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Metallic ferromagnetism in the systems with strongly correlated electrons

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The present paper considers the ground state ferromagnetic ordering in narrow-band models with strongly correlated electrons, in particular, in a single-band generalized Hubbard model with correlated hopping and interatomic exchange interaction, as well as in a double orbitally degenerate Hubbard model with correlated hopping. The effective Hamiltonians of these models are treated by means of variants of generalized Hartree-Fock approximations, in which the quasi-particle energy spectra are obtained. The ground state energy, critical electron concentration and magnetization are calculated for some types of density of states. The mechanisms of ferromagnetic ordering stability in the narrow-band materials are discussed.

Key words: *narrow energy band, ferromagnetism, ground state energy, magnetization*

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1. Introduction

The interest to the Hubbard model [1] and its generalizations has been resumed lately due to the intensive studies of the electrical and the magnetic properties of the materials with narrow energy bands.

The issue of the origin of ferromagnetism in the narrow-band materials still remains open, despite a great number of papers devoted to it (for review see [2,3]).

The most favorable situation for ferromagnetism is observed in the Hubbard model with a partially filled band and intra-atomic Coulomb repulsion energy $U \to \infty$. The extension of Nagaoka's result [4] to the case of finite number of holes (electrons) in the framework of various approximations leads to the conclusion that ferromagnetic solution in the Hubbard model is possible in some concentration region [5–10]. A considerable peculiarity of the results obtained in papers [6–8], similar

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in the ideology to the paper [5], is the presence in the single-particle energy spectrum of a spin-dependent shift of the band centers, which is responsible for the ferromagnetism stabilization. In fact, this is the "only" distinction [11] of the cited approximations from Hubbard-I approximation. The shape of the density of states essentially effects the ferromagnetism stability. This fact is emphasized in [8], as well as in papers [12,13].

At the same time, in a number of papers the question of ferromagnetic solution in the Hubbard model is disputed. It is generally agreed that in the Hubbard model the ferromagnetic ordering is not realized in the case of small electron concentration $n \ll 1$ (the gas limit) [14]. The extension of Nagaoka's theorem to the case of a system with a finite number of holes is not trivial whereas the thermodynamic limit for half-filling does not exist. It should be also noted that approximations [1,5,16,17] (and the above cited papers which follow the ideology of Roth) for the case of Mott-Hubbard insulator do not provide the Curie law for magnetic susceptibility [18]. At $n = 1$ and $U \to \infty$ the electrons are localized on the lattice sites and the equation for the magnetization should take the mean-field form, which can be obtained only if the unrealistic condition $w/zJ \to 0$ is satisfied. The absence of ferromagnetic solution has been also indicated in [15], where the calculation of magnetic susceptibility in the random phase approximation has been done.

Although there are arguments that corroborate the existence of ferromagnetism in the Hubbard model, this problem requires further studies. In addition, it has been repeatedly emphasized [19–24], that a consistent analysis of the correlation effects in the narrow bands should be carried out in the framework of generalized Hubbard model. Other matrix elements of electron-electron interactions, in particular, an inter-atomic exchange interaction [19,12,25–27] and correlated hopping [28,29] have to be taken into account at the investigation of ferromagnetic ordering in the narrow band materials.

It can be noted that the extension of the narrow band model to the case of a system with orbital degeneracy, which takes place in the transition metal compounds, can provide the additional mechanisms of ferromagnetism stabilization. At the same time, the majority of the results in the case of degenerated band (see for example [30–35]) are devoted only to a "standard" generalization of the degenerate Hubbard model. Besides, taking into account the correlated hopping essentially enriches the properties of the model (see [36–38]).

In this paper, the consideration of ferromagnetism in narrow bands in the case of strong electron-electron correlations is based on the variants of generalized Hartree-Fock approximation [24]. In the framework of this approach, in particular, the investigation of the metal-to-insulator transition at half-filling have been recently carried out [39]. In this case the obtained energy spectrum reproduces exact atomic and band limits, provides the correct behavior of the ground state energy, energy gap and polar states concentration. At the basis of these results, some peculiarities of narrow band materials have been interpreted.

The aim of this paper is to study the condition of ferromagnetism stabilization in the case of strong Coulomb correlations in generalized narrow-band models, which reflect some properties of real systems. In particular, the peculiarities of the models studied lie in accounting for the non-diagonal matrix elements of electron-electron interaction (correlated hopping and interatomic exchange interaction), as well as for the orbital degeneracy of the band.

2. Ferromagnetism in the single-band model

2.1. The effective Hamiltonian of generalized single-band model

In the case of strong Coulomb correlations we use a perturbation theory (in accordance with the method described in [40,41]), that lead [42] to effective Hamiltonian (EH) of the Mott-Hubbard metallic magnet (in the representation of X-operators [16]):

$$\begin{aligned} H &= -\mu \sum_i \left(X_i^{\uparrow} + X_i^{\downarrow} + 2X_i^2 \right) + {\sum_{ij\sigma}}' t_{ij}(n) X_i^{\sigma 0} X_j^{0\sigma} + {\sum_{ij\sigma}}' \tilde{t}_{ij}(n) X_i^{2\sigma} X_j^{\sigma 2} \\ &\quad + U \sum_i X_i^2 - {\sum_{ij\sigma}}' \frac{J(ij)}{2} \left((X_i^{\sigma} + X_i^2)(X_j^{\sigma} + X_j^2) + X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \right) \\ &\quad - {\sum_{ij\sigma}}' \frac{\tilde{J}(ij)}{2} \left(X_i^{\sigma} X_j^{\bar{\sigma}} - X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - 2X_i^0 X_i^2 \right). \end{aligned} \tag{1}$$

Here, μ is the chemical potential, $t_{ij}(n) = t_{ij}(1 - \tau_1 n)$, $\tilde{t}_{ij}(n) = t_{ij}(1 - \tau_1 n - 2\tau_2)$ are the hopping integrals in the lower Hubbard subband (hole subband) and upper Hubbard subband (doublon subband) respectively, $J(ij)$ is the integral of direct inter-atomic exchange, $\tilde{J}(ij) = 2(t'_{ij}(n))^2/U$ is the integral of indirect (through the polar states) exchange, $t'_{ij}(n) = t_{ij}(1 - \tau_1 n - \tau_2)$ is the hopping integral between the lower and upper Hubbard subbands. For convenience, the parameters of correlated hopping $\tau_1 = T_1(ij)/|t_{ij}|$ and $\tau_2 = T_2(ij)/|t_{ij}|$ are introduced. Here, t_{ij} is the band hopping integral for the nearest neighbors i and j, $T_1(ij)$ and $T_2(ij)$ are the integrals of correlated hopping of first type (it depends on the occupancy of the neighboring sites which are not involved in the hopping process) and second type (in such a hopping of electrons, doubly occupied lattice cites are involved) respectively.

It is worth-while to note that the small perturbation parameter at the obtaining of EH (1) is $t'_{ij}(n)/U$, which reduces the condition of transition to the EH in comparison to the Hubbard model, where the parameter is t_{ij}/U. The distinctions of the obtained EH (1) from generalized forms of $t - J$-models [17,40,43] are, firstly, concentration dependence of hopping integrals in lower and upper Hubbard subbands and non-equivalence of these integrals due to the correlated hopping being taken into account (i.e., the absence of electron-hole asymmetry; this fact has been also emphasized in [44]); secondly, unusual form (due to concentration dependence of hopping integral) of the indirect exchange integral. Although the EH (1) is very cumbersome, the mathematical treatment of the EH is essentially simplified and the interpretation of the results is clear from the viewpoint of physics.

2.2. The single-particle Green function and energy spectrum

We introduce the retarded Green function $G_{pp'}(E) = \langle\langle X_p^{0\sigma}|X_{p'}^{\sigma 0}\rangle\rangle$ and write the equation of motion in the case $n < 1$ when the processes with doublons can be neglected:

$$(E+\mu+zJ_{\text{eff}}n_\sigma)G_{pp'}(E) = \frac{\delta_{pp'}}{2\pi}\left\langle X_p^\sigma + X_p^0\right\rangle + \left\langle\left\langle \left[X_p^{0\sigma}, {\sum_{ij\sigma'}}' t_{ij}(n) X_i^{\sigma' 0} X_j^{0\sigma'}\right]\middle| X_{p'}^{\sigma 0}\right\rangle\right\rangle, \tag{2}$$

(in this case the exchange interaction is taken into account within the mean-field approximation, z is the number of nearest neighbor sites, $J_{\text{eff}} = J - \tilde{J}$). Similarly to [24,41], we apply the variant of generalized Hartree-Fock approach. To obtain a self-consistent equation for the Green function in accordance with the projection procedure we assume that

$$\left[X_p^{0\sigma}, {\sum_{ij\sigma'}}' t_{ij}(n) X_i^{\sigma' 0} X_j^{0\sigma'}\right] = \sum_j \epsilon^\sigma(pj) X_j^{0\sigma}, \tag{3}$$

where $\epsilon^\sigma(pj)$ is non-operator expression. After anticommutation of equation (3) with $X_k^{\sigma 0}$ we obtain:

$$\epsilon^\sigma(pk)(X_k^\sigma + X_k^0) = t(n)(X_p^\sigma + X_p^0)(X_k^\sigma + X_k^0) + t(n) X_k^{\sigma\bar{\sigma}} X_p^{\bar{\sigma}\sigma} - \delta_{pk} t(n) \sum_j X_k^{\bar{\sigma}0} X_j^{0\bar{\sigma}}. \tag{4}$$

Then, equation (2) can be rewritten in the form:

$$(E+\mu+zJ_{\text{eff}}n_\sigma)G_{pp'}(E) = \frac{\delta_{pp'}}{2\pi}\langle X_p^\sigma + X_p^0\rangle + \sum_{j\neq p} \epsilon^\sigma(pj)\langle\langle X_k^{0\sigma}|X_{p'}^{\sigma 0}\rangle\rangle + \epsilon_p^\sigma \langle\langle X_p^{0\sigma}|X_{p'}^{\sigma 0}\rangle\rangle, \tag{5}$$

The non-operator expressions $\epsilon^\sigma(pj)$, ϵ_p^σ can be obtained in the following way: the averages with quasi-bose operators are replaced by c-numbers (in this connection see our paper [42]), and to obtain the averages with quasi-fermi operators, the procedure of self-consistent calculation (using corresponding Green functions) is applied.

Here, we introduce the notations

$$\epsilon^\sigma(pj) = \alpha_\sigma t_{pj}(n), \qquad \epsilon_p^\sigma = \beta_\sigma(pi), \tag{6}$$

and after Fourier transformation of equation (5) we obtain the equation for Green function

$$G_{\mathbf{k}}^\sigma(E) = \frac{1}{2\pi}\frac{1-n_{\bar{\sigma}}}{E - E_{\mathbf{k}}^\sigma}\,, \tag{7}$$

where single-particle energy spectrum $E_{\mathbf{k}}^\sigma$ has the form

$$E_{\mathbf{k}}^\sigma = -\mu + \alpha_\sigma t_{\mathbf{k}}(n) + \beta_\sigma - zJ_{\text{eff}}n_\sigma\,. \tag{8}$$

Here, the coefficient of correlation band-narrowing is

$$\alpha_\sigma = 1 - n_{\bar\sigma} + \frac{n_{\bar\sigma} n_\sigma}{1 - n_{\bar\sigma}} = \frac{2 - n + \eta_\sigma m}{2} + \frac{n^2 - m^2}{2(2 - n + \eta_\sigma m)} \tag{9}$$

and the correlation shift of the band center is

$$\beta_\sigma = -\frac{1}{1 - n_{\bar\sigma}} \sum_{\mathbf{k}} t_{\mathbf{k}}(n) \langle X_i^{\bar\sigma 0} X_j^{0\bar\sigma} \rangle_{\mathbf{k}}\,, \tag{10}$$

n_σ is the concentration of electrons with spin σ, and the expressions

$$t_{\mathbf{k}}(n) = \frac{1}{N} \sum_{ij} t_{ij}(n) \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} = t(n)\gamma(\mathbf{k}), \qquad \gamma(\mathbf{k}) = \sum_{\mathbf{R}} \mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{R}}$$

are used (the sum goes according to the nearest neighbors to a site). We note that in distinction to the variant of projection method applied in [24], where in order to obtain β_σ the c-numbers representation has been used, in this work a spin-dependent correlation shift of the band center will be calculated self-consistently. The shape of bare density of states strongly effects the form of β_σ, which may essentially modify the condition of ferromagnetism stabilization in the model.

Analogously, in the case $n > 1$ for Green function $\tilde G^\sigma_{pp'}(E) = \langle\langle X_p^{\sigma 2} | X_{p'}^{2\sigma} \rangle\rangle$ we obtain after Fourier transformation

$$\tilde G^\sigma_{\mathbf{k}}(E) = \frac{1}{2\pi} \frac{n_\sigma}{E - \tilde E^\sigma_{\mathbf{k}}}, \tag{11}$$

where energy spectrum of the upper subband has the form

$$\tilde E^\sigma_{\mathbf{k}} = -\mu + \tilde\alpha_\sigma \tilde t_{\mathbf{k}}(n) + U + \tilde\beta_\sigma - zJ_{\mathrm{eff}}(1 - n_\sigma), \tag{12}$$

here $\tilde\alpha$ and $\tilde\beta$ are rewritten in the following way

$$\tilde\alpha_\sigma = \frac{n + \eta_\sigma m}{2} + \frac{n^2 - m^2}{2(n + \eta_\sigma m)}, \tag{13}$$

$$\tilde\beta_\sigma = -\frac{1}{n_\sigma} \sum_{\mathbf{k}} \tilde t_{\mathbf{k}}(n) \left\langle X_i^{2\sigma} X_j^{\sigma 2} \right\rangle_{\mathbf{k}}. \tag{14}$$

The obtained energy spectra (8) and (12) possess considerable peculiarities. Firstly, there is a correlation narrowing of the band, which is dependent on band-filling. Besides, the widths of subbands are non-equivalent due to the correlated hopping of electrons. Secondly, there is a spin-dependent correlation shift β_σ of subband center (the importance of similar subband shifts have also been emphasized in references [11,45]), which leads (see below) to the stabilization of ferromagnetic ordering.

2.3. The ground state energy and magnetization

Let us calculate the ground state energy of the system described by EH (1) in the case of $n < 1$. Like in [5,6] we use the expression for the ground state energy (per lattice site) in the form

$$\frac{E_0}{N} = \frac{1}{2N}\sum_{\sigma\mathbf{k}}\int\limits_{-\infty}^{\infty}\left(t_{\mathbf{k}}(n)+E\right)f(E)S^{\sigma}_{\mathbf{k}}(E)\mathrm{d}E \tag{15}$$

and concentration of electrons with spin σ

$$n_\sigma = \frac{1}{N}\sum_{\mathbf{k}}\int\limits_{-\infty}^{\infty} f(E)S^{\sigma}_{\mathbf{k}}(E)\mathrm{d}E, \tag{16}$$

here $f(E)$ is the Fermi distribution function, $S^{\sigma}_{\mathbf{k}}(E) = (1-n_{\bar{\sigma}})\delta(E-E^{\sigma}_{\mathbf{k}})$ is spectral density of the Green function.

In the case of simple forms of bare density of states (DOS), in particular, rectangular and semi-elliptical DOS, we have obtained an analytical expression for the ground state energy and concentration of electrons with spin σ. The calculation results show that in the ground state of single-band Hubbard model at $U \to \infty$ and rectangular DOS there is a degeneracy of the paramagnetic and saturated ferromagnetic states. To attain ferromagnetic ordering, the effective exchange parameter $zJ_{\text{eff}} > 0$ is necessary. Accordingly, in the case of rectangular DOS, the direct interatomic exchange interaction J which provides the ferromagnetic character of the effective exchange turns out to be a key parameter for ferromagnetism. Another situation is realized in the case of semi-elliptical DOS: at some critical concentration the saturated ferromagnetic state is realized (even without the exchange interaction). At the presence of $zJ_{\text{eff}}/w > 0$ the stability of ferromagnetic state rises (see figure 1) forasmuch as the difference $\Delta E_0^{\text{FM}}/Nw$ between the energy of the paramagnetic and ferromagnetic ground states increases. It is shown that the saturated ferromagnetic state at $n = 0.59$ is realized while using semi-elliptical DOS in the case of infinite-U Hubbard model. $zJ_{\text{eff}}/w > 0$ being taken into account leads to the decrease of critical concentration at which ferromagnetism occurs.

The effect of correlated hopping on the stability of ferromagnetic ordering is illustrated in figure 2 (for the case of semi-elliptical DOS). In the absence of effective exchange, ferromagnetic ordering is realized due to spin-dependent shifts of the subband center but the correlated hopping leads to the narrowing of the band and hereby suppresses the “translational” mechanism of ferromagnetism. The difference between the energies of paramagnetic and ferromagnetic states is reduced. At the same time, the reduction of $\Delta E_0^{\text{FM}}/Nw$ at the presence of an effective exchange leads to the occurrence of spontaneous magnetization at a lower electron concentration in comparison to the case of the system without correlated hopping. Therefore, at $zJ_{\text{eff}}/w > 0$ in the system where the correlated hopping is taken into account, the region of electron concentration with ferromagnetic ordering is slightly extended

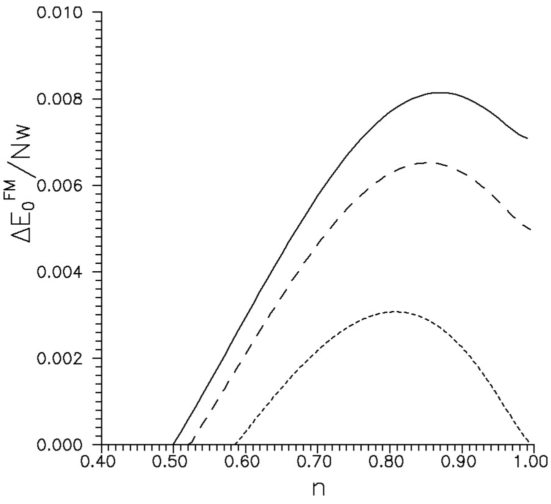

Figure 1. The effect of the effective exchange interaction on the concentration dependence of $\Delta E_0^{\mathrm{FM}}/Nw$ in the generalized Hubbard model at $\tau_1 = 0$. Solid curve: $zJ_{\mathrm{eff}}/w = 0.03$; long-dashed curve: $zJ_{\mathrm{eff}}/w = 0.02$; short-dashed curve: $zJ_{\mathrm{eff}}/w = 0$ (semi-elliptical DOS).

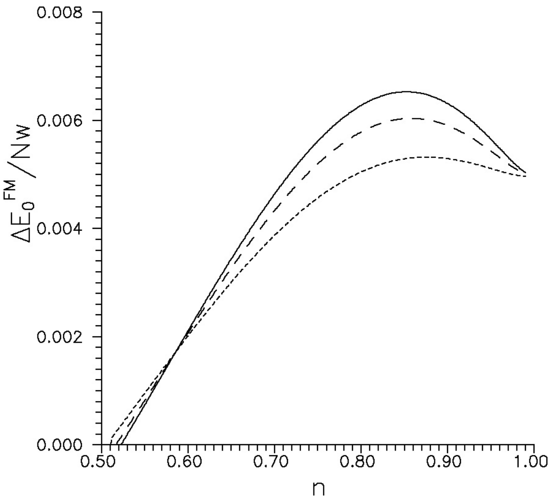

Figure 2. The effect of the correlated hopping on the concentration dependence of $\Delta E_0^{\mathrm{FM}}/Nw$ in the generalized Hubbard model at $zJ_{\mathrm{eff}}/w = 0.02$. Solid curve: $\tau_1 = 0$; long-dashed curve: $\tau_1 = 0.2$; short-dashed curve: $\tau_1 = 0.4$ (semi-elliptical DOS).

(see figure 2). Besides, in the case $n > 1$, the second type of correlated hopping (due to the occupancy of lattice sites involved in the hopping process) appears. This, firstly, destabilizes the "translational" tendency to the ferromagnetism yet more (this fact may provide the absence of ferromagnetic ordering if there is no exchange interaction in the system). Secondly, in the presence of an effective exchange $zJ_{\mathrm{eff}}/w > 0$ the magnetization curve is asymmetrical and the ferromagnetic region in the case $n > 1$ is wider in comparison with the case $n < 1$ (figure 3).

Concentration dependence of magnetization at $T = 0$ obtained by the minimization of ground state energy is illustrated in figure 3. We note that the concentration region most favorable for ferromagnetism is located around half-filling. At the same time, it is known that at $n = 1$ in the "standard" Hubbard model, the antiferromagnetic ordering is realized. In the model studied the competition of various types of magnetic ordering is described by the parameter of effective exchange J_{eff}. In our article we investigate only ferromagnetic situation when $J_{\mathrm{eff}} > 0$ (although if $2t^2/U > J$ then in the system the indirect anti-ferromagnetic exchange dominates, but this case is beyond the scope of this paper).

We note that the shape of non-interacting DOS (which corresponds to some lattice structure) substantially effects the critical electron concentration at which ferromagnetic ordering occurs as well as the electron concentration at which magnetic moment becomes saturated. By the numerical calculations of the ground state energy at the base of expression (15) and the subsequent minimization we have

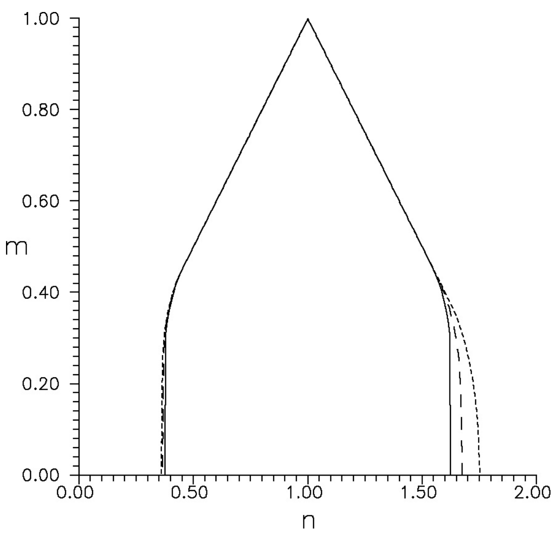

Figure 3. Concentration dependence of magnetization m (semi-elliptical DOS) at $zJ_{\mathrm{eff}}/w = 0.1$. Solid curve: $\tau_1 = \tau_2 = 0$; long-dashed curve: $\tau_1 = \tau_2 = 0.1$; short-dashed curve: $\tau_1 = 0.2; \tau_2 = 0.2$.

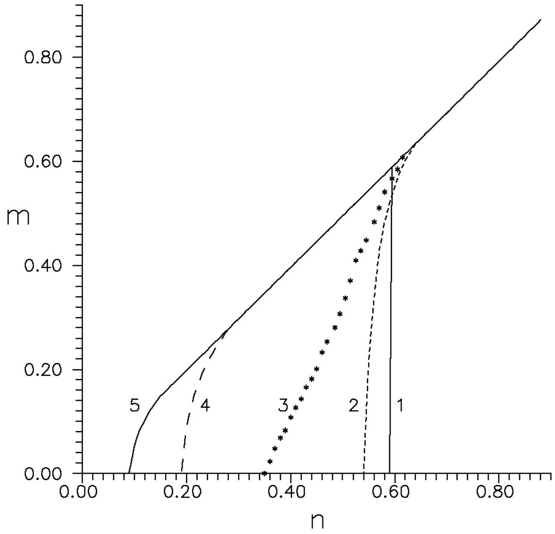

Figure 4. Concentration dependence of magnetization m in the infinite-U Hubbard model at various DOS (see table 1).

investigated the condition of ferromagnetism stabilization for various DOS. In particular, the numerical analysis has been carried out for DOS that corresponds to the simple cubic lattice [47]

$$\rho(\epsilon) = \begin{cases} A\sqrt{9-\epsilon^2} - C(1-\epsilon^2), & |\epsilon| \leqslant 1, \\ A\sqrt{9-\epsilon^2} - B\sqrt{1-(|\epsilon|-2)^2}, & 1 \leqslant |\epsilon| \leqslant 3, \end{cases} \tag{17}$$

(here $A = 0.10108$, $B = 0.12807$, $C = 0.02$); for DOS that corresponds to the body-centered cubic lattice [48]

$$\rho(\epsilon) = 2\sqrt{(}1-|\epsilon|)\ln^2\left(\frac{5.845}{|\epsilon|}\right)\left(16.6791 + 3.6364|\epsilon| + 2.4880|\epsilon|^2\right), \quad |\epsilon| \leqslant 1, \tag{18}$$

as well as for the DOS with the peak near the band-edge [12]

$$\rho(\varepsilon) = c\frac{\sqrt{w^2 - E^2}}{w + aE}\,, \tag{19}$$

with free parameter $c = (1 + \sqrt{1-a^2})/(\pi w)$. Changing the asymmetry parameter a, one can obtain both the semi-elliptical DOS ($a = 0$) and the DOS with the peak near the band-edge (a $\to$ 1).

The results of numerical calculations (in the infinite-U Hubbard model in order to compare with the results of other authors) of critical electron concentration are presented in table 1. The obtained concentration dependencies of magnetization for the above mentioned DOS are illustrated in figure 4. Our results agree with the well

Table 1. The critical electron concentrations for ferromagnetic ordering (single-band model).

Density of states	Appearance of magnetization	Saturation of magnetization
simple cubic lattice, sc (curve 2, figure 4)	$n_1 = 0.36$	$n_2 = 0.62$
body centered cubic lattice, bcc (curve 3, figure 4)	$n_1 = 0.55$	$n_2 = 0.64$
asymmetrical DOS		
$a = 0.3$ (curve 4, figure 4)	$n_1 = 0.20$	$n_2 = 0.31$
$a = 0.5$ (curve 5, figure 4)	$n_1 = 0.09$	$n_2 = 0.15$

known result for sc-lattice obtained by Roth [5]: at $n_1 = 0.36$ the ferromagnetic ordering occurs, and at $n_2 = 0.63$ the magnetic moment saturates. Similarly to the ideology of Roth the spectral density approximation (SDA) gives, in the case of sc-lattice, the following results: spontaneous magnetization occurs at $n_1 = 0.34$ and at $n_2 = 0.68$, ferromagnetic ordering reaches the saturation. In the case of bcc-lattice: the critical concentrations are $n_1 = 0.52$ and $n_2 = 0.68$, respectively. The Gutzwiller variational function method [9] gives only the critical concentration of saturated ferromagnetic state $n_2 = 0.68$ for sc- and bcc-lattices. Our results also agree with the results obtained using the expansion of one-particle Green functions by the coordination number [10].

It is worth-while to note that in the case of strong electron correlation and half-filled band (when the shifts of subband center vanish) the ferromagnetic ordering is stabilized only due to the interatomic exchange interaction (independently of the DOS used). Accordingly, the direct interatomic exchange in the single-band model being taken into account is very important.

3. Ferromagnetism in the double orbitally degenerate band

3.1. The effective Hamiltonian of the generalized double orbitally degenerate narrow-band model

Let us obtain the EH of the generalized double orbitally degenerate model using the canonical transformation of general Hamiltonian in the $X^{kl}_{\gamma i}$ representation (see [36]). In the case of strong Coulomb interaction ($U \gg |t_{ij}|$) and strong Hund's coupling (the energy of intra-atomic Coulomb interaction of electrons with different spin projections at different orbitals U' and intra-atomic exchange interaction of electrons with the same spin projection at different orbitals J_0 have the same order, $U' \gg U' - J_0$) at $n < 2$ one can neglect the states with the number of electrons greater than two and non-Hund's doubly occupied states. Generalizing the approach used in the previous section for the single-band model we use the perturbation expansion in the parameter $t'(n)/(U-J_0)$. In this case, $\gamma\sigma-0$ and $\sigma\sigma-\gamma\sigma$-subbands (here $\gamma=\alpha,\beta$ indicates the orbital) are separated by the energy gap and hence the EH of generalized double orbitally degenerate Hubbard model with correlated hopping has the form:

$$H = H_0 + H_{\mathrm{tr}} + \tilde{H}_{\mathrm{ex}} + H_{\mathrm{tr-ex}}\,, \tag{20}$$

where

$$\begin{aligned}
H_0 &= -\mu\sum_{i\sigma}\left(X_i^{\alpha\sigma}+X_i^{\beta\sigma}+2X_i^{\sigma\sigma}\right)+(U'-J_0)\sum_{i\sigma}X_i^{\sigma\sigma},\\
H_{\mathrm{tr}} &= {\sum_{ij\gamma\sigma}}' t_{ij}(n)X_i^{\gamma\sigma,0}X_j^{0,\gamma\sigma}+{\sum_{ij\gamma\sigma}}'\tilde{t}_{ij}(n)X_i^{\sigma\sigma,\gamma\sigma}X_j^{\gamma\sigma,\sigma\sigma},\\
\tilde{H}_{\mathrm{ex}} &= -\sum_{ij\gamma\sigma}\frac{\tilde{J}(ij)}{2}\left(X_i^{\gamma\sigma}X_i^{\bar{\gamma}\sigma}-X_i^{\gamma\sigma,\bar{\gamma}\sigma}X_i^{\bar{\gamma}\sigma,\gamma\sigma}-2X_i^{\sigma\sigma}X_j^{0}\right),\\
H_{\mathrm{tr-ex}} &= -\sum_{ijk\gamma\sigma}\frac{J_{\mathrm{tr-ex}}(ijk)}{2}(X_i^{\gamma\sigma,0}X_j^{\bar{\gamma}\sigma}X_k^{0,\gamma\sigma}-X_i^{\gamma\sigma,0}X_j^{\bar{\gamma}\sigma,\gamma\sigma}X_k^{0,\bar{\gamma}\sigma}\\
&\quad+X_i^{\sigma\sigma,\gamma\sigma}X_j^{\gamma\sigma,\bar{\gamma}\sigma}X_k^{\bar{\gamma}\sigma,\sigma\sigma}-X_i^{\sigma\sigma,\gamma\sigma}X_j^{\bar{\gamma}\sigma}X_k^{\gamma\sigma,\sigma\sigma}).
\end{aligned}$$

In the Hamiltonian (20) besides the atomic and the hopping terms one can distinguish the term $\tilde{H}_{\mathrm{ex}}$ which describes the indirect exchange interaction (kinetic super-exchange) as well as the term $H_{\mathrm{tr-ex}}$ that describes the indirect hopping. Similarly to the single-band case, the obtained EH has some peculiarities: the hopping processes in the lower and upper bands are non-equivalent (due to the correlated hopping being taken into account). At the same time, the effective exchange has the *ferromagnetic* character (in distinction from non-degenerate band) and stabilizes (see in the next section) the ferromagnetic ordering.

3.2. The single-particle Green function and energy spectrum

Let us write the model Hamiltonian of Mott-Hubbard narrow-band ferromagnet with orbital degeneracy (without the processes of indirect hopping which play here the secondary role). Such an approach makes it possible to investigate the effect of electron and doublon hopping as well as of the effective exchange interaction of electrons on the ferromagnetism stabilization.

In the case $n<1$ one can consider only lower $\alpha\gamma-0$ and $\beta\gamma-0$-subbands (such a situation takes place in the compound $\mathrm{Fe}_{1-x}\mathrm{Co}_x\mathrm{S}_2$ while changing the cobalt concentration). We write the equation of motion for the Green function $G_{pp'}^{\gamma\sigma}(E)=\langle\langle X_p^{0,\gamma\sigma}|X_{p'}^{\gamma\sigma,0}\rangle\rangle$ ($n<1$, the processes with double occupied states are neglected):

$$\begin{aligned}
(E+\mu+zJ_{\mathrm{eff}}\langle X_p^{\bar{\gamma}\bar{\sigma}}\rangle)G_{pp'}^{\gamma\sigma}(E) &= \frac{\delta_{pp'}}{2\pi}\langle X_p^{\gamma\sigma}+X_p^{0}\rangle\\
&\quad+\left\langle\left\langle\left[X_p^{0,\gamma\sigma},{\sum_{ij\gamma'\sigma'}}' t_{ij}(n)X_i^{\gamma'\sigma',0}X_j^{0,\gamma'\sigma'}\right]\middle|X_{p'}^{\gamma\sigma,0}\right\rangle\right\rangle,
\end{aligned} \tag{21}$$

(the exchange interaction is taken into account in the mean-field approximation). Similarly to the case of single-band model for obtaining a self-consistent equation we assume

$$\left[X_p^{0,\gamma\sigma}, {\sum_{ij\gamma'\sigma'}}' t_{ij}(n) X_i^{\gamma'\sigma',0} X_j^{0,\gamma'\sigma'}\right] = \sum_j \epsilon_\gamma^\sigma(pj) X_j^{\gamma 0,\sigma}\,, \tag{22}$$

here $\epsilon_\gamma^\sigma(pj)$ is the non-operator expression. After anticomutation of equation (22) with $X_k^{\gamma\sigma,0}$ we have:

$$\begin{aligned}\epsilon_\gamma^\sigma(pk)(X_k^{\gamma\sigma} + X_k^0) &= t_{pk}(n)(X_p^{\gamma\sigma} + X_p^0)(X_k^{\gamma\sigma} + X_k^0) \\ &+ t_{pk}(n) X_p^{\gamma\bar\sigma,\gamma\sigma} X_k^{\gamma\sigma,\gamma\bar\sigma} + t_{pk}(n) X_p^{\bar\gamma\bar\sigma,\gamma\sigma} X_k^{\gamma\sigma,\bar\gamma\bar\sigma} + t_{pk}(n) X_p^{\bar\gamma\sigma,\gamma\sigma} X_k^{\gamma\sigma,\bar\gamma\sigma} \\ &- \delta_{pk} \sum_j t_{pj}(n) \left(X_k^{\gamma\bar\sigma,0} X_j^{0,\gamma\bar\sigma} + X_k^{\bar\gamma\bar\sigma,0} X_j^{0,\bar\gamma\bar\sigma} + X_k^{\bar\gamma\sigma,0} X_j^{0,\bar\gamma\sigma}\right).\end{aligned} \tag{23}$$

According to (23) the equation (21) has the form:

$$\begin{aligned}(E + \mu + zJ_{\text{eff}}\langle X_p^{\bar\gamma\bar\sigma}\rangle) G_{pp'}^{\gamma\sigma}(E) &= \frac{\delta_{pp'}}{2\pi}\langle X_p^{\gamma\sigma} + X_p^0\rangle \\ &+ \sum_{j\neq p} \epsilon_\gamma^\sigma(pj) \left\langle\left\langle X_k^{0,\gamma\sigma} | X_{p'}^{\gamma\sigma,0}\right\rangle\right\rangle + \epsilon_\gamma^\sigma(p) \left\langle\left\langle X_p^{0,\gamma\sigma} | X_{p'}^{\gamma\sigma,0}\right\rangle\right\rangle.\end{aligned} \tag{24}$$

In [36], the connection between the Hubbard operators and Shubin-Wonsovsky configuration operators was established. For simplicity we assume that γ- and $\bar\gamma$-orbitals are equivalent ($n_{\gamma\sigma} = n_{\bar\gamma\sigma} = n_\sigma$), and replace in expression (23) quasi-bose averages by the c-numbers

$$\begin{aligned} X_i^{\gamma\sigma} &= n_\sigma, \qquad X_i^0 = 1 - n, \\ X_i^{\gamma\sigma,\gamma\bar\sigma} X_j^{\gamma\bar\sigma,\gamma\sigma} &= n_\sigma n_{\bar\sigma}, \quad X_i^{\gamma\sigma,\bar\gamma\sigma} X_j^{\bar\gamma\sigma,\gamma\sigma} = n_\sigma n_\sigma, \quad X_i^{\gamma\sigma,\bar\gamma\bar\sigma} X_j^{\bar\gamma\bar\sigma,\gamma\sigma} = n_\sigma n_{\bar\sigma},\end{aligned} \tag{25}$$

while the averages of quasi-fermi operators will be calculated self-consistently, hereby postulating the non-operator character of $\epsilon_\gamma^\sigma(pj)$, $\epsilon_\gamma^\sigma(\mathrm{p})$. We use the notations

$$\epsilon_\gamma^\sigma(pj) = \alpha_{\gamma\sigma} t_{pj}(n), \qquad \epsilon_\gamma^\sigma(p) = \beta_{\gamma\sigma}(pk), \tag{26}$$

and after Fourier transformation (24) we have the Green function in the form

$$G_{\mathbf{k}}^{\gamma\sigma}(E) = \frac{1}{2\pi} \cdot \frac{1 - n + n_\sigma}{E - E_{\mathbf{k}}^{\gamma\sigma}}\,, \tag{27}$$

where the single-particle energy spectrum of $(0 - \gamma\sigma)$–subband $E_{\mathbf{k}}^{\gamma\sigma}$ is

$$E_{\mathbf{k}}^{\gamma\sigma} = -\mu + \alpha_{\gamma\sigma} t_{\mathbf{k}}(n) + \beta_{\gamma\sigma} - zJ_{\text{eff}} n_\sigma. \tag{28}$$

Here, the band-narrowing due to electron correlation is

$$\alpha_{\gamma\sigma} = 1 - n + n_\sigma + \frac{2n_{\bar\sigma} n_\sigma + n_\sigma^2}{1 - n + n_\sigma}, \tag{29}$$

and correlated spin-dependent shift of the subband center is

$$\beta_{\gamma\sigma}=-\frac{1}{1-n+n_\sigma}\sum_{\mathbf{k}}t_{\mathbf{k}}(n)\big(\langle X_i^{\gamma\bar{\sigma},0}X_j^{0,\gamma\bar{\sigma}}\rangle_{\mathbf{k}}+\langle X_i^{\bar{\gamma}\bar{\sigma},0}X_j^{0,\bar{\gamma}\bar{\sigma}}\rangle_{\mathbf{k}}+\langle X_i^{\bar{\gamma}\sigma,0}X_j^{0,\bar{\gamma}\sigma}\rangle_{\mathbf{k}}\big)\,, \quad (30)$$

where n_σ is the electron concentration with spin σ at γ orbital; we assume the equality of orbitals, thus

$$n_\uparrow=\frac{n+m}{4},\qquad n_\downarrow=\frac{n-m}{4}\,. \quad (31)$$

Similarly to the case of non-degenerate band, the spin-dependent shift of the subband center will be calculated self-consistently and its form is strongly effected by the shape of non-interacting density of states.

In the case $n>1$, the doublon Green function has the form

$$\tilde{G}_{\mathbf{k}}^{\gamma\sigma}(E)=\frac{1}{2\pi}\frac{n_\sigma+n_{\sigma\sigma}}{E-\tilde{E}_{\mathbf{k}}^{\gamma\sigma}}, \quad (32)$$

where the single-particle energy spectrum is

$$\tilde{E}_{\mathbf{k}}^{\gamma\sigma}=-\mu+U-J_0+\tilde{\alpha}_{\gamma\sigma}\tilde{t}_{\mathbf{k}}(n)+\tilde{\beta}_{\gamma\sigma}-zJ_{\text{eff}}n_\sigma\,. \quad (33)$$

Here, the narrowing of the upper $(\gamma\sigma-\sigma\sigma)$-subband is

$$\tilde{\alpha}_{\gamma\sigma}=n_\sigma+n_{\sigma\sigma}+\frac{n_\sigma^2}{n_\sigma+n_{\sigma\sigma}}\,, \quad (34)$$

and the shift of the upper subband center is

$$\tilde{\beta}_{\gamma\sigma}=\frac{1}{n_\sigma+n_{\sigma\sigma}}\sum_{\mathbf{k}}\tilde{t}_{\mathbf{k}}(n)\left\langle X_i^{\sigma\sigma,\bar{\gamma}\sigma}X_j^{\bar{\gamma}\sigma,\sigma\sigma}\right\rangle_{\mathbf{k}}\,, \quad (35)$$

the concentration of electrons with spin σ and the concentration of Hund's states are as follows:

$$\begin{aligned}n_\uparrow &= \frac{2-n}{4}\left(1+\frac{m}{n}\right), \qquad n_\downarrow=\frac{2-n}{4}\left(1-\frac{m}{n}\right),\\ n_{\uparrow\uparrow} &= \frac{n-1}{2}\left(1+\frac{m}{n}\right), \qquad n_{\downarrow\downarrow}=\frac{n-1}{2}\left(1-\frac{m}{n}\right).\end{aligned} \quad (36)$$

The comparison of the expression for the band-narrowing coefficients and the shifts of the subband centers in the cases $n<1$ and $n>1$ shows that even in the "standard" degenerate Hubbard model ($t(n)=\tilde{t}(n)=t$) the electron-hole asymmetry with respect to $n=1$ is realized. The correlated hopping being taken into account is another factor that enhances this tendency.

3.3. The ground state energy and magnetization

To obtain of the ground state energy (per lattice site) we generalize the expressions (15) and (16) to the case of orbitally degenerate model:

$$\frac{E_0}{N} = \frac{1}{2}\sum_{\gamma\sigma\mathbf{k}} \int_{-\infty}^{\infty} (t_{\mathbf{k}}(n) + E)\, S_{\mathbf{k}}^{\gamma\sigma}(E)\mathrm{d}E. \tag{37}$$

The concentration of electrons with spin σ at the orbital γ is

$$n_\sigma = \frac{1}{N}\sum_{\mathbf{k}} \int_{-\infty}^{\infty} f(E) S_{\mathbf{k}}^{\gamma\sigma}(E)\mathrm{d}E, \tag{38}$$

$S_{\mathbf{k}}^{\gamma\sigma}(E) = (1 - n + n_\sigma)\delta(E - E_{\mathbf{k}}^{\gamma\sigma})$ is spectral density of the Green function.

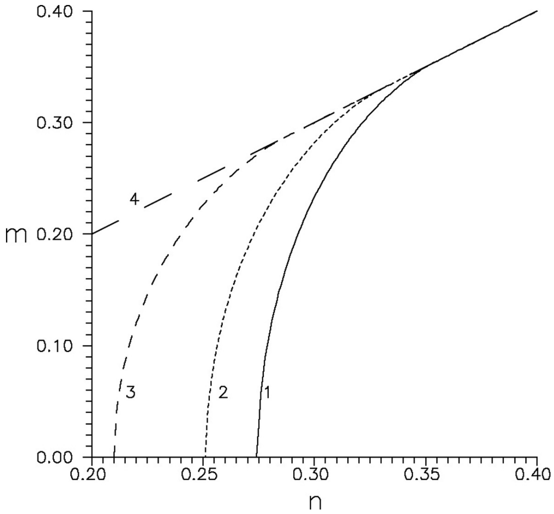

Figure 5. The concentration dependence of magnetization m at various values of the effective exchange parameter zJ_{eff}/w, $\tau_1 = \tau_2 = 0$ (semi-elliptical DOS). Curve 1: $zJ_{\text{eff}}/w = 0$, curve 2: $zJ_{\text{eff}}/w = 0.1$ curve 3: $zJ_{\text{eff}}/w = 0.3$. For convenience, the curve 4 that corresponds the saturated ferromagnetic state is added.

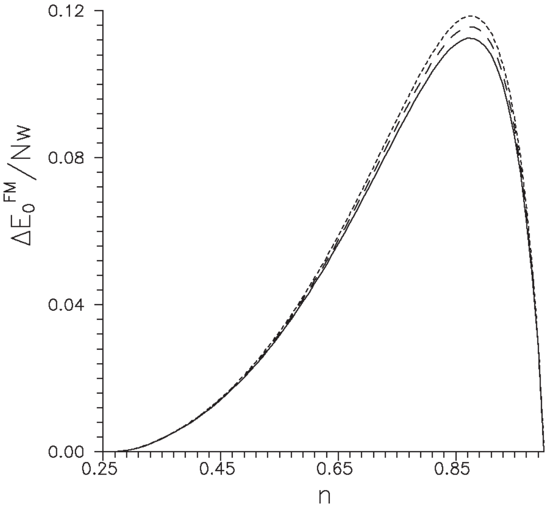

Figure 6. The concentration dependence of the difference between the energies of paramagnetic and ferromagnetic states at some values of the correlated hopping parameter τ_1, $zJ_{\text{eff}}/w = 0$, (semi-elliptical DOS). Upper curve: $\tau_1 = 0$; middle curve: $\tau_1 = 0.2$; lower curve: $\tau_1 = 0.5$.

Using the rectangular and semi-elliptical DOS we analytically obtain the system of expressions for the ground state energy (both for the case $n < 1$ and for $n > 1$). The results of ground state energy calculations show that the ground state of the double orbitally degenerate Hubbard model is ferromagnetic in the whole region of electron concentration even in the case of rectangular DOS. The ferromagnetic type effective exchange interaction enforces the stability of ferromagnetism (its role is most important in the case of $n = 1$), see figure 5 (for example the semi-elliptical DOS is used). Similarly to the case of single-band model, the correlated hopping suppresses the "translational" mechanisms of the ferromagnetic ordering, thus reducing the energy difference between the paramagnetic and ferromagnetic states (figure 6).

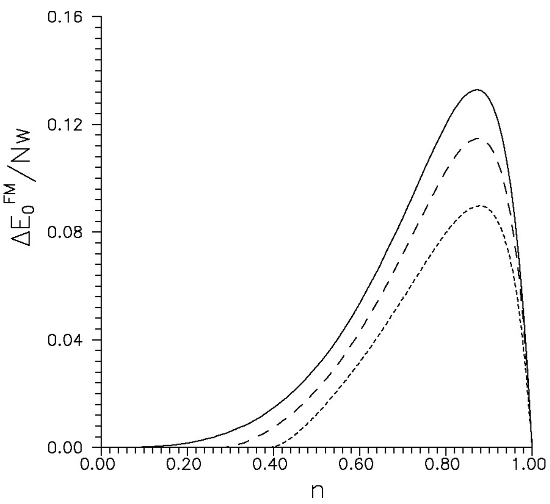

Figure 7. The concentration dependence of the difference between the energies of paramagnetic and ferromagnetic states for some types of DOS, $zJ_{\text{eff}}/w = 0$, $\tau_1 = 0$. Upper curve: rectangular DOS; middle curve: semi-elliptical DOS; lower curve: the DOS of a simple cubic lattice.

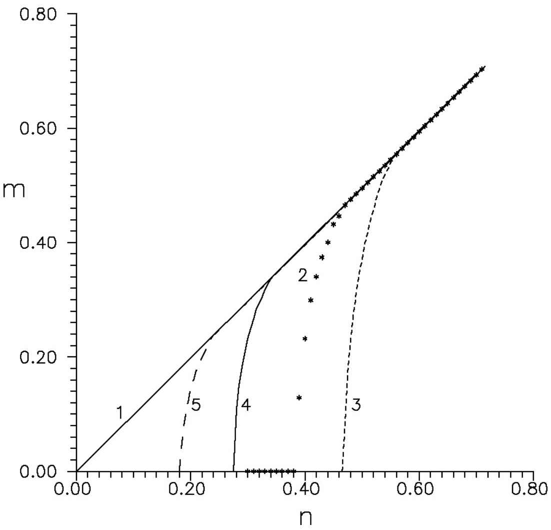

Figure 8. The concentration dependencies of magnetization m in the orbitally degenerate Hubbard model (in the case of strong Coulomb interaction and Hund's coupling) (see table 2). Curve 1: rectangular DOS; curve 2: sc-lattice; curve 3: bcc-lattice; curve 4: semi-elliptical DOS; curve 5: the DOS with asymmetry on the band-edge.

In the case of semi-elliptical DOS, the saturated ferromagnetic state is realized only in some concentration region. Even if $zJ_{\text{eff}}/w) = 0$ at the electron concentration $n_1 = 0.28$, the transition from paramagnetic to ferromagnetic state with non-saturated magnetic moment occurs. If the electron concentration reaches the value $n_2 = 0.35$ then the saturated ferromagnetic state is realized (see figure 5). The increase of an effective exchange interaction extends the region with ferromagnetic ordering. We emphasize that in the case of degenerate model the shape of DOS essentially effects the critical concentration n at which the ferromagnetic ordering appears (figure 7). At the base of ground state energy calculation (37) and its following minimization we have studied the effect of the DOS type on the ferromagnetism stability condition. In particular, numerical calculations were performed in the case of rectangular, semi-elliptical DOS, the DOS with asymmetry on the band edge [12] as well as the DOS of simple cubic [47] and body centered cubic [48]

Table 2. The critical electron concentrations for ferromagnetic ordering (double orbitally degenerate model).

Density of states	Appearance of magnetization	Saturation of magnetization
semi-elliptical DOS (curve 4, figure 8)	$n_1 = 0.28$	$n_2 = 0.35$
simple cubic lattice, sc (curve 2, figure 8)	$n_1 = 0.39$	$n_2 = 0.47$
body centered cubic lattice, bcc (curve 3, figure 8)	$n_1 = 0.47$	$n_2 = 0.56$
asymmetrical DOS $a = 0.3$ (curve 5, figure 8)	$n_1 = 0.19$	$n_2 = 0.23$

lattices. The results of these calculations (for the "standard" degenerate Hubbard model with strong correlations) are presented in table 2 and in figure 8 (note that these results for such a model have been obtained for the first time).

4. Discussion and conclusions

In the present paper the single-particle energy spectra are obtained in the framework of generalized Hartree-Fock approximation [24] by treating the effective Hamiltonians of generalized narrow-band models (in the case of strong electron correlation). This approach has been recently approved while investigating the metal-to-insulator transition at half-filling [39] (in this case the obtained energy spectrum reproduces exact atomic and band limits, provides the correct behavior of the ground state energy, energy gap and polar states concentration; at the basis of these results, some peculiarities of narrow band materials have been interpreted).

The obtained results show that ferromagnetic ordering can be stabilized by the "translational" mechanism, in particular, due to the peculiarities of the single-particle energy spectrum (we can observe the correlation narrowing of the subband and spin-dependent shifts of subband center). The ferromagnetic indirect exchange can also stabilize the magnetic ordering and is essential at half-filling of the band.

In the case of single-band model and rectangular DOS the direct inter-atomic exchange interaction is the key parameter for the saturated ferromagnetic ordering in the systems with strong correlations. In the framework of the proposed approach we have studied the effect of the shape of the DOS on the condition of ferromagnetism stability. In particular, we have calculated the ground state energy, magnetization, as well as the critical electron concentration at which the ferromagnetic ordering occurs and the magnetic moment saturates. Our results are in agreement with the results of other authors. Besides, our approach makes it possible to solve the problem of correct transition to the case of half-filled Mott-Hubbard ferromagnet, which takes place in some approximations [11].

We emphasize that in the case of strong electron correlations and half-filled single band, the ferromagnetic ordering is stabilized only via direct inter-atomic exchange interaction at the arbitrary non-interacting DOS.

The correlated hopping leads to the narrowing of the band and hereby the "translational" mechanism of ferromagnetism stabilization is suppressed at n close to half-filling. At the same time, if the $zJ_{\rm eff}/w > 0$, the region of ferromagnetic ordering in the systems with correlated hopping is wider (forasmuch as the difference between the energies of paramagnetic and ferromagnetic states is reduced and the exchange interaction effect is greater) than in the "standard" Hubbard model and magnetization curve has an asymmetrical character (due to correlated hopping).

In the case of double orbitally degenerate model with strong Hund's coupling it is shown that already rectangular DOS provides the ferromagnetic ordering due to correlation narrowing of the subband and spin-dependent shifts of subband center. The effective exchange of ferromagnetic type enforces this ferromagnetic tendency. In this paper we obtain critical concentrations for the degenerate system (for some types of the DOS) at which the magnetic moment arises and reaches saturation.

We want to emphasize the essential peculiarities of the results for a degenerate model. Firstly, the indirect (kinetic) exchange favors the ferromagnetism (at the same time one can take into account the direct inter-atomic interaction which stabilizes the ferromagnetism as well). Secondly, we can observe the above mentioned "translational" stabilization of ferromagnetism which can dominate at small electron concentrations. This last result is interesting in connection with the fact that in the ferromagnetic compounds $\mathrm{Fe}_{1-x}\mathrm{Co}_x\mathrm{S}_2$ and $\mathrm{Co}_{1-x}\mathrm{Ni}_x\mathrm{S}_2$ [49], where the partially filled double orbitally degenerate e_g-band is realized, the magnetization remains at a small doping ($x \simeq 0.05$), and the Curie temperature is considerably high. Forasmuch as the effective exchange at a small electron concentration n is reduced, the fact of the existence of a saturated magnetic moment may be interpreted based on the "translational" mechanism. Although in this paper we analyse only the case of ground state, our calculation of the Curie temperature (in the case of rectangular DOS) at a small electron concentration ($n < 0.3$) is in good agreement with experimental results of Jarett et al. [49]. Moreover, the concentration dependence of the difference between the energies of paramagnetic and ferromagnetic states (see figure 7) has a peak near the band-fillings $n = 0.7-0.8$ (this fact indicates that a similar maximum takes place in the concentration dependence of the Curie temperature). At the same time, the magnetization increases linearly (see figure 8). This result qualitatively describes the experimentally observed behavior of the concentration dependence of Curie temperature for the above mentioned metallic ferromagnets. A more detailed study of the non-zero temperature properties of the models and the comparison of the results with the experimentally observed ones will be presented elsewhere.

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References

1. Hubbard J., Proc. Roy. Soc. A, 1963, **276**, No. 1369, 238–257.
2. Vollhardt D., Blümer N., Held K., Kollar M., Schlipf J., Ulmke M., Wahle J., Advances in Solid State Physics, 1999, **38**, 383–398; Cond-mat/9804112.
3. Baberschke K., Donath M., Nolting W. (Eds.) Band-ferromagnetism. Ground state and finite-temperature phenomena. Springer, Berlin, 2001, 394 p.
4. Nagaoka Y., Phys. Rev., 1966, **147**, No. 1, 392–405.
5. Roth L.M., Phys. Rev, 1969, **184**, No. 2, 451–459.
6. Gaipel G., Nolting W., Phys. Rev. B, 1988, **38**, No. 4, 2608–2622.
7. Hermann T., Nolting W., J. Magn. Magn. Mater, 1997, **170**, No. 3, 253–276; Cond-mat/9702022.
8. Hermann T., Nolting W., Solid State Commun, 1997, **103**, 351–356; Cond-mat/9705305.
9. Shastry B.S., Krishnamurthy H.R., Anderson P.W., Phys. Rev. B, 1990, **41**, No. 4, 2375–2379.
10. Zarubin A.V., Irkhin V.Yu., Fiz. Tv. Tela, 1999, **41**, No. 6, 1057–1063 (in Russian).
11. Nolting W., Potthoff M., Herrmann T., Wegner T. Band-ferromagnetism. Ground state and finite-temperature phenomena. Springer, Berlin, 2001, 208–225.
12. Vollhardt D., Blümer N., Held K., Kollar M., Schlipf J., Ulmke M., Z. Phys. B, 1997, **103**, 283–292.
13. Ulmke M., Eur. Phys. J. B, 1998, **1**, No. 3, 301–304.
14. Kanamori J., Prog. Theor. Phys, 1963, **30**, No. 3, 275–289.
15. Kuz'min E.V., Fiz. Tv. Tela, 1997, **39**, No. 2, 193–203 (in Russian).
16. Hubbard J., Proc. Roy. Soc. A, 1965, **285**, No. 1403, 542–560.
17. Harris A.B., Lange R.V., Phys. Rev, 1967, **157**, No. 2, 295–314.
18. Kawabata A., Progr. Theor. Phys, 1972, **48**, No. 6, 1793–1808.
19. Didukh L.D., Fiz. Tv. Tela, 1977, **19**, No. 8, 1217–1222 (in Russian).
20. Kivelson S., Su W.P., Schrieffer J.R., Heeger A.J., Phys. Rev. Lett, 1987, **58**, No. 18, 1899–1902.
21. Campbell D.K., Gammel J.T., Loh E.Y., Phys. Rev. B, 1990, **42**, No. 1, 475–492.
22. Baeriswyl D., Horsch P., Maki K., Phys. Rev. Lett, 1988, **60**, No. 1, 70–70.
23. Hirsch J.E., Physica B, 1994, **199–200**, 366–372.
24. Didukh L.D., Zhurn. Fiz. Doslidzh, 1997, **1**, No. 2, 241–250 (in Ukrainian).
25. Hirsch J.E., Phys. Rev. B, 1989, **40**, No. 4, 2354–2361; Hirsch J.E., Phys. Rev. B, 1989, **40**, No. 13, 9061–9069; Hirsch J.E., Phys. Rev. B, 1999, **59**, No. 9, 6256–6265.
26. Ivanov V.A., Ukr. Fiz. Zhurn, 1991, **36**, No. 5, 751–757 (in Russian).
27. Hui-Quan Nie, Wei-Ying Zhou, Phys. Rev. B, 1997, **55**, No. 1, 59–62.
28. Amadon J.C., Hirsch J.E., Phys. Rev. B, 1996, **54**, No. 9, 6364–6375.
29. Kollar M., Vollhardt D., Phys. Rev. B, 2001, **63**, No. 1, 045107–045111.
30. Hirsch J.H., Phys. Rev. B, 1997, **56**, No. 17, 11022–11030.
31. Held K., Vollhardt D., Eur. Phys. J. B, 1998, **5**, No. 4, 473–478.
32. Meyer D., Nolting W., J. Phys.: Cond. Matter, 1999, **11**, No. 30, 5811–5825.
33. Bünemann J., Weber W., Gebhard F., Phys. Rev. B, 1998, **57**, No. 12, 6896–6916.
34. Okabe T., J. Phys. Soc. Jpn, 1996, **65**, No. 4, 1056–1064; Okabe T., Prog. Theor. Phys, 1997, **98**, No. 2, 331–348.
35. Kusakabe K., Aoki H., Phisica B, 1994, **194–196**, part I, 217–218.

36. Didukh L., Skorenkyy Yu., Dovhopyaty Yu., Hankevych V., Phys. Rev. B, 2000, **61**, No. 12, 7893–7908.
37. Didukh L., Skorenkyy Yu., Hankevych V., Kramar O., Phys. Rev. B, 2001, **64**, No. 14, 144428–144437.
38. Didukh L., Hankevych V., Kramar O., Skorenkyy Yu., J. Phys.: Cond. Matter, 2002, **14**, No. 4, 827–835.
39. Didukh L., Hankevych V., Phys. Stat. Sol. B, 1999, **211**, No. 2, 703–712; Didukh L., Skorenky Yu., Condens. Matt. Phys, 2000, **3**, No. 4(24), 787–798.
40. Didukh L.D., Stasyuk I.V., Ukr. Fiz. Zhurn, 1968, **13**, No. 6, 899–904.
41. Didukh L.D., Preprint Nat. Science Academy of Ukraine. Institute for Condensed Matter Physics; IFKS-92-9P, 1992, 32 p. (in Russian).
42. Didukh L., Kramar O., Condens. Matter Phys., 2003, **6**, No. 1(33), 145–158.
43. Chao K.A., Spałek J., Oles A., Phys. Lett. A, 1977, **64**, No. 2, 163–166.
44. Irkhin V.Yu. E-print Cond-mat/9705043, Los-Alamos, 1997, 4 p.
45. Stasyuk I.V., Danyliv O.D., Phys. Stat. Sol. B, 2000, **219**, 299–312.
46. Didukh L., Kramar O., Fiz. Nizk. Temp, 2002, **28**, No. 1, 42–50; Low Temp. Phys, 2002, **28**, No. 1, 30–36.
47. Tonegava T., Progr. Theor. Phys, 1974, **56**, No. 5, 1293–1311.
48. Jelitto J., J. Phys. Chem. Solids, 1969, **30**, No. 3, 609–626.
49. Jarrett H.S., Cloud W.H., Bouchard R.J., Butler S.R., Frederick C.G., Gillson J.L., Phys. Rev. Lett, 1968, **21**, No. 4, 617–620.

Металічний феромагнетизм в системах сильно скорельованих електронів

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В статті досліджено феромагнітне впорядкування в основному стані у вузькозонних моделях з сильно скорельованими електронами, зокрема, в узагальненій невиродженій моделі Габбарда з корельованим переносом та міжатомною обмінною взаємодією, та в узагальненій двократно орбітально виродженій моделі Габбарда з корельованим переносом. Для дослідження ефективних гамільтоніанів вказаних систем застосовано варіанти узагальненого наближення Гартрі-Фока, на основі яких отримано одночастинкові енергетичні спектри моделей. Для деяких форм густин станів, що відповідають певним типам ґраток, проведено розрахунок енергії основного стану, намагніченості та критичних концентрацій електронів, при яких магнітний момент виникає та досягає свого насичення. Обговорено можливі механізми стабілізації феромагнітного впорядкування в реальних вузькозонних матеріалах.

Ключові слова: *вузькі енергетичні зони, феромагнетизм, енергія основного стану, намагніченість*

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