Single–particle spectrum for a model of fermions interacting with two-level local excitations on a lattice: A dynamical CPA approach

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Abstract

The problem of motion of a single electron interacting with a periodic lattice of two-level systems is investigated within a spinless fermion model. The Green’s function is calculated in a single-site dynamical coherent potential approximation which is equivalent to DMFT. The picture of one-electron density of states is obtained for various values of the tunnel splitting and coupling between the electron and two-level system. The occurrence of a band splitting with increase of the coupling is demonstrated.

Key words: pseudospins, dynamical CPA, DMFT, two level systems

PACS: 71.10.Fd, 71.20.-b, 71.23.An

The problem of interaction of current carriers with local excitations is one of the classical problem of solid state physics [1]. Recently, the interest in this topic has been revived in connection with investigation of highly correlated electron systems, in particular high-$T_c$ superconductors where anharmonic lattice vibrations (i.e., those of apical oxygen) are assumed sometimes to play an important role [2,3,4,5,6]. The problem is relevant for both metals and semiconductors where the electron spectrum is essentially modified by the influence of local excitations.

Formally the local excitations can be described in terms of multi-level spectrum of a strongly anharmonic system. In the simplest case one can use a model of two-level system (TLS) which is formally described by pseudospin formalism. This model is widely used for two-level systems in metallic glasses [7,8,9,10], crystalline-electric field (CEF) excitations [11], dissipative systems with tunneling states [12].
In the present Letter we investigate the one-electron spectrum in this model by using well established method — single-site dynamical coherent potential approximation (DCPA) [13,14,15,16] which becomes equivalent to dynamical mean-field theory (DMFT) [17] in the limit of infinite dimensionality of the lattice ($d \to \infty$, which corresponds to Gaussian bare density of states for hypercubic lattice) or infinite nearest neighbor number ($z \to \infty$, Bethe lattice). In those limits the equivalence of both methods was demonstrated explicitly in [18]. From the practical point of view, DCPA differs from DMFT by that the former retains the shape of the bare density of states for finite $d$. Both the methods enable us to map a rather complicated TLS lattice problem onto a single-impurity problem which is readily solvable for one electron in empty conduction band.

We consider the spinless fermion model describing fermion-pseudospin interaction:

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j - \sum_i (\gamma_i \tau_i) n_i - \sum_i (h_i \tau_i) \tag{1}$$

where $c_i^\dagger, c_i$ are fermion creation and annihilation operators on a site $i$; $t_{ij}$ are transfer integrals, $n_i = c_i^\dagger c_i$, $\tau_i$ are pseudospin-1/2 operators; $\gamma_i$ is the vector of coupling between fermions and pseudospins, $h_i$ is pseudomagnetic field vector, the tunneling frequency being $\Omega_i = \Delta_i = \sqrt{(h_i h_i)}$.

Further on we consider translationally invariant case where site dependence of both coupling constants and tunnelling frequency is absent

$$H = \sum_k \epsilon_k c_k^\dagger c_k - \lambda \sum_i (\tau_i^+ + \tau_i^-) n_i - h_z \sum_i \tau_i^z \tag{2}$$

with $\epsilon_k$ being electron band spectrum, and we have put $\gamma_z = 0$ after pseudospin quantization axis rotation.

Note that the model (1,2) can be mapped onto various models in different regions of its parameter space. For example, at $\gamma_i = (0, 0, \gamma_z)$ and $h_i = (0, 0, h_z)$ we get the Falicov-Kimball model [19]. For large pseudospin values we obtain by using the Holstein-Primakoff representation the Holstein model [20,21] which is widely used to describe small polaron formation, in particular in molecular crystals.

We calculate the one-particle Green’s function in the case of single conduction electron,

$$G_k(z) = \langle \langle c_k c_k^\dagger \rangle \rangle_z = [z - \epsilon_k - \Sigma_k(z)]^{-1} \tag{3}$$
where $\Sigma_k(z)$ is the electron self-energy.

In the local self-consistent approximation (which corresponds to dynamical CPA and DMFT) the quantity $\Sigma_k(z)$ is replaced by the momentum-independent local self-energy, $\Sigma_k(z) \to \Sigma_{\text{loc}}(z)$ and the expression for the on-site Green’s function $G(z) = \sum_k G_k(z)$ takes the form

$$G(z) = R_0(z - \Sigma_{\text{loc}}(z)), \quad R_0(z) = \sum_k \frac{1}{z - \epsilon_k}. \quad (4)$$

The local self-energy is obtained from the solution of the auxiliary single-impurity problem, the corresponding model parameters being determined from the self-consistency condition $G(z) = G_{\text{loc}}(z)$. The local Green’s function is given by

$$G_{\text{loc}}^{-1}(z) = \left[R_{\text{loc}}^0(z)\right]^{-1} - \Sigma_{\text{loc}}(z) \quad (5)$$

where $R_{\text{loc}}^0(z)$ is the resolvent of the single-impurity problem, with the interaction at the impurity site being switched off. We obtain the self-consistency condition as

$$R_{\text{loc}}^0(z) = \frac{G(z)}{1 + G(z)\Sigma_{\text{loc}}(z)}. \quad (6)$$

Introducing $F(z)$ by $F(R_0(z)) = z$ to exclude $\Sigma_{\text{loc}}(z)$ from the expression (6), one can write down the self-consistency condition in a more familiar form

$$[R_{\text{loc}}^0(z)]^{-1} = z - F(G(z)) + G^{-1}(z), \quad (7)$$

if one prefers a DMFT-like formulation (see [17]).

Further on we solve the auxiliary single-impurity problem with the Hamiltonian on the fictitious one-dimensional lattice

$$H = \sum_{n=0}^{\infty} \epsilon_n c_n^\dagger c_n + \sum_{n=0}^{\infty} \epsilon_{n,n+1} [c_n^\dagger c_{n+1} + \text{h.c.}]$$

$$-\lambda c_0^\dagger c_0 (\tau^+ + \tau^-) - h_z \tau^z \quad (8)$$

by using the method described in [22] to find $G_{\text{loc}}(z)$ for a single current carrier. Here $\epsilon_n$ and $\epsilon_{n,n+1}$ are on-site energy levels and transfer integrals, respectively, for that fictitious lattice, $n$ enumerates the lattice sites. Then we write down
the on-site impurity scattering matrix for the pseudospin projection $\alpha$,

$$t_\alpha(z) = \frac{\lambda^2 R^{\text{loc}}_0(z - \alpha \Delta)}{1 - \lambda^2 R^{\text{loc}}_0(z - \alpha \Delta) R^{\text{loc}}_0(z)},$$

(9)

and introduce the average $T$-matrix

$$t(z) = \sum_{\alpha = \pm} P_\sigma t_\alpha(z),$$

(10)

$$P_\sigma = \frac{1}{2} [1 + \sigma \tanh(\beta \Delta/2)], \quad \Delta = h_z, \quad \beta = \frac{1}{T}$$

to obtain the standard expression

$$\Sigma^{\text{loc}}(z) = \frac{t(z)}{1 + R^{\text{loc}}_0(z) t(z)},$$

(11)

As follows from the above treatment, $G^{\text{loc}}(z)$ can be considered as a solution to the problem of scattering by the random substitutional impurity in the lattice with the bare resolvent $R^{\text{loc}}_0(z)$. In such a case, the quantity $\lambda^2 R^{\text{loc}}_0(z - \alpha \Delta)$ has the meaning of the random dynamical scattering potential for the impurity distribution $P_\alpha$.

For the lattice model the quantity $\Sigma^{\text{loc}}(z)$ calculated under the assumption $R^{\text{loc}}_0(z) = R_0(z)$ corresponds to the average single-site $T$-matrix approximation (ATA), and the fully self-consistent solution corresponds to CPA for the disordered alloy problem [23]. This analogy enables us to use bonding and anti-bonding state classification.

We use the semielliptic bare density of states (the Bethe lattice with infinite nearest-neighbor number which corresponds to DMFT situation),

$$N(\epsilon) = \frac{2}{\pi D^2} \sqrt{D^2 - \epsilon^2},$$

(12)

$D$ being bare half-bandwidth, and organize our numerical procedure as follows. For a given $R^{\text{loc}}_0(z)$ we calculate $\Sigma^{\text{loc}}(z)$ from (11), and then $G(z)$ from (3,4). Using the self-consistency condition in the form (6) or (7) we recompute updated $R^{\text{loc}}_0(z)$ for the next step of the iteration procedure. The iteration process rapidly converges in a few steps. We also calculate $G^{\text{loc}}(z)$ from (5), but for the first iteration only.

As an initial condition for the iteration process we choose $R^{\text{loc}}_0(z) = R_0(z)$. In that situation $G^{\text{loc}}(z)$ obtained at the first iteration gives us an exact solution of the single-impurity problem on a lattice with the bare resolvent $R_0(z)$ (i.e.,
As for the first iteration lattice $G(z)$, it has clear meaning of that calculated within the average single-site $T$-matrix approximation, speaking in an alloy analogy language.

Basing on the above consideration, we discuss the following three approximations (a) single impurity site in the lattice (b) dynamical ATA and (c) dynamical CPA.

The results of calculations for zero temperature are shown in Figs. 1-2. One can see that with increasing $\lambda$ formation of bonding and anti-bonding states takes place, which is clearly marked in the cases (a) and (b). It should be noted that, unlike the scattering by static impurity potential (where bonding and anti-bonding states occur depending on the potential sign), dynamical nature
Fig. 2. The same data as in Fig. 1 for $\Delta = 0.25$

of scattering in our model results in coexistence of both the state types.

In the case (a) and for $0 < \Delta < D$, the critical values $\lambda_{c,b}$ and $\lambda_{c,a}$ of the coupling parameter $\lambda$ for the occurrence of bonding and anti-bonding states are given by

$$
\lambda_{c,b} = \left[ R_0(E_b) R_0(E_b - \Delta) \right]^{-1/2},
\lambda_{c,a} = \left[ R_0(E_t) R_0(E_t + \Delta) \right]^{-1/2}.
$$

(13)

Here $E_b$ and $E_t$ are lower and upper bare conduction band edges, respectively, and we have taken into account that the quantities $\text{Im} R_0(E_b)$, $\text{Im} R_0(E_b - \Delta)$, $\text{Im} R_0(E_t)$ and $\text{Im} R_0(E_t + \Delta)$ are equal to zero. Provided that the bare DOS has a property

$$
N(E_b + D + \epsilon) = N(E_t - D - \epsilon),
$$

(14)
(e.g., bare DOS is symmetric) the following equalities hold

\[
\text{Re} R_0(E_b - \Delta) = -\text{Re} R_0(E_t + \Delta), \\
\text{Re} R_0(E_b) = -\text{Re} R_0(E_t),
\]

we have

\[ \lambda_{c,a} = \lambda_{c,b}, \]  

(15)

and hence in this case bonding and anti-bonding states appear in the spectrum simultaneously. For semielliptical bare DOS (12) we put

\[ E_b = -E_t = D \]

(16)

to obtain

\[ \lambda_{c,a} = \lambda_{c,b} = \frac{D}{2} \left[ \left(1 + \frac{\Delta}{D}\right) + \sqrt{\left(1 + \frac{\Delta}{D}\right)^2 - 1} \right]^{1/2}. \]

(17)

In the dynamical ATA (case (b)) and for \(0 < \Delta < D\), we derive

\[ \lambda_{c,b} = \sqrt{-\frac{2D - \Delta}{R_0(E_b)}}, \quad \lambda_{c,a} = \sqrt{\frac{2D + \Delta}{R_0(E_t)}} \]

(18)

where the conditions \(\text{Im} R_0(E_b) = 0, \text{Im} R_0(E_t) = 0, R_0(E_b) < 0\) and \(R_0(E_t) > 0\) have been used. Here \(\lambda_{c,b}\) and \(\lambda_{c,a}\) are critical couplings for the situation where bonding and anti-bonding state subbands have been already fully formed (e.g., the subbands are decoupled from a resonant state subband). Provided that the condition (15) takes place, one has

\[ \lambda_{c,b} \leq \lambda_{c,a} \]

(19)

and a bonding state subband appears in the spectrum at lower value of \(\lambda\) being compared with that for anti-bonding state subband formation. For semielliptical bare DOS (12,17) we obtain

\[ \lambda_{c,b} = D \sqrt{1 - \frac{\Delta}{2D}}, \quad \lambda_{c,a} = D \sqrt{1 + \frac{\Delta}{2D}}. \]

(20)

For small \(\Delta\) (Fig.1) the case (c) differs from the case (b) by a more smooth DOS behavior, which is a result of the full self-consistency in this approach. For
large \( \lambda \) we obtain in DCPA a quite rich structure owing to intrinsic impurity dynamics at \( \Delta \neq 0 \), along with the standard band splitting. One can see from Figs.1,2 that DCPA describes the formation of the energy gap in the band centre rather adequately, whereas dynamical ATA yields resonance states in the “pseudogap” even at large \( \lambda \). From analogy with disordered binary alloys one can assume that such a behavior is owing to lack of self-consistency in dynamical ATA (cf. the consideration of Hubbard-III-like approximation in strongly correlated systems \cite{24}). At the same time, dynamical ATA gives a reasonable picture of bonding and anti-bonding states formation.

The non-zero values of the critical values (13,19) are connected with the square-root energy behavior of the bare DOS at the band edges. One can expect that in the case of a rectangle-like bare DOS (e.g., two-dimensional case which may be also qualitatively described by DMFT) the bonding and anti-bonding states will occur at arbitrarily small \( \lambda \). A similar situation near the Fermi level is expected in the case of finite band filling in the rigid-band approximation.

The effective mass renormalization in our model is due to band narrowing. We obtain

\[
\frac{m^*}{m} = 1 - \left| \frac{\partial \text{Re} \Sigma^{\text{loc}}(E)}{\partial E} \right|_{E=E^*} \leq 2.
\]

Thus in our two-level situation the bandwidth renormalization does not exceed the value of two, and at large \( \lambda \) only two subbands survive in the spectrum. At the same time, in the standard problem of small phonon polaron (which was also considered in DMFT \cite{25} ) increasing electron-phonon interaction results in many-fold splitting of electron band.

To conclude, numerical results even in the simplest particular case of our model demonstrate a rather rich and non-trivial spectrum picture. Investigations of the general model (1,2) seem to be of interest.

The work was supported in part by Grant No. 4640.2006.2 (Support of Scientific School) from the Russian Basic Research Foundation.

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