FERROMAGNETISM AND METAL–INSULATOR TRANSITION IN HUBBARD MODEL WITH CORRELATED HOPPING*

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In this paper both the metal–insulator transition and ferromagnetic ordering stabilization have been studied in the framework of the Hubbard model with correlated hopping and inter-atomic exchange interaction. The energy spectrum of the model has been calculated, expressions for the energy gap in the paramagnetic state, the ground state energy, the criterion of the ferromagnetism stabilization, the magnetization of system have been obtained and analyzed.

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1. Introduction

To describe the concentration dependency of the physical properties of real materials the Hubbard model [1] has to be generalized by taking into account the non-diagonal matrix elements of Coulomb interaction [2–5]. In the case of strong and intermediate inter-atomic interactions the correlated hopping leads to the electron-hole asymmetry [4,6] and the renormalization of width of energy subbands. In this paper both the metal–insulator transition (MIT) and ferromagnetic ordering stabilization have been studied in the framework of the Hubbard model with correlated hopping and inter-atomic exchange interaction. To this end recently proposed variant [7] of the generalized Hartree–Fock approximation has been applied.

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2. The energy spectrum of generalized Hubbard model

We start with the Hamiltonian of the narrow-band model with correlated hopping of electrons and inter-atomic exchange interaction [4, 7]:

$$\begin{aligned} H &= H_0 + H_1 + H_1'; \qquad (1)\\ H_0 &= -\mu \sum_{i\sigma} \left(X_i^{\sigma} + X_i^{2}\right) + U \sum_i X_i^2 - \mu_{\rm B} h \sum_i (X_i^{\uparrow} - X_i^{\downarrow}) \\ &\quad + \frac{J}{2} \sum_{ij\sigma} \Big(X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} + (X_i^{\sigma} + X_i^{2})(X_j^{\sigma} + X_j^{2}) \Big), \\ H_1 &= \sum_{ij\sigma, i\neq j} t_{ij}(n) X_i^{\sigma 0} X_j^{0\sigma} + \sum_{ij\sigma, i\neq j} \tilde{t}_{ij}(n) X_i^{2\bar{\sigma}} X_j^{\bar{\sigma}2}, \\ H_1' &= \sum_{ij\sigma, i\neq j} t_{ij}'(n) \left(X_i^{\bar{\sigma}0} X_j^{\sigma 2} - X_i^{\sigma 0} X_j^{\bar{\sigma}2} + \text{H.c.} \right), \end{aligned}$$

here X_i^{kl} denotes the Hubbard operators, μ is chemical potential, U is the energy of intra-atomic Coulomb interaction, J is the parameter of the inter-atomic exchange interaction, h is the external magnetic field,

$$t_{ij}(n) = t_{ij}(1 - n\tau_1), \qquad (2)$$

$$t_{ij}'(n) = t_{ij}(1 - n\tau_1 - \tau_2), \qquad (3)$$

$$\tilde{t}_{ij}(n) = t_{ij}(1 - n\tau_1 - 2\tau_2), \qquad (4)$$

are the effective concentration-dependent hopping integrals [4]. Other notations are as usual.

The single particle energy spectrum calculated with use of the variant [7] of generalized Hartree–Fock approximation in Fourier representation has the form:

$$\begin{aligned} E_{1,2}^{\sigma}(\boldsymbol{k}) &= -\mu - \eta_\sigma h + \frac{U}{2} - \frac{(n + \eta_\sigma m)}{2} zJ + \frac{(\epsilon^{\sigma} + \tilde{\epsilon}^{\sigma})}{2} t(\boldsymbol{k}) \\ &\quad \mp \frac{1}{2} \sqrt{[U - ((\epsilon^{\sigma} - \tilde{\epsilon}^{\sigma}) t(\boldsymbol{k}))]^2 + 4\epsilon_1^{\sigma} \epsilon_2^{\sigma} t(\boldsymbol{k})^2}. \qquad (5) \end{aligned}$$

Here the non-operator coefficients $\epsilon^{\sigma}(pi)$, $\tilde{\epsilon}^{\sigma}(pi)$, ϵ_1^{σ} and ϵ_2^{σ}, calculated by the method of work [4, 7], can be written as functions of the electron concentration n, system magnetization m, hole (c) and doublon (d) concentrations and the correlated hopping parameters τ_1, τ_2 (the values d and c are connected by the relation $c - d = 1 - n$).

3. MIT in a paramagnetic half-filled band

Let us consider the MIT in paramagnetic state at electron concentration $n = 1$. From the energy spectrum (5) we find the energy gap width:

$$\Delta E = E_2(-w) - E_1(w) = -2w(1-2d)(1-\tau_1-\tau_2) + \frac{Q_1+Q_2}{2},$$
$$Q_{1,2} = \left((U \mp 2\tau_2 Cw)^2 + (1-\tau_1-2\tau)^2 w^2\right)^{\frac{1}{2}}, \quad C = 1-2d+4d^2. \quad (6)$$

When the correlation strength $\frac{U}{w}$ reaches its critical value $(\frac{U}{w})_c$ the energy gap opens and the metal–insulator transition occurs. The correlated hopping leads to the decrease of the $(\frac{U}{w})_c$. It is important to note, that the used approach allows to reproduce the exact results, found in the special case of the model with correlated hopping [8–11]. At $t'_{\boldsymbol{k}} = 0$ from (6) we obtain $U_c = w + \tilde{w}$, where $2w = 2z|t_{ij}|$ is the width of lower subband, $2\tilde{w} = 2z|\tilde{t}_{ij}|$ is the width of upper subband, z is the number of nearest neighbour to a site. In the paramagnetic ground state one can find the expression for the doublon concentration. The increase of τ_1, τ_2 leads to the decrease of d at fixed values of $\frac{U}{w}$. At the increase of $\frac{U}{w}$ in the point of MIT the slope of $d(\frac{U}{w})$ dependence changes. For the case $\tau_1 = \tau_2 = 0$ (Hubbard model) the obtained results agree with corresponding result of work [12]. The ground state energy in the metallic and insulating states is also calculated. The dependencies of the ground state energy on $\frac{U}{w}$ for different values of τ also change its slope in the point of MIT. The increase of the correlated hopping parameters τ_1, τ_2 leads both for the decrease of kinetic energy of electrons (the band narrowing), and for the decrease of potential energy (decrease of the doublon concentration). Thus the correlated hopping significantly influence the ground state energy in the region of MIT. At $\tau_1 = \tau_2 = 0$ (Hubbard model) the obtained values of the ground state energy lies within the interval determined in the paper [13].

4. The ground state ferromagnetism

Let us consider the ground state ferromagnetism in the model. In the limiting case of Hubbard model ($\tau_1 = \tau_2 = 0$) for the case of half-filling we obtain the condition of ferromagnetism stability in the form:

$$4d\frac{U}{2w} + \frac{zJ}{2w} > 4d(1-2d)(3-4d). \quad (7)$$

From equation (7) one can see that in the case of large $\frac{U}{2w}$ when $d \to 0$ the critical value of the interatomic exchange interaction tends to zero, on the absence of interatomic Coulomb interaction ($U \to 0$ and $d \to \frac{1}{4}$) the critical value of zJ is equal to the width of the energy band. One can also see

that the interatomic exchange is the key parameter for the ferromagnetism realization.

In the case of strong intra-atomic Coulomb interaction the energy spectrum (5) describes non-hybridized upper and lower Hubbard subbands. It is important to investigate the case $n \neq 1$ when system is metallic despite of strong interaction. In the ground state the equation

$$\frac{zJ}{2(1-n\tau_1)w} = 1 - \frac{n^2-m^2}{(2-n)^2-m^2}\left(1 - \frac{8(1-n)(2-n)}{(2-n)^2-m^2}\right) \tag{8}$$

determines the magnetization of system at $n < 1$ and corresponding equation at $n > 1$ is

$$\frac{zJ}{2(1-n\tau_1-\tau_2)w} = 1 - \frac{(2-n)^2-m^2}{n^2-m^2}\left(1 - \frac{8(1-n)n}{n^2-m^2}\right). \tag{9}$$

At increase of correlated hopping the region of ferromagnetism becomes wider. The taking into account correlated hopping leads to the concentration dependent bandwidth renormalization. Thus for the same values of the energy parameters the state of system at $n < 1$ can be paramagnetic and at $n > 1$-ferromagnetic. Note that real ferromagnetic transition metals have more than half-filled $3d$-band. The paramagnet–ferromagnet transition can realize both at the change of the electron concentration and at the change of energy parameters of the system. The calculated dependencies of magnetization on external magnetic field and temperature agree very well with experimental results of work [14] for the system $CoS_{2-x}Se_x$.

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