Conditions of ferromagnetic ordering in a model with Anderson-Hubbard centers: effective Hamiltonian approach

O Kramar, L Didukh, and Yu Skorenkyy

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

E-mail: kramar@tu.edu.te.ua

Abstract. A model of strongly correlated electron system in which magnetic impurity levels are hybridized with conduction band has been considered. The effective Hamiltonian has been constructed for the case of strong Coulomb correlation on basis of configurational representation of Hamiltonian with Hubbard X-operators describing the localized spin subsystem. Criteria for the ferromagnetic ordering stabilization have been found in partial case of partially filled band for arbitrary temperatures and Curie temperature has been calculated. For the partial case of weak effective exchange the formula for the Curie temperature reproducing the well-established results has been calculated analytically. The electron concentration region favorable for ferromagnetic ordering is determined by hybridization through effective exchange integral.

1. Introduction

Theoretical investigations of electrical and magnetic properties of a "quantum dot" have originated from the pioneering paper [1]. Since then, many generalizations and extensions of the Anderson model have been developed and used for description of heavy fermion [2] and quantum dot systems [3]-[5]. One of the first generalizations of the single impurity Anderson model [1] for the case of periodically spaced Anderson-Hubbard centers has been proposed in papers [6, 7]. It has been proven in the framework of the periodic Anderson model (PAM) 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 forth order of the hybridization parameter $V(i\mathbf{k})$ and also the indirect hopping of the current carriers takes place, being dependent on the hybridization parameter squared. Recent years have seen a renewed interest to the periodic Anderson model in connection with quantum dot systems and their promising properties. Electric conductivity of the system with quantum dots modelled by single- and double-impurities Anderson models has been studied in series of papers and transport properties were found to be spin-dependent [8, 9]. In this work the effective Hamiltonian of PAM is obtained by canonical transformation method. It allows the derivation of the Hamiltonians for partial cases in controllable manner. As a test of the approach applicability, the ferromagnetic ordering condition in a partial case of the model are studied.

2. Configurational representation of Hamiltonian

Following papers [6, 10], we start from the model of Anderson-Hubbard material which describe localized $(d-)$ subsystem hybridized with conduction $(c-)$ band. Coulomb and exchange interactions within the localized subsystem are the most conveniently described in the configurational representation of Hubbard X-operators.

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

Here operator X_i^{kl} describes transition of site i from state $|l\rangle$ to state $|k\rangle$, $c_{\mathbf{k}\sigma}^+$ $(c_{\mathbf{k}\sigma})$ are creation (annihilation) operators for band electrons. Energy parameters of the model are the chemical potential μ, the energy of intra-site Coulomb repulsion of electrons U, the direct inter-site exchange interaction $J(ij)$, hybridization parameters $V(i\mathbf{k})$ and $V(ij\mathbf{k},-\mathbf{k})$. Let us introduce the dimensionless parameters which describe relative hybridization:

$$
\frac{V(\mathbf{k}i)}{E_F - E_d} \equiv v_{\tilde{h}}(i\mathbf{k}), \quad \frac{V(i\mathbf{k})}{E_d + U - E_F} \equiv v_{\tilde{d}}(\mathbf{k}i),
$$

$$
\frac{V(\mathbf{k},-\mathbf{k}ij)}{2(E_F - E_d)} \equiv v_{2\tilde{h}}(\mathbf{k},-\mathbf{k}ij),
$$

$$
\frac{V(ij,-\mathbf{k}\mathbf{k})}{2(E_d + U - E_F)} \equiv v_{2\tilde{d}}(ij,-\mathbf{k}\mathbf{k}),
$$

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

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 [11]). The $X-$operator representation of the Anderson-like Hamiltonian is also suitable for mathematical treatment within Green function method.

3. 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 $V(i\mathbf{k})$ and $V(ij\mathbf{k}, -\mathbf{k})$

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

where the unitary operator constituents are determined from equations

$$[S_{\tilde{h}}, H_0] + H_{\tilde{h}} = 0, \qquad [S_{\tilde{d}}, H_0] + H_{\tilde{d}} = 0,$$

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

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

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 forth order of magnitude has the following form (we take $V(i\mathbf{k})$ to be first order of magnitude, $V(ij\mathbf{k}, -\mathbf{k})$ the second order, H_0 of the zeroth order)

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

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

$$\tilde{H} = \tilde{H}_0 + H_1' + H_{cd}, \tag{4}$$

where

$$\begin{aligned}
\tilde{H}_0 &= H_0 + {\sum_{ij\sigma}}' t_0(ij)X_i^{\sigma 0}X_j^{0\sigma} + {\sum_{ij\sigma}}' t_2(ij)X_i^{2\sigma}X_j^{\sigma 2} - \\
&- \frac{1}{2}{\sum_{ij\sigma}}' \tilde{J}(ij)\left(X_i^{\sigma}X_j^{\bar{\sigma}} - X_i^{\sigma\bar{\sigma}}X_j^{\bar{\sigma}\sigma} - X_i^0 X_j^2\right), \\
H_1' &= {\sum_{ij}}' t_{02}(ij)\left(X_i^{2\downarrow}X_j^{0\uparrow} - X_i^{2\uparrow}X_j^{0\downarrow}\right) + h.c., \\
H_{cd} &= \sum_{ikk'} J_1(ikk'i)(c_{\mathbf{k}\uparrow}^+ c_{\mathbf{k}'\uparrow}(X_i^{\uparrow} + X_i^0) + c_{\mathbf{k}\downarrow}^+ c_{\mathbf{k}'\downarrow}(X_i^{\downarrow} + X_i^0) - \\
&- c_{\mathbf{k}\downarrow}^+ c_{\mathbf{k}'\uparrow}X_i^{\uparrow\downarrow} - c_{\mathbf{k}\downarrow}^+ c_{\mathbf{k}'\uparrow}X_i^{\downarrow\uparrow}) + \sum_{ikk'} J_2(ikk'i)(c_{\mathbf{k}\uparrow}^+ c_{\mathbf{k}'\uparrow}(X_i^{\downarrow} + X_i^2) + \\
&+ c_{\mathbf{k}\downarrow}^+ c_{\mathbf{k}'\downarrow}(X_i^{\uparrow} + X_i^2) + c_{\mathbf{k}\downarrow}^+ c_{\mathbf{k}'\uparrow}X_i^{\uparrow\downarrow} + c_{\mathbf{k}\downarrow}^+ c_{\mathbf{k}'\uparrow}X_i^{\downarrow\uparrow}).
\end{aligned}$$

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), $J_1(i\mathbf{kk'}i)$ and $J_2(i\mathbf{kk'}i)$ are hybridization exchange integrals.

$$t_0(ij) = \sum_{k<k_F} \frac{V(i\mathbf{k})V(\mathbf{k}j)}{E_d - \epsilon_\mathbf{k}}, \qquad t_2(ij) = \sum_{k>k_F} \frac{V(i\mathbf{k})V(\mathbf{k}j)}{E_d + U - \epsilon_\mathbf{k}},$$

$$t_{02}(ij) = \frac{1}{2}\left(t_0(ij) + t_2(ij)\right),$$

$$J_1(ikk'i) = \frac{V(ik)V(k'i)}{2}\left(\frac{1}{\epsilon_{\mathbf{k}} - E_d} + \frac{1}{\epsilon_{\mathbf{k'}} - E_d}\right),$$

$$J_2(ikk'i) = \frac{V(ik)V(k'i)}{2}\left(\frac{1}{\epsilon_{\mathbf{k}} - E_d - U} + \frac{1}{\epsilon_{\mathbf{k'}} - E_d - U}\right).$$

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 t^4/U^3) than direct exchange interactions. In the case of strong correlation $U \gg w_d$ (here w_d is $d-$band halfwidth) and
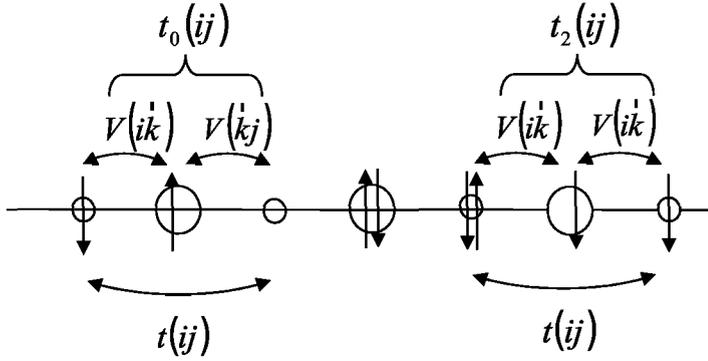
Figure 1. Hybridization and band hopping processes.

$n < 1$ the effective Hamiltonian of localized electron subsystem has the form:

$$H_{eff} = (E_d - \mu)\sum_i \left(X_i^\uparrow + X_i^\downarrow\right) + \sum_{ij\sigma} t_0(ij)X_i^{\sigma 0}X_j^{0\sigma} - \frac{J_{eff}}{2}\sum_{ij\sigma}' \left(X_i^{\sigma\sigma}X_j^{\sigma\sigma} + X_i^{\sigma\bar\sigma}X_j^{\bar\sigma\sigma}\right). \quad (5)$$

In distinction from standard $t - J$ Hamiltonian the hopping amplitude is substantially renormalized as it represents an indirect hopping here. In other respects the Hamiltonian (5) is very simple and allows for analytical calculations. The simplest analytical approach of choice is the decoupling of equation of motions, similar to the first step of work [3].

4. Condition of ferromagnetic ordering

The energy spectrum obtained within projection procedure [12] 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

$$n_\uparrow = \frac{1 - n_\downarrow}{2w_d}\int\limits_{-w_d}^{w_d}\frac{dt}{\exp(\frac{-\mu_\uparrow + t}{\Theta}) + 1}, \qquad n_\downarrow = \frac{1 - n_\uparrow}{2w_d}\int\limits_{-w_d}^{w_d}\frac{dt}{\exp(\frac{-\mu_\downarrow + t}{\Theta}) + 1}, \qquad (6)$$

where shifted chemical potential $\mu_\sigma = \mu + zJ_{eff}n_\sigma$. Equation for system magnetization has the form

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

At $n \to 0$ the above equation reproduces the corresponding molecular field equation. The obtained equation has the ferromagnetic solution determined by the condition

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

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 ([13]). Equalizing left and right sides of the inequality (8) we obtain the equation for Curie temperature. Let us take $\Theta_C \ll w_d$. Then

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

where the ground state system magnetization is

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

If the band is less than half-filled, one has $\Theta_C = zJ_{eff}/2$ 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. From figs. 2,3 one can see that the ferromagnetic ordering is quite stable for electron
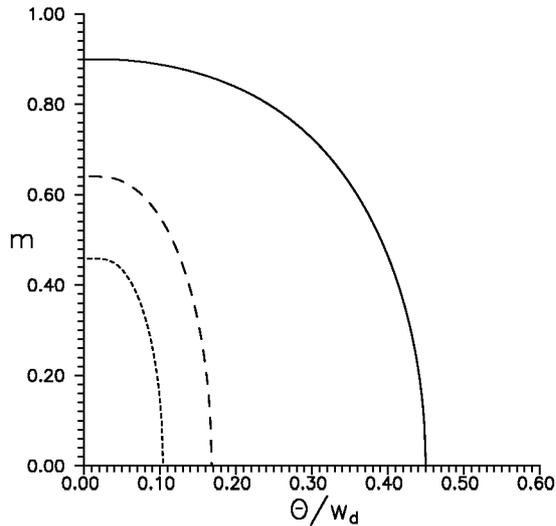
Figure 2. Temperature dependence of magnetization at $n = 0.9$. $zJ_{eff}/w_d = 1$ for solid curve, $zJ_{eff}/w_d = 0.5$ for dashed curve, $zJ_{eff}/w = 0.4$ for dotted curve.
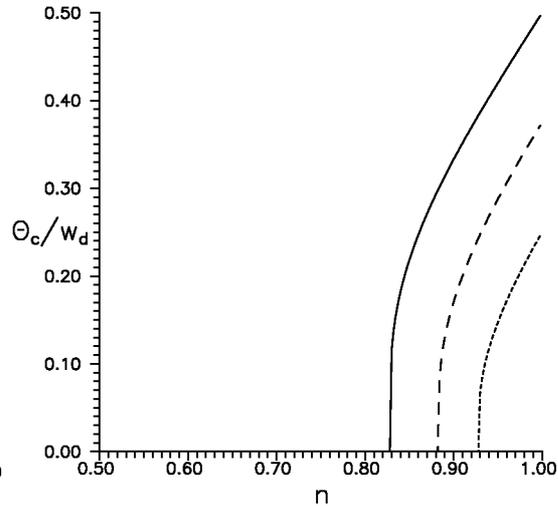
Figure 3. Concentration dependence of Curie temperature. $zJ_{eff}/w_d = 1$ for solid curve, $zJ_{eff}/w_d = 0.75$ for dashed curve, $zJ_{eff}/w = 0.5$ for dotted curve.

concentrations $n > 0.5$, in agreement with the results of paper [14]. The electron concentration region favorable for ferromagnetic ordering is considerably widened by hybridization through effective exchange integral. Summarizing, we note that taking $c - d$ hybridization into account as a perturbation leads to effective Hamiltonian in which the indirect hopping in (σ-0)- and ($\uparrow\downarrow$-$\bar{\sigma}$)-subbands and indirect $c - d$-exchange interaction are enhanced.

References

[1] Anderson P.W. 1961 *Phys. Rev.* **124**, 41.

[2] Hewson A.C. *The Kondo Problem to Heavy Fermions, Cambridge University Press*, New York, N.Y., 1993.

[3] Fransson J., Eriksson O., and Sandalov I. 2002 *Physical Review Letters* **88**, 226601.

[4] Braun M., Struck P.R., and Burkard G. 2011 *Phys. Rev. B* **84**, 115445.

[5] Zhen-Gang Zhu and Berakdar J. 2011 *Phys. Rev. B* **84**, 165105.

[6] Didukh L.D., Stasyuk I.V. 1968 *Fiz. Metal. Metaloved.* **26**, 582 [in Russian].

[7] Didukh L.D., Stasyuk I.V. 1968 *Ukr. Fiz. Zhurn.* **13**, 1774 [in Russian].

[8] Ping Zhang et al. 2002 *Phys. Rev. Lett.* **89**, 286803.

[9] Dias da Silva L. 2008 *Phys. Rev. B.* **78**, 153304.

[10] Didukh L.D., Didukh V.D., and Stasyuk I.V. 1975 *Ukr. Fiz. Zhurn.* **20**, 97 [in Russian].

[11] Fazekas P. *Lecture notes on electron correlation and magnetism*, Singapore, World Scientific Publishing, 1999.

[12] Didukh L. 2000 *Acta Physica Polonica (B).* **31**, 3097.

[13] Didukh L., Kramar O., and Skorenkyy Yu. in *New Developments in Ferromagnetism Research*, Ed.: Murray V.N., Nova Science Publishers, Inc, 2006.

[14] Meyer D., Nolting W. 2000 *Eur. Phys. Journ.* **18**, 385.