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2002 J. Phys.: Condens. Matter 14 827

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Itinerant ferromagnetism of systems with double orbital degeneracy

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Received 25 June 2001, in final form 5 December 2001

Published 18 January 2002

Online at stacks.iop.org/JPhysCM/14/827

Abstract

In this paper we study the ground state ferromagnetism in a doubly orbitally degenerate Hubbard model generalized by taking into account correlated hopping and inter-atomic exchange interaction. We find that an important role in the stabilization of ferromagnetism is played by the intra- and inter-atomic exchange interactions as well as correlated hopping, which allows us to describe the metallic paramagnetic–ferromagnetic transition with a realistic relationship between the above-mentioned exchange interactions. The expression for magnetization and the criterion of ferromagnetic ground state stability are derived. The obtained results are compared with some experimental data for magnetic materials.

1. Introduction

The Stoner–Wohlfarth [1, 2] theory has been used widely for the description of band electron magnetism. This theory of itinerant magnetism is based on the mean-field treatment of the exchange interaction among band electrons. Calculations in this model depend essentially on the shape and peculiarities of the density of states; in particular, it is known that the incomplete ferromagnetism in this model is absent if the density of states is rectangular [2].

In the papers [3, 4] the generalizations of this theory for the single-band case were carried out by taking into consideration within a Hubbard-like tight-binding Hamiltonian certain matrix elements of electron–electron interaction which provide new mechanisms of ferromagnetism stabilization in metallic ferromagnets. The main result of these works is that the inter-atomic exchange interaction plays an essential role for the appearance of a ferromagnetic state with partial polarization. It has also been shown [5] that correlated hopping enhances the tendency to ferromagnetism in the case of a less than half-filled band versus a more than half-filled band. Moreover, due to an additional mechanism of correlated hopping the opposite behaviour can be realized [4] (in this connection see also section 2).

However, the presence of band degeneracy is essential for itinerant ferromagnetism. This view was originated in the work of Slater [6] and van Vleck [7], where it was argued that the presence of orbital degeneracy and Hund's rule exchange interaction leads to so-called 'atomic ferromagnetism'; in such a situation translational motion of electrons forces the spins of electrons on nearest-neighbour atoms to align in parallel. This is confirmed by the fact that ferromagnetism in metals has only been found in systems that have atoms with valence electrons in degenerate orbitals that can support an atomic magnetic moment through Hund's rule. Therefore, the extension of the theory proposed in works [3, 4] for systems with orbital degeneracy is a relevant and important task, to which this paper is devoted.

We start from the following generalization [8] of the Hubbard model for an orbitally degenerate band taking into account the matrix element of electron–electron interaction, which describes intersite hoppings of electrons (correlated hopping), and inter-atomic exchange:

$$\begin{aligned}
H = & -\mu \sum_{i\gamma\sigma} a_{i\gamma\sigma}^+ a_{i\gamma\sigma} + \sum'_{ij\gamma\sigma} a_{i\gamma\sigma}^+ \left(t_{ij} + \sum_{k\gamma'} J(i\gamma k\gamma' j\gamma k\gamma') n_{k\gamma'} \right) a_{j\gamma\sigma} \\
& + U \sum_{i\gamma} n_{i\gamma\uparrow} n_{i\gamma\downarrow} + U' \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} + (U' - J_0) \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\sigma} \\
& + J_0 \sum_{i\sigma} a_{i\alpha\sigma}^+ a_{i\beta\bar{\sigma}}^+ a_{i\alpha\bar{\sigma}} a_{i\beta\sigma} + \frac{J}{2} \sum'_{ij\gamma\sigma\sigma'} a_{i\gamma\sigma}^+ a_{j\gamma\sigma'}^+ a_{i\gamma\sigma'} a_{j\gamma\sigma}
\end{aligned} \quad (1.1)$$

where μ is the chemical potential, $a_{i\gamma\sigma}^+$, $a_{i\gamma\sigma}$ are the creation and destruction operators of an electron of spin σ ($\sigma = \uparrow, \downarrow$; $\bar{\sigma}$ denotes spin projection which is opposite to σ) on site i and in orbital γ ($\gamma = \alpha, \beta$ denotes two possible orbital states), $n_{i\gamma\sigma} = a_{i\gamma\sigma}^+ a_{i\gamma\sigma}$ is the number operator of electrons of spin σ and in orbital γ on site i , $n_{i\gamma} = n_{i\gamma\uparrow} + n_{i\gamma\downarrow}$; t_{ij} is the hopping integral of an electron from orbital γ of site j to orbital γ of site i (we neglect the electron hoppings between orbitals α and β). In real systems electron hoppings between different orbitals can exist; in addition the hopping integrals are anisotropic for e_g orbitals. However, we assume for simplicity $t_{ij}^{\alpha\beta} = t_{ij} \delta_{\alpha\beta}$. This assumption is a conventional approach in this field (for example, see [8–13] and references therein), and simplifies considerably the analysis of properties of the model under consideration.

$$J(i\gamma k\gamma' j\gamma k\gamma') = \iint \varphi_{\gamma'}^*(\mathbf{r} - \mathbf{R}_i) \varphi_{\gamma}(\mathbf{r} - \mathbf{R}_j) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |\varphi_{\gamma'}(\mathbf{r}' - \mathbf{R}_k)|^2 d\mathbf{r} d\mathbf{r}' \quad (1.2)$$

(φ_{γ} is the Wannier function), U is the intra-atomic Coulomb repulsion of two electrons of the opposite spins at the same orbital (we assume that it has the same value for orbitals α and β), U' is the intra-atomic Coulomb repulsion of two electrons of the opposite spins at the different orbitals, J_0 is the intra-atomic exchange interaction energy which stabilizes the Hund states forming the atomic magnetic moments and J is the inter-atomic exchange interaction. The primes at sums in equation (1.1) signify that $i \neq j$.

In Hamiltonian (1.1) we rewrite the sum $\sum'_{ijk\gamma\gamma'\sigma} J(i\gamma k\gamma' j\gamma k\gamma') a_{i\gamma\sigma}^+ n_{k\gamma'} a_{j\gamma\sigma}$ in the form

$$\begin{aligned}
& \sum'_{ij\gamma\sigma} (J(i\gamma i\gamma j\gamma i\gamma) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\gamma\bar{\sigma}} + \text{h.c.}) + \sum'_{ij\gamma\sigma} (J(i\gamma i\bar{\gamma} j\gamma i\bar{\gamma}) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\bar{\gamma}} + \text{h.c.}) \\
& + \sum'_{ij\gamma\gamma'\sigma} \sum_{\substack{k \neq i \\ k \neq j}} J(i\gamma k\gamma' j\gamma k\gamma') a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{k\gamma'}
\end{aligned} \quad (1.3)$$

($\bar{\gamma} = \beta$ if $\gamma = \alpha$, and $\bar{\gamma} = \alpha$ when $\gamma = \beta$). The first and second sums of equation (1.3) describe the hoppings of electrons which are correlated by electron occupation of sites involved in the hopping process. The third sum describes the hoppings of an electron between states $|i\gamma\sigma\rangle$ and

$|j\gamma\sigma\rangle$ which are dependent on the occupation number n_k of other sites ($k \neq i$, $k \neq j$). Let us take into account the influence of occupation of these sites in the Hartree–Fock approximation:

$$\sum'_{ij\gamma\gamma'\sigma} \sum_{\substack{k \neq i \\ k \neq j}} J(i\gamma k\gamma' j\gamma k\gamma') a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{k\gamma'} \simeq n \sum'_{ij\gamma\sigma} T(ij) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} \quad (1.4)$$

where $n = \langle n_{i\alpha} + n_{i\beta} \rangle$ is the average number of electrons per site,

$$T(ij) = \sum_{\substack{k \neq i \\ k \neq j}} J(i\gamma k\gamma' j\gamma k\gamma') \quad (1.5)$$

we have supposed that $J(i\gamma k\alpha j\gamma k\alpha) = J(i\gamma k\beta j\gamma k\beta)$ and $T(ij)$ have the same value for orbitals α and β . Assuming that states α and β are equivalent, denote

$$J(i\gamma i\bar{\gamma} j\gamma i\bar{\gamma}) = t'_{\alpha\alpha}(ij) = t'_{\beta\beta}(ij) = t'_{ij} \quad (1.6)$$

$$J(i\gamma i\gamma j\gamma i\gamma) = t''_{\alpha\alpha}(ij) = t''_{\beta\beta}(ij) = t''_{ij}. \quad (1.7)$$

So we can rewrite Hamiltonian (1.1) in the following form:

$$\begin{aligned} H = & -\mu \sum_{i\gamma\sigma} a_{i\gamma\sigma}^+ a_{i\gamma\sigma} + \sum'_{ij\gamma\sigma} t_{ij}(n) a_{i\gamma\sigma}^+ a_{j\gamma\sigma} + \sum'_{ij\gamma\sigma} (t'_{ij} a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\bar{\gamma}} + \text{h.c.}) \\ & + \sum'_{ij\gamma\sigma} (t''_{ij} a_{i\gamma\sigma}^+ a_{j\gamma\sigma} n_{i\gamma\bar{\sigma}} + \text{h.c.}) + U \sum_{i\gamma} n_{i\gamma\uparrow} n_{i\gamma\downarrow} + U' \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\bar{\sigma}} \\ & + (U' - J_0) \sum_{i\sigma} n_{i\alpha\sigma} n_{i\beta\sigma} + J_0 \sum_{i\sigma} a_{i\alpha\sigma}^+ a_{i\beta\bar{\sigma}}^+ a_{i\alpha\bar{\sigma}} a_{i\beta\sigma} + \frac{J}{2} \sum'_{ij\gamma\sigma\sigma'} a_{i\gamma\sigma}^+ a_{j\gamma\sigma'}^+ a_{i\gamma\sigma'} a_{j\gamma\sigma} \end{aligned} \quad (1.8)$$

with the effective hopping integral $t_{ij}(n) = t_{ij} + nT(ij)$ being concentration dependent in consequence of taking into account the correlated hopping $T(ij)$. To characterize the value of correlated hopping we use the dimensionless parameters τ (defined by $t_{ij}(n) = t_{ij}(1 - n\tau)$), $\tau' = \frac{t'_{ij}}{|t_{ij}|}$ and $\tau_2 = \frac{t''_{ij}}{|t_{ij}|}$.

The typical range of the parameters in Hamiltonian (1.8) is $U \geq U' > J_0 > t_{ij} > t'_{ij} \sim t''_{ij} \geq T(ij) > J$ (see [14–17]). However, different materials can be characterized by completely different values of these parameters. Realistic values for the transition metals and their compounds are $U \approx 2\text{--}5$ eV, $J_0 \approx 0.5\text{--}1$ eV, $t_{ij} \approx 0.1\text{--}0.3$ eV and $J \approx 0.02\text{--}0.03$ eV [15–17].

Within the mean-field theory in the Fourier representation we obtain for the single-particle Green function

$$\langle\langle a_{p\gamma\sigma} | a_{p'\gamma\sigma}^+ \rangle\rangle_{\mathbf{k}} = \frac{1}{2\pi} \frac{1}{E - E_{\gamma\sigma}(\mathbf{k})} \quad (1.9)$$

where the single-particle energy spectrum is

$$E_{\gamma\sigma}(\mathbf{k}) = -\mu_{\gamma\sigma} + t_{\mathbf{k}}(n\gamma\sigma) \quad (1.10)$$

with the shifted chemical potential

$$\mu_{\gamma\sigma} = \mu - \beta'_{\gamma} - \beta''_{\gamma\sigma} - n_{\gamma\bar{\sigma}} U - n_{\bar{\gamma}\bar{\sigma}} U' - n_{\bar{\gamma}\sigma} (U' - J_0) + zJ n_{\gamma\sigma} \quad (1.11)$$

here the shifts of subband centres are

$$\beta'_{\gamma} = \frac{2}{N} \sum'_{ij\sigma} t'(ij) \langle a_{i\bar{\gamma}\sigma}^+ a_{j\bar{\gamma}\sigma} \rangle \quad \beta''_{\gamma\sigma} = \frac{2}{N} \sum'_{ij} t''(ij) \langle a_{i\gamma\bar{\sigma}}^+ a_{j\gamma\bar{\sigma}} \rangle \quad (1.12)$$

(N is the number of lattice sites). The hopping integral, which is spin and concentration dependent, reads as

$$t_k(n\gamma\sigma) = t_k \left(1 - \tau n - 2\tau' n_{\bar{\gamma}} - 2\tau_2 n_{\gamma\bar{\sigma}} - \frac{zJ}{w} \sum_{\sigma'} \langle a_{i\gamma\sigma'}^+ a_{j\gamma\sigma'} \rangle \right). \quad (1.13)$$

t_k is the Fourier transform of the hopping integral t_{ij} , $2w = 2z|t_{ij}|$ is the bandwidth with z being the number of nearest neighbours to a site, $n_{\gamma\sigma} = \langle n_{i\gamma\sigma} \rangle$ and $n_{\gamma} = \langle n_{i\gamma} \rangle$.

The dependence of effective hopping integral on electron concentration and magnetization and the presence of a spin-dependent shift of the subband centre are the essential distinctions of the single-particle energy spectrum of the model described by Hamiltonian (1.8) from the spectrum of the two-band Hubbard models.

The mean-field approach is often criticized for its simplism. Unfortunately, the treatment of this model with so many parameters into the framework of other methods (for example, dynamical mean-field theory or exact diagonalization) is very complicated. At the same time it is interesting and important to find how the orbital degeneracy with intra-atomic Hund's rule coupling and 'off-diagonal' matrix elements of electron–electron interaction (correlated hopping and inter-atomic direct exchange interaction) in the aggregate shows itself in the metallic ferromagnetism problem. Therefore, our consideration of the metallic ferromagnetism problem is the development of the theory following the ideas proposed in papers [3] (which are based on the mean-field treatment of electron–electron interactions). We assume that the mean-field approximation can give the qualitatively correct physical picture in the case of the intermediate electron–electron correlations. This approach leads to results which agree qualitatively with those of the papers (see e.g. [9–13]), where the authors used other methods to treat electron correlations in less complicated Hamiltonians, and are in agreement with experimental data. In particular, the approach we use allows us to avoid the problem of Curie temperature overestimation, and to explain the peculiarities of ferromagnetic properties (electron–hole asymmetry of the concentration dependence of magnetization and of Curie temperature) for some transition metals and their compounds (in this connection see [18], and also section 2).

2. Results and discussion

The concentration of electrons with spin σ on orbital γ is

$$n_{\gamma\sigma} = \int_{-\infty}^{+\infty} \rho(\epsilon) f(E_{\gamma\sigma}(\epsilon)) d\epsilon. \quad (2.1)$$

Here $\rho(\epsilon)$ is the density of states, $f(\epsilon)$ is the Fermi distribution function and $E_{\gamma\sigma}(\epsilon)$ is obtained from the respective formula (1.10) substituting $t_k \rightarrow \epsilon$.

In the case of zero temperature and rectangular density of states we obtain

$$n_{\gamma\sigma} = \frac{\varepsilon_{\gamma\sigma} + w}{2w} \quad (2.2)$$

where the value $\varepsilon_{\gamma\sigma}$ is the solution of the equation $E_{\gamma\sigma}(\varepsilon) = 0$. One can obtain that $\varepsilon_{\gamma\sigma} = \frac{\mu_{\gamma\sigma}}{\alpha_{\gamma\sigma}}$, where $\alpha_{\gamma\sigma} = 1 - \tau n - 2\tau' n_{\bar{\gamma}} - 2\tau_2 n_{\gamma\bar{\sigma}} - \frac{zJ}{w} \sum_{\sigma'} n_{\gamma\sigma'} (1 - n_{\gamma\sigma'})$.

The shifts of subband centres are

$$\beta'_{\gamma} = -2\tau' w \sum_{\sigma} n_{\bar{\gamma}\sigma} (n_{\bar{\gamma}\sigma} - 1) \quad \beta''_{\gamma\sigma} = -2\tau_2 w n_{\gamma\bar{\sigma}} (n_{\gamma\bar{\sigma}} - 1). \quad (2.3)$$

From equation (2.2) we derive the formula for magnetization ($m < n$):

$$m = \sum_{\gamma} (n_{\gamma\uparrow} - n_{\gamma\downarrow}) = \pm \frac{2}{\sqrt{zJ}} \sqrt{(1+n-n^2/4)zJ + (U+J_0) + [2(n\tau_1-1) + (4-n)\tau_2]w} \quad (2.4)$$

where $\tau_1 = \tau + \tau'$; here we have assumed that the distribution of electrons between orbitals is uniform ($n_{\alpha\sigma} = n_{\beta\sigma}$). Note that magnetization (2.4) does not depend on the parameter of intra-atomic Coulomb interaction U' . This parameter leads to chemical potential renormalization, which is independent of magnetic moment (this can be seen also from the expression for ground state energy). Similarly, in the work [9] it has been argued that this parameter does not play a decisive role in metallic ferromagnetism of the transition metal compounds.

From equation (2.4) we obtain the condition of spin polarization

$$\frac{U + J_0}{2w} + \frac{zJ}{8w} [4 + n(4 - n) - m^2] + n\tau_1 + \frac{1}{2}\tau_2(4 - n) > 1. \quad (2.5)$$

For the case of $J = 0$ from equation (2.5) we obtain a generalization of the Stoner criterion which takes into account the orbital degeneracy and correlated hopping

$$(U + J_0)\rho(\epsilon_F) > 1 - n\tau_1 - \frac{1}{2}\tau_2(4 - n). \quad (2.6)$$

Note that equations (2.4)–(2.6) coincide with the expressions which can be found from the ground state energy calculations.

Analysis of the expressions for ground state energy and magnetization (2.4) shows that for the values of inter-atomic exchange interaction $J > 0$ at the point of the transition from a paramagnetic metal to a ferromagnetic metal the magnetization changes continuously, and for $J = 0$ it has a jump: namely, in the former case the transition from a paramagnetic state to a partially polarized ferromagnetic state occurs; in the latter the transition from a paramagnetic state to a fully polarized ferromagnetic state (saturated ferromagnetic state, $m = n$) is obtained. Similar results have been obtained in a single-band model [4, 5, 19]. Thus, taking into account the inter-atomic exchange interaction allows us to obtain a partially polarized ferromagnetic state in the two-band Hubbard model with symmetrical density of states; the partially polarized ferromagnetic state has been obtained by the authors of [10], using the special feature of the density of states.

The magnetization defined by equation (2.4) is plotted in figure 1 as a function of electron concentration n at different values J_0/w . These dependences qualitatively agree with results of [10] obtained by use of the Gutzwiller variational function method. From figure 1 one can see that nature of the ground state of the system depends strongly on the values of system parameters; small changes of J_0 can lead to the transition from a paramagnetic state to a ferromagnetic one at some values of electron concentration and energy parameters (this result agrees with the results of works [11, 12]); note that at some values of parameters the state of the system can be fully polarized. The transition to the ferromagnetic state is also possible with the increase of n . A similar transition with the increase of electron concentration has been found by the authors of [20].

Taking into account correlated hopping leads to the appearance of a peculiar kinetic mechanism of ferromagnetic ordering stabilization. This mechanism is caused by the presence of a spin-dependent shift of the subband centres, being the consequence of correlated hopping (which is similar to the shift of subband centres in consequence of inter-atomic direct exchange interaction). The influence of correlated hopping on the behaviour of the system is illustrated in figure 2. In distinction from the two-band Hubbard model there is an asymmetry of the cases $n < 2$ and $n > 2$. One can see also that both mechanisms of correlated hopping favour ferromagnetism but their concentration dependences are different: if $\tau_2 > \tau_1$ then the systems with the electron concentration $n < 2$ are more favourable to ferromagnetism than the systems with $n > 2$, and vice versa. With the increase of parameter τ_1 the region of ferromagnetic ordering moves towards larger values of electron concentration n , and with increasing τ_2 to smaller values of n . Note that taking into account the correlated hopping

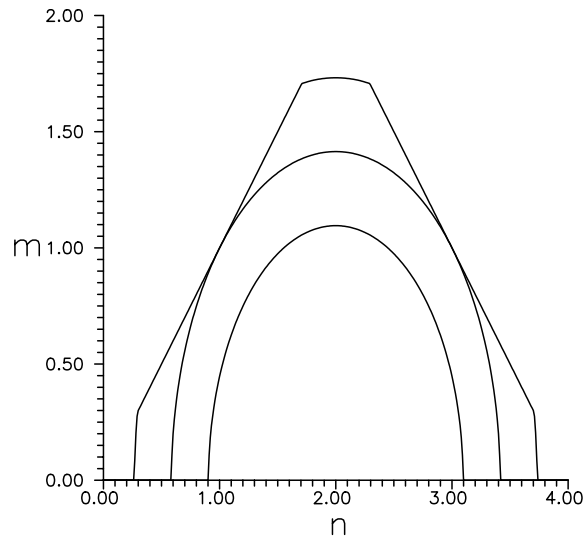


Figure 1. The magnetization m as a function of n at $U/w = 1.5$ and $\tau_1 = \tau_2 = 0$, $zJ/w = 0.05$. The upper curve corresponds to $J_0/w = 0.25$, the middle curve corresponds to $J_0/w = 0.2$ and the lower one corresponds to $J_0/w = 0.16$.

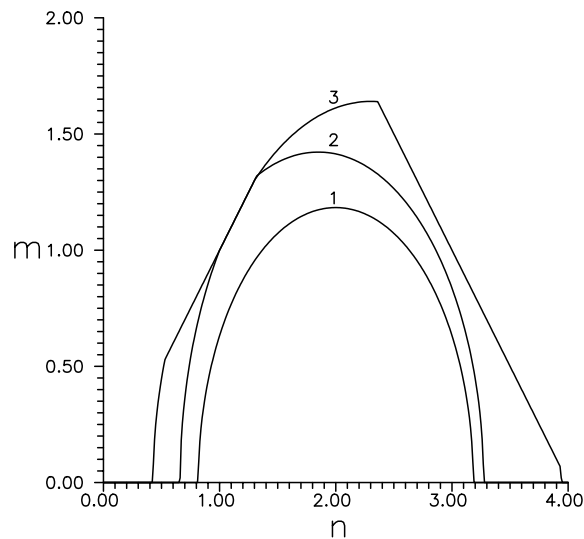


Figure 2. The magnetization m as a function of n at $U/w = 1.5$, $zJ/w = 0.05$ and $J_0/w = 0.17$. Curve 1 corresponds to $\tau_1 = \tau_2 = 0$, curve 2 to $\tau_1 = 0$, $\tau_2 = 0.015$, and curve 3 to $\tau_1 = 0.015$, $\tau_2 = 0$.

enriches significantly the set of curves (illustrating the $m(n)$ dependences), which qualitatively describe the experimental Slater–Pauling curves [21] for ferromagnetic alloys.

In figure 3 the dependences of critical values of J_0/w for ferromagnetism stabilization on electron concentration at different values of zJ/w are plotted. It is important to note that at $zJ = 0$ the critical value of J_0/w does not depend on the electron concentration. This can be explained by the following arguments: in the absence of inter-atomic exchange the mechanism which stabilizes ferromagnetism is a translational motion of electrons which enforces the spins

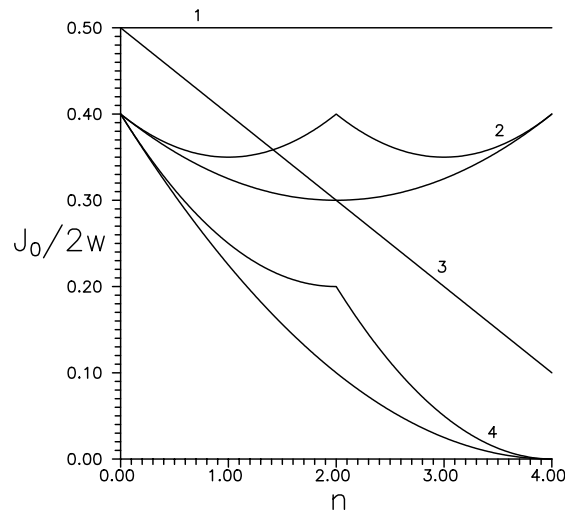


Figure 3. The critical values of J_0/w as a function of n at $U/w = 1$, $\tau_2 = 0$. Curve 1 corresponds to $zJ/w = 0$, $\tau_1 = 0$, curves 2 to $zJ/w = 0.05$, $\tau_1 = 0$, curve 3 to $zJ/w = 0$, $\tau_1 = 0.1$, and curves 4 to $zJ/w = 0.05$, $\tau_1 = 0.1$. The region below the lower line of curves 2 and 4 corresponds to the paramagnetic ordering of spins, above the upper line to the full polarization of spins and between the lines to the partial polarization.

of sites involved in the hopping process to align in parallel because of Hund's rule coupling. Note also the essential difference of the situation where the system is described by non-zero values of correlated hopping: since correlated hopping renormalizes the bandwidth and makes it dependent on the concentration, the behaviour of the critical value of J_0/w becomes asymmetrical relative to half-filling. The increase of zJ/w decreases significantly the critical value of J_0/w (in the same way as the correlated hopping does). The inverse dependence of critical values of zJ/w and J_0/w (which indicates the destabilization of ferromagnetic ordering at the increase of J_0/w) at some electron concentrations has been obtained in work [11] with use of the exact diagonalization method for the even number of sites in one-dimensional chains, but that result depends sensitively on the number of lattice sites and the boundary conditions.

Thus, our result shows that both the intra-atomic Hund's rule coupling and inter-atomic direct exchange interaction stabilize ferromagnetic ordering in systems with orbital degeneracy. In the absence of correlated hopping and J (J_0) the values of J_0 (J) required for ferromagnetism are of the same order as the bandwidth. Taking into consideration both intra- and inter-atomic exchange interactions as well as correlated hopping leads to more realistic critical values of the mentioned exchange interactions, allowing us to describe real materials. Note also that the critical values of J_0 and J decrease with the increase of Coulomb interaction parameter U . A qualitatively similar picture has been obtained by the authors of [13].

Figure 4, which is plotted with use of equation (2.4) at $U/w = 1.2$, $zJ/w = 0.012$, $J_0/w = 0.3$, $\tau_1 = 0$ and $\tau_2 = 0.14$ (these values of the parameters agree with the estimations mentioned in section 1), reproduces the behaviour of the magnetization observed in the systems $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ and $\text{Co}_{1-x}\text{Ni}_x\text{S}_2$ with changing electron concentration in the 3d band [22]. In these crystals the same subsystem of electrons is responsible for both conductivity and localized magnetic moment formation. The noted compounds have the cubic pyrite structure, so the 3d band is split into two subbands: a doubly degenerate e_g band and a triply degenerate t_{2g} band; the t_{2g} band is completely filled and the e_g band is partially filled (the e_g band filling changes from zero to unity in the compound $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ and from unity to two in the compound

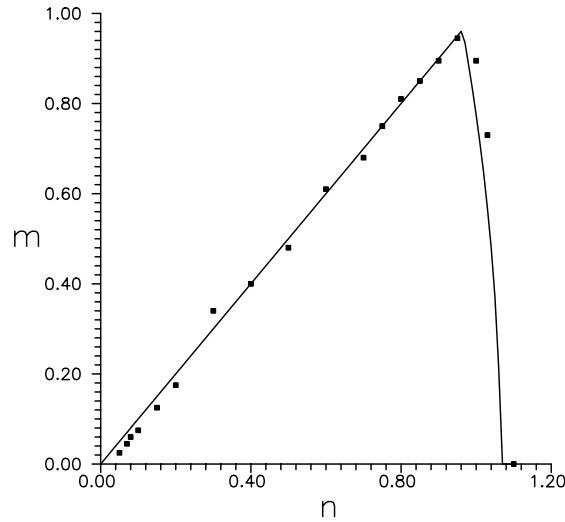


Figure 4. The magnetization m as a function of n at $U/w = 1.2$, $zJ/w = 0.012$, $J_0/w = 0.3$, $\tau_1 = 0$ and $\tau_2 = 0.14$. The experimental points for $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ and $\text{Co}_{1-x}\text{Ni}_x\text{S}_2$ are shown.

$\text{Co}_{1-x}\text{Ni}_x\text{S}_2$). One should describe the e_g band of these compounds by a doubly orbitally degenerate model.

The unusual peculiarity of the system $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ is the presence of ferromagnetic ordering at very small values of electron concentration $n = x \simeq 0.05$ [22]. Ferromagnetism in this compound has been studied within a single-band model in [23–25]. The authors of work [23, 24] have proposed an approximation for the description of $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ in the non-degenerate Hubbard model with $U = \infty$ which provides the ferromagnetic solution even at very small electron concentration (in this connection see also [25]). However, in accordance with the Kanamori theory [26] at very small n we should obtain the gas limit where ferromagnetism does not occur. We also suggest that the degeneracy of the e_g band is essential for the description of ferromagnetic ordering in this system. Our results allow us to obtain the ferromagnetism for small values of electron concentration induced by correlated hopping τ_2 in the presence of the inter-atomic exchange interaction (see figure 4). Thus, we believe that the correlated hopping mechanism in the presence of the inter-atomic exchange interaction allows a more natural explanation of the origin of ferromagnetism in the $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ system at very small x .

3. Conclusions

In this paper we have investigated the ground state ferromagnetism in a doubly orbitally degenerate Hubbard model generalized by taking into account correlated hopping and inter-atomic exchange interaction. We have found that intra-atomic Hund's rule coupling, inter-atomic direct exchange interaction and correlated hopping act cooperatively, stabilizing ferromagnetic order in systems with orbital degeneracy. The transition from the paramagnetic phase to the ferromagnetic one occurs at values of interaction parameters which are of the same order as the bandwidth, and with density of states without peculiarities. For the values of inter-atomic exchange interaction $J > 0$ the transition from a paramagnetic state to a partially polarized ferromagnetic state occurs, and for $J = 0$ the transition from a paramagnetic state to a fully polarized ferromagnetic state (saturated ferromagnetic state) is realized.

Taking into account the correlated hopping leads to the appearance of the specific mechanism due to the spin-dependent shift of the subband centres, which stabilizes ferromagnetic ordering. At values of the correlated hopping parameters $\tau_2 > \tau_1$ in the system with concentration of electrons $n < 2$ the situation for ferromagnetic ordering is more favourable than for the system with $n > 2$; at $\tau_2 < \tau_1$ the opposite behaviour is found.

The calculated dependence of magnetization on concentration of electrons qualitatively describes the experimental Slater–Pauling curves for ferromagnetic alloys. At some values of the model parameters the experimental dependence of magnetization for the systems $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ and $\text{Co}_{1-x}\text{Ni}_x\text{S}_2$ with change of electron concentration in the e_g band is reproduced theoretically. The correlated hopping mechanism of ferromagnetism stabilization allows us to explain the ferromagnetism in the systems $\text{Fe}_{1-x}\text{Co}_x\text{S}_2$ at small concentrations $x \simeq 0.05$.

Acknowledgments

VH is grateful to Professor W Nolting (Humboldt-Universität, Berlin) for hospitality during the workshop *242nd W E Heraeus Seminar on Ground-State and Finite-Temperature Band Ferromagnetism (Berlin, 2000)*, where some of the results considered in this paper were discussed. The authors thank Professor D Vollhardt, Professor W Weber and Dr Bünemann for valuable discussions. VH acknowledges a fellowship of the Cabinet of Ministers of Ukraine for outstanding young researchers.

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