

# FERROMAGNETISM IN SPIN SUBSYSTEM HYBRIDIZED WITH CONDUCTION BAND IN ANDERSON-HUBBARD-TYPE MODEL

L. Didukh, O. Kramar and Yu. Skorenky

Ternopil National Technical University, Physics Department, 56 Ruska Str., 46001 Ternopil, Ukraine



## Abstract

Magnetic ordering mechanisms in spin subsystem of a model with Anderson-Hubbard centers have been studied. Besides the spin-spin interactions and strong on-site Coulomb interaction, the model takes into account the hybridization with conduction band which results in the indirect hopping and indirect exchange interaction. Our results show that in the considered model the effects of localization are enhanced due to reduced values of indirect hopping integrals in comparison with standard  $s-d$ -model.

## Polar model of narrow band materials with Anderson-type centers

In recent years the progress of modern technologies has been associated with the synthesis of new materials with unique electrical and magnetic properties. Among these, very promising ones are materials with quantum dots where an "atom" of impurity is placed in the array of narrow band conductor. Theoretical investigations of electrical and magnetic properties of a "quantum dot" have originated from the pioneering paper [1]. In papers [2, 3] a generalization of the single impurity Anderson model [1] for the case of periodically spaced Anderson-Hubbard centers has been proposed (nowadays known as the periodic Anderson model). It has been proven in the framework of the periodic Anderson model that in the regime of strong intra-atomic interaction of localized magnetic moments the indirect (through the conduction band) exchange interaction occurs, which is proportional to the fourth order of the hybridization parameter  $V(\mathbf{ik})$  and also the indirect hopping of the current carriers takes place, being dependent on the hybridization parameter squared. In papers [4, 5], within single- and double-impurity Anderson models the electric conductivity of the system with quantum dots has been studied. In paper [5] the Coulomb interaction and band-localized states hybridization have been taken into account and the dependence of the conductivity on the magnitude of Coulomb interaction of the localized electrons have been found. From the paper [4] the conclusion can be drawn that the magnetic ordering in itinerant subsystem plays an important role in the spin-dependent transport.

Let us formulate the model of Anderson-Hubbard material, which generalizes the models proposed in papers [2, 6] and takes into account peculiarities of the correlation effects in narrow bands.

The peculiarity of configuration representation are the diagonal form of the on-site Coulomb repulsion term and association of the effects related to intra-atomic correlation to translation processes.

Let us write the Hamiltonian in  $X$ -operator representation

$$\begin{aligned} H &= H_0 + H_{\tilde{h}} + H_{\tilde{d}} + H_{2\tilde{h}} + H_{2\tilde{d}} + H_{\tilde{h}\tilde{d}}, \\ H_0 &= (E_d - \mu) \sum_i (X_i^\uparrow + X_i^\downarrow + 2X_i^2) + U \sum_i X_i^2 + \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \\ &\quad - \sum_{ij\sigma} \frac{J(ij)}{2} \left( (X_i^\sigma + X_j^\sigma)(X_i^\sigma + X_j^\sigma) + X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \right), \\ H_{\tilde{h}} &= \sum_{i\mathbf{k}\sigma} (\eta_{i\sigma} V(\mathbf{k}i) c_{\mathbf{k}\sigma}^\dagger X_i^{0\sigma} + h.c.), \\ H_{\tilde{d}} &= \sum_{i\mathbf{k}\sigma} (V(\mathbf{k}i) c_{\mathbf{k}\sigma}^\dagger X_i^{2\sigma} + h.c.), \\ H_{2\tilde{h}} &= 2 \sum_{ijk} (V(ij\mathbf{k}, -\mathbf{k}) X_i^{\uparrow 0} X_j^{\downarrow 0} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + h.c.), \\ H_{2\tilde{d}} &= 2 \sum_{ijk} (V(ij\mathbf{k}, -\mathbf{k}) X_i^{2\uparrow} X_j^{2\downarrow} c_{-\mathbf{k}\uparrow} c_{\mathbf{k}\downarrow} + h.c.), \\ H_{\tilde{h}\tilde{d}} &= 2 \sum_{ijk} (V(ij\mathbf{k}, -\mathbf{k}) (X_i^{\uparrow 0} X_j^{2\downarrow} c_{-\mathbf{k}\uparrow} c_{\mathbf{k}\downarrow} - X_i^{\downarrow 0} X_j^{2\uparrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) + h.c.). \end{aligned} \quad (1)$$

Here operator  $X_i^{kl}$  describes transition of site  $i$  from state  $|l\rangle$  to state  $|k\rangle$ ,  $\mu$  is the chemical potential,  $U$  denotes the energy of intra-site Coulomb repulsion of electrons,  $J(ij)$  stands for the direct inter-site exchange interaction.

Let us write the parameters which describe relative hybridization:

$$\begin{aligned} \frac{V(\mathbf{k}i)}{E_F - E_d} &\equiv v_{\tilde{h}}(\mathbf{k}i), & \frac{V(\mathbf{k}i)}{E_d + U - E_F} &\equiv v_{\tilde{d}}(\mathbf{k}i), \\ \frac{V(\mathbf{k}, -\mathbf{k}ij)}{2(E_F - E_d)} &\equiv v_{2\tilde{h}}(\mathbf{k}, -\mathbf{k}ij), \\ \frac{V(ij, -\mathbf{k}\mathbf{k})}{2(E_d + U - E_F)} &\equiv v_{2\tilde{d}}(ij, -\mathbf{k}\mathbf{k}), \\ \frac{V(ij, -\mathbf{k}\mathbf{k})}{2E_d + U - E_F} &\equiv v_{\tilde{h}\tilde{d}}(ij, -\mathbf{k}\mathbf{k}). \end{aligned}$$

If one of the parameters  $v_x$  ( $x = \tilde{h}, \tilde{d}, 2\tilde{h}, 2\tilde{d}, \tilde{h}\tilde{d}$ ) satisfies the condition  $v_x \ll 1$  then one can apply the perturbation theory to the hybridization interaction terms  $H_x$  (we note, that the configuration representation of the Hamiltonian is most appropriate for this purpose).

In the case when  $E_d + U - E_F \gg E_F - E_d$  (or opposite case) one can neglect corresponding translation processes in the Hamiltonian. These conclusions are in accordance with estimation of the hybridization matrix elements in the model of heavy fermions (see monograph [7]). The  $X$ -operator representation of the Anderson-type Hamiltonian is also suitable for mathematical treatment within Green function method.

## Canonical transformation and effective Hamiltonian

According to the methodology of effective Hamiltonian derivation we assume that parameters characterizing the relative value of hybridization are small enough and perform the canonical transformation which excludes the terms of the first order in hybridization parameters  $V(\mathbf{ik})$  and  $V(ij\mathbf{k}, -\mathbf{k})$

$$\tilde{H} = e^{(S_{\tilde{h}} + S_{\tilde{d}} + S_{2\tilde{h}} + S_{2\tilde{d}})} H e^{-(S_{\tilde{h}} + S_{\tilde{d}} + S_{2\tilde{h}} + S_{2\tilde{d}})}, \quad (2)$$

where the unitary operator constituents are determined by equations

$$\begin{aligned} [S_{\tilde{h}}, H_0] + H_{\tilde{h}} &= 0, & [S_{\tilde{d}}, H_0] + H_{\tilde{d}} &= 0, \\ [S_{2\tilde{h}}, H_0] + \frac{1}{2} [S_{\tilde{h}}, H_{\tilde{h}}]' - H_{2\tilde{h}} &= 0, \\ [S_{2\tilde{d}}, H_0] + \frac{1}{2} [S_{\tilde{d}}, H_{\tilde{d}}]' - H_{2\tilde{d}} &= 0, \end{aligned}$$

which exclude the negligible processes. In above equations a prime by the Poisson bracket means that the terms  $\frac{1}{2} [S_{\tilde{d}}, H_{\tilde{d}}]'$  having the same operator structure as  $H_2$ , are included.

In this way the equation (2) up to the fourth order of magnitude has the following form (we take  $V(\mathbf{ik})$  to be first order of magnitude,  $V(ij\mathbf{k}, -\mathbf{k})$  the second order,  $H_0$  of the zeroth order)

$$\begin{aligned} \tilde{H} &= H + [S_{\tilde{h}}, H] + \frac{1}{2} [S_{\tilde{h}}, [S_{\tilde{h}}, H_0]] + \frac{1}{6} [S_{\tilde{h}}, [S_{\tilde{h}}, [S_{\tilde{h}}, H]]] + \\ &\quad + \frac{1}{24} [S_{\tilde{h}}, [S_{\tilde{h}}, [S_{\tilde{h}}, \frac{1}{6} [S_{\tilde{h}}, [S_{\tilde{h}}, [S_{\tilde{h}}, H_0]]]]]] + \dots \end{aligned} \quad (3)$$

Let us take into account that spin-spin interaction between localized magnetic moments and indirect hopping in localized subsystem attribute only to terms of the fourth order of magnitude. Thus, we can neglect the processes of double creation or annihilation of electrons on the same site and the interaction of BCS-type in the itinerant subsystem. The resulting effective Hamiltonian has the form

$$\tilde{H} = \tilde{H}_0 + H'_1 + H_{cd}, \quad (4)$$

where

$$\begin{aligned} \tilde{H}_0 &= H_0 + \sum_{ij\sigma} t_0(ij) X_i^{\sigma 0} X_j^{0\sigma} + \sum_{ij\sigma} t_2(ij) X_i^{2\sigma} X_j^{\sigma 2} - \\ &\quad - \sum_{ij\sigma} \frac{J(ij)}{2} \left( (X_i^\sigma + X_j^\sigma)(X_i^\sigma + X_j^\sigma) + X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} \right), \\ H'_1 &= \sum_{ij} t_{02}(ij) (X_i^{2\downarrow} X_j^{0\uparrow} - X_i^{2\uparrow} X_j^{0\downarrow}) + h.c., \\ H_{cd} &= \sum_{i\mathbf{k}\mathbf{k}'} J_1(i\mathbf{k}\mathbf{k}') (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} (X_i^\uparrow + X_i^0) + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\downarrow} (X_i^\downarrow + X_i^0) - \\ &\quad - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\uparrow} X_i^{\uparrow\downarrow} - c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow} X_i^{\downarrow\uparrow}) + \sum_{i\mathbf{k}\mathbf{k}'} J_2(i\mathbf{k}\mathbf{k}') (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} (X_i^\downarrow + X_i^2) + \\ &\quad + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\downarrow} (X_i^\uparrow + X_i^2) + c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\uparrow} X_i^{\uparrow\downarrow} + c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow} X_i^{\downarrow\uparrow}). \end{aligned}$$

In the above formulae  $t_0(ij)$ ,  $t_2(ij)$ ,  $t_{02}(ij)$  are the integrals of indirect hopping through the sites with localized electrons (cation subsystem in transition metal compounds, quantum dots, etc),  $J_1(i\mathbf{k}\mathbf{k}')$  and  $J_2(i\mathbf{k}\mathbf{k}')$  are hybridization exchange integrals.

$$\begin{aligned} t_0(ij) &= \sum_{\mathbf{k}<\mathbf{k}_F} \frac{V(\mathbf{ik})V(\mathbf{k}j)}{E_d - \epsilon_{\mathbf{k}}}, & t_2(ij) &= \sum_{\mathbf{k}>\mathbf{k}_F} \frac{V(\mathbf{ik})V(\mathbf{k}j)}{E_d + U - \epsilon_{\mathbf{k}}}, \\ t_{02}(ij) &= \frac{1}{2} (t_0(ij) + t_2(ij)), \\ J_1(i\mathbf{k}\mathbf{k}') &= \frac{V(\mathbf{ik})V(\mathbf{k}'i)}{2} \left( \frac{1}{\epsilon_{\mathbf{k}} - E_d} + \frac{1}{\epsilon_{\mathbf{k}'} - E_d} \right), \\ J_2(i\mathbf{k}\mathbf{k}') &= \frac{V(\mathbf{ik})V(\mathbf{k}'i)}{2} \left( \frac{1}{\epsilon_{\mathbf{k}} - E_d - U} + \frac{1}{\epsilon_{\mathbf{k}'} - E_d - U} \right). \end{aligned}$$

The magnitudes of these parameters can essentially renormalize the bare band hopping integral and enhance localization effects. In fig. 1 the mechanisms of the band and hybridization hoppings are shown. Due to the substantial overlapping of the wave functions of conduction electrons one should expect that not only indirect hopping renormalizes the band hopping but also hybridization exchange has greater magnitude (of order of  $\frac{t^2}{U}$ ) than direct exchange interactions.

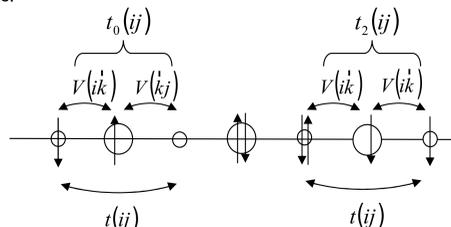


Fig.1. Hybridization and band hopping processes.

In the case of strong correlation  $U \gg w_d$  and  $n < 1$  the effective Hamiltonian of localized electron subsystem has the form:

$$\begin{aligned} H_{eff} &= (E_d - \mu) \sum_i (X_i^\uparrow + X_i^\downarrow) + \sum_{ij\sigma} t_0(ij) X_i^{\sigma 0} X_j^{0\sigma} \\ &\quad - \frac{J_{eff}}{2} \sum_{ij\sigma} (X_i^{\sigma\sigma} X_j^{\sigma\sigma} + X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma}) \end{aligned} \quad (5)$$

## Conditions of ferromagnetic ordering

The energy spectrum obtained within projection procedure [8] in the Green function method  $E_{\mathbf{k}} = -\mu - t_0(\mathbf{k}) + zn_{\sigma} J_{eff}$  allows us to calculate the mean numbers of spin-up and spin-down electrons

$$n_{\uparrow} = \frac{1 - n_{\downarrow}}{2w_d} \int_{-w_d}^{w_d} \frac{dt}{\exp(-\frac{\mu+t}{\Theta}) + 1}, \quad n_{\downarrow} = \frac{1 - n_{\uparrow}}{2w_d} \int_{-w_d}^{w_d} \frac{dt}{\exp(-\frac{\mu+t}{\Theta}) + 1}, \quad (6)$$

where shifted chemical potential  $\mu_{\sigma} = \mu - zJ_{eff}n_{\sigma}$ .

Equation for system magnetization has the form

$$\exp\left(\frac{zJ_{eff}m}{\Theta}\right) = \frac{\sinh\left(\frac{2(1-n)w_d}{(2-n)\Theta}\right) \sinh\left(\frac{w_d}{\Theta} - \frac{w_d}{\Theta} \frac{2(1-n)}{(2-n+m)}\right)}{\sinh\left(\frac{2(1-n)w_d}{(2-n+m)\Theta}\right) \sinh\left(\frac{w_d}{\Theta} - \frac{w_d}{\Theta} \frac{2(1-n)}{(2-n-m)}\right)}. \quad (7)$$

At  $n \rightarrow 0$  the above equation reproduces the corresponding molecular field equation, so the eq. (7) is correct. The obtained equation has the ferromagnetic solution determined by the condition

$$zJ_{eff} > \frac{2(1-n)w_d}{(2-n)^2} \left[ \coth\left(\frac{(1-n)w_d}{(2-n)\Theta}\right) - \coth\left(\frac{w_d}{2\Theta} - \frac{(1-n)w_d}{(2-n)\Theta}\right) \right]. \quad (8)$$

For zero temperature this yields the inequality  $zJ_{eff} > \frac{4(1-n)}{(2-n)^2} w_d$  which is in agreement with the condition of ferromagnetic ordering stabilization in polar model with strong interaction ([9]). Equalizing left and right sides of the inequality (8) we obtain the equation for Curie temperature value. Let us take  $\Theta_C \ll w_d$  (this condition actually corresponds to  $J_{eff} \ll w_d$ ). Then

$$\frac{\Theta_C}{w_d} = \frac{(1-n)}{(2-n) \ln \frac{2-n}{m_0}}, \quad (9)$$

where the ground state system magnetization is

$$m_0 = \left[ (2-n)^2 - \frac{4(1-n)w_d}{zJ_{eff}} \right]^{\frac{1}{2}}. \quad (10)$$

If the band is less than half-filled, one has  $\Theta_C = \frac{zJ}{2}$  from eq. (9), in agreement with the above considerations. It is interesting to note that in eq. (9) Curie temperature value is proportional to the conduction band width, though ferromagnetic ordering is stabilized by exchange mechanism. One can see from eq. (10) that the saturation can be reached only for half-filled band.

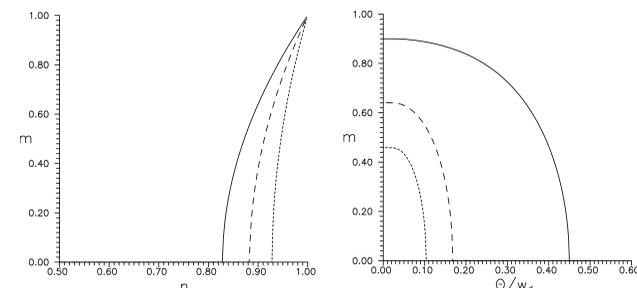


Fig.2. Ground state magnetization concentration dependence.  $zJ_{eff}/w_d = 1$  for solid curve,  $zJ_{eff}/w_d = 0.75$  for dashed curve,  $zJ_{eff}/w_d = 0.5$  for dotted curve.

Fig.2. Temperature dependence of magnetization at  $n = 0.9$ .  $zJ_{eff}/w_d = 1$  for solid curve,  $zJ_{eff}/w_d = 0.5$  for dashed curve,  $zJ_{eff}/w_d = 0.4$  for dotted curve.

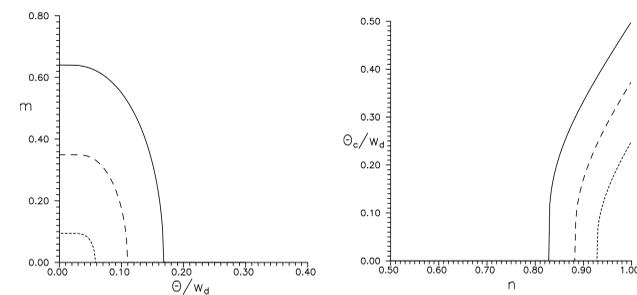


Fig.4. Temperature dependence of magnetization at  $zJ_{eff}/w_d = 0.5$ .  $n = 0.9$  for solid curve,  $n = 0.85$  for dashed curve,  $n = 0.83$  for dotted curve.

Fig.5. Concentration dependence of Curie temperature.  $zJ_{eff}/w_d = 1$  for solid curve,  $zJ_{eff}/w_d = 0.75$  for dashed curve,  $zJ_{eff}/w_d = 0.5$  for dotted curve.

From our results the following conclusions can be drawn. Taking  $c-d$  hybridization into account as perturbation leads to effective Hamiltonian in which the following effects are manifested. The first, the indirect hopping in  $(\sigma-0)$ - and  $(\uparrow\downarrow-\bar{\sigma})$ -subbands. The second, the pair creation of holes and doublons. The third, indirect  $c-d$ -exchange interaction. The fourth, indirect exchange interaction and indirect hopping between localized magnetic moments. In our opinion, the proposed approach is applicable for a wide class of ferromagnetic systems.

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