Energy spectrum and metal-insulator transition in system with Anderson-Hubbard centers

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Abstract. Energy spectrum of a model of narrow-band metal into which the periodically spaced Anderson-Hubbard centers are introduced has been studied. Hybridization with conduction band results in the indirect exchange interaction which is different from the interactions between localized magnetic moments and strong on-site Coulomb interaction. To study effect of the lattice deformation under the external pressure (or the self-contraction of the lattice) on electrical properties of the system, the phonon term and elastic energy have been taken into account. The equilibrium values of lattice strain and chemical potential have been calculated self-consistently for non-zero temperatures. Within the Green function approach, the energy spectrum has been calculated as function of model parameters, temperature and external pressure. Our results show that there exists a threshold value of the external pressure above which energy gap value decreases rapidly with temperature and system becomes a correlated metal.

1. Introduction

In recent years the metal-insulator transition problem has been intensively studied in the framework of periodic Anderson model [1-4]. Methods developed for investigation of Hubbard model, namely dynamical mean field theory (DMFT) [1,2], Gutzwiller variational method [3,4], exact diagonalization [4], spectral density approximation and modified alloy analogy [5] have been applied to clarify the role of hybridization in destabilization of Mott insulator. It has been found that the width of the Mott gap is renormalized by hybridization effects [2], and the increase of temperature leads to the gap closure [1], however the pressure-temperature phase diagram has not been built so far. To complement the results cited above, we have considered a model of the periodically spaced Anderson-Hubbard centers hybridized with conduction band which takes into account the lattice elastic energy also and allows to describe the effect of the external pressure on energy spectrum of the system.

2. The model Hamiltonian

We start from the model of Anderson-Hubbard material which generalizes the models [6, 7] and take into account the peculiarities of correlation effects in narrow energy bands. The Hamiltonian contains terms describing localized (*d*) subsystem and band (*s*) subsystem as well as their hybridization

$$H = -\mu\sum_{i\sigma}\left(c_{i\sigma}^{+}c_{i\sigma} + d_{i\sigma}^{+}d_{i\sigma}\right) + E_d\sum_{i\sigma}d_{i\sigma}^{+}d_{i\sigma} + E_b(u)\sum_{i\sigma}c_{i\sigma}^{+}c_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} +$$
$$+ H_s + H_{sd} + \sum_{\vec{q}f}\hbar\omega_f(\vec{q})b_{\vec{q}f}^{+}b_{\vec{q}f} + \frac{1}{2}NV_0C\overline{u}^2, \qquad (1)$$
$$H_s = \sum_{ij\sigma}t_{ij}(u)c_{i\sigma}^{+}c_{i\sigma},$$
$$H_{sd} = V(u)\sum_{i\sigma}\left(c_{i\sigma}^{+}d_{i\sigma} + d_{i\sigma}^{+}c_{j\sigma}\right),$$

where $d_{i\sigma}^{+}$, $d_{i\sigma}$ are creation and annihilation operators for spin σ electron on i^{th} center in localized (*d*) state; $c_{i\sigma}^{+}$, $c_{i\sigma}$ are operators of band electron creation and annihilation, $b_{\vec{q}f}$ operators describe phonon subsystem. The parameters of hybridization of band and localized states $V(u) = V - gu$ and electron hopping $t_{ij}(u) = t_{ij}\left(1 + \frac{BV_0}{2w}u\right)$ are renormalized due to the lattice strain *u* (values of parameters *g*, *B*, V_0, *C* depend on the narrow-band compound [8]), other notations are usual.

The model Hamiltonian (1) takes into account basic processes and interactions in a narrow non-degenerate band, namely electron hoppings (H_s term), intra-site Coulomb repulsion (the fifth sum), interatomic exchange (the fourth sum), the hybridization of band and localzed states (H_{sd} term). The terms "localized" and "band" used here can have different sense depending on the peculiarities of the material under consideration. If a transition metal is studied then the localized subsystem are *3d*-electrons and band subsystem is formed by *s-p*-electrons. For the case of narrow band oxides, *3d* electrons form the localized sybsystem and band states correspond to both *3d* electrons of transition metal and *2p* of oxygen sybsystem, in rare earth compounds one has localized *f*-electrons and band *s-p-d*-electrons.

3. Lattice self-contraction and metal-insulator transition

We use the Green function method for calculation and write the equation for localised electron $\left\langle\left\langle d_{p\uparrow}\middle|d_{p'\uparrow}^{+}\right\rangle\right\rangle$ and band electron $\left\langle\left\langle c_{p\uparrow}\middle|c_{p'\uparrow}^{+}\right\rangle\right\rangle$ Green functions. To break off the chain of equation we apply a projection procedure [9]

$$\left[c_{p\uparrow}; H_{sd}\right] = \sum_i \varepsilon_{pj}d_{j\uparrow}; \qquad (2)$$

$$\left[d_{p\uparrow}; H_{sd}\right] = \sum_j \xi_{pj}c_{j\uparrow}, \qquad (3)$$

$$\left\langle\left\langle n_{p\downarrow}d_{p\uparrow}\middle|d_{p'\uparrow}^{+}\right\rangle\right\rangle \cong \left\langle n_{p\downarrow}\right\rangle\left\langle\left\langle d_{p\uparrow}\middle|d_{p'\uparrow}^{+}\right\rangle\right\rangle \qquad (4)$$

and analogous decouplings in the equations for functions $\left\langle\left\langle c_{p\uparrow}\middle|d_{p'\uparrow}^{+}\right\rangle\right\rangle$ and $\left\langle\left\langle d_{p\uparrow}\middle|c_{p'\uparrow}^{+}\right\rangle\right\rangle$. Solving the equations with respect to band and localised electrons Green functions we obtain the energy spectrum

$$E_{1,2} = -\mu + \frac{E_d + E_b(u)}{2} + \frac{U\left\langle n_{p\downarrow}\right\rangle}{2} + \frac{t_{\vec{k}}(u)}{2}$$
$$\mp\frac{1}{2}\sqrt{\left(E_d - E_b(u) + U\left\langle n_{p\downarrow}\right\rangle - t_{\vec{k}}(u)\right)^2 + 4(V(u))^2} \qquad (5)$$

for localized electrons and standard band spectrum for itinerant ones. The spectrum (5), calculated using simple projection procedure, is equivalent to the corresponding results of Gutzwiller variational

approach [3, 4]. The distinctive feature of the present result and results of papers [3, 4] from the results of paper [5] is the presence of hybridization gap even in the formal limit of U=0.
Both the bandwidth and band center position cal be changed by the external pressure application. The equilibrium value of the lattice strain can be found from a minimum condition for Gibbs function

$$G = F + PV = F + NPV_0(1+\overline{u}), \tag{6}$$

as

$$\overline{u} = -\frac{1}{V_0 C}\left(\frac{S}{N}\sum_{\vec{k}\sigma}\left\langle c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}\right\rangle + \frac{BV_0}{2w}\frac{1}{N}\sum_{\vec{k}\sigma} t_{\vec{k}}\left\langle c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}\right\rangle - \frac{PV_0}{CV_0}\right. . \tag{7}$$

To find $\left\langle c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}\right\rangle$, determined by the spectral function of band electrons, we first calculate the chemical potential from the condition $\sum_i \left(\left\langle d^+_{k\sigma} d_{k\sigma}\right\rangle + \left\langle c^+_{i\sigma} c_{i\sigma}\right\rangle\right) = nN$. For the transtion to be initiated the equilibrium value of lattice strain has to be equal $\overline{u} = -(W - w_c)/(S - 0.5BV_0) < 0$.
After numerical calculation with model rectangular density of states at non-zero temperature we obtain from equation (7) the monotonic dependence of equilibrium lattice strain on temperature. As lattice contracts at the increase of temperature, it induces the metallization of the system. Following the paper [8] we take parameter values $1/CV_0 = 0.05eV^{-1}$; $BV_0 = -3eV$, S=0.4 *eV*; W=2,2 *eV*; $w = 2$ *eV*; U=5 *eV* and obtain the pressure-temperature phase diagram shown in figure 1.

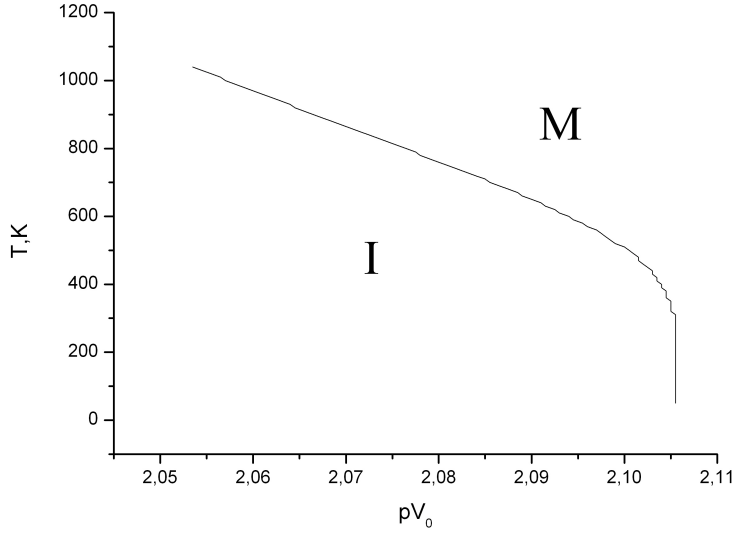

Figure 1. The pressure-temperature phase diagram of metal-insulator transition in the model.

4. Conclusions

In the simple model of narrow band compound with Anderson-Hubbard centers taking into account lattice elastic energy a destabilization of the low temperature insulator phase can be easily described. The increase of temperature leads to the transition from insulating to metallic state, contrary to the Hubbard model at integer filling. Qualitatively, the obtained temperature dependence of the hybridization gap agrees with the corresponding result of DMFT [1]. No matter how weak, the hybridization of band and localized states provide a sufficient mechanism for localization effects to dominate in a wide temperature-pressure ranges. Insulator or correlated metal phases in the phase diagram and the Coulomb repulsion-to-bandwidth or localized level energy-to-bandwith ratios, where both the bandwidth and localized levels position can be substantially changed by the external pressure or chemical substitution can in principle be estimated from the expreimental data on the basis of the

considered model. There also exists a threshold value of the external pressure, above which the system is metallic to the lowest temperature.

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