EXTENDED HOLSTEIN POLARON MASS

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

1. Introduction

A model of a polaron with a long-range "density-displacement" type interaction was introduced in Ref. [1] by Alexandrov and Kornilovitch. The model by itself represents an extension of the large Fröhlich polaron (LFP) model [2] to a discrete ionic crystal lattice or an extension of the Holstein polaron model (HM) [3] to a case where an electron interacts with many ions of the lattice due to the long-range electron-phonon interaction. Subsequently, the model was named an extended Holstein model (EHM) [4]. In the model, a polaron has an internal structure different from those of both HM polaron and LFP. In the HM, a carrier is coupled to intramolecular vibrations and self-trapped on a single site. The size of a Holstein polaron is the same as the size of the phonon cloud, both are about the lattice constant. In the case of large Fröhlich 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 size of a polaron in EHM is about the lattice constant, but its phonon cloud spreads over the whole crystal. As was shown in Ref. [1] in the strong-coupling limit of EHM, a polaron consists of an electron localized on a site **n** and the phonon cloud spread over other lattice sites **m**. The mass enhancement of such a quasiparticle increases exponentially with coupling as in the standard *small polaron theory*. In EHM, one has to work with a new situation where the electron wave function size in a polaron and the size of a lattice deformation surrounding an electron are different. The former is the atomic size, while the latter is spread over the whole crystal. According to Ref. [1], we use the term *small polaron* for such a quasiparticle (for an alternative viewpoint, see Ref. [4]). Within the model, a renormalized mass appears to be much smaller as compared with that in the ordinary Holstein model. Conclusions of [1] were confirmed later on by other authors [4–6]. In addition, Fehske, Loos, and Wellein [4] investigated electron-lattice correlations, a single-particle spectral function, and the optical conductivity of a polaron in EHM in strong and the weak coupling regimes by means of the 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 [7, 8]. All numerical and analytical results in [1] were obtained in the nonadiabatic or near-nonadibatic regime. In work [9], 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. Work [1, 9] considered an electron interacting with vibrations of ions of an upper chain which are polarized perpendicularly to the chain. This case mimics $high - T_c$ cuprates, where the in-plane (CuO_2) carriers

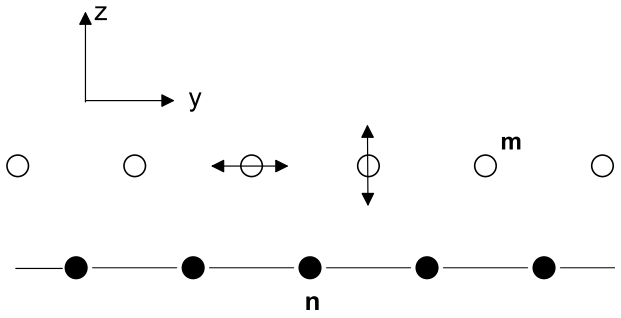

Fig. 1. Electron hops on a lower chain and interacts with vibrations of ions of the upper infinite chain via a density-displacement type force $f_{\mathbf{m},\alpha}(\mathbf{n})$. The distances between chains and between ions are assumed equal to 1

are strongly coupled with the c-axis polarized vibrations of *apical* oxygen ions [10]. A more realistic case where *apical* ions vibrate in all directions and their effect on the mass of a small polaron in EHM were studied in [11]. At the same time, polarons were experimentally recognized as quasiparticles in novel materials, in particular, in superconducting cuprates and manganites with colossal magnetoresistance [12–20]. In the previous papers [9, 11], the mass renormalization of an electron due to the formation of a small polaron 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 the strong coupling regime and compare it with that in the ordinary Holstein model. In addition, the effect of polarized vibrations and their contributions to the mass of a polaron are discussed within EHM.

2. The Model

We consider an electron performing the hopping motion on a lower chain consisting of 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 [5, 6]. So, the motion of an electron is always one-dimensional, but vibrations of upper chain's ions are isotropic and two-dimensional.

The Hamiltonian of the model is

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

where

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

is the electron hopping energy,

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

is the Hamiltonian of vibrating ions, and

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

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

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

and

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

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

3. Strong Coupling and Nonadiabatic Limit

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

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

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

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

$$= t\sum_{\mathbf{n}\neq\mathbf{n_i}} A_{\mathbf{n}}(\mathbf{u}_{\mathbf{m},\alpha}) \tag{8}$$

with $i = 0, \pm1, \pm2, \ldots, \pm(N-1), \pm N$. Further, we omit the argument $\mathbf{u}_{\mathbf{m},\alpha}$ of $A_{\mathbf{n}}$, but keep in mind that it depends on them. The common tool to investigate (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 $A_{\mathbf{n}} = \widetilde{A}_{\mathbf{n}_i}$ if $\mathbf{n} = \mathbf{n}_i$, where

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

and zero otherwise. In the first order in the hopping integral t, we are looking for a solution of system (8) as a single column matrix $\left(A_{\mathbf{n}_{-N}}, A_{\mathbf{n}_{(-N+1)}}, \ldots, A_{\mathbf{n}_{(N-1)}}, A_{\mathbf{n}_N}\right)^T$ (T stands for a transposed matrix) which is a linear combination of $\widetilde{A}_{\mathbf{n}_i}$:

$$\left(A_{\mathbf{n}_{-N}}, A_{\mathbf{n}_{(-N+1)}}, \ldots, A_{\mathbf{n}_{(N-1)}}, A_{\mathbf{n}_N}\right)^T =$$

$$= \alpha_{-N}\left(\widetilde{A}_{\mathbf{n}_{-N}}, 0, \ldots, 0\right)^T + \alpha_i\left(0, \ldots, \widetilde{A}_{\mathbf{n}_i}, \ldots, 0\right)^T +$$

$$+\alpha_{-N}\left(0, \cdots, 0, \widetilde{A}_{\mathbf{n}_N}\right)^T. \tag{10}$$

Substituting (10) into the system of equations (8), we get a system of linear equations for the coefficients $\alpha_{-N}, \alpha_{-N+1}, \cdots, \alpha_{N-1}, \alpha_N$,

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

where

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

The system of equations (11) have a square $(2N+1)\times(2N+1)$ matrix. Diagonal elements of the matrix are products of (9) and (12). Then we introduce the Born–von Karman boundary condition $\widetilde{A}_{\mathbf{n}_{-N}} = \widetilde{A}_{\mathbf{n}_N}$ which ensures the translation invariance of the system and enables us rewrite the system of equations (11) as

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

Here, $\widetilde{E} = E - N'\hbar\omega/2 - E_{\mathrm{p}}$, N' is the number of ions in the upper chain,

$$\widetilde{t}_{k,k'} = t\frac{\int\widetilde{A}_{\mathbf{n}_k}\widetilde{A}_{\mathbf{n}_{k'}}d\mathbf{u}_{\mathbf{m},\alpha}}{\int|\widetilde{A}_{\mathbf{n}_k}|^2 d\mathbf{u}_{\mathbf{m},\alpha}} \tag{14}$$

are the renormalized hopping integrals and

$$E_{\mathrm{p}} = E_{\mathrm{p}}(\mathbf{n}_i) = \sum_{\mathbf{m},\alpha}\frac{\mathbf{f}^2_{\mathbf{m},\alpha}(\mathbf{n}_i)}{2M\omega^2} \tag{15}$$

is the polaronic shift which is independent of $\mathbf{n}_i$. Expressing all nondiagonal elements $\widetilde{t}_{k,k'}$ of the matrix through $\widetilde{t} = \widetilde{t}_{1,2}$, we find

$$\widetilde{E}\alpha_i - \widetilde{t}\sum_{k\neq i}\widetilde{g}^2_{i,k}\alpha_k = 0 \tag{16}$$

and

$$\widetilde{g}^2_{i,k} = -(1/2M\hbar\omega^3)\times$$

$$\times\sum_{\mathbf{m},\alpha}\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}_i)(\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}_{i+1}) - \mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}'k)). \tag{17}$$

It appears that the matrix of the system of equations (16) is symmetric. Then the system of equations is separated into block 2×2 diagonal matrix equations that couple only α_i and α_{i+1} as

$$\begin{pmatrix}\widetilde{E} & -\widetilde{t}e^{-\widetilde{g}^2_{i,i+1}}\\ -\widetilde{t}e^{-\widetilde{g}^2_{i,i+1}} & \widetilde{E}\end{pmatrix}\begin{pmatrix}\alpha_i\\ \alpha_{i+1}\end{pmatrix} = 0. \tag{18}$$

From (18), we obtain a secular equation for the energy

$$\begin{vmatrix}E - N'\hbar\omega/2 + E_{\mathrm{p}} & -\widetilde{t}\\ -\widetilde{t} & E - N'\hbar\omega/2 + E_{\mathrm{p}}\end{vmatrix} = 0. \tag{19}$$

The energy levels of the system are found as

$$E_{\pm} = N'\hbar\omega/2 - E_{\mathrm{p}} \pm \tilde{t} \tag{20}$$

The evaluation of (14) with regard for (9) results in

$$\widetilde{t} = te^{-g^2}, \tag{21}$$

where

$$g^2 = \frac{1}{2M\hbar\omega^3}\sum_{\mathbf{m},\alpha}\left(\mathbf{f}^2_{\mathbf{m},\alpha}(\mathbf{n}) - \mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n})\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}+\mathbf{a}).\right). \tag{22}$$

Formulas (15) and (21) are the main analytical results of the present work.

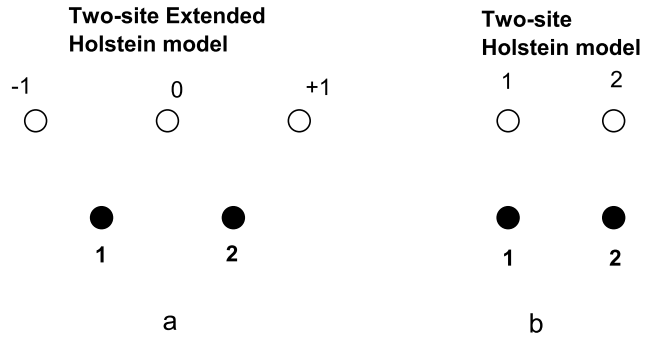

Fig. 2. Schematic representation of the extended Holstein model and the ordinary Holstein model for a two-site system. The electron on site **1** interacts (a) with sites $m = -1$ and $m = 0$ and (b) with only site $m = 1$ of the ion chain, in the extended Holstein model and the Holstein model, respectively

4. Results

Analytical expressions for the polaronic shift (15) and the renormalized hopping integral (21) were obtained early in Ref. [1] by using the canonical Lang–Firsov transformation. Work [1] studied the renormalization of the effective mass of an electron due to only z-polarized vibrations of the upper chain. However, a role of y-polarized vibrations of the upper chain and their influence on the mass renormalization in EHM was not discussed, and no quantitative results were presented. In this section, we calculate the small polaron mass in EHM for both density-displacement type interactions (5) and (6). Moreover, we calculate the mass of a small polaron in EHM with two-dimensional isotopic vibrations of ions of the upper chain as well. In our model, the electron-phonon coupling constant $\lambda = E_{\rm p}/2t$, and the polaron mass

$$m_{\rm p} = \frac{\hbar^2}{2\widetilde{t}a^2} = m^* \exp[g^2], \tag{23}$$

where $m^* = \hbar^2/2ta^2$ is the bare electron band mass. One can express the polaron mass in terms of λ and t/ω (parameter of nonadiabaticity) as

$$m_{\rm p}/m^* = e^{2\gamma\lambda t/\hbar\omega}, \tag{24}$$

where

$$\gamma_{\rm EHM} = 1 - \frac{\sum_{\mathbf{m},\alpha} \mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}) \cdot \mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n}+\mathbf{a})}{\sum_{\mathbf{m},\alpha} \mathbf{f}^2_{\mathbf{m},\alpha}(\mathbf{n})}. \tag{25}$$

The dimensionless parameter γ in the exponent of (24) depends on the type of interacting force and the geometry of a lattice. For the ordinary Holstein model, it is always equal to 1 ($\gamma_{\rm HM} = 1$). So the ratio of small polaron masses in EHM and ordinary HM is given by

$$\frac{m_{\rm p,EHM}}{m_{\rm p,HM}} = \exp\left[2\lambda(\gamma_{\rm EHM} - \gamma_{\rm HM})\frac{t}{\hbar\omega}\right]. \tag{26}$$

We would like to stress that the model yields a less renormalization of the effective mass than the Holstein model. This is true not only for c-axis polarized vibrations of *apical* oxygen ions, but for their isotropic vibrations as well [11]. For simplicity, let us first consider z-polarized vibrations of ions of the upper chain and only nearest-neighbors interactions, as in Fig. 2,a. In this case, our model yields $E_{\rm p} = f^2_{\mathbf{0}z}(\mathbf{1})/M\omega^2$ and the mass renormalization $m_{\rm p}/m^* = \exp(E_{\rm p}/2\hbar\omega)$, while the Holstein model with the local interaction, Fig. 2,b, for the same $E_{\rm p}$ yields $m_{\rm p}/m^* = \exp(E_{\rm p}/\hbar\omega)$.

The factor 1/2 in the exponent provides much lighter small polarons in EHM as compared with those within the Holstein model. If one considers the Coulomb-like interaction with the whole upper chain, one gets the factor $\gamma_z = 0.28$ [6] instead of 0.5 in the exponent, which means an even less renormalized effective mass. The results for the mass of a nonadiabatic small polaron in EHM with the only z-polarized vibrations of ions in comparison with those of HM are presented in Fig. 3.

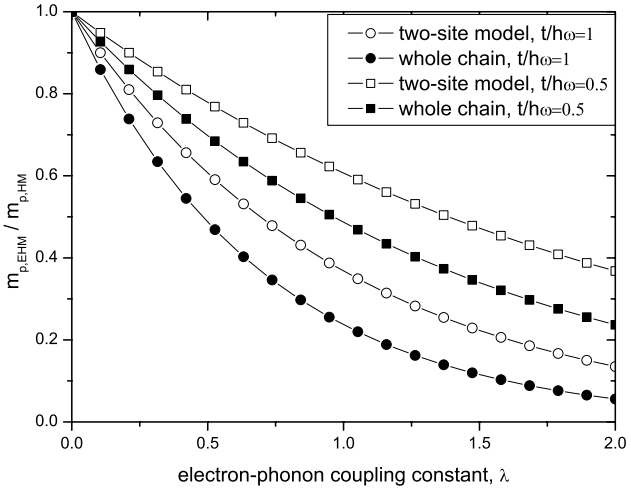

Fig. 3. Ratio of the masses of nonadiabatic small polarons in EHM and HM with the only $z-$ polarized vibrations of ions as a function of the electron-phonon coupling constant λ at different values of $t/\hbar\omega$. Open (filled) circles and squares show γ calculated within two models (for a whole chain)

Now we discuss the influence of y-polarized vibrations of the upper chain on the small polaron mass in EHM. In this case, the density-displacement type interaction force (5) is longer ranged than (6), as it decays as r^{-2},

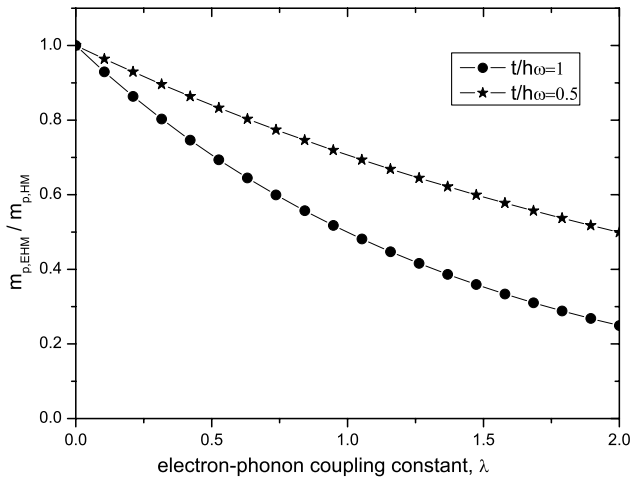

Fig. 4. The mass ratio for nonadiabatic small polarons in EHM and HM with only $y-$ polarized vibrations of ions as a function of the electron-phonon coupling constant λ at different values of $t/\hbar\omega$

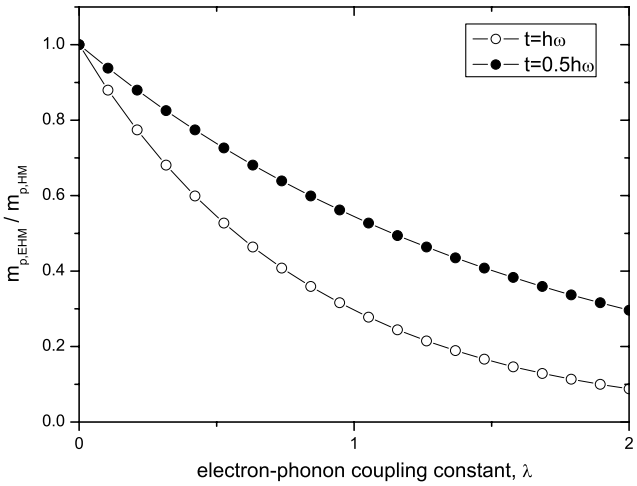

Fig. 5. The mass ratio for nonadiabatic small polarons in EHM and HM with vector vibrations of ions as a function of the electron-phonon coupling constant λ at different values of $t/\hbar\omega$

while force (6) decays as r^{-3}. For a lattice in Fig. 1, one finds $\gamma_y = 0.652657$. The results for the mass of a small polaron in EHM with only $y-$ polarized vibrations of the upper chain and their comparison with those of HM are given in Fig. 4.

The comparison of curves in Figs. 3 and 4 shows that the effective mass of an electron is more renormalized with y-polarized vibrations of ions than with z-polarized vibrations. For example, at $\lambda = 1$ and $t/\hbar\omega = 1$, $m_{\mathrm{p,EHM},z} \simeq 1.77m^*$, while $m_{\mathrm{p,EHM},y} \simeq 3.68m^*$. If we switch-on both z- and y-polarized vibrations, then each of them contributes to the mass renormalization. The overall effect of both contributions of vibrations of ions to a small polaron mass in EHM depends on the ratio κ_z/κ_y. In the case where $\kappa_z = \kappa_y$, ions are isotropic oscillators. The calculations of (25) with a vector $\mathbf{f_m}(\mathbf{n})$ force (taking both (5) and (6) into account) yields $\gamma = 0.392008$. This result shows that a nonadiabatic small polaron in EHM remains lighter than a small polaron of HM. The comparison of the results of EHM with two-dimensional vector vibrations of ions and ordinary HM is given in Fig. 5. For the illustrative purpose, the calculated masses of small polarons (i) for each type of ions vibrations in EHM and (ii) in HM are presented in Table 1 at the same polaron shift. As many experiments with cuprates show, the polaron mass is of the order of $\sim (2 \div 5)m^*$ [21]. In our model, such values of m_{p} can be explained in the $\kappa_z \geq \kappa_y$ limit.

T a b l e 1. Calculated masses of polarons for the same polaron shift with *z*- and *y*-polarized two-dimensional vector vibrations of ions in EHM. The fifth column presents the polaron mass in HM

λ	$t/\hbar\omega = 0.50$			
	$m_{\mathrm{p},z}$	$m_{\mathrm{p},y}$	$m_{\mathrm{p,EHM}}$	$m_{\mathrm{p,HM}}$
1	1.33213	1.92064	1.47995	2.71828
2	1.77457	3.68885	2.19025	7.38906
3	2.36396	7.08494	3.24146	20.0855
4	3.14910	13.6076	4.79720	54.5982
5	4.19501	26.1353	7.09961	148.413
λ	$t/\hbar\omega = 0.75$			
	$m_{\mathrm{p},z}$	$m_{\mathrm{p},y}$	$m_{\mathrm{p,EHM}}$	$m_{\mathrm{p,HM}}$
1	1.53752	2.66175	1.80041	4.48169
2	2.36396	7.08494	3.24146	20.0855
3	3.63462	18.8584	5.83594	90.0171
4	5.58829	50.1963	10.5071	403.429
5	8.59209	133.610	18.9130	1808.04

It should be emphasized than the full polaron mass m_{p} can be presented as a product of $m_{\mathrm{p},z}$ and $m_{\mathrm{p},y}$: $m_{\mathrm{p}} = m_{\mathrm{p},z} \times m_{\mathrm{p},y}$ (see Table 2). However, the full polaron shift E_{p} is given as the sum of $E_{\mathrm{p},z}$ and $E_{\mathrm{p},y}$: $E_{\mathrm{p}} = E_{\mathrm{p},z} + E_{\mathrm{p},y}$. The same is true for the electron-phonon coupling constant λ: $\lambda = \lambda_z + \lambda_y$, $\lambda_z = E_{\mathrm{p},z}/2t = \delta_{E,z}\lambda$ and $\lambda_y = E_{\mathrm{p},y}/2t = \delta_{E,y}\lambda$. Here, λ_z and λ_y are the electron-phonon coupling constants due to only z- and y-polarized vibrations of ions of the upper chain, respectively, and

$$\delta_{E,z} = \frac{E_{\mathrm{p},z}}{E_{\mathrm{p}}} = \frac{\sum_{\mathbf{m}} f^2_{\mathbf{m},z}(\mathbf{n})}{\sum_{\mathbf{m}} (f^2_{\mathbf{m},z}(\mathbf{n}) + f^2_{\mathbf{m},y}(\mathbf{n}))}, \qquad (27)$$

$$\delta_{E,y} = \frac{E_{\mathrm{p},y}}{E_{\mathrm{p}}} = \frac{\sum_{\mathbf{m}} f^2_{\mathbf{m},y}(\mathbf{n})}{\sum_{\mathbf{m}} (f^2_{\mathbf{m},z}(\mathbf{n}) + f^2_{\mathbf{m},y}(\mathbf{n}))} \tag{28}$$

are the relative contributions of z- and y-polarized vibrations to a full polaron shift. In the case of isotropic vibrations of the upper chain ions and $\kappa_z = \kappa_y$, we find $\delta_{E,z} = 0.712393$ and $\delta_{E,y} = 0.287603$ (within HM, $\delta_{E,z} = \delta_{E,y} = 0.5$). As one can see, the main contribution to a full polaron shift comes from z polarized vibrations. In general, $\delta_{E,\alpha}$ ($\alpha = z, y$) depends (i) on the ratio κ_z/κ_y, (ii) on the type (range) of interaction forces $\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n})$, and (iii) on a lattice geometry. For the ordinary Holstein model, $\delta_{E,\alpha}$ depends only on the ratio κ_z/κ_y. As far as the effects of polarized vibrations on a small polaron in HM and EHM are concerned, there are qualitative and quantitative differences that can be seen in the following:

– in the Holstein model: polarized vibrations of both types contribute to the mass renormalization and a full polaron shift $m_{\mathrm{p},z} = m_{\mathrm{p},y}$, $E_{\mathrm{p},z} = E_{\mathrm{p},y}$ if $\kappa_z = \kappa_y$.

– in the extended Holstein model: as in HM, both types of polarized vibrations contribute to the mass renormalization and to a full polaron shift but now with a different weights. $m_{\mathrm{p},z} \neq m_{\mathrm{p},y}$ and $E_{\mathrm{p},z} \neq E_{\mathrm{p},y}$ even if $\kappa_z = \kappa_y$. z-polarized vibrations of ions give rise to a mobile polaron, while y-polarized vibrations give rise to a heavy polaron. When both types of polarization are switched on, the full polaron shift is mainly determined by the z contribution $\simeq 71\%$, and the value of $m_{\mathrm{p},z}$ exceeds that of $m_{\mathrm{p},y}$ (Table 2). So, the anisotropic properties of a polaron due to polarized vibrations are more pronounced in EHM.

T a b l e 2. Calculated masses of polarons in EHM with regard for z-, y-polarized, and two-dimensional vector vibrations of ions

λ	$t/\hbar\omega = 0.50$			
	$m_{\mathrm{p},z}$	$m_{\mathrm{p},y}$	$\frac{m_{\mathrm{p},z}-m_{\mathrm{p},y}}{m_{\mathrm{p},y}}$	$m_{\mathrm{p}} = m_{\mathrm{p},z} \times m_{\mathrm{p},y}$
1	1.22667	1.20648	0.01673	1.47995
2	1.50471	1.45560	0.03374	2.19025
3	1.84577	1.75615	0.05103	3.24146
4	2.26415	2.11877	0.06861	4.79720
5	2.77735	2.55626	0.08649	7.09961
λ	$t/\hbar\omega = 0.75$			
	$m_{\mathrm{p},z}$	$m_{\mathrm{p},y}$	$\frac{m_{\mathrm{p},z}-m_{\mathrm{p},y}}{m_{\mathrm{p},y}}$	$m_{\mathrm{p}} = m_{\mathrm{p},z} \times m_{\mathrm{p},y}$
1	1.35859	1.32520	0.02520	1.80041
2	1.84577	1.75615	0.05103	3.24146
3	2.50765	2.32725	0.07752	5.83594
4	3.40688	3.08408	0.10467	10.5071
5	4.62856	4.08702	0.13250	18.9130

5. Conclusion

We have solved the extended Holstein model with a long-range density-displacement type interaction in the strong coupling limit and in the nonadiabatic regime. We have found the mass of a small polaron in the extended Holstein model and compared it with that in the ordinary Holstein model. It is established that y-polarized vibrations of ions give a more renormalization of the polaron mass than z-polarized vibrations. In general, both y- and z-polarized vibrations contribute to the mass renormalization. The overall effect of both types of polarized vibrations depends (i) on the ratio κ_z/κ_y, (ii) on the type (range) of interaction forces $\mathbf{f}_{\mathbf{m},\alpha}(\mathbf{n})$, and (iii) on a lattice geometry. In the limit $\kappa_z \geq \kappa_y$, it is found that a small polaron in EHM is lighter than a small Holstein polaron in the nonadiabatic regime.

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МАСА ПОЛЯРОНУ В РОЗШИРЕНІЙ МОДЕЛІ ХОЛСТЕЙНА

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Р е з ю м е

Вивчено перенормування маси електрона в результаті утворення малого полярону в межах розширеної моделі Холстейна. Передбачається, що електрон рухається по одномірному ланцюжку іонів і взаємодіє з коливаннями іонів сусіднього ланцюжка внаслідок далекодійних сил. Шляхом прямих обчислень отримано перенормовану масу недіабатичного малого полярону в межах сильного зв'язку. Отримані результати порівняно з аналітичними результатами Холстейна. Обговорено вплив коливань іонів з різними поляризаціями на масу малого полярону.