Polaronic states in a slab of a polar crystal

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The ground state and the first excited state of the polaron confined in a slab of a polar crystal are investigated. Both the bulk longitudinal-optical and the surface optical (SO) modes are included in our consideration of the electron-phonon interaction. The polaron self-energy due to either mode of phonon is calculated as a function of the thickness of the slab. It is found that the SO-phonon contribution changes the behavior of the polaron self-energy qualitatively. Instead of monotonically increasing with the slab thickness it increases to a maximum at the beginning and then decreases to the bulk value as its limit when the thickness increases indefinitely. A number of other interesting features are also discussed.

I. INTRODUCTION

There has been great interest in recent years in the electronic properties in heterostructures and superlattices of insulators and semiconductors. The electron states in such structures are well described by means of a square-well potential.[1] The square-well model works not only for the conduction electron but also for the exciton[2] and impurity[3] states in a thin film of semiconductor crystal.

The phonon-electron interaction in a dielectric film was first considered in the context of electron energy gain and loss spectra.[4] Since the electronic polarizability was not properly included in this early work, a more careful treatment of the interactions between electron and optical-phonon modes in a slab of crystal had been given.[5] Only the Hamiltonian operators for electron interactions with the bulk longitudinal-optical (LO) phonon and with the surface optical (SO) phonon were derived because it had been established experimentally that the bulk transverse optical (TO) phonon would not participate in the energy exchange between the electron and the slab.[6] It is further shown in Ref. 5 that the electron—LO-phonon interaction is equivalent to Fröhlich operator in the limit of thick slab, and the electron—SO-phonon interaction operator leads to the classical result of image charge method for an external electron interacting with the polarization eigenmodes in the semi-infinite crystal.

The ground-state energy of the polaron has been calculated as a function of the slab thickness.[7] With only the LO-phonon—electron interaction included, it is found that the polaron energy increases monotonically with increasing thickness and slowly approaches the bulk value as its limit. A completely different approach,[8] however, yields qualitatively different results. The variation of the polaron energy is not a monotonic function of the slab thickness. The most obvious cause for this discrepancy may be attributed to the surface phonon, although it has already been suggested (in Ref. 7) to be responsible for the slow rise of the polaron energy to its limiting bulk value.

In this paper, we calculate the energy levels of the ground and the first excited states of a polaron confined in a slab of arbitrary thickness. Interactions of the electron with both the LO and SO modes are included. It is found that the total electron self-energy increases rapidly with the thickness to a maximum and then decreases slowly to the limit of bulk value as the thickness approaches infinity. After the total Hamiltonian is written down, the energy levels are calculated for several III-V and II-VI compounds. The electron self-trapping energy is calculated by second-order perturbation as a function of the slab thickness. Our results are finally discussed with conclusions.

II. THE HAMILTONIAN

Consider a slab of polar crystal with thickness $2d$. As shown in Fig. 1, the slab occupies the space for $|z| \leq d$ and when $|z| > d$, the space is a vacuum. For simplicity, we assume that the effective-mass approximation is valid.

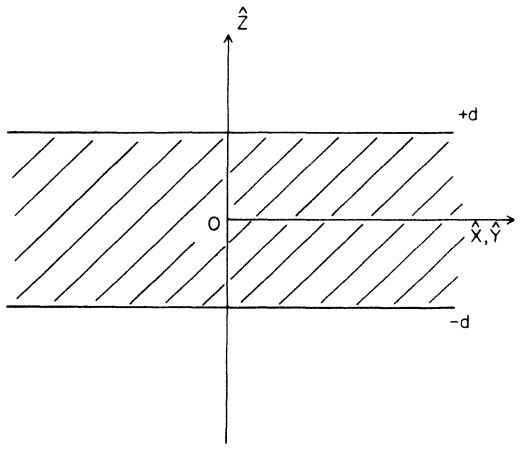

FIG. 1. Geometry of the polar crystal slab.

Then the problem is approximately the motion of a particle of mass m^* in a square well of width $2d$. Therefore, we have the total Hamiltonian

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

The first term is the Hamiltonian of the electron in the rigid lattice of the slab and is given by

$$H_e=\begin{cases} -\dfrac{\hbar^2}{2m^*}\nabla^2, & |z|\le d \\ -\dfrac{\hbar^2}{2m_e}\nabla^2+V_0, & |z|>d , \end{cases} \tag{2}$$

where m^* is the effective mass of the electron and m_e is the free-electron rest mass, V_0 is a parameter related to the work function or the height of the potential barrier at the surface. The second term in (1) represents the free-polarization Hamiltonian. We note that the phonons in this geometry are traveling waves in the xy plane and standing waves in the z direction. Thus,

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

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

$$H_{\rm SO}=\sum_{\mathbf{q},p}\hbar\omega_{{\rm S}p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q}) , \tag{3b}$$

where $a^{\dagger}_{m,p}$ ($a_{m,p}$) is the creation (annihilation) operator for the LO phonon of frequency $\omega_{\rm LO}$ and wave vector $\mathbf{k}$, and $b^{\dagger}_{p}$ (b_p) creates (annihilates) a SO phonon of frequency $\omega_{{\rm S}p}$ and wave vector $\mathbf{q}$. The phonon modes are specified by the subscripts, namely, the parity p referring to the mirror symmetry, with respect to the plane $z=0$, and the z component m of the wave vector $\mathbf{k}$ measured in the unit of $\pi/2a$. For even parity, p is positive and m is odd; while for odd parity, p is negative and m is even. It should be noted that the wave vector $\mathbf{k}$ of the LO phonon is limited by Brillouin-zone boundary, namely, $m\pi/2d\le\pi/2a$ or $m\le d/a$. Hence m can be any integer within the range $1\le m\le D/2$. The phonon frequencies are expressed in terms of the TO-phonon frequency by

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

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

where ϵ_0 is the static dielectric constant and ϵ_∞ is the optical dielectric constant.

The last two terms in (1) are the electron-phonon interaction Hamiltonian operators and are directly taken from Ref. 5. Thus,

$$H_{e\text{-LO}}=\begin{cases} \displaystyle\sum_{\mathbf{k}}\left[B^*e^{i\mathbf{k}\cdot\rho}\left[\sum_{m=1,3,\ldots}\frac{\cos[(m\pi/2d)z]}{[k^2+(m\pi/2d)^2]^{1/2}}a^{\dagger}_{m,+}(\mathbf{k})+\sum_{m=2,4,\ldots}\frac{\sin[(m\pi/2d)z]}{[k^2+(m\pi/2d)]^{1/2}}a^{\dagger}_{m,-}(k)\right]+\text{h.c.}\right], & |z|\le d , \\ 0, & |z|>d , \end{cases} \tag{5}$$

$$H_{e\text{-SO}}=\sum_{q}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C^*e^{-i\mathbf{q}\cdot\rho}[G_+(q,z)b^{\dagger}_{+}(\mathbf{q})+G_-(q,z)b^{\dagger}_{-}(\mathbf{q})]+\text{H.c.}\} . \tag{6}$$

where ρ and $\mathbf{k}$ are two-dimensional vectors in the xy plane, and

$$B^*=i\left[\frac{4\pi e^2}{V}\hbar\omega_{\rm LO}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2} , \tag{7}$$

$$C^*=i\left[\frac{2\pi e^2}{A}\hbar\omega_{\rm TO}(\epsilon_0-\epsilon_\infty)\right]^{1/2} , \tag{8}$$

with A and V the surface area and volume of the crystal slab. The functions G are defined by

$$G_+(q,z)=\begin{cases} \dfrac{\cosh(qz)/\cosh(qd)}{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|\le d \\ \dfrac{e^{-q|z|}/e^{-qd}}{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|>d \end{cases} \tag{9a}$$

$$G_-(q,z)=\begin{cases} \dfrac{\sinh(qz)/\sinh(qd)}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|\le d \\ \dfrac{e^{-q|z|}/e^{-qd}}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|>d \end{cases} \tag{9b}$$

This Hamiltonian appears to be exceedingly complicated and approximations must be sought. It has been shown in Ref. 1 that the energy levels obtained for a finite square well are not very different from those for an infinite square well. Therefore, we shall set the wave functions to be identically zero for $z \geq d$. Next, we note that a unitary transformation U has been constructed[9] to eliminate the electron coordinate ρ in the xy plane, that is

$$U=\exp\left[i\rho\cdot\left[\mathbf{K}_{||}-\sum_{\mathbf{k},m,p}\mathbf{k}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})-\sum_{\mathbf{q},p}\mathbf{q}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})\right]\right], \tag{10}$$

where $\mathbf{K}_{||}$ is the projection of the total momentum of the polaron in xy plane.

After some algebra, we find the transformed Hamiltonian

$$H^{*}=U^{-1}HU=H_0+H_1\ , \tag{11}$$

where we have purposely written the new Hamiltonian into two parts so that perturbation method can be applied. The "unperturbed" Hamiltonian is

$$H_0=\frac{\hbar^2}{2m^{*}}K_{||}^2+\frac{\hbar^2}{2m^{*}}\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})(k^2+\kappa_{\mathrm{L}}^2)+\frac{\hbar^2}{2m^{*}}\sum_{\mathbf{q},p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})(q^2+\kappa_{Sp}^2)-\frac{\hbar^2}{2m^{*}}\frac{d^2}{dz^2}\ , \tag{12}$$

where κ_{L} and κ_{Sp} are the polaron wave vectors defined by

$$\hbar^2\kappa_{\mathrm{L}}^2/2m^{*}=\hbar\omega_{\mathrm{LO}}\ , \tag{13a}$$

$$\hbar^2\kappa_{Sp}^2/2m^{*}=\hbar\omega_{Sp}\ . \tag{13b}$$

The "perturbation" Hamiltonian is

$$H_1=\frac{\hbar^2}{2m^{*}}\left[\left[\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\right]^2-\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})k^2\right]+\frac{\hbar^2}{2m^{*}}\left[\left[\sum_{\mathbf{q},p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})\mathbf{q}\right]^2-\sum_{\mathbf{q},p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})q^2\right]$$
$$-\frac{\hbar^2}{m^{*}}\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\cdot\mathbf{K}_{||}-\frac{\hbar^2}{m^{*}}\sum_{\mathbf{q},p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})\mathbf{q}\cdot\mathbf{K}_{||}$$
$$-\frac{\hbar^2}{m^{*}}\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\,b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})\mathbf{k}\cdot\mathbf{q}+H^{*}_{e\text{-LO}}+H^{*}_{e\text{-SO}}\ . \tag{14}$$

The first two terms in (14) represent the interactions between virtual phonons emitted and reabsorbed by the recoiled electron and are generally small quantities.[10] The third and fourth terms are also small quantities as long as $\mathbf{K}_{||}$ is small, which is generally the case in practice. The next two terms stand for the interactions between the LO and SO phonons and are, of course, small. The last two terms are the electron-phonon interaction Hamiltonians after the transformation, and are small in case of weak coupling. They differ from the original expression only by the oscillation factors involving ρ and are given by

$$H^{*}_{e\text{-LO}}=\sum_{\mathbf{k}}\left[B^{*}\left[\sum_{m=1,3,\ldots}\frac{\cos[(m\pi/2d)z]}{[k^2+(m\pi/2d)^2]^{1/2}}a^{\dagger}_{m,+}(\mathbf{k})+\sum_{m=2,4,\ldots}\frac{\sin[(m\pi/2d)z]}{[k^2+(m\pi/2d)^2]^{1/2}}a^{\dagger}_{m,-}(\mathbf{k})\right]+\mathrm{H.c.}\right], \tag{15}$$

$$H^{*}_{e\text{-SO}}=\sum_{\mathbf{q}}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C^{*}[G_{+}(\mathbf{q},z)b^{\dagger}_{+}(\mathbf{q})+G_{-}(\mathbf{q},z)b^{\dagger}_{-}(\mathbf{q})]+\mathrm{H.c.}\}\ . \tag{16}$$

From what we have discussed above, H_1 is generally small for the case of weak coupling. Therefore, we shall treat it as a small perturbation in the present work.

III. PERTURBATION METHOD

The unperturbed equation

$$H_0\psi=E_0\psi \tag{17}$$

can be solved by splitting the Hamiltonian H_0 into two parts:

$$H_0=H_z+H_{||}\ , \tag{18}$$

$$H_z=-\frac{\hbar^2}{2m^{*}}\frac{d^2}{dz^2},\quad |z|\leq d\ , \tag{18a}$$

$$H_{||}=\frac{\hbar^2K_{||}^2}{2m^{*}}+\frac{\hbar^2}{2m^{*}}\left[\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})(k^2+\kappa_{\mathrm{L}}^2)+\sum_{\mathbf{q},p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})(q^2+\kappa_{Sp}^2)\right]. \tag{18b}$$

The motion along z direction is just the infinite square-well problem with the well-known solutions. That is,

$$H_z\phi_n(z)=E_n\phi_n(z)\ , \tag{19}$$

$$E_n=\frac{\pi^2\hbar^2n^2}{8m^*d^2},\quad n \text{ a positive integer} \tag{19a}$$

$$\phi_n(z)=\begin{cases}\dfrac{1}{\sqrt{d}}\sin\left[\dfrac{n\pi}{2d}(z+d)\right], & |z|\le d\\ 0, & |z|>d\ .\end{cases} \tag{19b}$$

We note, however, that we are considering the conduction electron. Even in the nearly-free-electron model, the quantum number n in (19a) is limited by the band width, namely, $E_0\le(\hbar^2/2m^*)(\pi/a)^2$, where a is the lattice spacing constant. Thus we have

$$n\le\frac{2d}{a}=D\ , \tag{20}$$

where D is the slab thickness in the unit of a, or the number of molecular layers in the slab. The motion parallel to the xy plane can be solved most easily in the phonon number representation. We have

$$H_{\|}\,|\,N_{m,p}(\mathbf{k}),N_{Sp}(\mathbf{q})\rangle=E_{\|}\,|\,N_{m,p}(\mathbf{k}),N_{Sp}(\mathbf{q})\rangle \tag{21}$$

$$E_{\|}=\frac{\hbar^2}{2m^*}\left[K_{\|}^2+\sum_{\mathbf{k},m,p}(k^2+\kappa_L^2)N_{m,p}(\mathbf{k})+\sum_{\mathbf{q},p}(q^2+\kappa_{Sp}^2)N_{Sp}(\mathbf{q})\right], \tag{21a}$$

where $N_{m,p}(\mathbf{k})$ and $N_{Sp}(\mathbf{q})$ are the number of LO and SO phonons, respectively. Putting together all these results, we have the unperturbed polaron energies and wave functions

$$E_0=E_z+E_{\|}\ , \tag{22a}$$

$$\psi_{n,m,p}(z,\mathbf{k},\mathbf{q})=\phi_n(z)\,|\,N_{m,p}(\mathbf{k}),N_{Sp}(\mathbf{q})\rangle\ . \tag{22b}$$

To calculate the perturbation energy, we assume, for simplicity, that there is no real phonon present in the polaron states. This is valid in the low-temperature limit. It is obvious that in the zero-phonon state, the expectation value of H_1 vanishes. Since only the last two terms of H_1 are nondiagonal, they are the only terms we have to include in our second-order perturbation calculation. In the following, we give all the nonvanishing matrix elements between n, zero-phonon state and n', one-phonon state. The calculation is tedious but straightforward, and will not be reproduced here. We have

$$\langle n,0\,|\,H_1\,|\,n',\mathbf{k}+\rangle=\frac{B}{d}\int_{-d}^{d}\sin\left[\frac{n\pi(z+d)}{2d}\right]\sin\left[\frac{n'\pi(z+d)}{2d}\right]\frac{\cos[(m\pi/2d)z]}{[k^2+(m\pi/2d)^2]^{1/2}}dz$$
$$=\pm\frac{2nB}{\pi[k^2(m\pi/2d)^2]^{1/2}}\left[\frac{1}{(n'+m)^2-n^2}-\frac{1}{(n'-m)^2-n^2}\right], \tag{23a}$$

where $m=1,3,5,\ldots$, $n'-n=0,\pm2,\pm4,\ldots$, and $+$ $(-)$ sign applies when $(m+1)/2$ is odd (even). We have

$$\langle n,0\,|\,H_1\,|\,n',\mathbf{k}-\rangle=\frac{B}{d}\int_{-d}^{d}\sin\left[\frac{n\pi(z+d)}{2d}\right]\sin\left[\frac{n'\pi(z+d)}{2d}\right]\frac{\sin[(m\pi/2d)z]}{[k^2+(m\pi/2d)^2]^{1/2}}dz$$
$$=\pm\frac{2nB}{\pi[k^2(m\pi/2d)^2]^{1/2}}\left[\frac{1}{(n'+m)^2-n^2}-\frac{1}{(n'-m)^2-n^2}\right], \tag{23b}$$

where $+$ $(-)$ sign applies when $m/2$ is even (odd), $m=2,4,6,\ldots$, $n'-n=\pm1,\pm3,\pm5,\ldots$,

$$\langle n,0\,|\,H_1\,|\,n',\mathbf{q}+\rangle=\frac{C}{d}\int_{-d}^{d}\sin\left[\frac{n\pi(z+d)}{2d}\right]\sin\left[\frac{n'\pi(z+d)}{2d}\right]\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}G_+(q,z)dz$$
$$=\frac{Ce^{-qd}}{d}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}\frac{\sinh(qd)}{\cosh(qd)}\left[\frac{q}{q^2+[(n'-n)\pi/2d]^2}-\frac{q}{q^2+[(n'+n)\pi/2d]^2}\right]$$
$$\times\frac{1}{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}\left[\frac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, \tag{23c}$$

where $n'-n=0,\pm2,\pm4,\ldots$,

$$\langle n,0\,|\,H_1\,|\,n',\mathbf{q}-\rangle=\frac{C}{d}\int_{-d}^{d}\sin\left[\frac{n\pi(z+d)}{2d}\right]\sin\left[\frac{n'\pi(z+d)}{2d}\right]\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}G_-(q,z)dz$$
$$=-\frac{Ce^{-qd}}{d}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}\frac{\cosh(qd)}{\sinh(qd)}\left[\frac{q}{q^2+[(n'-n)\pi/2d]^2}-\frac{q}{q^2+[(n'+n)\pi/2d]^2}\right]$$
$$\times\frac{1}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}\left[\frac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, \tag{23d}$$

TABLE I. Characteristic parameters used in the numerical calculation. All the parameters are taken from Ref. 11 except for the lattice constant a, which is taken from Ref. 12. Energy is measured in meV, length in Å, and m^* in the free-electron rest mass.

	ϵ_0	ϵ_∞	$\hbar\omega_{LO}$ (meV)	$\hbar\omega_{TO}$ (meV)	m^*	a (Å)	α
InAs	14.61	11.80	30.20	27.14	0.023	6.058	0.0525
InP	12.29	9.56	43.27	38.18	0.076	5.869	0.1136
GaAs	12.83	10.90	36.70	33.83	0.0657	5.654	0.0681
InSb	17.88	15.68	24.50	22.94	0.0138	6.479	0.0217
GaSb	15.69	14.44	29.80	28.59	0.0470	6.095	0.0256
ZnSe	8.33	5.90	30.50	25.67	0.1710	5.669	0.4317
ZnTe	9.86	7.28	15.50	21.91	0.1600	6.103	0.3320
CdTe	10.23	7.21	20.80	17.46	0.0910	6.478	0.3158

where $n'-n=\pm1,\pm3,\pm5,\ldots$.

From Eqs. (21a) and (23), we can write down directly the second-order correction to the polaron energy. The calculation is again straightforward, and we give the results:

$$\Delta E=\Delta E_{k+}+\Delta E_{k-}+\Delta E_{q+}+\Delta E_{q-}\ , \tag{24}$$

where

$$\Delta E_{k+}=-\sum_{n',\mathbf{k},m}\frac{|\langle n,0|H_1|n',\mathbf{k}+\rangle|^2}{E_{n'_{\mathbf{k}}}-E_{n0}}$$

$$=-\alpha\hbar\omega_{LO}\frac{8D\kappa_L a}{\pi^4}\sum_{n',m}\frac{n^2\{1/[(n'+m)^2-n^2]-1/[(n'-m)^2-n^2]\}^2}{m^2+n^2-(n')^2+(D\kappa_L a/\pi)^2}\ln\left|\frac{m^2}{(n')^2-n^2+(D\kappa_L a/\pi)^2}\right|\ , \tag{24a}$$

where $n'-n=0,\pm2,\pm4,\ldots$ and $m=1,3,5,\ldots$. We have

$$\Delta E_{k-}=-\sum_{n',\mathbf{k},m}\frac{|\langle n,0|H_1|n'\mathbf{k}-\rangle|^2}{E_{n'\mathbf{k}}-E_{n0}}$$

$$=-\alpha\hbar\omega_{LO}\frac{8D\kappa_L a}{\pi^4}\sum_{n',m}\frac{n^2\{1/[(n'+m)^2-n^2]-1/[(n'-m)^2-n^2]\}^2}{m^2+n^2-(n')^2-(D\kappa_L a/\pi)^2}\ln\left|\frac{m^2}{(n')^2-n^2+(D\kappa_L a/\pi)^2}\right|\ , \tag{24b}$$

with $n'-n=\pm1,\pm3,\pm5,\ldots$ and $m=2,4,6,\ldots$,

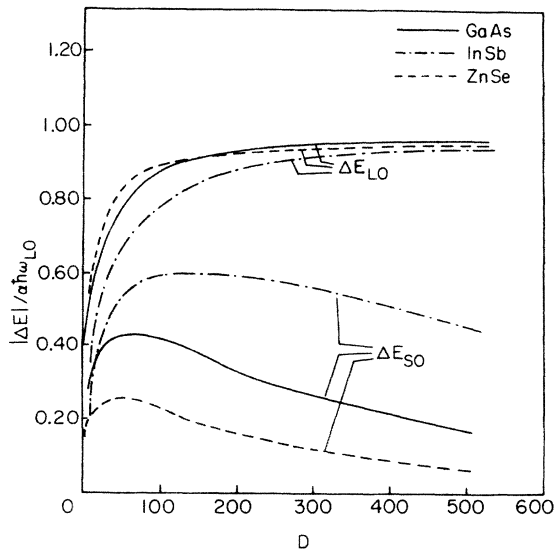

FIG. 2. LO and SO self-energy vs slab thickness D.

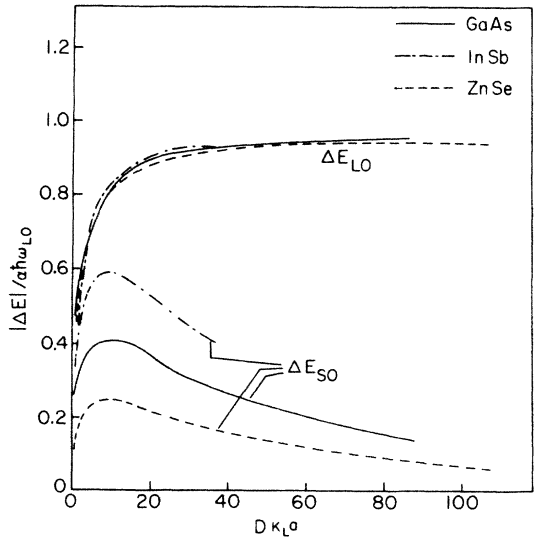

FIG. 3. LO and SO self-energy vs slab thickness $D\kappa_L a$.

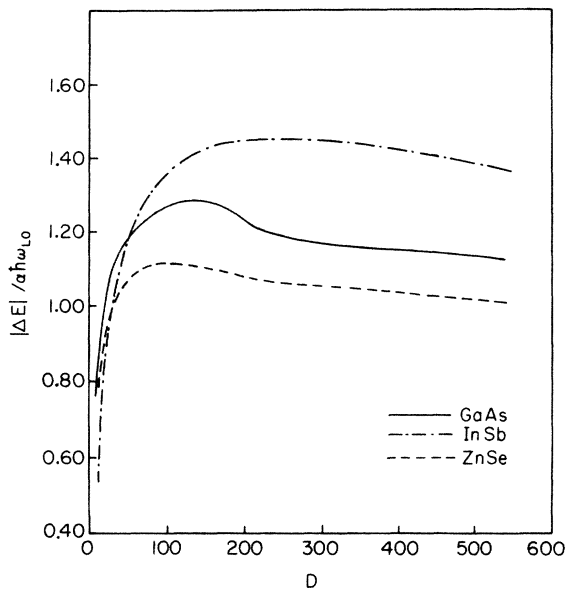

FIG. 4. Total self-energy as a function of the thickness D.

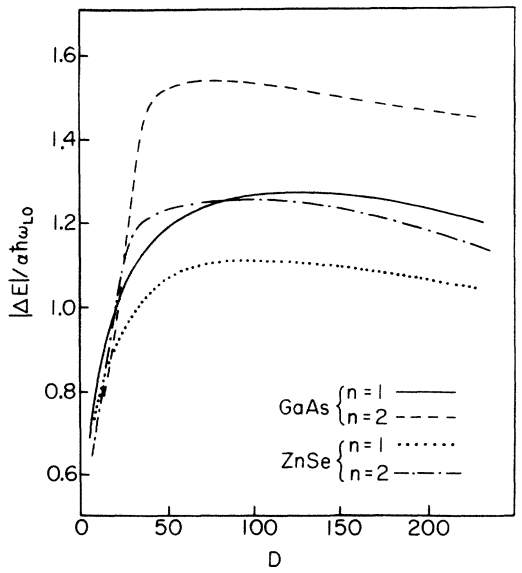

FIG. 5. Comparison of self-energy correction to different polaron energy levels in a slab.

$$\Delta E_{q+}=-\sum_{n',\mathbf{q}}\frac{|\langle n,0|H_1|n,\mathbf{q}+\rangle|^2}{E_{n'\mathbf{q}}-E_{n0}}$$

$$=-\alpha\hbar\omega_{\mathrm{LO}}\frac{8D\kappa_{\mathrm{L}}a}{\pi^4}\epsilon_0^{1/2}\epsilon_\infty^{3/2}$$

$$\times\sum_{n'}\int_0^{D\pi/2}\left[e^{-x}\sinh(x)\tanh^2(x/2)\left[\frac{x}{x^2+(n'-n)^2\pi^2}-\frac{x}{x^2+(n'+n)^2\pi^2}\right]^2 dx\right]$$

$$\times(\{x^2+(D\kappa_{\mathrm{S}+}a)^2+[(n')^2-n^2]\pi^2\}[(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}]^{3/2}$$

$$\times[(\epsilon_0+1)-(\epsilon_0-1)e^{-x}]^{1/2})^{-1}\,, \tag{24c}$$

TABLE II. Polaron energies in a slab of thickness $D=20$ for several compounds. Energies are in the unit of $\alpha\hbar\omega_{\mathrm{LO}}$ unless otherwise specified.

	n	$\lvert\Delta E_{\mathrm{LO}}\rvert/\alpha\hbar\omega_{\mathrm{LO}}$	$\lvert\Delta E_{\mathrm{SO}}\rvert/\alpha\hbar\omega_{\mathrm{LO}}$	$\lvert\Delta E\rvert/\alpha\hbar\omega_{\mathrm{LO}}$	$\lvert\Delta E\rvert$ (meV)	E_n (meV)	$\lvert\Delta E\rvert/(E_2-E_1)$ (%)
InAs	1	0.53	0.34	0.87	1.37	111.47	0.41
	2	0.38	0.44	0.82	1.30	445.89	0.39
InP	1	0.65	0.35	1.00	4.92	35.94	4.56
	2	0.51	0.49	1.01	4.94	143.77	4.58
GaAa	1	0.62	0.35	0.98	2.44	44.80	1.87
	2	0.47	0.49	0.96	2.40	179.20	1.78
InSb	1	0.47	0.37	0.85	0.45	162.43	0.092
	2	0.34	0.47	0.81	0.43	649.71	0.088
GaSb	1	0.59	0.42	1.01	0.77	53.89	0.48
	2	0.44	0.57	1.00	0.76	215.56	0.47
ZnSe	1	0.68	0.23	0.91	11.95	17.12	23.26
	2	0.58	0.33	0.91	12.03	68.49	23.42
ZnTe	1	0.67	0.28	0.95	8.04	15.79	16.97
	2	0.56	0.40	0.96	8.13	63.16	17.16
CdTe	1	0.63	0.27	0.89	5.87	24.64	7.94
	2	0.47	0.37	0.84	5.54	98.56	7.49

with $n'-n=0,\pm2,\pm4,\ldots$,

$$\Delta E_{q-}=-\sum_{n',\mathbf{q}}\frac{|\langle n,0|H_1|n,\mathbf{q}-\rangle|^2}{E_{n'\mathbf{q}}-E_{n0}}$$

$$=-\alpha\hbar\omega_{\mathrm{LO}}\frac{8Da\kappa_{\mathrm{L}}}{\pi^4}\epsilon_0^{1/2}\epsilon_\infty^{3/2}$$

$$\times\sum_{n'}\int_0^{D\pi/2}\left[e^{-x}\sinh(x)\coth^2(x/2)\left[\frac{x}{x^2+(n'-n)^2\pi^2}-\frac{x}{x^2+(n'+n)^2\pi^2}\right]^2 dx\right]$$

$$\times(\{x^2+(D\kappa_{\mathrm{S}-}a)^2+[(n')^2-n^2]\pi^2\}[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^{3/2}[(\epsilon_0+1)+(\epsilon_0-1)e^{-x}]^{1/2})^{-1}\,, \tag{24d}$$

with $n'-n=\pm1,\pm3,\pm5,\ldots$.

In these equations, we have defined the variable $x=2qd$ and the dimensionless coupling constant for the electron—LO-phonon interaction

$$\alpha=\frac{m^*e^2}{\hbar^2\kappa_{\mathrm{L}}}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]. \tag{25}$$

$\kappa_{\mathrm{S}+}$ ($\kappa_{\mathrm{S}-}$) is the wave number of even- (odd-) parity SO phonon and has been defined by (14b). All the summation and integrals can only be evaluated numerically.

IV. RESULTS AND DISCUSSIONS

Using the formulas (24), we have computed the ground-state and the first-excited-state energies of the polaron for several III-V and II-VI compounds. As the experimental observations are made on slow polarons, we have set $K_{\|}=0$. The characteristic parameters employed in our numerical computation are listed in Table I. The electron self-energy, as given by (24), contains two parts, the LO and SO contributions defined by

$$\Delta E_{\mathrm{LO}}=\Delta E_{k+}+\Delta E_{k-}\,, \tag{26a}$$

$$\Delta E_{\mathrm{SO}}=\Delta E_{q+}+\Delta E_{q-}\,. \tag{26b}$$

They are plotted in Fig. 2 as functions of the thickness D. It is observed that they both increase quickly with D at the beginning. As D increases further, we find that ΔE_{LO} increases monotonically at reduced rate and approaches the bulk limit slowly as is found in Ref. 7. On the other hand, ΔE_{SO} rises to a maximum value and then decreases to zero in the limit of infinite thickness. What is more interesting is that when the unit of length is changed from the lattice constant a to the polaron size κ_{L}^{-1}, the variation of ΔE_{LO} with D becomes almost independent of the material while the maximum self-energy ΔE_{SO} occurs at around 10 for different compounds we have calculated. Figure 3 depicts this situation.

To see how the electron self-energy changes with the thickness of the slab, both the LO and SO contributions are combined and plotted in Fig. 4. It is seen that for all the three compounds, the self-energy increases rapidly to the maximum and then decreases slowly to the limit of the bulk value. This unexpected behavior is, of course, due entirely to the SO-phonon interaction, and is therefore qualitatively different from the previous results.[7,8]

In Fig. 5, we show the electron self-energy in the excited states for GaAs and ZnSe. The ground-state self-energy is also plotted for comparison purposes. Only when $D<20$ does the polaron in the ground state have bigger self-energy correction than it does in the excited state. When the slab is thicker than 20 layers or so, however, the polaron in the excited state has bigger self-energy correction than in the ground state. This is again caused by the SO phonon as can be seen from our numerical work which reveals a number of interesting features. Absolute values of the various energies of polaron in different states are tabulated for several compounds in Table II. We take the thickness $D=20$, for which the self-energy corrections to the ground state and excited state are comparable.

We notice first that the LO self-energy correction to the ground state is larger than that to the excited state for all the compounds, while the opposite is true in case of the SO self-energy. Secondly, we see that while the size of the dimensionless self-energy is roughly the same for all the compounds, the absolute size is much larger for II-VI compounds than for III-V compounds. The reason is simply that the electron-phonon coupling constant α for the II-VI compounds is about an order of magnitude larger than that for the III-V compounds as shown in Table I. Finally, we also notice that in II-VI compounds, the polaron energy levels are generally lower and more dense than those in III-V compounds. Therefore the self-energy contribution can be rather significant in case of II-VI compounds and must be taken into account in the analysis of polaron energy levels for these compounds.

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