Study of the specific heat for the binary alloy in the CPA+DMFT method.

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The thermodynamic properties of strongly correlated system with binary type of disorder are investigated using the combination of the coherent potential approximation and dynamical mean-field theory. The specific heat has a peak at small temperatures for the concentrations close to the filling of system. This peak is associated with the local moment formation due to Coulomb interaction. The linear coefficient to the specific heat is divergent and the system stays in the non-Fermi-liquid regime.

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INTRODUCTION

The investigation of the properties of real materials from first principles is one of the challenging problems in condensed matter physics. Over the last half of century the methods within density functional theory framework recommended themselves as very successful at describing the wide band compounds. Concurrently the coherent potential approximation (CPA) was developed to treat the effects of disorder in alloys and real materials that are far from perfect crystal stoichiometry. The physics of transition metal alloys and steels are defined by the doping components and hence it is highly desirable to have a method that can treat on equal footing disorder distributions for half-filling and constructed magnetic phase diagram. In the same years, Bhatt and Fisher almost two decades ago where they combined coherent potential approximation with dynamical mean field theory to treat problem of disorder and interacting electrons simultaneously. Later on they studied in details the thermodynamic properties for the Anderson-Hubbard model with different type of disorder distributions for half-filling and constructed magnetic phase diagram. In the same time, important quantity that gives an access to the many thermodynamic properties of real materials. Therefore, the understanding of its behavior upon doping, temperature, pressure or other external parameters is of high importance for physics of alloys. In the present paper we investigate the specific heat in the disordered Hubbard model with the local binary disorder as a function of temperature and doping. This will allow one for better explanation of the steel’s and alloy’s properties.

METHOD

The Hubbard-type Hamiltonian of the binary alloy system \( A_x B_{1-x} \) with substitutional type of disorder can be written as

\[
H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} (\varepsilon_{i\sigma} - \mu) n_{i\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow}, \tag{1}
\]

where \( c_{i\sigma}^\dagger (c_{i\sigma}) \) is a creation (annihilation) operator and \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) (\( i, j, \sigma \) are the site and spin indexes). Therefore, the first term is responsible for the transfer of the electrons from one site to other with the hopping amplitude \( t_{ij} \). The second term contains \( \varepsilon_{i\sigma} \) and \( \mu \) that are one site and chemical potentials. The former is equal to either \( \varepsilon_A \) or \( \varepsilon_B \) (case of so-called diagonal disorder) with the probability \( x_A \) or \( x_B \) \( (x_A + x_B = 1) \). The last term of this Hamiltonian is an interacting contribution, like in conventional Hubbard model, but different for the different atomic species, \( U_A \) or \( U_B \), depending on atom
remaining on site $i$. $x_A(x_B)$ is a concentration of the atoms of type $A$ ($B$).

The complexity of the above Hubbard-type Hamiltonian is high enough to be solved directly but one can follow the effective medium ideology applied in coherent potential approximation for disordered systems and later in dynamical mean-field theory to treat correlated problem. In this case an action for the effective medium problem is

$$S_{med} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{k\sigma} c_k^\dagger(\tau) G_{med}^{-1}(k, \tau - \tau') c_k(\tau')$$

with Green function of effective medium

$$G_{med}^{-1}(k, i\omega_n) = i\omega_n + \mu - H(k) - \Sigma(i\omega_n),$$

where $\beta = 1/T$ is an inverse temperature, $i\omega_n = (2n - 1)\pi/\beta$ are fermionic Matsubara frequencies and $H(k)$ is a Fourier transform of the kinetic term of the Hamiltonian. The self-energy, $\Sigma(i\omega_n)$, is a pure local quantity that contains the information about disorder and local on-site interaction and has to be determined self-consistently.

One can easily write an impurity action embedded in the effective medium by subtracting the local self-energy on site and adding back the exact interaction

$$S_{imp}^\alpha = S_{med} - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\alpha^\dagger(\tau) \Sigma(\tau - \tau') c_\alpha(\tau') + U_\alpha \int_0^\beta d\tau n_\alpha^\dagger(\tau)n_\alpha(\tau)$$

with $\alpha = \{A, B\}$. The sites distinct from $\alpha$ can be integrated out exactly because they enter quadratically in action and it now becomes

$$S_{imp}^\alpha = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\alpha^\dagger(\tau) G_\alpha^{-1}(\tau - \tau') c_\alpha(\tau') + U_\alpha \int_0^\beta d\tau n_\alpha^\dagger(\tau)n_\alpha(\tau)$$

with bath Green function

$$G_\alpha^{-1}(i\omega_n) = G_{med}^{-1}(i\omega_n) + \Sigma(i\omega_n).$$

The self-consistency condition requires that the impurity Green function embedded in effective medium has to coincide with the local medium Green function and in case of alloy it can be written as properly weighted sum of Green functions for different atomic species

$$\sum_{\alpha=A,B} x_\alpha G_\alpha(i\omega_n) = \sum_k G_{med}(k, i\omega_n)$$

where

$$G_\alpha(\tau - \tau') \equiv - \langle Tc(\tau)c^\dagger(\tau') \rangle_{S_{imp}^\alpha}.$$ 

One should note that the effective impurity Green functions can be evaluated with any suitable technique. Above set of equations has to be iterated until self-consistency with respect to self-energy is reached.

The measurable quantities in presence of disorder are evaluated in the usual CPA way and are regarded as weighted sum of the local values

$$\langle A \rangle = \sum_\alpha x_\alpha \langle A_\alpha \rangle,$$

where $\alpha$ subscribe means that this is an average of operator $A$ for the certain type of atom in effective medium. Therefore the internal energy of the system can be written as

$$E \equiv \langle H \rangle = \frac{1}{\beta} \sum_{n,k} H(k) G_{med}(k, i\omega_n)e^{i\omega_n 0^+} + \sum_\alpha x_\alpha U_\alpha \langle n_\alpha^\dagger n_\alpha \rangle$$

where $\langle n_\alpha^\dagger n_\alpha \rangle$ correlator can be calculated within segment version of hybridization expansion continuous-time quantum Monte Carlo method [10] (CT-QMC) at no additional cost.

**RESULTS AND DISCUSSIONS**

We carried out the calculations of the specific heat for the binary alloy using the CT-QMC method [10]. In this case the the interaction contribution to the internal energy can be easily calculated with high precision and what is also important in our study that the low temperatures can be accessed. The specific heat was evaluated as $C_v = \partial E(T)/\partial T$. The conventional Bethe lattice is explored with the half-bandwidth, $D=1$, and in following all energy quantities will be expressed in units of half-bandwidth. The total occupation was fixed to $n=0.3$ and the Coulomb interactions are equal, $U_A=U_B=2$, in order to deal with only disorder due to local potentials of the different species: $\varepsilon_A=-0.5, \varepsilon_B=0.5$.

The results of the calculations for various alloy concentrations, $x$, are presented on the Fig.1 (hereafter the concentration $x \equiv x_A$ will be used for simplicity keeping in mind that $x_A + x_B = 1$). One can clearly see common features of the specific heat at different concentrations. At small temperature $C_v$ has small value that increases with temperature and at about 0.2-0.3 it has a large peak that is connected with the thermal activation of incoherent states [11]. After the specific heat is decreasing with temperature and has an universal behavior at temperatures that are much larger than other energy
FIG. 1: Specific heat versus temperature for various alloy concentrations (see colorcoding on the figure). Total occupation is $n=0.3$, Coulomb interactions are $U_A=U_B=2$, local potentials are $\varepsilon_A=-\varepsilon_B=-0.5$. The curves are shifted up as 0.06$x$ to make the picture more clear.

detailed explanation and analysis of the specific heat and spectral functions...
The temperature dependence of the linear coefficient to the specific heat, $\gamma(T)=C_v(T)/T$, is plotted on the Fig. 5 for the concentration $x=0.3$. One can clearly see that in non-interacting case (red squares) the linear coefficient is constant at small temperatures, and hence, the system is in Fermi liquid regime even in the presence of the relatively large disorder, $\varepsilon_B - \varepsilon_A=1$. In interacting case the situation is different, $\gamma$ is divergent at small temperatures [18] and therefore the system is in non-Fermi-liquid state. This result is consistent with the results of Dobrosavljević and Kotliar who found similar divergent behavior of the linear coefficient in the model with random hoppings and associated it also with the local moments formation [19].

To summarize, we have studied the temperature and concentration dependence of the electronic specific heat in the binary alloy with Coulomb correlations. At very low temperatures the specific heat has the small peak which exists at the concentrations close to the per site filling of the system, $x \approx n$. The local magnetic moments are formed and as a consequence the peak in the specific heat appears due to additional degrees of freedom. The weakly correlated binary alloy can be driven to the strongly correlated regime with change of concentration, and hence, the magnetic properties can be tuned by concentration [13]. Additional analysis of the linear coefficient to specific heat shows non-Fermi-liquid behavior of correlated binary alloy.

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