomic Coulomb interaction of the electrons, and their mutual stability depends on the magnitude of interorbital interactions. On the other hand, ferromagnetic ordering is due to interatomic exchange interactions.

In the case of antiferromagnetic, charge and orbital order the system is nonmetallic in the low temperature phase and an insulator-metal transition occurs simultaneously with the transition to the disordered state. On the contrary, for the ferromagnetic state the insulator-metal transition temperature is always lower than the Curie temperature.

In this work we investigated in detail two cases (i) identical bands, (ii) one of the bands very narrow. There are important differences in the behaviour of the system for the two cases.

We found that the properties of the ferro- and antiferromagnetic orderings in the case (i) are very similar to those of the one-band extended Hubbard model [4, 5], whereas in the case (ii) — to those of the modified Zener model [19, 20]. Moreover, in the case (ii) in the orbital-ordered state, there exists additionally charge-ordering (contrary to the case (i)) i. e. the number of electrons per atom in the one sublattice differs from that in the other.

In the present case of half-filled bands, magnetic and charge or orbital orderings exclude mutually. For  $n \neq 2$  it follows from the ground state analysis of the two-band Hubbard model [21, 22] that the situation has to be quite different. In that model, if  $n = 1$ , the ferromagnetic and orbital orderings occur simultaneously and the orbital ordering temperature is always higher than the Curie temperature [16].

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