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Small polaron mass with a long range density–displacement type interaction

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ABSTRACT

In this work renormalization of the effective mass of an electron due to a small polaron formation is studied within the framework of the extended Holstein model. It is assumed that an electron moves along the one-dimensional chain of ions and interacts with ions vibrations of a neighboring chain via a long-range density–displacement type force. By means of the exact calculations a renormalized mass of a nonadiabatic small polaron is obtained at strong coupling limit. The obtained results compared with the mass of small polaron of ordinary Holstein model. The effect of ions vibrations polarization on the small polaron mass is addressed.

1. Introduction

Polarons have been extensively studied since a seminal paper of Landau [1]. They are divided into the small and large polarons in accordance with the size of their wave function. In the first case a carrier is coupled to intramolecular vibrations and self-trapped on a single site. Its size is the same as the size of the phonon cloud, both are about the lattice constant. In the case of large polarons the size of a polaron is also the same as the size of the phonon cloud, but the polaron extends over many lattice constants. The properties of large polarons in the effective mass approximation have been studied in greater detail by Pekar [2], Fröhlich [3], Feynman [4], Devreese [5] and other authors. When the electron–phonon coupling is relatively strong, $\lambda = E_p/D > 1$, all electrons in the Bloch band are "dressed" by phonons. In this regime the electron kinetic energy, which is less than the half-bandwidth (D), is small compared with the potential energy due to a local lattice deformation, E_p, caused by the electrons themselves. Here the finite bandwidth is essential and the effective mass approximation cannot be applied. The electron is called a *small polaron* in this regime. The main features of small polarons were understood by Tjablikov [6], Yamashita and Kurosava [7], Sewell [8], Holstein [9] and his school [10,11], Lang and Firsov [12], Eagles [13] and others and described within the framework of Holstein model (HM) in several review papers and textbooks [5,14–18]. In Ref. [19] the polaron model with a long-range "density–displacement" type force was introduced by Alexandrov and Kornilovitch. The model by itself represents an extension of the Fröhlich polaron model to a discrete ionic crystal lattice or extension of the Holstein polaron model to a case when an electron interacts with many ions of a lattice with longer ranged electron–phonon interaction. Subsequently, the model was named as the extended Holstein model (EHM) [20]. In the model polaron has an internal structure different from the internal structure of a polaron in ordinary Holstein model. The size of a polaron in EHM is about the lattice constant, but its phonon cloud spreads overthe whole crystal. Within the model a renormalized mass appears to be much smaller compared with that in the ordinary Holstein model. Conclusions of Ref. [19] were confirmed later by other authors [20–22]. Besides that Fehske et al. [20] investigated the electron–lattice correlations, single-particle spectral function and optical conductivity of a polaron in EHM in the strong and weak coupling regimes by means of an exact Lancroz diagonalization method. Other properties of EHM such as the ground state spectral weight, the average kinetic energy and the mean number of phonons by means of the variational and quantum Monte Carlo simulation approaches were studied in Refs. [23,24]. All numerical and analytical results in Ref. [19], were obtained in the nonadiabatic or near-nonadiabatic regimes. In the work [25] we extended this model to the adiabatic limit and found that the mass of a polaron in EHM is much less renormalized than the mass of a small Holstein polaron in this limit as well. Refs. [19,25] considered an electron interacting with ions vibrations of an upper chain,

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polarized perpendicular to the chain. This case mimics *high* $-T_c$ cuprates, where the in-plane (CuO_2) carriers are strongly coupled with the *c*-axis polarized vibrations of the *apical* oxygen ions [26]. A more realistic case when the *apical* ions vibrate in all directions and its effect on a mass of a small polaron in EHM was studied in Ref. [27]. At the same time polarons were experimentally recognized as quasiparticles in the novel materials, in particular, in the superconducting cuprates and colossal magnetoresistance manganites [28]. In the previous papers of the author [25,27] mass renormalization of an electron due to a small polaron formation in EHM was restricted only to a simple two-site model. Here we extend these studies for a many-site system and derive an analytical expression for the mass of a nonadiabatic small polaron in EHM in a strong coupling regime and compare it with the those of small polarons in an ordinary Holstein model.

2. The model

We consider an electron performing hopping motion on a lower chain consisting of the static sites, but interacting with all ions of an upper chain via a long-range density–displacement type force, as shown in Fig. 1, similar to a case considered in Refs. [21,22] . So, the motion of an electron is always one-dimensional, but a vibration of the upper chain's ions is isotropic and two-dimensional one.

The Hamiltonian of the model is

$$H = H_e + H_{ph} + H_{e-ph}, \tag{1}$$

where

$$H_e = -t\sum_{\mathbf{n}}(c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}+\mathbf{a}} + H.c.) \tag{2}$$

is the electron hopping energy,

$$H_{ph} = \sum_{\mathbf{m},\alpha}\left(-\frac{\hbar^2\partial^2}{2M\partial\mathbf{u}^2_{\mathbf{m},\alpha}} + \frac{M\omega^2\mathbf{u}^2_{\mathbf{m},\alpha}}{2}\right) \tag{3}$$

is the Hamiltonian of the vibrating ions,

$$H_{e-ph} = \sum_{\mathbf{n},\mathbf{m},\alpha}\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n})\cdot\mathbf{u}_{\mathbf{m},\alpha}c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}} \tag{4}$$

describes interaction between the electron that belongs to a lower chain and the ions of an upper chain. Here $c^{\dagger}_{\mathbf{n}}(c_{\mathbf{n}})$ is a creation (destruction) operator of an electron on a cite $\mathbf{n}$, $\mathbf{u}_{\mathbf{m},\alpha}$ is the $\alpha = y,z$-polarized displacement of the $\mathbf{m}$-th ion and $\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n})$ is an interacting density–displacement type force between an electron on a site $\mathbf{n}$ and the α polarized vibration of the $\mathbf{m}$-th ion. M is the mass of the vibrating ions and ω is their frequency. An explicit form of y and z coordinates of interacting force are

$$f_{\mathbf{m},y}(\mathbf{n}) = \frac{\kappa_y|\mathbf{n}-\mathbf{m}+\mathbf{a}/2|}{(|\mathbf{n}-\mathbf{m}+\mathbf{a}/2|^2+b^2)^{3/2}} \tag{5}$$

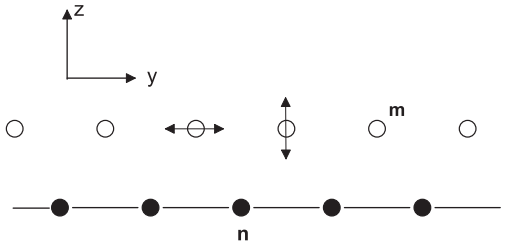

Fig. 1. An electron hops on a lower chain and interacts with the ions vibrations of an upper infinite chain via a density–displacement type force $f_{\mathbf{m},\alpha}(\mathbf{n})$. The distances between the chains and between the ions are assumed equal to 1.

and

$$f_{\mathbf{m},z}(\mathbf{n}) = \frac{\kappa_z b}{(|\mathbf{n}-\mathbf{m}+\mathbf{a}/2|^2+b^2)^{3/2}}, \tag{6}$$

where κ_y and κ_z are some coefficients. The distance along the chain $|\mathbf{n}-\mathbf{m}|$ is measured in the units of a lattice constant $|\mathbf{a}| = 1$. The distance between the chains is $b = 1$ too.

3. Strong coupling and nonadiabatic limit

In the strong coupling limit ($\lambda = E_p/D > 1$) and the nonadiabatic approximation wave function of the system is presented as a superposition of the normalized Wannier functions $W(\mathbf{r}-\mathbf{n})$, localized on the site $\mathbf{n}$,

$$\Psi = \sum_{\mathbf{n}} A_{\mathbf{n}}(\mathbf{u}_{\mathbf{m},\alpha})\mathbf{W}(\mathbf{r}-\mathbf{n}). \tag{7}$$

For a convenience we consider the $2N+1$ ions in a lower chain. Then Schrödinger equation $H\Psi = E\Psi$ is reduced to a system of the coupled second order differential equations with respect to the *infinite* number of the vibrational coordinates $\mathbf{u}_{\mathbf{m},\alpha}$

$$\left(E - H_{ph} - \sum_{\mathbf{m},\alpha}\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}_i)\cdot\mathbf{u}_{\mathbf{m},\alpha}\right)A_{\mathbf{n}_i}(\mathbf{u}_{\mathbf{m},\alpha}) = t\sum_{\mathbf{n}\neq\mathbf{n}_i}A_{\mathbf{n}}(\mathbf{u}_{\mathbf{m},\alpha}) \tag{8}$$

with $i = 0, \pm1, \pm2, \ldots, \pm(N-1), \pm N$. Further we omit an argument $\mathbf{u}_{\mathbf{m},\alpha}$ of $A_{\mathbf{n}}$, but keep in mind that it depends on them. The common tool to investigate Eq. (8) is a perturbation approach with respect to the hopping integral. In the zero order ($t = 0$) the system is $(2N+1)$-fold degenerate with the electron localized, for example, on site $\mathbf{n}_i$, so that $A_{\mathbf{n}} = \tilde{A}_{\mathbf{n}_i}$ if $\mathbf{n} = \mathbf{n}_i$ where

$$\tilde{A}_{\mathbf{n}_i} = \exp\left[-\frac{M\omega}{2\hbar}\sum_{\mathbf{m},\alpha}\left(\mathbf{u}_{\mathbf{m},\alpha} + \frac{\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}_i)}{M\omega^2}\right)^2\right] \tag{9}$$

and zero otherwise. In the first order to a hopping integral t we are looking for a solution of the system (8) as a single column matrix $(A_{\mathbf{n}_{-N}}, A_{\mathbf{n}_{(-N+1)}}, \ldots, A_{\mathbf{n}_{(N-1)}}, A_{\mathbf{n}_N})^T$ (T—standing for a transpose matrix) which is the linear combinations of $\tilde{A}_{\mathbf{n}_i}$ as

$$\begin{aligned}\left(A_{\mathbf{n}_{-N}}, A_{\mathbf{n}_{(-N+1)}}, \ldots, A_{\mathbf{n}_{(N-1)}}, A_{\mathbf{n}_N}\right)^T &= \alpha_{-N}\left(\tilde{A}_{\mathbf{n}_{-N}}, 0, \ldots, 0\right)^T \\ &+\alpha_i\left(0, \ldots, \tilde{A}_{\mathbf{n}_i}, \ldots, 0\right)^T \\ &+\alpha_{-N}\left(0, \ldots, 0, \tilde{A}_{\mathbf{n}_N}\right)^T.\end{aligned} \tag{10}$$

Substituting Eq. (10) into the system of Eq. (8) one gets a system of the linear equations with respect to the coefficients $\alpha_{-N}, \alpha_{-N+1}, \ldots, \alpha_{N-1}, \alpha_N$.

$$E(\mathbf{n}_i)\tilde{A}_{\mathbf{n}_i}\alpha_i - t\sum_{k\neq i}\tilde{A}_{\mathbf{n}_{i+k}}\alpha_{i+k} = 0, \tag{11}$$

where

$$E(\mathbf{n}_i) = \left(E - H_{ph} - \sum_{\mathbf{m},\alpha}\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}_i)\cdot\mathbf{u}_{\mathbf{m},\alpha}\right). \tag{12}$$

The system of Eq. (11) has a square $(2N+1)\times(2N+1)$ matrix. The diagonal elements of the matrix are the product of Eqs. (9) and (12). Next we introduce the *Born-von Karmana* boundary conditions $\tilde{A}_{\mathbf{n}_{-N}} = \tilde{A}_{\mathbf{n}_N}$ which ensures a translation invariance of the system and enables us rewrite the system of Eq. (11) as

$$\tilde{E}\alpha_i - \sum_{k\neq i}t_{i,k}\alpha_k = 0. \tag{13}$$