Ferromagnetic ordering in a generalized Hubbard model: weak intra-atomic interaction limit

L. Didukh

Ternopil State Technical University, Department of Physics
56 Rus’ka Str., Ternopil UA–282001, Ukraine
Tel.: +380352251946, Fax: +380352254983
E-mail: didukh@tu.edu.te.ua

Abstract

In the present work ferromagnetic ordering in the Hubbard model generalized by taking into account the inter-atomic exchange interaction and correlated hopping in partially filled narrow band is considered. Expressions for the magnetization and Curie temperature as functions of model parameters and band filling are obtained in the case of weak intra-atomic Coulomb interaction. Condition of ferromagnetic state realization is found. The obtained results indicate the important role of correlated hopping. pacs71.10.Fd, 71.30.+h, 71.27.+a

1 Introduction

In spite of great attention payed to investigation of ferromagnetism in narrow energy bands [1]-[7], where the same system of electrons is responsible both for conductivity and for magnetic ordering (the transition 3d-metals, ferromagnetic sulphides, oxides and selenides with metallic type of conductivity) the problem still remains open [8, 9].

There are some experimental results for the disulphides of transition metals which can be interpreted on the basis of itinerant mechanism of ferromagnetism. In these compounds the dependence of Curie temperature on the number of magnetic moments is non-typical from point of view of exchange mechanism of ferromagnetism. In $Fe_xCo_{1-x}S_2$ [10] where electron concentration $n$ changes from 0 to 1 in doubly degenerate $e_g$ -subband the Curie temperature increases with decrease of electron concentration at $0.75 < n < 1$.

Although the consistent theory of ferromagnetic ordering in transition metal compounds can be constructed only in the model including the orbital degeneracy of the band, the qualitative character of observed properties can be interpreted in the framework of generalized model of non-degenerate band [11].
2 The Hamiltonian

The simplest model for description of the magnetic properties of narrow-band materials is the Hubbard model [12], but this model contains only diagonal matrix elements of Coulomb interaction in site representation, that not give rise to metallic ferromagnetism except in special situations such as a single hole in a half-filled band [13] or a special lattice geometry [7]. The importance of non-diagonal matrix elements of Coulomb interaction was pointed out in papers [14, 8].

We write the Hamiltonian of system of $s$-electrons in the following form [15, 16]

$$H = -\mu \sum_i a_{i\sigma}^+ a_{i\sigma} + \sum'_{ij\sigma} t_{ij}(n) a_{i\sigma}^+ a_{j\sigma} + \sum'_{ij\sigma} (T_2(ij) a_{i\sigma}^+ a_{j\sigma} n_{i\bar{\sigma}} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum'_{ij\sigma\sigma'} J a_{i\sigma}^+ a_{j\sigma} n_{i\bar{\sigma}} a_{j\bar{\sigma}},$$

where $a_{i\sigma}^+$, $a_{i\sigma}$ - creation and destruction operators of electron on site $i$, $\sigma = \uparrow, \downarrow$, $n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$, $n = (n_{i\uparrow} + n_{i\downarrow})$, $\mu$ - chemical potential, $t_{ij}(n) = t(ij) + T_1(ij)$ is the effective hopping integral between nearest neighbours, $t_{ij}$ is the hopping integral of an electron from site $j$ to site $i$, $T_1(ij)$ and $T_2(ij)$ are the parameters of correlated hopping [16] of electron, $U$ is the intraatomic Coulomb repulsion and $J$ is the exchange integral for the nearest neighbours. The prime by second sum in Eq. (1) signifies that $i \neq j$.

The peculiarities of the model described by the Hamiltonian (1) is taking into consideration the influence of sites occupation on the electron hoppings (correlated hopping), and the exchange integral. The correlated hopping, firstly, renormalize the initial hopping integral (it becomes concentration- and spin-dependent) and, secondly, lead to an independent on quasimomentum shift of the band center, dependent on magnetic ordering. Taking into account the quantity of second order $J$ is on principle necessary to describe ferromagnetism in this model [14, 8, 17]. In this paper we do not take into account the inter-atomic Coulomb interaction, which is important in the charge ordering state (this ordering type go beyond this article).

To characterize the value of correlated hopping we introduce dimensionless parameters $\tau_1 = \frac{T_1(ij)}{|t_{ij}|}$, $\tau_2 = \frac{T_2(ij)}{|t_{ij}|}$.

3 Weak intra-atomic interaction

To simplify the consideration we use model Hamiltonian (1). If intra-atomic Coulomb interaction is weak ($U < |t_{ij}(n)|$) then we can take into account the electron-electron interaction in the Hartree-Fock approximation:

$$n_{i\uparrow} n_{i\downarrow} = n_{\uparrow} n_{\downarrow} + n_{\downarrow} n_{\uparrow},$$

$$a_{i\sigma}^+ n_{i\bar{\sigma}} a_{j\sigma} = n_{\bar{\sigma}} a_{i\sigma}^+ a_{j\sigma} + \langle a_{i\sigma}^+ a_{j\sigma} \rangle n_{i\bar{\sigma}},$$

where the average values $\langle n_{i\sigma} \rangle = n_{\sigma}$ are independent of site number (we suppose that distributions of electron charge and magnetic momentum are homogenous). Taking into account (2) we can write Hamiltonian (1) in the following form:

$$H = \sum'_{ij\sigma} \epsilon_{\sigma}(ij) a_{i\sigma}^+ a_{j\sigma},$$

(3)
where

\[ \epsilon_\sigma(ij) = -\mu + \beta_\sigma + n_\sigma U + zn_\sigma J + t_{ij}(n\sigma); \] (4)

\[ \beta_\sigma = \frac{2}{N} \sum_{ij} T_2(ij) \langle a_{i\sigma}^+ a_{j\sigma}^\prime \rangle, \] (5)

\[ t_{ij}(n\sigma) = t_{ij}(n) + 2n_\sigma T_2(ij). \] (6)

The dependences of effective hopping integral on electron concentration and magnetization, a being of the spin-dependent displacement of band center are the essential distinction of single-particle energy spectrum in the model described by Hamiltonian (3) from the spectrum in the Hubbard model for weak interaction. An use of (3) allows, in particular, to explain the peculiarities of dependence of binding energy on atomic number in transition metals and also essentially modifies theory of ferromagnetism in a collective electron model.

4 Ferromagnetic ordering in weak intra-atomic interaction limit

After the transition to Fourier representation we obtain for the Green function

\[ \braket{a_{p\sigma}|a_{p'\sigma}}_k = \frac{1}{2\pi} \frac{1}{E - \epsilon_\sigma(k)} \] (7)

where the energy spectrum is

\[ \epsilon_\sigma(k) = -\mu + \beta_\sigma + n_\sigma U - zn_\sigma J + t(n\sigma)\gamma(k); \] (8)

here the spin-dependent shift of the band center is

\[ \beta_\sigma = \frac{2}{N} \sum_{ij} T_2(ij) \langle a_{i\sigma}^+ a_{j\sigma}^\prime \rangle, \] (9)

\[ \gamma(k) = \sum_R e^{ikR}, \] the spin and concentration dependent hopping integral is

\[ t(n\sigma) = t(n) + 2n_\sigma T_2. \] (10)

The concentration of electrons with spin \( \sigma \) is

\[ n_\sigma = \int_{-\infty}^{+\infty} \rho(\epsilon) f(\epsilon) d\epsilon. \] (11)

Here \( \rho(\epsilon) \) is the density of states, \( f(\epsilon) \) is the Fermi distribution function. Let us assume the rectangular density of states:

\[ \rho(\epsilon) = \frac{1}{N} \sum_k \delta(\epsilon - \epsilon(k)) = \frac{1}{2w} \theta(\epsilon^2 - w^2) \] (12)
Then in the case of zero temperature we obtain:

\[ n_\sigma = \int_{-\infty}^{+\infty} \rho(\epsilon) \theta(-E_\sigma(\epsilon))d\epsilon = \frac{1}{2w} \int_{-w}^{w} \theta(-E_\sigma(\epsilon))d\epsilon = \frac{1}{2w} \int_{-w}^{\epsilon_\sigma} d\epsilon, \]  

(13)

where \( \epsilon_\sigma = w(2n_\sigma - 1) \). The value \( \epsilon_\sigma \) is the solution of the equation \( E_\sigma(\epsilon) = 0 \) from which we obtain \( \epsilon_\sigma = \frac{\mu_\sigma}{\alpha_\sigma} \), where \( \mu_\sigma = \mu - \beta_\sigma + zn_\sigma J - n_\theta U \) and \( \alpha_\sigma = 1 - 2\tau_2 n_\theta \).

The system parameters are related by the equation

\[ m(zJ + u) + \beta_\downarrow - \beta_\uparrow = 2m(1 - \tau_2). \]  

(14)

The shift of band center is obtained from

\[ \beta_\sigma = \frac{2}{N} \sum_{ij} T_2(ij) \langle a^+_i a_j \rangle = -\tau_2 \frac{\epsilon_\sigma}{2} \int_{-w}^{\epsilon_\sigma} d\epsilon = -\tau_2 wn_\sigma(n_\theta - 1). \]  

(15)

One can see that

\[ \beta_\downarrow - \beta_\uparrow = 2\tau_2 mw(1 - n). \]  

(16)

From the equation (14) one can see that in less than half-filled band correlated hopping leads to the stabilisation of ferromagnetism as well as inter-atomic exchange interaction and intra-atomic Coulomb interaction; the larger is electron concentration \( n \) the smaller is the critical value of exchange integral for occurrence of ferromagnetism. These our results are in accordance with the results of paper [8].

From (14) and (16) we obtain the condition of ferromagnetic ordering realization:

\[ \frac{zJ + U}{2w} + \tau_2(2 - n) > 1. \]  

(17)

Here we use the notation

\[ w = w(n) = z|t_0|(1 - \tau_1 n) \]  

(18)

where \( t_0 \) is the band hopping integral.

In the case of non-zero temperatures the equation for magnetization is

\[ \exp\left(\frac{-mJ_{eff}}{\theta}\right) = \frac{\sinh((1 - n_\uparrow)\alpha_\uparrow w/\theta)\sinh(n_\downarrow\alpha_\downarrow w/\theta)}{\sinh((1 - n_\downarrow)\alpha_\downarrow w/\theta)\sinh(n_\uparrow\alpha_\uparrow w/\theta)}, \]  

(19)

where the effective exchange integral is

\[ J_{eff} = zJ + U + 2zT_2(1 - n) \]  

(20)

The expression for Curie temperature can be obtained from equation (19) at \( m \to 0 \). If \( \tau_1 = \tau_2 = 0 \) then we obtain

\[ \theta_C = \frac{w_0}{2} \arctanh\left(\frac{2w_0}{zJ + U}\right) \]  

(21)

If \( \tau_1 = \tau_2 = 1/2 \) then

\[ \theta_C = \frac{w_0n(2 - n)(1 - \frac{n}{2})}{4} \arctanh\left(\frac{w_0(1 - \frac{n}{2})}{zJ + U + (1 - n)(1 - \frac{n}{2})w_0}\right) \]  

(22)

It is important that at some values of parameters the Curie temperature can increase with the decrease of the electron concentration.
5 Discussion and Conclusions

The analysis of obtained in this paper energy spectrum (8) shows that both intraatomic Coulomb repulsion $U$ and exchange integral $J$ favor spin polarization. Furthermore, taking into account the correlated hopping leads to the spin-dependent shift of the band center and to the band narrowing, which also give rise to ferromagnetism. These our results are in accordance with the results of paper [8].

The peculiarities of the energy spectrum (8) lead to concentration dependence of the Curie temperature. In particular, the concentration dependent shift (16) of the band centers at $n < 1$ is positive, at $n > 1$ is negative. According to this fact the Curie temperature at decreasing $n$ from 1 can increase and at $n > 1$ can decrease. The obtained dependence qualitatively agrees with the experimental data on Fe$_x$Co$_{1-x}$S$_2$ [10]. The proposed approach can be extended to all values of $n$, and the peculiarities of ferromagnetic ordering in Co$_x$Ni$_{1-x}$S$_2$ where this concentration changes from 1 to 2 can be explained.

In conclusion, taking into consideration both correlated hopping and inter-atomic exchange interaction essentially modify the $s-$band model and favours the ferromagnetic ordering.

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