# Giant enhancement of anisotropy by electron-phonon interaction

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Anisotropic electron-phonon interaction is shown to lead to the anisotropic polaron effect. The resulting anisotropy of the polaron band is an exponential function of the electron-phonon coupling and might be as large as $10^3$. This also makes anisotropy very sensitive to small changes of coupling and implies wide variations of anisotropy among compounds of similar structure. The isotope effect on mass anisotropy is predicted. Polaron masses are obtained by an exact quantum Monte Carlo method. Implications for high-temperature superconductors are briefly discussed. [S0163-1829(99)00221-0]

In an anisotropic crystal, electron-phonon interaction (EPI) is anisotropic too. This is of minor importance in a metal with a high carrier density and weak EPI. The carrier mass is renormalized as $m^*_\alpha = m_{0\alpha}(1+\gamma_\alpha\lambda)$, where $\lambda$ is the electron-phonon coupling constant and $\gamma_\alpha \sim 1$ a numerical coefficient corresponding to direction $\alpha$. At $\lambda \ll 1$ mass renormalization is small and EPI has little effect on the band anisotropy which is governed by bare anisotropy of the rigid lattice. The situation is qualitatively different in a semiconductor with a low carrier density and strong EPI $\lambda \geqslant 1$. Under these conditions formation of small (lattice) polarons is expected.[1–3] A general property of *small* polarons is an exponential renormalization of mass $m^*_\alpha \propto \exp(\gamma_\alpha \lambda/\overline{\omega})$, where $\overline{\omega}$ is the dimensionless phonon frequency.[4] Now the mass anisotropy $m^*_\alpha/m^*_\beta \propto \exp[(\gamma_\alpha - \gamma_\beta)\lambda/\overline{\omega}]$ is an *exponential* function of $\lambda$, $\overline{\omega}$, and the form of EPI (through $\gamma_\alpha s$). This simple relation hints several possible effects. (i) Anisotropy may be very large if $\lambda \geqslant 1$ and $\overline{\omega} \leqslant 1$. (ii) Anisotropy is very sensitive to small changes of $\lambda$ caused, e.g., by doping (due to changes in screening). This also implies that different compounds that are similar in structure and have close $\lambda$ may nevertheless have very different anisotropies. (iii) The dependence on phonon frequency is strong, hence the *isotope effect* on anisotropy. Thus anisotropic EPI may have profound effect on electronic properties of doped semiconductors.

The anisotropic case has been little touched in the polaron literature. Kahn considered the large (continuum) Fröhlich polaron with bare anisotropy and isotropic EPI and found that the polaron is *less* anisotropic than the bare carrier.[5] Recently Caprara and Del Prete found an *enhancement* of anisotropy by a factor $\approx 2$ in the vicinity of a saddle point of the bare spectrum.[6] Both studies were weak-coupling perturbational. In the strong-coupling regime the Lang-Firsov transformation[7] leads quite naturally to a strongly anisotropic polaron but we are not aware of any specific applications of this method. Also we are not aware of any previous numerical studies of the anisotropic case. Almost all the recent activity in the polaron field has been directed to the paradigmatic Holstein model[8] where EPI is local and the effect is absent.

The recently developed quantum Monte Carlo (QMC) algorithms[9,10] have opened the possibility to calculate the polaron effective mass exactly. The methods also allow studies of infinite lattices and arbitrary forms of electron-phonon interaction including anisotropic. In this paper we apply the method of Ref. 10, based on Feynman's integration of phonons,[11,12] to two models with anisotropic EPI. The first one is a simple two-dimensional (2D) model where the enhancement of anisotropy is weak. The second model is a three-dimensional (3D) one with long-range EPI. Here we will find a very large enhancement and confirm the existence of the effects mentioned in the beginning.

Let us begin with the simplest possible 2D model with anisotropic EPI (see Fig. 1). The lattice consists of two interpenetrating square sublattices **n** (crosses) and **m** (circles). The sites **n** are fixed in their positions but sites **m** can vibrate along $z$ direction (up-down), $\xi_{\mathbf{m}}$ being the internal coordinates. All **m** are uncoupled and have the same frequency $\omega$ and mass $M$. The carrier moves in the sublattice **n** by hopping between nearest neighbors with amplitudes $t_{\mathbf{nn}'}$. The carrier at a site **n** attracts the two nearest sites **m** (above and below) with *force* $\kappa$. The model Hamiltonian is

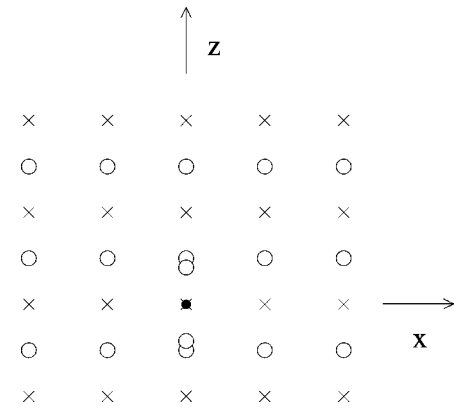


FIG. 1. The two-dimensional lattice (positioned in the plane $xz$) of the model (2). The carrier (bullet) hops between **n** sites (crosses) but interacts with **m** sites (circles) which vibrate along $z$ direction. Two **m** sites are shifted from their equilibrium positions by some distance forming a small polaron. The three-dimensional lattice of the model (4) is obtained by repeating the whole figure along $y$ direction perpendicular to the sheet plane.

 

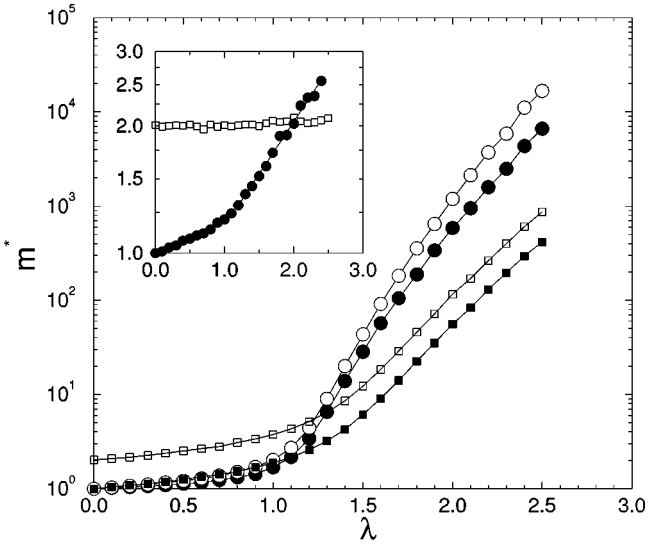


FIG. 2. Polaron masses in the model (2) for $t_\perp = t$ (circles) and in the 2D Holstein model for $t_\perp/t = 0.5$ (squares). $\bar{\omega} = 1.0$ in both cases. Open (filled) symbols are $m_z^*$ ($m_x^*$). Inset: anisotropy $m_z^*/m_x^*$ for the model (2) (circles) and Holstein model (squares).

$$H = -\sum_{\langle \mathbf{n}\mathbf{n}' \rangle} t_{\mathbf{n}\mathbf{n}'} c_{\mathbf{n}}^\dagger c_{\mathbf{n}'} + \sum_{\mathbf{m}} \left( \frac{\hat{p}_{\mathbf{m}}^2}{2M} + \frac{M\omega^2}{2} \xi_{\mathbf{m}}^2 \right) - \sum_{\langle \mathbf{n}\mathbf{m} \rangle} f_{\mathbf{m}}(\mathbf{n}) c_{\mathbf{n}}^\dagger c_{\mathbf{n}} \xi_{\mathbf{m}}, \tag{1}$$

$$f_{\mathbf{m}}(\mathbf{n}) = \kappa(\delta_{\mathbf{n},\mathbf{m}-\mathbf{z}/2} - \delta_{\mathbf{n},\mathbf{m}+\mathbf{z}/2}), \tag{2}$$

where $\hat{p}_{\mathbf{m}} = -i\hbar\partial/\partial\xi_{\mathbf{m}}$. The hopping integral in $x$ and $z$ directions are $t$ and $t_\perp$, respectively. The model is characterized by the dimensionless frequency $\bar{\omega} = \hbar\omega/t$, the bare anisotropy ratio $m_{0z}/m_{0x} = t/t_\perp$, and the coupling constant $\lambda \equiv [\Sigma_{\mathbf{m}} f_{\mathbf{m}}^2(0)]/(2M\omega^2 D) = 2\kappa^2/(2M\omega^2 D)$, where $D$ is half of the bare bandwidth. If the carrier interacted only with *one* neighboring **m** site then Eq. (2) would have described the 2D Holstein model. Polaron masses of the latter model for $\bar{\omega} = 1.0$ and $t_\perp = 0.5\,t$, obtained with QMC, are shown in Fig. 2 (main picture, squares). At $\lambda > 1.5$ both $m_z^*$ and $m_x^*$ increase exponentially as $\propto \exp(4.2\lambda)$. However, the ratio $m_z^*/m_x^*$ remains constant as a function of $\lambda$ and equal to the bare anisotropy 2.0 (see inset, squares). Thus the local interaction of the Holstein model does not enhance bare anisotropy.

The behavior of the model (2) is different. While the renormalization of both masses is similar to the Holstein case, $m_z^*$ now grows faster than $m_x^*$ even for $t_\perp = t$ (see Fig. 2, main picture, circles). The ratio $m_z^*/m_x^*$ grows exponentially as $\propto \exp(0.58\lambda)$ in the small-polaron regime $\lambda > 1.2$ (see the inset in Fig. 2, circles). The physical reason for the difference is as follows. In the small-polaron regime the carrier is mostly confined to a single lattice site **n** and both nearest **m** ions are shifted by some distance $d$ from their equilibrium positions (see Fig. 1). Tunneling along $x$ direction occurs when two neighboring **m** ions on the right (or left) get shifted fluctuationally by $d$ which creates a potential well on the neighboring **n** site, similar to the one the electron is already in. However, for the tunneling along $z$ direction to become possible only one **m** ion must be shifted by $d$ but another, the one which is forming the current potential well, must be shifted by the *double* distance $2d$. This process is less probable and requires more time to occur. That is why, although the lattice deformation extends in $z$ direction, it is more mobile in $x$ direction.

The simple model considered illustrates the two generic properties of strong anisotropic electron-phonon interaction: (i) it makes the spectrum anisotropic, and (ii) anisotropy is an exponential function of coupling. However, the actual enhancement is modest in this model, $m_z^*/m_x^* \approx 2$ for $\lambda = 2.0$ when the masses themselves are already huge, $m^* \sim 10^3$. In order to understand under which conditions anisotropy can be larger one has to consider how the form of electron-phonon interaction, i.e., the shape of the function $f_{\mathbf{m}}(\mathbf{n})$ affects mass enhancement of the small polaron. Within the path-integral approach the inverse polaron mass is the second moment of the end-to-end distribution of imaginary-time paths with open boundary conditions.[10] Each path includes in its statistical weight a phonon induced factor $e^A$ where $A$ is the action of the retarded self-interaction.[11] Essentially, $A$ depends on the forces $f_{\mathbf{m}}(\mathbf{n})$ via combinations

$$\Phi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{m}} f_{\mathbf{m}}(\mathbf{r}_1) f_{\mathbf{m}}(\mathbf{r}_2). \tag{3}$$

Here **r** is the carrier position on a path, i.e., one of **n**. Normally, the function $\Phi(\mathbf{r})$ is the largest at $\mathbf{r} = 0$ and decays monotonically at large **r**. What matters for polaron mass are the *gradients* $\nabla\Phi(\mathbf{r})$ in the corresponding direction. The smaller the gradient the less the action changes upon the increase of $\mathbf{r}_1 - \mathbf{r}_2$, the more likely such a change will be accepted by the Monte Carlo process, the larger the second moment of the resulting end-to-end distribution. Thus a steep (smooth) $\Phi(\mathbf{r})$ leads to a large (small) effective mass.

For the Holstein model [for which $f_{\mathbf{m}}(\mathbf{n}) = \kappa\delta_{\mathbf{mn}}$] function (3) is the lattice delta function $\Phi(\mathbf{r}_1 - \mathbf{r}_2) = \kappa^2 \delta_{\mathbf{r}_1\mathbf{r}_2}$ which is a steep function. Therefore in the small-polaron regime the weight of paths with nonzero $\mathbf{r}_1 - \mathbf{r}_2$ is exponentially small leading to an exponentially small second moment. For the model (2) the $x$ and $z$ cross sections of $\Phi(\mathbf{r})$ are shown in Fig. 3(a). One can see that due to negative values at $(x = 0, z = \pm 1)$ the gradient in $z$ direction is larger than in $x$ direction. This is the reason for the enhanced $m_z^*$. There are cases where $\nabla\Phi(\mathbf{r})$ in one direction is much smaller than in the Holstein model or than in model (2). Consider again a lattice with the topology of Fig. 1. Elementary geometrical considerations show that $\nabla_x\Phi(\mathbf{r})$ is small when (i) the distance between chains **n** and **m** is large; (ii) interaction with *distant* **m** ions is included. When these conditions are fulfilled one should expect a much lighter $x$ mass than in the Holstein case. At the same time $\nabla_z\Phi(\mathbf{r})$ is *always* big at the origin. Indeed, by definition $\Phi(0,0)$ is positive but $\Phi(0,\pm 1)$ is negative [because $f_{\mathbf{m}}(0,0)$ and $f_{\mathbf{m}}(0,1)$ have different signs for **m** ions with $\mathbf{m} = (x, 1/2)$]. Therefore the $z$ mass is of the order of the Holstein mass and, consequently, a large anisotropy $m_z^*/m_x^*$ might follow. One should add, that if **m** ions were allowed to move along $x$ direction it would have increased $m_x^*$ and decreased $m_z^*$. A predominant interaction with a single phonon polarization is essential for

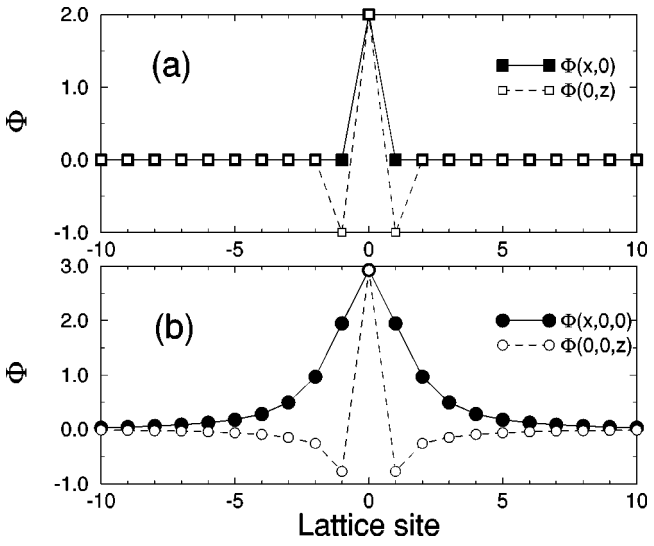


FIG. 3. Function $\kappa^{-2}\Phi(\mathbf{r})$ [Eq. (3)] for: (a) the 2D model (2); (b) the 3D model (4).

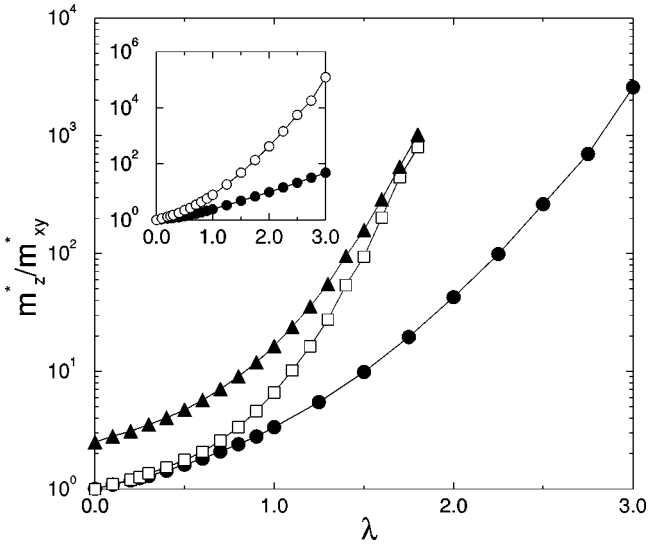


FIG. 4. Mass anisotropy of the model (4). Circles: $\bar{\omega}=1.0$, $t_\perp=0.25\,t$; squares: $\bar{\omega}=0.5$, $t_\perp=0.25\,t$; triangles: $\bar{\omega}=0.5$, $t_\perp=0.1\,t$. Inset: masses $m^*_{xy}$ (filled circles) and $m^*_z$ for $\bar{\omega}=1.0$, $t_\perp=0.25\,t$.

a large anisotropy. Finally, it is not difficult to see that in 3D the difference between $\nabla_z\Phi(\mathbf{r})$ and $\nabla_x\Phi(\mathbf{r})$ would be even bigger than in 2D.

We now consider a 3D model where all the above factors are present. The lattice structure is obtained from the one depicted in Fig. 2, by repeating it along *y* direction which is perpendicular to the sheet plane. The distance between neighboring **n** and **m** *planes* is equal to the lattice constant in *x* and *y* directions (i.e., the lattice constant in *z* direction is *twice* the one in *xy* plane). The EPI has the form

$$f_{\mathbf{m}}(\mathbf{n})=\kappa\frac{m_z-n_z}{|\mathbf{m}-\mathbf{n}|^3}e^{-\frac{|\mathbf{m}-\mathbf{n}|}{R}}, \tag{4}$$

which is the *z* projection of the Coulomb force with a screening radius *R*. This model is designed to describe the layered structure of high-$T_c$ superconductors, **n** sites (crosses) representing the copper-oxygen planes, and **m** sites (circles) the apical oxygens.[13] Its 1D (one **n** chain and one **m** chain) and 2D (one **n** plane and one **m** plane) versions were considered in Ref. 14 (see also Ref. 10). There was found a much reduced polaron mass, as compared with the Holstein model. Here we consider the full 3D problem. Due to the low *c*-axis conductivity of the cuprates screening in *z* direction is poor and *R* is large. We use $R=10$ lattice constants in *x* direction. For this interaction $\lambda=2.93\kappa^2/(2M\omega^2D)$. Function $\Phi(\mathbf{r})$ for this model is shown in Fig. 3(b).

Effective masses of model (4) for $\bar{\omega}=1.0$ and $t_\perp=0.25\,t$, obtained with the exact QMC, are shown in the inset of Fig. 4. There is a striking difference in λ dependences of $m^*_{xy}$ and $m^*_z$. While $m^*_{xy}$ grows much slower than the Holstein mass, which is consistent with previous findings in one and two dimensions, $m^*_z$ grows similar to the Holstein case. For example, for $\lambda=2.0$ $m^*_z=420\,m_{0x}$ while $m^*_x=10\,m_{0x}$, for $\lambda=2.5$ $m^*_z=5600\,m_{0x}$ while $m^*_x=21\,m_{0x}$, etc. As a result, the mass anisotropy increases sharply with coupling reaching 2500 for $\lambda=3.0$ (see the main picture in Fig. 4, circles). Basically, we are dealing with a new situation when two types of polarons are present at the same time. In *z* direction the carrier is the Holstein small polaron with a small size of lattice deformation (of the order of one lattice constant), localization of the carrier within this local deformation, and a very large effective mass. In *xy* plane the lattice deformation is larger than both the lattice constant and the localization area of the carrier, and the polaron is much more mobile (such a quasiparticle was named small Fröhlich polaron in Ref. 14). It is interesting to note fits $m^*_z/m_{0x}=\exp(1.26\lambda+0.88\lambda^2)$ and $m^*_z/m^*_{xy}=\exp(0.42\lambda+0.71\lambda^2)$. The quadratic terms in the exponents are unusual. We were unable to establish if this is the true asymptotic behavior or the dependencies approach a pure exponential growth at larger λ.

We continue to study the model (4) by changing its parameters. A general property of the small polaron is that its mass increases as the phonon frequency decreases because the lattice deformation becomes less mobile, $m^*_\alpha \propto\exp(\gamma_\alpha\lambda/\bar{\omega})$. In our case $\gamma_z>\gamma_{xy}$. Therefore one should expect much stronger change of $m^*_z$ than of $m^*_{xy}$ with frequency. Figure 4 shows $m^*_z/m^*_{xy}$ for $\bar{\omega}=0.5$ and $t_\perp=0.25\,t$ (squares). One can see that in this case the anisotropy is much bigger than when $\bar{\omega}=1.0$. This implies the existence of the *isotope effect on mass anisotropy* in systems with strong long-range anisotropic electron-phonon interaction. Another model parameter is the bare anisotropy $t_\perp/t$. It has been found to be of minor importance. In short, it is a constant factor which is carried throughout the whole λ interval. Figure 4 shows $m^*_z/m^*_{xy}$ for $\bar{\omega}=0.5$ and $t_\perp=0.1\,t$ which corresponds to the bare anisotropy $m_{0z}/m_{0xy}=2.5$ (triangles). The plot is very close to the one with $t_\perp=0.25\,t$, the small difference resulting from the latter case being more adiabatic than $t_\perp=0.1\,t$.

Layered high-$T_c$ superconductors seem to be a good candidate for the effect described. Indeed, in the cuprates the carrier density is low, EPI is obviously anisotropic and *strong*, as revealed by isotope substitution[15,16] and neutron-scattering[17] experiments. Moreover, coupling to *c*-axis polarized phonons is strong.[18] At the same time, a number of unusual *c*-axis properties[19] — anomalously low

interlayer hopping (large $m_z^*$), anomalously large mass anisotropy, large variation of anisotropy among different cuprates — are reproduced in our model calculation. Although other effects, such as the pairing of carriers, have been shown to account for some *c*-axis anomalies of the cuprates,[20] the effect of strong anisotropic EPI seems to be worth further studying. For instance, the puzzling exponential increase of *c*-axis plasma frequency with doping and the exponential decrease of anisotropy with doping observed in YBCO and other cuprates[19] can be explained easily by the present mechanism if one assumes that extra holes screen the long-range EPI and thereby reduce $\lambda$.[20]

In summary, it has been argued that strong anisotropic electron-phonon interaction in general enhances the anisotropy of the carrier band. The effect is strongest when (i) the interaction is predominantly with one phonon polarization only; (ii) the interaction is long-range; (iii) the dimensionality is three; (iv) the distance between planes is large. The mass anisotropy is an exponential function of coupling which results in the large value of anisotropy and in wide variations among different compounds of similar structure. The bare anisotropy is irrelevant for the effect. With decreasing phonon frequency the mass anisotropy increases drastically. This amounts to isotope shift of the mass anisotropy. Possible candidates for the effect are layered high-$T_c$ superconductors.

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