Impurity states in a polar-crystal slab

You-Cheng Li and Ling-Feng Zheng
Institute of Theoretical Physics, Hebei Normal University, Shijiazhuang, Hebei, People's Republic of China

Shi-Wei Gu
Center of Theoretical Physics, Chinese Center for Advanced Science and Technology (World Laboratory) Beijing, People's Republic of China
and Department of Physics, Jiao Tong University, Shanghai, People's Republic of China
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The ground state and the first excited state of a bound polaron in a polar crystal slab are investigated by means of the Lee-Low-Pines variation technique. Both the electron–LO-phonon interaction and the electron–surface-optical-phonon interaction are taken into account. For an impurity located at different positions in the slab, the self-energy and the effective mass as well as the transition energies are evaluated as functions of slab thickness. It is found that, in our approximate calculations, the position of the shallow-doped impurity in the slab will produce an impact only on that part of the bound polaron's energy associated with motion parallel to the xy plane. Consequently, it will exert a great influence on the transition energies.

I. INTRODUCTION

In recent years, much interest has been shown in the study of semiconductor superlattice systems because of their wide applications. As an elementary problem, understanding of the role of impurities in a polar-crystal slab would be of particular importance from a technological point of view.

Since the subject was first studied, impurity states in thin films of semiconductor crystals have been described by using a square-well model.[1] A number of theoretical papers[2–6] have discussed the issue of the "hydrogenic" binding of an electron to a donor impurity in a polar crystal slab or in a semiconductor quantum well.

In order to investigate the properties of an electron bound to a shallow dopant impurity in a polar slab, the interactions between the electron and the phonon modes of an ionic crystal slab must be dealt with correctly. According to the microscopic approach, in which the electronic polarization particularly due to the ionic motion was introduced,[7] the bulk transverse-optical (TO) modes would not make any contribution to the energy exchange between electrons and slab. Such a conclusion has also been established experimentally.[8] But then the bulk longitudinal-optical (LO) and the surface-optical (SO) modes should be included in the electron-phonon interactions, since for both of them there exist polarization charge densities in the volume and the surface of the slab.

The electron–LO-phonon interaction operator, in the limit of infinite thickness, is equivalent to the interaction operator of the bulk Fröhlich Hamiltonian.[9] By considering the interaction energy of a classical electron external to the slab and the SO polarization field, it is found that the electron–SO-phonon interaction operator leads to the result of classical image-charge theory. The electron–SO-phonon interaction should be taken into account as the electron inside the slab approaches the surface, even if the amplitudes of the SO modes decrease exponentially on moving away from the surface.

Most of the early studies have concentrated on the interaction of LO modes and concluded that such an interaction tended to increase the impurity binding energy and the polaron's effective mass.[5,10] Licari and Evrard[7] deduced the Hamiltonian operators of the electron-phonon system in a polar crystal slab with both SO and LO modes included. They illustrated that the effect of the SO phonons on the electron surface-state formation in semiconductors might give a binding energy deeper than previously expected. Based on the same consideration of the electron-phonon interactions as in Ref. 7, for a weak-coupling case, Gu and Sun[11] made a numerical calculation of the self-energy of a polaron bound to the shallow dopant impurity located at the slab center by using a perturbation method.

In this paper, a further investigation of a bound polaron confined in a polar crystal slab with arbitrary thickness is made by means of the Lee-Low-Pines variation technique.[12] The interactions of both LO and SO modes are taken into account, and the effective Hamiltonian of the electron-phonon system is derived. The self-energy as well as the effective mass, for GaAs as an example, are calculated as functions of the slab thickness. It is shown that the electron–SO-phonon interaction also increases the self-energy and the effective mass just as LO modes do.

We assume the impurity to be located in three different positions inside the polar slab instead of at the center. Our calculations show that the impurity position will exert obvious influence only on that part of the polaron's energy associated with motion parallel to the xy plane. Consequently, it will produce an impact on the transition energy between different impurity states. If the donor is located closer to the slab center, the transition energy for the quantum number $l=1$ will be larger and for $l=2$ will be smaller.

The formalism of this paper is suitable not only for weak- but also for intermediate-coupling bound polarons.

II. THE HAMILTONIAN

Consider a polar crystal slab with thickness $2d$. As shown in Fig. 1, the space for $|z| \leq d$ is occupied by the crystal and for $|z| > d$ the space is a vacuum. The shallow doped impurity is located at the point z_i in the z direction. We assume that the effective-mass approximation is valid and that the potential barrier in the slab surface is approximately, infinity, i.e., the tunneling of electrons through the surface is neglected. Then the problem may approximately be the motion of an electron of mass m^* in the infinite square-well potential of width $2d$. So, the Hamiltonian of the electron-phonon system can be written as

$$H = H_e + H_{\rm ph} + H_{e\text{-LO}} + H_{e\text{-SO}} \ . \tag{1}$$

The first term is the Hamiltonian of the shallow donor, given by

$$H_e = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \frac{\hbar^2 K_\rho^2}{2m^*} - \frac{e^2}{\epsilon_\infty r'}, \quad |z| \leq d \tag{2a}$$

where $r' = [\rho^2 + (z - z_i)^2]^{1/2}$, $\mathbf{K}_\rho$ and $\boldsymbol{\rho}$ are the wave vector and the position vector of the electron in the xy plane, respectively, m^* is the band mass of the electron, ϵ_∞ is the optical dielectric constant and $-e^2/\epsilon_\infty r'$, is the Coulomb potential. In order to solve the energy eigenequation of H(1), we introduce the plane Coulomb potential[13] with the parameter λ and rewrite H_e as

$$H_e = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \left[\frac{\hbar^2 K_\rho^2}{2m^*} - \frac{e^2\lambda}{\epsilon_\infty \rho}\right] + \left[\frac{e^2\lambda}{\epsilon_\infty \rho} - \frac{e^2}{\epsilon_\infty r'}\right] . \tag{2b}$$

As will be seen later, λ can be determined by perturbation theory.

The second term in (1) represents the phonon-field Hamiltonian and is given by

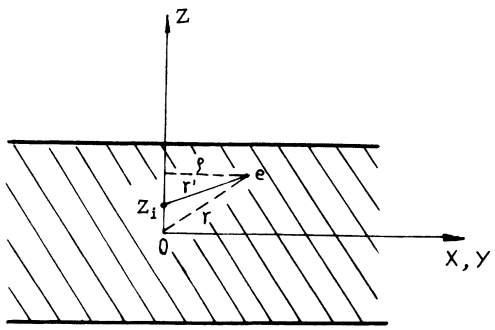

FIG. 1. Geometry of the polar crystal slab.

$$H_{\rm ph} = H_{\rm LO} + H_{\rm SO} \ , \tag{3a}$$

$$H_{\rm LO} = \sum_{\mathbf{k},m,p} \hbar\omega_{\rm LO} a^\dagger_{m,p}(\mathbf{k}) a_{m,p}(\mathbf{k}) \ . \tag{3b}$$

$$H_{\rm SO} = \sum_{\mathbf{q},p} \hbar\omega_{Sp} b^\dagger_p(\mathbf{q}) b_p(\mathbf{q}) \ , \tag{3c}$$

where $a^\dagger_{m,p}(\mathbf{k})$ $[a_{m,p}(\mathbf{k})]$ is the creation (annihilation) operator for the LO phonon with frequency $\omega_{\rm LO}$ and $\mathbf{k}$ is the two-dimensional projection on the xy plane of the wave vector. $b^\dagger_p(\mathbf{q})$ $[b_p(\mathbf{q})]$ is the corresponding operator for the SO phonon with frequency ω_{Sp} and wave vector $\mathbf{q}$. The phonon modes are specified by subscripts p and m. The parity index p, taking the value $+$ and $-$, refers to the mirror symmetry with respect to the plane $z=0$. The index m is the quantum number denoting the z component of the LO-phonon wave vector. For even parity (p takes $+$), m is odd and for odd parity (p takes $-$), m is even. The phonon frequencies can be expressed in terms of the transverse optical (TO) phonon frequency $\omega_{\rm TO}$ by

$$\omega^2_{\rm LO} = (\epsilon_0/\epsilon_\infty)\omega^2_{\rm TO} \ , \tag{4a}$$

$$\omega^2_{S\pm} = \frac{(\epsilon_0+1) \mp (\epsilon_0-1)e^{-2qd}}{(\epsilon_\infty+1) \mp (\epsilon_\infty-1)e^{-2qd}}\omega^2_{\rm TO} \ , \tag{4b}$$

where ϵ_0 is the static dielectric constant.

In (1), the last two terms are the electron–LO-phonon and the electron–SO-phonon interaction Hamiltonian operators and are directly taken from Ref. 7,

$$H_{e\text{-LO}} = \sum_{\mathbf{k}} \left[B^* e^{-i\mathbf{k}\cdot\boldsymbol{\rho}} \left(\sum_{m=1,3,\ldots} \frac{\cos\left[\frac{m\pi}{2d}z\right]}{\left[k^2 + \left[\frac{m\pi}{2d}\right]^2\right]^{1/2}} a^\dagger_{m,+}(\mathbf{k}) + \sum_{m=2,4,\ldots} \frac{\sin\left[\frac{m\pi}{2d}z\right]}{\left[k^2 + \left[\frac{m\pi}{2d}\right]^2\right]^{1/2}} a^\dagger_{m,-}(\mathbf{k}) \right) + \text{H.c.} \right], \quad |z| \leq d \tag{5a}$$

$$H_{e\text{-SO}} = \sum_{\mathbf{q}} \left[\frac{\sinh(2qd)}{q}\right]^{1/2} e^{-qd}\{C^* e^{-i\mathbf{q}\cdot\boldsymbol{\rho}}[G_+(q,z)b^\dagger_+(\mathbf{q}) + G_-(q,z)b^\dagger_-(\mathbf{q})] + \text{H.c.}\} \ , \tag{5b}$$

where

$$B^*=i\left[\frac{4\pi e^2}{V}\hbar\omega_{\mathrm{LO}}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\right]^{1/2}, \tag{6a}$$

$$C^*=i\left[\frac{2\pi e^2}{A}\hbar\omega_{\mathrm{TO}}(\epsilon_0-\epsilon_\infty)\right]^{1/2}, \tag{6b}$$

$$G_+=\frac{\cosh(qz)/\cosh(qd)}{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}} \times\left[\frac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, \quad |z|\le d \tag{7a}$$

$$G_-=\frac{\sinh(qz)/\sinh(qd)}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}} \times\left[\frac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, \quad |z|\le d . \tag{7b}$$

In the above equations, A and V are the surface area and the volume of the slab respectively. We take N as the slab thickness in the unit of the lattice spacing constant a, namely, we have $Na=2d$. According to the Brillouin-zone boundary limitation $m\pi/2d\le\pi/2a$, m can be any integer within the range $1\le m\le N/2$.

III. THE EFFECTIVE HAMILTONIAN

We adopt the variation technique developed by Lee *et al.*[12] to deal with the Hamiltonian (1). For the sake of convenience, first, we perform the unitary transformations twice to H (1) with

$$U_1=\exp\left[-i\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\cdot\boldsymbol{\rho} -i\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})b_p(\mathbf{q})\mathbf{q}\cdot\boldsymbol{\rho}\right], \tag{8}$$

and

$$U_2=\exp\left[\sum_{\mathbf{k},m,p}[a^\dagger_{m,p}(\mathbf{k})f_{m,p}(\mathbf{k})-a_{m,p}(\mathbf{k})f^*_{m,p}(\mathbf{k})] +\sum_{\mathbf{q},p}[b^\dagger_p(\mathbf{q})g_p(\mathbf{q})-b_p(\mathbf{q})g^*_p(\mathbf{q})]\right], \tag{9}$$

where $f^*_{m,p}$, $f_{m,p}$, g^*_p, and g_p are the variational parameters determined by minimizing the energy subsequently. After some tedious but straightforward algebra, we obtain the transformed Hamiltonian and separate it into two parts for applying the perturbation method later on. That is

$$\mathcal{H}=U_2^{-1}U_1^{-1}HU_1U_2=\mathcal{H}_0+\mathcal{H}_1 , \tag{10}$$

where

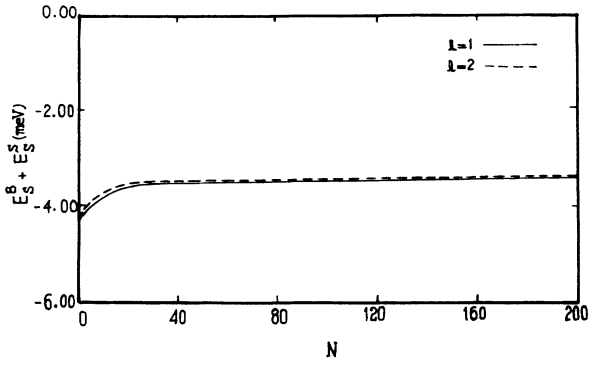

FIG. 2. Self-energy vs slab thickness N in units of the lattice-spacing constant a.

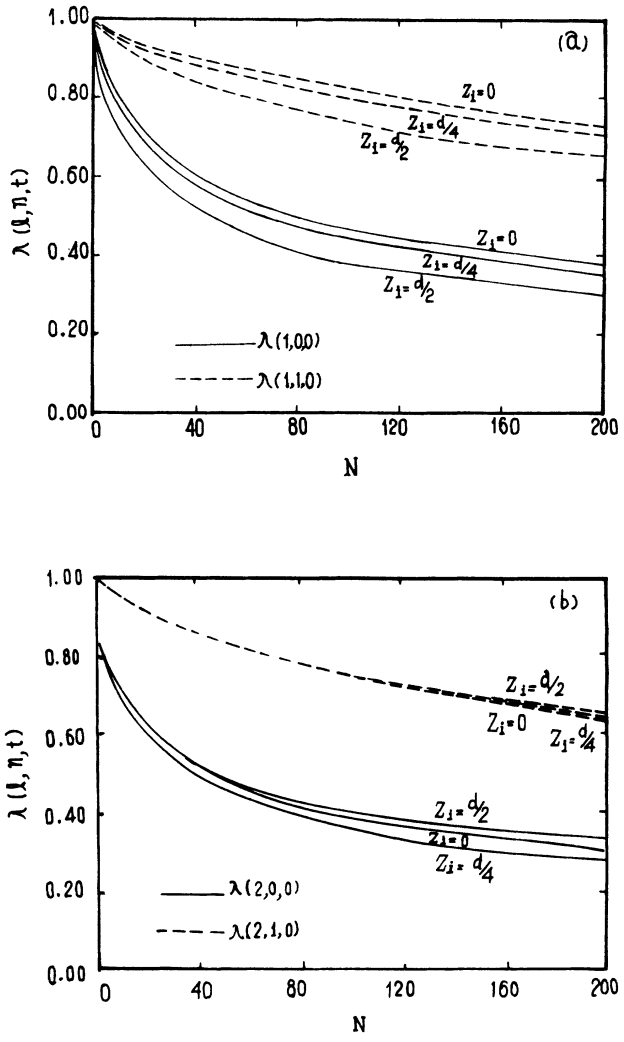

FIG. 3. (a) The variational parameter λ vs slab thickness N (for $l=1$). (b) The variational parameter λ vs slab thickness N (for $l=2$).

$$
\begin{aligned}
\mathcal{H}_0 = & -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+\frac{\hbar^2 K_\rho^2}{2m^*}-\frac{e^2\lambda}{\epsilon_\infty \rho}+\frac{\hbar^2}{2m^*}\left[\sum_{\mathbf{k},m,p} a^\dagger_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}+\sum_{\mathbf{q},p} b^\dagger_p(\mathbf{q})b_p(\mathbf{q})\mathbf{q}\right]^2 \\
& +\frac{\hbar^2}{2m^*}\left[\left[\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\mathbf{k}\right]^2+\left[\sum_{\mathbf{q},p}|g_p(\mathbf{q})|^2\mathbf{q}\right]^2\right]+\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\left[\hbar\omega_{\mathrm{LO}}+\frac{\hbar^2}{2m^*}\mathbf{k}^2-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{k}\right] \\
& +\sum_{\mathbf{q},p}|g_p(q)|^2\left[\hbar\omega_{Sp}+\frac{\hbar^2}{2m^*}\mathbf{q}^2-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{q}\right] \\
& +\frac{\hbar^2}{m^*}\left[\left[\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\right]\left[\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\mathbf{k}\right]+\left[\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})b_p(\mathbf{q})\mathbf{q}\right]\left[\sum_{\mathbf{q},\mathrm{p}}|g_p(\mathbf{q})|^2\mathbf{q}\right]\right] \\
& +\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\left[\hbar\omega_{\mathrm{LO}}-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{k}\right]+\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})b_p(\mathbf{q})\left[\hbar\omega_{Sp}-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{q}\right] \\
& +\sum_{\mathbf{k}}\left[B\left[\sum_{m=1,3,\ldots}^{N/2}\frac{\cos\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}f_{m,+}(\mathbf{k})+\sum_{m=2,4,\ldots}^{N/2}\frac{\sin\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}f_{m,-}(\mathbf{k})\right]+\mathrm{H.c.}\right] \\
& +\sum_{\mathbf{q}}\left[\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C[G_+(q,z)g_+(\mathbf{q})+G_-(q,z)g_-(\mathbf{q})]+\mathrm{H.c.}\}\right] \\
& +\sum_{\mathbf{k}}\sum_{m=1,3,\ldots}^{N/2}\left\{a^\dagger_{m,+}(k)\left[B^*\sum_{m=1,3,\ldots}^{N/2}\frac{\cos\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}\right.\right. \\
& \qquad \left.\left.+f_{m,+}(\mathbf{k})\left[\hbar\omega_{\mathrm{LO}}-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{k}+\frac{\hbar^2}{2m^*}\mathbf{k}^2+\frac{\hbar^2}{m^*}\mathbf{k}\cdot\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\mathbf{k}\right]\right]+\mathrm{H.c.}\right\} \\
& +\sum_{\mathbf{k}}\sum_{m=2,4,\ldots}^{N/2}\left\{a^\dagger_{m,-}(\mathbf{k})\left[B^*\sum_{m=2,4,\ldots}^{N/2}\frac{\sin\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}\right.\right. \\
& \qquad \left.\left.+f_{m,-}(\mathbf{k})\left[\hbar\omega_{\mathrm{LO}}-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{k}+\frac{\hbar^2}{2m^*}\mathbf{k}^2+\frac{\hbar^2}{m^*}\mathbf{k}\cdot\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\mathbf{k}\right]\right]+\mathrm{H.c.}\right\} \\
& +\sum_{\mathbf{q}}\left\{b^\dagger_+(\mathbf{q})\left[C^*\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}G_+(q,z)\right.\right. \\
& \qquad \left.\left.+g_+(\mathbf{q})\left[\hbar\omega_{S+}-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{q}+\frac{\hbar^2}{2m^*}\mathbf{q}^2+\frac{\hbar^2}{m^*}\mathbf{q}\cdot\sum_{\mathbf{q},p}|g_p(\mathbf{q})|^2\mathbf{q}\right]\right]+\mathrm{H.c.}\right\} \\
& +\sum_{\mathbf{q}}\left\{b^\dagger_-(\mathbf{q})\left[C^*\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}G_-(q,z)\right.\right. \\
& \qquad \left.\left.+g_-(\mathbf{q})\left[\hbar\omega_{S-}-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{q}+\frac{\hbar^2}{2m^*}\mathbf{q}^2+\frac{\hbar^2}{m^*}\mathbf{q}\cdot\sum_{\mathbf{q},p}|g_p(\mathbf{q})|^2\mathbf{q}\right]\right]+\mathrm{H.c}\right\}, \qquad (10a)
\end{aligned}
$$

$$\mathcal{H}_1=\left[\frac{\lambda}{\rho}-\frac{1}{r'}\right]\frac{e^2}{\epsilon_\infty}+\frac{\hbar^2}{2m^*}\left[\left[\sum_{\mathbf{k},m,p}a_{m,p}(\mathbf{k})f^*_{m,p}(\mathbf{k})\mathbf{k}\right]\left[\sum_{\mathbf{k},m,p}a_{m,p}(\mathbf{k})f^*_{m,p}(\mathbf{k})\mathbf{k}\right]+\text{H.c.}\right]$$
$$+\frac{\hbar^2}{m^*}\left[\left[\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})f_{m,p}(\mathbf{k})\mathbf{k}\right]\left[\sum_{\mathbf{k},m,p}a_{m,p}(\mathbf{k})f^*_{m,p}(\mathbf{k})\mathbf{k}\right]\right]$$
$$+\frac{\hbar^2}{2m^*}\left[\left[\sum_{\mathbf{q},p}b_p(\mathbf{q})g^*_p(\mathbf{q})\mathbf{q}\right]\left[\sum_{\mathbf{q},p}b_p(\mathbf{q})g^*_p(\mathbf{q})\mathbf{q}\right]+\text{H.c.}\right]+\frac{\hbar^2}{m^*}\left[\left[\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})g_p(\mathbf{q})\mathbf{q}\right]\left[\sum_{\mathbf{q},p}b_p(\mathbf{q})g^*_p(\mathbf{q})\mathbf{q}\right]\right]$$
$$+\frac{\hbar^2}{m^*}\left[\left[\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\right]\left[\sum_{\mathbf{k},m,p}a_{m,p}(\mathbf{k})f^*_{m,p}(\mathbf{k})\mathbf{k}\right]+\left[\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})f_{m,p}(\mathbf{k})\mathbf{k}\right]\left[\sum_{\mathbf{k},m,p}a^\dagger_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\right]\right]$$
$$+\frac{\hbar^2}{m^*}\left[\left[\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})b_p(\mathbf{q})\mathbf{q}\right]\left[\sum_{\mathbf{q},p}b_p(\mathbf{q})g^*_p(\mathbf{q})\mathbf{q}\right]+\left[\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})g_p(\mathbf{q})\mathbf{q}\right]\left[\sum_{\mathbf{q},p}b^\dagger_p(\mathbf{q})b_p(\mathbf{q})\mathbf{q}\right]\right]. \tag{10b}$$

With the physical assumption that successive virtual phonons around the electron are emitted individually in the field, i.e., there is no interaction between different phonons; we omit those terms including the factor $(a^\dagger_{m,p}a_{m,p}b^\dagger_p b_p)$ in the transformed $\mathcal{H}$.

From the form of Hamiltonian (10), the wave function of the system can be written as

$$|\Psi(z,\boldsymbol{\rho},\mathbf{k},\mathbf{q})\rangle=|\Phi(z,\boldsymbol{\rho})\rangle\,|N_{m,p}(\mathbf{k}),N_{Sp}(\mathbf{q})\rangle\ , \tag{11}$$

where $\Phi(z,\boldsymbol{\rho})$ is the wave function of the electron moving inside the slab and $|N_{m,p}(\mathbf{k}),N_{Sp}(\mathbf{q})\rangle$ is the wave function of the phonon field in the particle number representation. $N_{m,p}(\mathbf{k})$ and $N_{Sp}(\mathbf{q})$ are the numbers of the LO phonon and SO phonon respectively. Within the limitation of low temperature, few phonons will be excited and then we assume that there is no real phonon present in the phonon ground state. Hence, we take $|0,0\rangle$ as the wave function for the phonon system, which satisfies

$$a_{m,p}(\mathbf{k})\,|0,0\rangle=b_p(\mathbf{q})\,|0,0\rangle=0\ . \tag{12}$$

So, the wave function of the state with no phonon present is given by

$$|\Psi_0(z,\boldsymbol{\rho},\mathbf{k},\mathbf{q})\rangle=|\Phi(z,\boldsymbol{\rho})\rangle\,|0,0\rangle\ . \tag{13}$$

And the energy-expected value of $\mathcal{H}$ in such a state is

$$E=\langle\Psi_0|\mathcal{H}|\Psi_0\rangle=\langle\Phi(z,\boldsymbol{\rho})|F|\Phi(z,\boldsymbol{\rho})\rangle\ , \tag{14}$$

where we set

$$F=\langle 0,0|\mathcal{H}|0,0\rangle=F(z,\boldsymbol{\rho},f_{m,p},f^*_{m,p},g_p,g^*_p)\ . \tag{15}$$

From Eq. (10), we obtain

$$F=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+\left[\frac{\hbar^2}{2m^*}\mathbf{K}^2_\rho-\frac{e^2\lambda}{\epsilon_\infty\rho}\right]+\frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{r'}\right]$$
$$+\sum_{\mathbf{k}}\left[B\left[\sum_{m=1,3,\ldots}^{N/2}\frac{\cos\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}f_{m,+}(\mathbf{k})+\sum_{m=2,4,\ldots}^{N/2}\frac{\sin\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}f_{m,-}(\mathbf{k})\right]+\text{H.c.}\right]$$
$$+\sum_{\mathbf{q}}\left[\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C[G_+(q,z)g_+(\mathbf{q})+G_-(q,z)g_-(\mathbf{q})]+\text{H.c.}\}\right]$$
$$+\frac{\hbar^2}{2m^*}\left[\left[\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\mathbf{k}\right]^2+\left[\sum_{\mathbf{q},p}|g_p(\mathbf{q})|^2\mathbf{q}\right]^2\right]$$
$$+\sum_{\mathbf{k},m,p}|f_{m,p}(\mathbf{k})|^2\left[\hbar\omega_{\text{LO}}+\frac{\hbar^2}{2m^*}\mathbf{k}^2-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{k}\right]$$
$$+\sum_{\mathbf{q},p}|g_p(\mathbf{q})|^2\left[\hbar\omega_{Sp}+\frac{\hbar^2}{2m^*}\mathbf{q}^2-\frac{\hbar^2}{m^*}\mathbf{K}_\rho\cdot\mathbf{q}\right]. \tag{16}$$

According to the consideration in Ref. 12, if it is noted that the only preferred direction in the xy plane is the direction of $\mathbf{K}_\rho$, we may conveniently introduce two parameters η_1 and η_2 as

$$\sum_{\mathbf{k},m,p} |f_{m,p}(\mathbf{k})|^2 \mathbf{k}=\eta_1 \mathbf{K}_\rho ,$$

$$\sum_{\mathbf{q},p} |g_p(\mathbf{q})|^2 \mathbf{q}=\eta_2 \mathbf{K}_\rho . \tag{17}$$

Inserting (17) into (16), and from

$$\frac{\delta F}{\delta f_{m,p}}=\frac{\delta F}{\delta f^*_{m,p}}=\frac{\delta F}{\delta g_p}=\frac{\delta F}{\delta g^*_p}=0 ,$$

we obtain

$$f_{m,+}(\mathbf{k})=-\frac{B^*\cos\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}\Big/\left[\hbar\omega_{\mathrm{LO}}+\frac{\hbar^2\mathbf{k}^2}{2m^*}-\frac{\hbar^2\mathbf{K}_\rho\cdot\mathbf{k}}{m^*}(1-\eta_1)\right] , \tag{18a}$$

$$f_{m,-}(\mathbf{k})=-\frac{B^*\sin\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}\Big/\left[\hbar\omega_{\mathrm{LO}}+\frac{\hbar^2\mathbf{k}^2}{2m^*}-\frac{\hbar^2\mathbf{K}\rho\cdot\mathbf{k}}{m^*}(1-\eta_1)\right] , \tag{18b}$$

$$g_+(\mathbf{q})=-C^*\left[\frac{\sinh(2qd)}{q}\right]^{1/2} e^{-qd}G_+(q,z)\Big/\left[\hbar\omega_{S+}+\frac{\hbar^2\mathbf{q}^2}{2m^*}-\frac{\hbar^2\mathbf{K}_\rho\cdot\mathbf{q}}{m^*}(1-\eta_2)\right] , \tag{18c}$$

$$g_-(\mathbf{q})=-C^*\left[\frac{\sinh(2qd)}{q}\right]^{1/2} e^{-qd}G_-(q,z)\Big/\left[\hbar\omega_{S-}+\frac{\hbar^2\mathbf{q}^2}{2m^*}-\frac{\hbar^2\mathbf{K}_\rho\cdot\mathbf{q}}{m^*}(1-\eta_2)\right] . \tag{18d}$$

$f^*_{m,p}(\mathbf{k})$ and $g^*_p(\mathbf{q})$ can be easily expressed as the conjugate formulas of Eqs. (18a)–(18d).

It is necessary to point out that we are interested only in the slow electron always observed in experiments, namely, we can set $\mathbf{K}_\rho\approx 0$. By putting (18a)–(18d) and their conjugate formulas into (17) and expanding them to the first power of $\mathbf{K}_\rho$, η_1 and η_2 are given by

$$\eta_1=\alpha C_1(z)/[1+\alpha C_1(z)] , \tag{19}$$

where

$$C_1(z)=\frac{8}{Nau_l}\left[\sum_{m=1,3,\ldots}^{N/2}\cos^2\left[\frac{m\pi}{2d}z\right]I_m+\sum_{m=2,4,\ldots}^{N/2}\sin^2\left[\frac{m\pi}{2d}z\right]I_m\right] , \tag{19a}$$

and

$$I_m=\int_0^\infty \frac{x^3dx}{(1+x^2)^3\left[x^2+\left[\frac{m\pi}{Nau_l}\right]^2\right]} . \tag{19b}$$

$$\eta_2=\alpha C_2(z)/[1+\alpha C_2(z)] , \tag{20}$$

where

$$C_2(z)=4\epsilon_\infty^{3/2}\epsilon_0^{1/2}(Nau_l)^3(I_{N+}+I_{N-}) , \tag{20a}$$

and

$$I_{N+}=\int_0^{N\pi/2}\frac{(\sinh x)e^{-x}x^2}{[(Nau_{S+})^2+x^2]^3}\left[\frac{\cosh(xz/2d)}{\cosh(x/2)}\right]^2\times\frac{1}{[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^2}\times\left[\frac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-x}}\right]^{1/2}dx , \tag{20b}$$

$$I_{N-}=\int_0^{N\pi/2}\frac{(\sinh x)e^{-x}x^2}{[(Nau_{S-})^2+x^2]^3}\left[\frac{\sinh(xz/2d)}{\sinh(x/2)}\right]^2\times\frac{1}{[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^2}\times\left[\frac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-x}}\right]^{1/2}dx . \tag{20c}$$

In the above equations, we define the variable $x=2qd$ and the dimensionless coupling constant of the electron–LO-phonon interaction as

$$\alpha=\frac{m^*e^2}{\hbar^2u_l}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right] . \tag{21}$$

In addition, the polaron wave vectors u_l and u_{Sp} are defined as

$$u_l^2=\frac{2m^*\hbar\omega_{\mathrm{LO}}}{\hbar^2},\quad u_{Sp}^2=\frac{2m^*\hbar\omega_{Sp}}{\hbar^2} . \tag{22}$$

We take the variation minimum of F as the effective Hamiltonian of the electron-phonon system in a polar crystal slab, namely,

$$H_{\text{eff}}=\min F \ .$$

Also for a slow electron, considering Eqs. (17)–(20), we have

$$H_{\text{eff}}=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+\frac{\hbar^2}{2m^*}\mathbf{K}_\rho^2\left[1-\frac{\alpha C_1(z)}{[1+\alpha C_1(z)]^2}-\frac{\alpha C_2(z)}{[1+\alpha C_2(z)]^2}+\left[\frac{\alpha C_1(z)}{1+\alpha C_1(z)}\right]^2+\left[\frac{\alpha C_2(z)}{1+\alpha C_2(z)}\right]^2\right]$$
$$-\frac{e^2\lambda}{\epsilon_\infty\rho}+V_I^{(B)}(z)+V_I^{(S)}(z)+\frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{r'}\right], \tag{23}$$

where $V_I^{(B)}(z)$ and $V_I^{(S)}(z)$ are the effective potentials due respectively to the electron–LO-phonon interaction and the electron–SO-phonon interaction. After some direct calculations, they are derived as

$$V_I^{(B)}(z)=-\alpha\hbar\omega_{\text{LO}}\frac{4}{Nau_l}\left[\sum_{m=1,3,\ldots}^{N/2}\cos^2\left[\frac{m\pi}{2d}z\right]\frac{u_l^2}{\left[\frac{m\pi}{2d}\right]^2-u_l^2}\ln\frac{m\pi}{Nau_l}\right.$$
$$\left.+\sum_{m=2,4,\ldots}^{N/2}\sin^2\left[\frac{m\pi}{2d}z\right]\frac{u_l^2}{\left[\frac{m\pi}{2d}\right]^2-u_l^2}\ln\frac{m\pi}{Nau_l}\right], \tag{23a}$$

$$V_I^{(S)}(z)=-\alpha\hbar\omega_{\text{LO}}\epsilon_\infty^{3/2}\epsilon_0^{1/2}2(Nau_l)(I_{N1}+I_{N2}) \ , \tag{23b}$$

where

$$I_{N1}=\int_0^{N\pi/2}\frac{(\sinh x)e^{-x}}{(Nau_{S+})^2+x^2}\left[\frac{\cosh(xz/2d)}{\cosh(x/2)}\right]^2$$
$$\times\frac{1}{[(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}]^2}$$
$$\times\left[\frac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-x}}\right]^{1/2}dx \ , \tag{23c}$$

$$I_{N2}=\int_0^{N\pi/2}\frac{(\sinh x)e^{-x}}{(Nau_{S-})^2+x^2}\left[\frac{\sinh(xz/2d)}{\sinh(x/2)}\right]^2$$
$$\times\frac{1}{[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^2}$$
$$\times\left[\frac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-x}}\right]^{1/2}dx \ . \tag{23d}$$

IV. THE EFFECTIVE MASS AND ENERGIES

In light of the expression of H_{eff} (23), we have set

$$(M^*)^{-1}(z)=(m^*)^{-1}\left[1-\frac{\alpha C_1(z)}{[1+\alpha C_1(z)]^2}\right.$$
$$-\frac{\alpha C_2(z)}{[1+\alpha C_2(z)]^2}$$
$$+\left[\frac{\alpha C_1(z)}{1+\alpha C_1(z)}\right]^2$$
$$\left.+\left[\frac{\alpha C_2(z)}{1+\alpha C_2(z)}\right]^2\right] . \tag{24}$$

Because $\alpha C_1(z)\ll 1$ and $\alpha C_2(z)\ll 1$ as shown in our calculations, the bound polaron's effective mass M^* can be approximately evaluated by

$$M^*(z)=m^*[1+\alpha C_1(z)+\alpha C_2(z)] \ , \tag{25}$$

where $C_1(z)$ and $C_2(z)$ are given by (19a) and (20a), respectively.

Since it is exceedingly complicated to get the exact solution of the eigenfunction of H_{eff} (23), an approximate wave function should be found. To solve the eigenenergy in the state without any real phonon present, first, H_{eff} is rewritten and separated into three parts:

$$H_{\text{eff}}=H_z+H_{2\text{D}}+H_1$$
$$=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+\left[\frac{\hbar^2K_\rho^2}{2M^*}-\frac{e^2\lambda}{\epsilon_\infty\rho}\right]+V_I^{(B)}(z)$$
$$+V_I^{(S)}(Z)+\frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{r'}\right], \tag{26}$$

where

$$H_z=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+V_I^{(B)}(z)+V_I^{(S)}(z) \ , \tag{26a}$$

$$H_{2\text{D}}=\frac{\hbar^2K_\rho^2}{2M^*}-\frac{e^2\lambda}{\epsilon_\infty\rho} \ , \tag{26b}$$

$$H_1=\frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{r'}\right] . \tag{26c}$$

As illustrated in Ref. 13, for a thin slab, the difference between λ/ρ and $1/r'$ ($r'=[\rho^2+(z-z_i)^2]^{1/2}$) can be made very small by choosing an applicable value of λ.

Therefore we treat H_1 (26c) as a perturbation and take

$$H_0 = H_z + H_{2D}$$

as the unperturbed Hamiltonian.

The variation of the effective mass M^* with coordinate z is so small that it can be approximately taken as a constant independent of z. Hence, according to Eqs. (26a) and (26b), the motion parallel to the xy plane can be separated from the motion along the z direction. Consequently, the wave function of the electron motion referring to the unperturbed H_0 can be written as

$$|\Phi_{l,n,t}(z,\rho)\rangle = |\phi_l(z)\rangle\,|\phi_{n,t}(\rho)\rangle\ , \tag{27}$$

where l and n,t are respectively the quantum number in the z direction and in the xy plane.

Compared with the kinetic energy of the electron motion along z direction, even for the intermediate coupling bound polaron, the effective potentials $V_I^{(B)}$ and $V_I^{(S)}$ can all be neglected due to their very small value. Then we will regard the electron as a particle moving in an infinite square-well potential along the z direction. The solutions are well known and given by

$$H_z\phi_l(z) = E_l\phi_l(z)\ , \tag{28a}$$

$$\phi_l(z) = \begin{cases} \dfrac{1}{\sqrt{d}}\sin\left[\dfrac{l\pi}{2d}(z+d)\right], & |z| \le d \\ 0, & |z| > d \end{cases} \tag{28b}$$

$$E_l = \frac{\pi^2\hbar^2 l^2}{8m^* d^2}\ , \tag{28c}$$

where the quantum number l is a positive integer and, for the conduction electron, is limited by the bandwidth, i.e., $E_l \le (\pi^2\hbar^2)/(2m^*a^2)$. Thus we have $l \le 2d/a = N$.

H_{2D}, (26b), is just the Hamiltonian of a two-dimensional hydrogenlike atom and then the solutions of the electron motion parallel to the xy plane are expressed as[14]

$$H_{2D}\phi_{n,t}(\rho) = E_{n,t}\phi_{n,t}(\rho)\ , \tag{29a}$$

$$\phi_{n,t}(\rho) = \frac{1}{\sqrt{2\pi}}e^{it\phi}\left[\frac{(n-|t|)!}{[(n+|t|)!]^3(2n+1)}\left[\frac{2\lambda}{(n+\frac{1}{2})a_0}\right]^2\right]^{1/2} \times\left[\frac{2\rho\lambda}{(n+\frac{1}{2})a_0}\right]^{|t|}\exp\left[-\frac{\rho\lambda}{(n+\frac{1}{2})a_0}\right]L_{n+|t|}^{2|t|}\left[\frac{2\rho\lambda}{(n+\frac{1}{2})a_0}\right], \tag{29b}$$

$$E_{n,t} = -\frac{\lambda^2 M^* e^4}{2\epsilon_\infty^2\hbar^2(n+\frac{1}{2})^2}\ , \tag{29c}$$

where the quantum number $n = 0,1,2,\ldots$, $t = 0, \pm1, \pm2, \ldots$ and $|t| \le n$; the parameter $a_0 = (\epsilon_\infty\hbar^2)/(M^*e^2)$; $L_{n+|t|}^{2|t|}$ Is the Laguerre polynomial. Since $\alpha C_1, \alpha C_2 \ll 1$, we take $M^*(z)$ as its expected value referring to $\phi_l(z)$ to simplify our calculation.

According to the perturbation method,[13] the expected value of the perturbation term H_1 referring to $\Phi_{l,n,t}$ should be set zero in a thin slab, i.e.,

$$\bar{H}_1(\lambda) = \langle\Phi_{l,n,t}|H_1|\Phi_{l,n,t}\rangle = 0\ .$$

So, the parameter λ can be determined by

$$\lambda(l,n,t) = \frac{\frac{1}{d}\int_{-d}^{d}\sin^2\left[\frac{l\pi}{2d}(z+d)\right]dz\int_0^\infty \frac{\rho}{[\rho^2+(z-z_i)^2]^{1/2}}|\phi_{n,t}(\rho)|^2 d\rho}{\int_0^\infty |\phi_{n,t}(\rho)|^2 d\rho} \tag{30}$$

By solving the eigenequation of the unperturbed term H_0

$$H_0|\Phi_{l,n,t}(z,\rho)\rangle = E_0|\Phi_{l,n,t}(z,\rho)\rangle\ , \tag{31}$$

the total energy of the bound polaron in the zero-phonon state is obtained

$$E_0 = E_l + E_{n,t} + E_s^B + E_s^S\ , \tag{32}$$

where E_s^B and E_s^S are the self-energies and come respectively from the expected values of $V_I^{(B)}$ and $V_I^{(S)}$. They are given by

$$E_s^B=\langle\phi_l(z)\,|\,V_l^{(B)}(z)\,|\,\phi_l(z)\rangle$$
$$=-\frac{2\alpha\hbar\omega_{\mathrm{LO}}u_l}{Na}\left[\sum_{m=1}^{N/2}\frac{1}{\left[\left(\frac{m\pi}{Na}\right)^2-u_l^2\right]}\ln\left(\frac{m\pi}{Nau_l}\right)+\frac{1}{2}\frac{1}{\left[\left(\frac{l\pi}{Na}\right)^2-u_l^2\right]}\ln\left(\frac{l\pi}{Nau_l}\right)\right], \tag{33a}$$

$$E_s^S=\langle\phi_l(z)\,|\,V_l^{(S)}(z)\,|\,\phi_l(z)\rangle$$
$$=-\alpha\hbar\omega_{\mathrm{LO}}\epsilon_0^{1/2}\epsilon_\infty^{3/2}Nau_l(I_{P1}+I_{P2}), \tag{33b}$$

where

$$I_{P1}=\int_0^{N\pi/2}\frac{(\sinh x)e^{-x}}{[(Nau_{S+})^2+x^2]}\frac{1}{\cosh^2(x/2)}\times\left[\frac{l^2\pi^2\sinh x}{x(x^2+l^2\pi^2)}+1\right]\times\frac{1}{[(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}]^2}\times\left[\frac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-x}}\right]^{1/2}dx, \tag{34a}$$

$$I_{P2}=\int_0^{N\pi/2}\frac{(\sinh x)e^{-x}}{[(Nau_{S-})^2+x^2]}\frac{1}{\sinh^2(x/2)}\times\left[\frac{l^2\pi^2\sinh x}{x(x^2+l^2\pi^2)}-1\right]\times\frac{1}{[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^2}\times\left[\frac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-x}}\right]^{1/2}dx. \tag{34b}$$

In these equations, α, u_l, and u_{Sp} are defined by Eqs. (21) and (22), and the variable $x=2qd$.

To investigate the absorption and emission of energy, we also give the calculations of the transition energies between different impurity states such as

$$\Delta E_{100}^{110}=E_{110}-E_{100},\quad \Delta E_{200}^{210}=E_{210}-E_{200}, \tag{35}$$

where $E_{lnt}=E_l+E(l,n,t)$ in which $E(l,n,t)$ represents $E_{n,t}$ with well quantum number l.

V. RESULTS AND DISCUSSION

According to the formulas obtained in Sec. IV and taking GaAs as an example, we have computed the energies and the effective mass of the bound polaron in a polar crystal slab. In our calculations, we assume that the shallow doped impurity is located at the positions of $z_i=0$, $d/4$, and $d/2$. Because experimental observations are always made on slow electrons, we also set $\mathbf{K}_\rho\approx 0$. The characteristic parameters of crystal GaAs are listed in Table I.

In the low-temperature limit, for a thin slab, the energy of the bound polaron in the state without any real phonon present can be expressed as

$$E=E_l+E_{n,t}+E_s^B+E_s^S.$$

E_l is the energy of the polaron within an approximately infinite square-well potential along the z direction. Since it is well known to all, we are not going into its details here.

The electron self-energy contains two parts, E_s^B and E_s^S, which are brought out, respectively, by LO- and SO-phonon contributions. The total self-energy is plotted in Fig. 2 as the function of the slab thickness N. For a very thin slab the self-energy is mainly attributed to the SO-phonon contribution, and due to the attractive action of SO modes its absolute value is larger than other theoretical results excluding the electron–SO-phonon interaction. When the slab thickness approaches zero, the self-energy tends to the surface limit of E_s^S. By the increasing of N, the SO-phonon contribution rapidly decreases and the LO-phonon contribution becomes the dominant one. In the limit of infinite thickness, the self energy slowly approaches the bulk limit value E_s^B. Figure 2 also shows that there is no obvious difference of the self-energy between the ground state ($l=1$) and the first excited state ($l=2$). In this paper, the self-energy is derived as the unperturbed terms and its second-order perturbation correction is proportional to the square of the coupling constant α. So, the formalism of our paper would also be suitable for the intermediate coupling polaron besides the weak one.

From Eq. (30), we can see that different positions of the donor will exert influence only on the determination of λ. As the only term relating to the value of λ, $E_{n,t}$, the energy of the bound polaron associated with motion parallel to the xy plane, will certainly depend on the donor position z_i besides the quantum numbers l, n, and t. For z_i being taken as 0, $d/4$, and $d/2$, respectively, Figs. 3(a)–3(b) give the description of the variation of λ with the slab thickness N and Figs. 4(a)–4(b) give that of $E_{n,t}$. In these figures, we choose $l=1,2$, $n=0,1$ and $t=0$.

TABLE I. Characteristic parameters of crystal GaAs. All the parameters are taken from Refs. 16 and 17. Energy is measured in meV, length in Å, and m^* in units of the free-electron rest mass.

ϵ_0	ϵ_∞	$\hbar\omega_{\mathrm{LO}}$ (meV)	$\hbar\omega_{\mathrm{TO}}$ (meV)	m^*	a (Å)	α
12.83	10.90	36.70	33.83	0.0657	5.654	0.0681

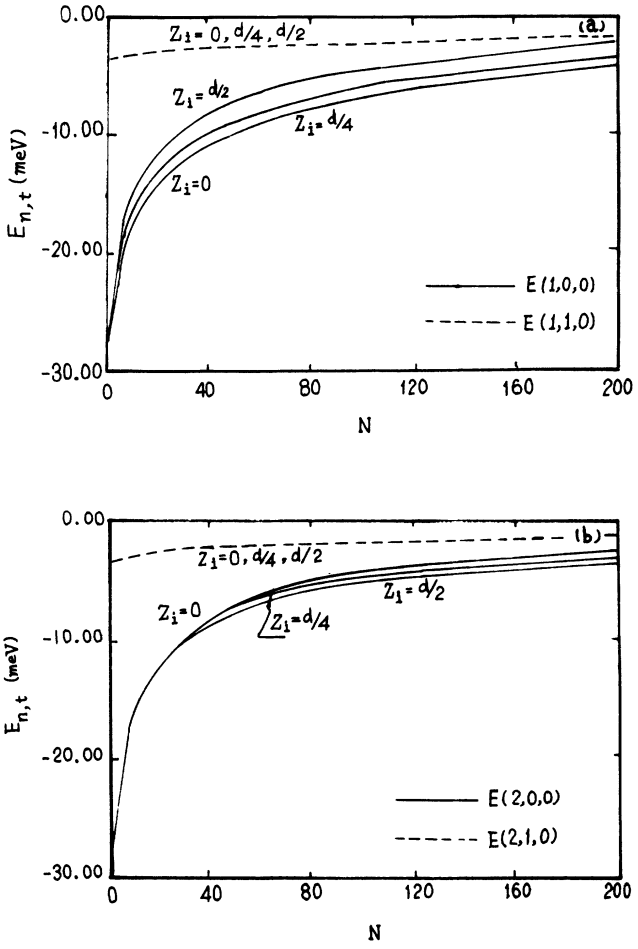

FIG. 4. (a) Energy in the xy plane ($E_{n,t}$) vs slab thickness N (for $l=1$). (b) Energy in the xy plane ($E_{n,t}$) vs slab thickness N (for $l=2$).

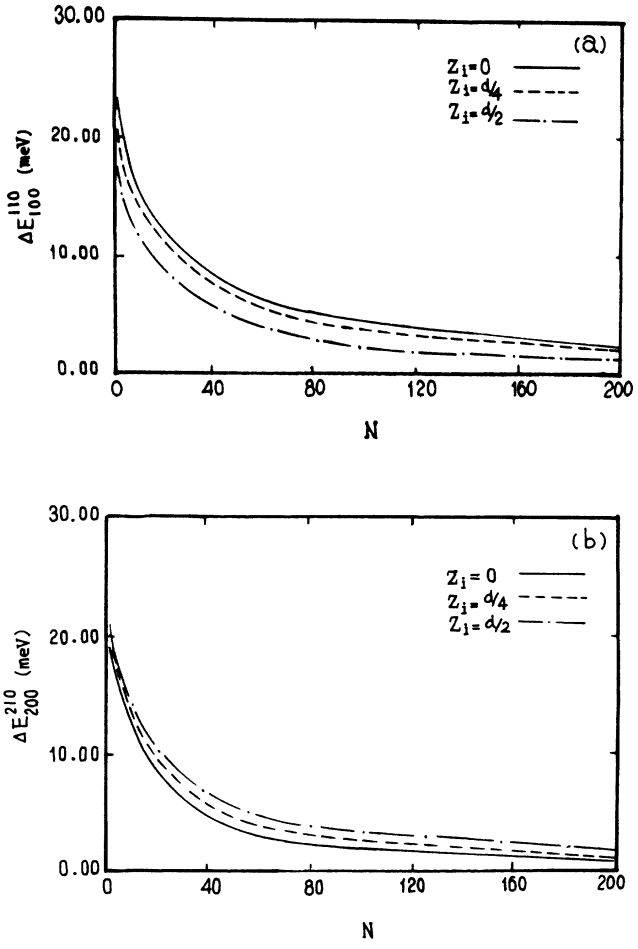

FIG. 5. (a) The transition energy ΔE^{110}_{100} vs slab thickness N. (b) The transition energy ΔE^{210}_{200} vs slab thickness N.

In Figs. 4(a)–4(b), we notice first that according to the varying features of λ, for a fixed value of z_i, $E_{n,t}$ increases monotonically at a reduced rate as the slab gets thicker. Secondly, the great difference among the curves is mainly owing to the different quantum number n. The absolute values of $E_{n,t}$ for $n=1$ are much smaller than that for $n=0$ in a very thin slab. With the thickness N increasing, such a difference will become smaller and disappear in the limit of infinite thickness.

Comparing the curves of $E_{n,t}$ with different z_i, we find that the various z_i brings obvious difference among the curves for $n=0$, while for $n=1$ the influence of z_i will not exist. Whether n is small or big, for the very thin slab, the donor position z_i will not produce impact on the value of $E_{n,t}$.

Figures 5(a)–5(b) depict a situation in which the transition energies (ΔE^{110}_{100} and ΔE^{210}_{200}) change with the slab thickness N. It is obvious that for various values of z_i the transition energies decrease monotonically with the increase of N, namely, the thinner the slab is, the larger the transition energy will be. Corresponding to the varying features of $E_{n,t}$, only when N is relatively bigger does the difference among the transition energies brought out by different z_i become obvious. And as N tends to zero, such a difference will disappear. By comparing Fig. 5(a) with Fig. 5(b), it should merit attention that with the located donor being closer to the center of the slab the transition energy for $l=1$ (ΔE^{110}_{100}) will be getting larger,

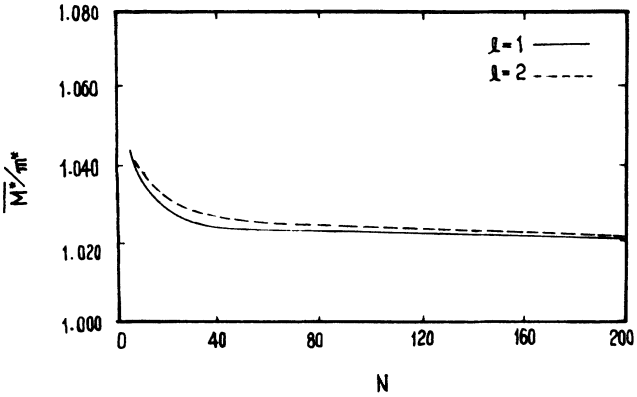

FIG. 6. The effective mass of the bound polaron vs slab thickness N.

while for that for $l=2$ (ΔE_{200}^{210}) will be getting smaller.

With consideration of $\alpha C_1(z) \ll 1$ and $\alpha C_2(z) \ll 1$, the effective mass of the bound polaron as the function of z is approximately given by (25). For a slab with thickness N, we calculate the expected value of $M^*(z)$ referring to the wave function in z direction. That is

$$\overline{M^*} = \langle \phi_l(z) \mid M^*(z) \mid \phi_l(z) \rangle \ .$$

Figure 6 shows us the variation of $\overline{M^*}/m^*$ with the slab thickness N, where m^* is the band mass of the electron. If the slab is thinner the effective mass will be bigger, and as thickness N increases, it will decrease monotonically. Comparing the theoretical results without SO modes included[15] with ours, we find that the electron–SO-phonon interaction increases the effective mass. In the two-dimensional limit, SO phonons will produce a bigger correction to the effective mass than in the bulk limit.

In addition, from Fig. 6, it is also noted that only at the middle range of N is there a little difference between the two curves with quantum number $l=1$ and $l=2$. This implies that the influence of various states on the effective mass can be neglected.

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