DIAGRAMMATIC APPROACH FOR THE ANDERSON-HOLSTEIN MODEL

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***Abstract**: We develop a strong-coupling approach to investigate the Anderson-Holstein model with strong repulsion on impurity centers. We derive the relation between electron propagators and correlation functions and prove that for the impurity electrons the latter is identical to the mass operator of the conduction electrons. Strong electron-phonon interaction determines formation of polarons with heavy clouds of phonons surrounding impurity electrons. We demonstrate the existence of a collective excitation mode of these clouds and obtain the dependence of its energy on the hybridization of the impurity with band states. Hybridization is shown to cause softening of the collective mode and its total suppression at sufficiently large values of the hybridization parameter.*

***Key words:** strongly correlated electron system, Dyson equation, Green's function, polaron, phonon clouds.*

We investigate the interaction of strongly correlated electrons with optical phonons in the frame of Anderson –Holstein model. The electron-phonon interaction and on-site Coulomb repulsion are considered to be strong. By using the Lang-Firsov canonical transformation this problem has been transformed to the problem of mobile polarons.

A new diagram technique is used in order to handle the strong Coulomb repulsion of the electrons and the existence of the phonon clouds surrounding electrons. In the perturbation approach we shall use the generalized Wick theorem proposed in [1-5] for strongly correlated systems. The generalized theorem will be employed for the impurity subsystem and the standard theorem will be used for the conduction electrons and the optical phonons.

We introduce the normal finite temperature Matsubara Green's functions for the conduction and impurity electrons in the interaction representation. In addition, there exist also propagators of the phonon clouds [5].

We henceforth assume that the system is in the paramagnetic state. The Fourier representation of the phonon cloud propagator can then be obtained using Laplace approximation. In the strong-coupling limit, $\alpha >> 1$, the propagator takes the following form [5]

$$\Phi(i\Omega) \approx \frac{2\omega_c}{\Omega^2 + \omega_c^2}, \omega_c = \alpha\omega_0, \qquad (1)$$

where ω_0 is the frequency of the optical phonons. This expression describes the harmonic propagator of the collective mode of phonons belonging to the polaron cloud and having the collective frequency ω_c. Thus, Eq. (1) defines the concept of free collective oscillations of the phonon clouds surrounding the polarons.

The Laplace approximation for the strong-coupling limit $\alpha >> 1$ also serves to prove the relation:

$$\Phi_0(\tau_1\tau_2 \mid \tau_3\tau_4) \approx \Phi_0(\tau_1 \mid \tau_3)\overline{\Phi}_0(\tau_2 \mid \tau_4) + \overline{\Phi}_0(\tau_1 \mid \tau_4)\Phi_0(\tau_2 \mid \tau_3).$$

This equation and its generalization for the many time arguments is considered as the Wick theorem for the phonon clouds in strong coupling polaron regime.

We shall investigate the process of renormalization of the phonon clouds propagators caused by the hybridization of impurity and band electron states.

The diagram series for the normal propagator $\Phi(\tau-\tau')$ can be put in the form of Dyson equation

$$\Phi(\tau-\tau') = \Phi^{(0)}(\tau-\tau') + \iint d\tau_1 d\tau_2 \Phi^{(0)}(\tau-\tau_1)\Pi(\tau_1-\tau_2)\Phi^{(0)}(\tau_2-\tau').$$

Here $\Pi(\tau)$ is the full polarization operator.

In the Fourier representation we have

$$\Phi(i\Omega) = \Phi^{(0)}(i\Omega) + \Phi^{(0)}(i\Omega)\Pi(i\Omega)\Phi(i\Omega), \Phi(i\Omega) = \Phi^{(0)}(i\Omega)/(1-\Phi^{(0)}(i\Omega)\Pi(i\Omega)).$$

Using the expression (1) we then find $\Phi(i\Omega) = \dfrac{2\omega_c}{\Omega^2 + \omega_c^2 - 2\omega_c \Pi(i\Omega)}$.

The pole of this equation determines the renormalization of the collective phonon frequency ω_c:

$$E^2 - \omega_c^2 + 2\omega_c \Pi(E) = 0. \qquad (2)$$

From the equation (2), for the case $T = 0$, we can determine the dependence of the collective mode energy E on the hybridization parameter V.

The results of numerical calculations are presented in Fig. 1.

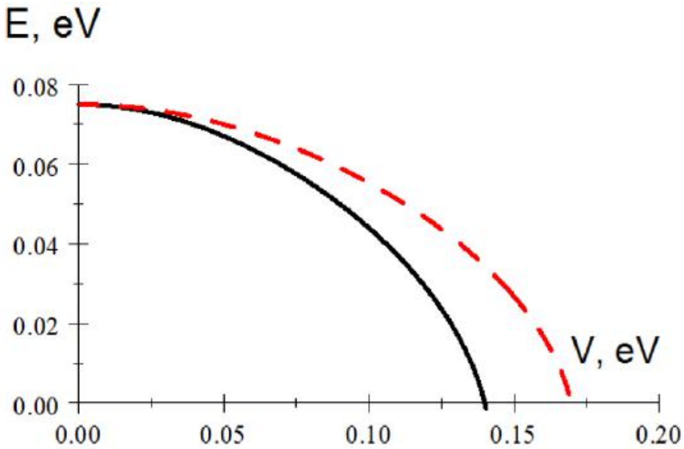

Fig. 1. Energy E of the collective mode vs hybridization V, for different band widths $W = 0.5eV$ (continuous line) and $W = 1eV$ (dashed line). The other parameters are: $\omega_c = 0.075eV, U = 5.85,$ and $\varepsilon_f = -0.095eV$ (U, ε_f is the renormalized on-site Coulomb repulsion of impurity electrons and local impurity energy respectively).

According to this results the renormalized energy E of collective mode of phonon clouds decreases with increasing the value of V and becomes equal to zero at the critical value V_c

$$V_c = \sqrt{\hbar\omega_c W / \ln\left|(W - \varepsilon_f)(W + U + \varepsilon_f) / \varepsilon_f (U + \varepsilon_f)\right|}.$$

It is clear the for larger energy band W the critical value V_c increases.

Thus we make the conclusion that the collective mode is suppressed by hybridization.

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