PHYSICAL REVIEW B VOLUME 35, NUMBER 18 15 JUNE 1987-II

Exciton in a slab of polar crystal

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(Received 24 September 1986)

In this paper, a weak-coupling exciton-phonon system in a polar-crystal slab is studied. A unitary transformation to the Hamiltonian is carried out, the effective Hamiltonian of the exciton-phonon system is obtained by variational technique. The variation of the self-energy and the induced potential with the thickness of the slab is calculated. Eventually, the ground-state and the first-excited-state energy of the exciton in the slab for different thicknesses of the slab are calculated by the variational method.

I. INTRODUCTION

Because of the practical interest in the technological development of heterostructures and superlattices, there has been great interest in recent years in the electronic properties in a slab.[1–9] Many properties of a crystal slab relate to the behavior of the exciton in the slab; so it is very important and very interesting to study the behavior of the exciton in a polar-crystal slab. The exciton in a polar-crystal slab is different from that in a three-dimensional polar crystal, and their behavior is very different. That is because, on the one hand, the homogeneity along the direction normal to the slab plane is destroyed, and on the other hand, in the polar slab the interaction of the electron (hole) with the surface-optical phonons must be considered. In their study of the exciton in a slab, Lee and Lin[2] restricted the crystal to nonpolar crystal, and did not consider the interaction of the exciton with phonons. In fact, in the polar-crystal slab, this part of the interaction has a great influence on the behavior of the exciton. In this paper we investigate, for the first time, the exciton-phonon system in the polar-crystal slab, taking account of the interaction of the electron (hole) with the phonons which include the bulk longitudinal-optical phonons and the surface-optical phonons.[3]

Licari and Evrard[3] have developed the Frölich Hamiltonian for the interaction of the electron with phonons in a polar-crystal slab. The Hamiltonian includes the interaction of the electron with the bulk longitudinal-optical (LO) phonons and the interaction of the electron with the surface-optical (SO) phonons. However, in his study of the polaron in a polar slab, Licari[4] only took account of the interaction of the electron with the bulk LO phonons. Taking account of both the interaction of the electron with the bulk LO phonons and the interaction of the electron with the SO phonons, Liang and Gu *et al.*[5] have further studied the polaron in the polar slab. In this paper, both the interaction of the electron with the bulk LO phonons and the interaction of the electron with the SO phonons are being considered, the behavior of the exciton-phonon system in the polar-crystal slab is investigated. In Sec. II, after the Hamiltonian of the polaron in the polar slab has been extended, the Hamiltonian of the exciton-phonon system in the polar slab is obtained. In Sec. III, after a unitary transformation is carried out, the Hamiltonian is divided into an unperturbed part and perturbing part, and the unperturbed part of the Hamiltonian is solved. In Sec. IV, extending the perturbative method which was used by Liang *et al.*,[5] and using the perturbative-variational method,[10] we obtain the effective Hamiltonian of the exciton in the slab. The effective Hamiltonian includes the self-energy and the induced potential, which are produced by the interaction of the electron (hole) with the phonons. In Sec. V, using as an example the II-VI compound GaAs, in which the coupling of the electron with the phonons is weak, we perform the numerical evaluation. Furthermore, with the variational method, the ground-state and the first-excited-state energies of the exciton in the slab for different thicknesses of the polar-crystal slab are obtained. In the last section, the results are analyzed and discussed.

II. THE HAMILTONIAN

Consider a slab of polar crystal with thickness $2d$. As shown in Fig. 1, the slab occupies the space for $|z| \le d$, and when $|z| > d$, the space is a vacuum.

Now we will give the Hamiltonian of the Wannier exciton-phonon system in the polar-crystal slab. For simplicity, suppose the electron in the Wannier exciton is in the parabolic monoconduction band, and the hole is in the parabolic monovalence band. In the effective-mass ap-

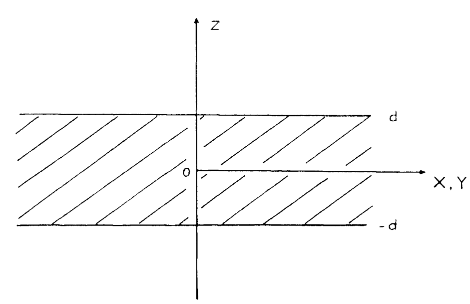

FIG. 1. Geometry of the polar-crystal slab.

proximation, the electron (hole) can be considered as a free particle moving in a square potential well. A zero point of energy being chosen properly, the Hamiltonian of the moving electron and hole in the polar-crystal slab can be written as[1]

$$H_e=\begin{cases}\dfrac{P_{ez}^2}{2m_e}+\dfrac{P_e^2}{2m_e}, & |z_e|\le d\\ \dfrac{P_{ez}^2}{2m_0}+\dfrac{P_e^2}{2m_0}+V_0, & |z_e|>d\end{cases} \tag{1}$$

$$H_h=\begin{cases}\dfrac{P_{hz}^2}{2m_h}+\dfrac{P_h^2}{2m_h}, & |z_h|\le d\\ \dfrac{P_{hz}^2}{2m_0}+\dfrac{P_h^2}{2m_0}+V_0', & |z_h|>d\end{cases} \tag{2}$$

where m_e and m_h are the band mass of the electron and the hole, respectively; m_0 the mass of the electron in the vacuum; V_0 and V_0' the depth of the potential well; P_{ez}, P_e, P_{hz}, and P_h the momentum of the electron and the hole in the z direction and the x-y plane, respectively.

The interaction between the electron and the hole is[11]

$$H_{e\text{-}h}=-\frac{e^2}{\epsilon_\infty|r_e\text{-}r_h|}, \tag{3}$$

where ϵ_∞ is the optical dielectric constant of the polar crystal.

With the interaction of the exciton with the phonons not being considered, the Hamiltonian of the exciton in the slab can be written as

$$H_{ex}=H_e+H_h+H_{e\text{-}h}. \tag{4}$$

In the polar-crystal slab, we only consider the coupling of the electron (hole) with the bulk longitudinal-optical (LO) phonons and the coupling of the electron (hole) with the surface-optical (SO) phonons, but we need not consider the coupling of the electron (hole) with the bulk transverse-optical (TO) phonons.[12] For the exciton being studied, the Hamiltonian of the phonon field can be written as[3]

$$H_{\text{ph}}=H_{\text{LO}}+H_{\text{SO}}, \tag{5a}$$

$$H_{\text{LO}}=\sum_{\mathbf{k},m,p}a^\dagger_{\mathbf{k},m,p}a_{\mathbf{k},m,p}\hbar\omega_{\text{LO}}, \tag{5b}$$

$$H_{\text{SO}}=\sum_{\mathbf{q},p}b^\dagger_{\mathbf{q},p}b_{\mathbf{q},p}\hbar\omega_{\text{SO}}, \tag{5c}$$

where $\mathbf{k}$ and $\mathbf{q}$ are the two-dimensional wave vectors of LO and SO phonons, respectively, m is the quantum number of the z component of the wave vector of the bulk LO mode, $m=1,2,3,\ldots,N/2$. $p=\pm$ is the parity (+ is even or − is odd). m is an even number when $p=-$, and m is an odd number when $p=+$. $a^\dagger_{\mathbf{k},m,p}$ ($a_{\mathbf{k},m,p}$) and $b^\dagger_{\mathbf{q},b}$ ($b_{\mathbf{q},p}$) are creation (annihilation) operators for the LO and SO phonons, respectively. ω_{LO} is the frequency of the LO phonons, ω_{SO} the frequency of the SO phonons, ω_{SO} is determined by the equation[3]

$$\omega_{S\pm}^2=\omega_{\text{TO}}^2\frac{(\epsilon_0+1)\mp(\epsilon_0-1)e^{-2qd}}{(\epsilon_\infty+1)\mp(\epsilon_\infty-1)e^{-2qd}}, \tag{6a}$$

$$\omega_{\text{LO}}^2=\omega_{\text{TO}}^2(\epsilon_0/\epsilon_\infty). \tag{6b}$$

ω_{TO} is the frequency of the bulk transverse-optical phonons, ϵ_0 the static dielectric constant.

The Hamiltonian $H_{e\text{-LO}}$ of the electron—LO-phonon interaction and Hamiltonian $H_{e\text{-SO}}$ of the electron-SO-phonon interaction developed by Licari and Evrard[3] can be written as

$$H_{e\text{-LO}}=\sum_{k}\left[B^*e^{-i\mathbf{k}\cdot\rho_e}\left[\sum_{m=1,3,\ldots}\frac{\cos\left[\dfrac{m\pi z_e}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}a^\dagger_{\mathbf{k},m,p}+\sum_{m=2,4,\ldots}\frac{\sin\left[\dfrac{m\pi z_e}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}a^\dagger_{\mathbf{k},m,p}\right]+\text{H.c.}\right], \tag{7}$$

$$H_{e\text{-SO}}=\sum_{\mathbf{q}}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C^*e^{-i\mathbf{q}\cdot\rho_e}[G_+(q,z_e)b^\dagger_{\mathbf{q},+}+G_-(q,z_e)b^\dagger_{\mathbf{q},-}]+\text{H.c.}\}. \tag{8}$$

We can extend (7) and (8) easily,[11] and can get the hole-phonon interaction Hamiltonians $H_{h\text{-LO}}$ and $H_{h\text{-SO}}$

$$H_{h\text{-LO}}=-\sum_{\mathbf{k}}\left[B^*e^{-i\mathbf{k}\cdot\rho_h}\left[\sum_{m=1,3,\ldots}\frac{\cos\left[\dfrac{m\pi z_h}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}a^\dagger_{\mathbf{k},m,p}+\sum_{m=2,4,\ldots}\frac{\sin\left[\dfrac{m\pi z_e}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi z_h}{2d}\right]^2\right]^{1/2}}a^\dagger_{k,m,p}\right]+\text{H.c.}\right], \tag{9}$$

$$H_{h\text{-SO}}=-\sum_{\mathbf{q}}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C^*e^{-i\mathbf{q}\cdot\rho_h}[G_+(q,z_h)b^\dagger_{\mathbf{q},+}+G_-(q,z_h)b^\dagger_{\mathbf{q},-}]+\text{H.c.}\}, \tag{10}$$

where

$$B^*=i\left[\frac{4e^2}{V}\hbar\omega_{\rm LO}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2}, \tag{11}$$

$$C^*=i\left[\frac{2e^2}{A}\hbar\omega_{\rm TO}(\epsilon_0-\epsilon_\infty)\right]^{1/2}, \tag{12}$$

$$G_+(z,q)=\begin{cases}\dfrac{\cosh(qz)/\cosh(qd)}{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|\le d\\[2ex] \dfrac{e^{-q|z|}/e^{-qd}}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)-(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|>d\end{cases} \tag{13}$$

$$G_-(q,z)=\begin{cases}\dfrac{\sinh(qz)/\cosh(qd)}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|\le d\\[2ex] \dfrac{e^{-q|z|}/e^{-qd}}{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}\left[\dfrac{(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-2qd}}{(\epsilon_0+1)+(\epsilon_0-1)e^{-2qd}}\right]^{1/4}, & |z|>d\,.\end{cases} \tag{14}$$

$\boldsymbol{\rho}_e$ ($\boldsymbol{\rho}_h$) is the projection of the electron (hole) position vector onto the x-y plane. A is the surface area of the slab and V the volume of the slab.

Summarizing the above, we can obtain the Hamiltonian H of the exciton-phonon system very naturally,

$$H=H_e+H_h+H_{e\text{-}h}+H_{\rm ph}+H_{e\text{-LO}}+H_{e\text{-SO}}+H_{\rm h\text{-}LO}+H_{h\text{-SO}}\,. \tag{15}$$

In the x-y plane, we introduce the center-of-mass coordinate:

$$\mathbf{R}=s_1\boldsymbol{\rho}_e+s_2\boldsymbol{\rho}_h,\quad \boldsymbol{\rho}=\boldsymbol{\rho}_e-\boldsymbol{\rho}_h,\quad s_1=m_e/M,\quad s_2=m_h/M,\quad M=m_e+m_h,\quad \mu=m_em_h/M\,.$$

Hence (15) can be rewritten as

$$\begin{aligned}H={}&\frac{P_{ez}^2}{2m_e}+\frac{P_{hz}^2}{2m_h}+\frac{P^2}{2M}+\frac{p^2}{2\mu}-\frac{e^2}{\epsilon_\infty[\rho^2+(z_e-z_h)^2]^{1/2}}+\sum_{\mathbf{k},m,p}a^\dagger_{\mathbf{k},m,p}a_{\mathbf{k},m,p}\hbar\omega_{\rm LO}+\sum_{\mathbf{q},p}b^\dagger_{\mathbf{q},p}b_{\mathbf{q},p}\hbar\omega_{\rm SO}\\&+\sum_{\mathbf{k},m}\{B^*[W_{k,m,+}(z_e,z_h;\rho)a^\dagger_{\mathbf{k},m,+}+W_{k,m,-}(z_e,z_h;\rho)a^\dagger_{\mathbf{k},m,-}]e^{-i\mathbf{k}\cdot\mathbf{R}}+\text{H.c.}\}\\&+\sum_{\mathbf{q}}\left[\frac{\sinh(2ad)}{q}\right]^{1/2}e^{-qd}\{C^*[V_{q,+}(z_e,z_h;\rho)b^\dagger_{\mathbf{q},+}+V_{q,-}(z_e,z_h;\rho)b^\dagger_{\mathbf{q},-}]e^{-i\mathbf{q}\cdot\mathbf{R}}+\text{H.c.}\}\,,\end{aligned} \tag{16}$$

where

$$W_{k,m,+}(z_e,z_h;\rho)=\frac{\cos\left[\dfrac{m\pi z_e}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}e^{-is_2\mathbf{k}\cdot\boldsymbol{\rho}}-\frac{\cos\left[\dfrac{m\pi z_h}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}e^{is_1\mathbf{k}\cdot\boldsymbol{\rho}},\quad m=1,3,\ldots \tag{17}$$

$$W_{k,m,-}(z_e,z_h;\rho)=\frac{\sin\left[\dfrac{m\pi z_e}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}e^{-is_2\mathbf{k}\cdot\boldsymbol{\rho}}-\frac{\sin\left[\dfrac{m\pi z_h}{2d}\right]}{\left[k^2+\left[\dfrac{m\pi}{2d}\right]^2\right]^{1/2}}e^{is_1\mathbf{k}\cdot\boldsymbol{\rho}},\quad m=2,4,\ldots \tag{18}$$

and

$$V_{q,\pm}(z_e,z_h;\rho)=G_\pm(q,z_e)e^{-is_2\mathbf{q}\cdot\boldsymbol{\rho}}-G_\pm(q,z_h)e^{is_1\mathbf{q}\cdot\boldsymbol{\rho}}\,. \tag{19}$$

III. UNITARY TRANSFORMATION

It is easy to prove that the projection of the total momentum of the exciton-phonon system onto the x-y plane, $\hbar\mathbf{K}_{\parallel}$,

$$\hbar\mathbf{K}_{\parallel}=\mathbf{P}_{\parallel}+\sum_{\mathbf{k},m,p}a^\dagger_{\mathbf{k},m,p}a_{\mathbf{k},m,p}\hbar\mathbf{K}+\sum_{\mathbf{q},p}b^\dagger_{\mathbf{q},p}b_{\mathbf{q},p}\hbar\mathbf{q}\,, \tag{20}$$

commutes with the Hamiltonian H, hence $\hbar\mathbf{K}_{\parallel}$ is a constant of the motion. Therefore we can introduce the following unitary transformation in order to eliminate $\mathbf{R}$, the coordinate of the exciton center of mass in the x-y plane:[13]

$$U=\exp\left[i\mathbf{K}_{\parallel}\cdot\mathbf{R}-i\sum_{\mathbf{k},m,p}a^{\dagger}_{\mathbf{k},m,p}a_{\mathbf{k},m,p}\mathbf{k}\cdot\mathbf{R}-i\sum_{\mathbf{q},p}b^{\dagger}_{\mathbf{q},p}b_{\mathbf{q},p}\mathbf{q}\cdot\mathbf{R}\right]. \tag{21}$$

After some algebraic manipulations, we find the transformed Hamiltonian

$$\mathcal{H}=U^{-1}HU=\mathcal{H}_0+\mathcal{H}_1 . \tag{22a}$$

$$\mathcal{H}_0=\frac{\hbar^2K_{\parallel}^2}{2M}+H_{2D}+\frac{P_{ez}^2}{2m_e}+\frac{P_{hz}^2}{2m_h}+\frac{\hbar^2}{2M}\sum_{\mathbf{k},m,p}a^{\dagger}_{\mathbf{k},m,p}a_{\mathbf{k},m,p}(k^2+u_l^2)+\frac{\hbar^2}{2M}\sum_{\mathbf{q},p}b^{\dagger}_{\mathbf{q},p}b_{\mathbf{q},p}(q^2+u_{\mathrm{SO}}^2), \tag{22b}$$

$$\begin{aligned}\mathcal{H}_1=&\frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{[\rho^2+(z_e-z_h)^2]^{1/2}}\right]+\frac{\hbar^2}{2M}\left[\sum_{\mathbf{k},m,p}a^{\dagger}_{\mathbf{k},m,p}a_{\mathbf{k},m,p}\mathbf{k}\right]^2-\sum_{\mathbf{k},m,p}a^{\dagger}_{\mathbf{k},m,p}a_{\mathbf{k},m,p}k^2\\&+\frac{\hbar^2}{2M}\left[\sum_{\mathbf{q},p}b^{\dagger}_{\mathbf{q},p}b_{\mathbf{q},p}\mathbf{q}\right]^2-\sum_{\mathbf{q},p}b^{\dagger}_{\mathbf{q},p}b_{\mathbf{q},p}q^2-\frac{\hbar^2}{M}\sum_{\mathbf{k},m,p}a^{\dagger}_{\mathbf{k},m,p}a_{\mathbf{k},m,p}\mathbf{k}\cdot\mathbf{K}_{\parallel}-\frac{\hbar^2}{M}\sum_{\mathbf{q},p}b^{\dagger}_{\mathbf{q},p}b_{\mathbf{q},p}\mathbf{q}\cdot\mathbf{K}_{\parallel}\\&+\frac{\hbar^2}{M}\sum_{\mathbf{k},\mathbf{q},m,p}a^{\dagger}_{\mathbf{k},m,p,}a_{\mathbf{k},m,p}b^{\dagger}_{\mathbf{q},p}b^{\dagger}_{\mathbf{q},p}b_{\mathbf{q},p}\mathbf{k}\cdot\mathbf{q}+\mathcal{H}_{e,h\text{-LO}}+\mathcal{H}_{e,h\text{-SO}} .\end{aligned} \tag{22c}$$

where

$$H_{2D}=\frac{p^2}{2\mu}-\frac{\lambda e^2}{\epsilon_\infty\rho}, \tag{22d}$$

$$\mathcal{H}_{e,h\text{-LO}}=\sum_{\mathbf{k},m}\{B^*[W_{k,m,+}(z_e,z_h;\rho)a^{\dagger}_{\mathbf{k},m,+}+W_{k,m,-}(z_e,z_h;\rho)a^{\dagger}_{\mathbf{k},m,-}]+\mathrm{H.c.}\}, \tag{22e}$$

$$\mathcal{H}_{e,h\text{-SO}}=\sum_{\mathbf{q}}\left[\frac{\sinh(2qd)}{q}\right]^{1/2}e^{-qd}\{C^*[V_{q,+}(z_e,z_h;\rho)b^{\dagger}_{\mathbf{q},+}+V_{q,-}(z_e,z_h;\rho)b^{\dagger}_{\mathbf{q},-}]+\mathrm{H.c.}\}, \tag{22f}$$

and

$$\frac{\hbar^2u_l^2}{2M}=\hbar\omega_{\mathrm{LO}},\quad\frac{\hbar^2u_{\mathrm{SO}}^2}{2M}=\hbar\omega_{\mathrm{SO}} . \tag{22g}$$

Equation (22d) is the Hamiltonian of a two-dimensional hydrogenlike atom system, where λ is a variational parameter which can be determined with the perturbative-variational method.[10]

Under conditions of the weak electron- (hole-) phonon coupling in the thin slab, we can consider $\mathcal{H}_0$ as the unperturbed Hamiltonian, and $\mathcal{H}_1$ as the perturbing Hamiltonian.[14]

For simplicity, and without losing generality, we discuss the slow exciton. For a slow exciton, the first term in $\mathcal{H}_0$, the translational energy of the exciton in the x-y plane, can be neglected. Then, the unperturbed Hamiltonian $\mathcal{H}_0$ (22b) can be divided into three parts,

$$\mathcal{H}_0=H_{2D}+H_{\perp}+H_{\parallel} , \tag{23}$$

where the first term is the internal motion energy of the exciton on the x-y plane. It has the form of the two-dimensional hydrogenlike atom system. The second term is the Hamiltonian of the electron (hole) moving along the z direction. The third term is the Hamiltonian of the phonon field. We will give their eigenfunctions and eigenenergies separately.

We first give the solution of the two-dimensional hydrogen atom system; the eigenenergy and eigenfunction are[15]

$$E(n)=-e^2\lambda^2/\epsilon_\infty 2a_0(n+\tfrac{1}{2})^2 , \tag{24}$$

$$\begin{aligned}\phi_{n,l}(\rho,\lambda)&=\frac{1}{\sqrt{2\pi}}e^{il\varphi}R_{n,l}(2\rho/(n+\tfrac{1}{2})a_0')\\&=\frac{1}{\sqrt{2\pi}}e^{il\varphi}\left[\frac{(n+|l|)!^3(2n+1)}{(n-|l|)!}\left[\frac{(n+\frac{1}{2})a_0'}{2}\right]\right]^{-1/2}\left[\frac{2\rho}{(n+\frac{1}{2})a_0'}\right]^{|l|}e^{-\rho/(n+\frac{1}{2})a_0'}L^{2|l|}_{n+|l|}\left[\frac{2\rho}{(n+\frac{1}{2})a_0'}\right],\end{aligned} \tag{25}$$

where $L_p^q(\rho)$ is the Laguerre polynomial; $\lambda a_0'=a_0=\epsilon_\infty\hbar^2/\mu e^2$; the principal quantum number $n=0,1,2,\ldots$; for a given n, the angular momentum quantum number $1=0,\pm1,\pm2,\ldots,\pm n$.

Now consider the eigenfunctions and eigenenergies of the exciton moving in the z direction:

$$H_\perp = \begin{cases} \frac{P_{ez}^2}{2m_e} + \frac{P_{hz}^2}{2m_h}, & |z_e|,|z_h| \le d \\ \frac{P_{ez}^2}{2m_0} + \frac{P_{hz}^2}{2m_0} + V_0 + V_0', & |z_e|,|z_h| > d . \end{cases} \tag{26}$$

For simplicity, in (26) suppose V_0 and $V_0' \to \infty$, i.e., suppose the electron (hole) are moving in a one-dimensional infinite-depth square potential well. The eigenfunctions and eigenenergies[16] are

$$|\phi_{l_1}(z_e)\phi_{l_2}(z_h)\rangle = \begin{cases} \frac{1}{d}\sin\left[\frac{l_1\pi}{2d}(z_e+d)\right]\sin\left[\frac{l_2\pi}{2d}(z_h+d)\right], & |z_e|,|z_h| \le d \\ 0, \quad |z_e|,|z_h| > d , \end{cases} \tag{27}$$

$$E_{l_1 l_2} = \frac{\pi^2\hbar^2 l_1^2}{8m_e d^2} + \frac{\pi^2\hbar^2 l_2^2}{8m_h d^2} \quad (l_1,l_2 = 1,2,3,\ldots,N) . \tag{28}$$

In the following, we give the eigenfunctions and eigenenergies of the phonon field,

$$H_\parallel = \frac{\hbar^2}{2M}\sum_{\mathbf{k},m,p} a_{\mathbf{k},m,p}^\dagger a_{\mathbf{k},m,p}(k^2+u_l^2) + \frac{\hbar^2}{2M}\sum_{\mathbf{q},p} b_{\mathbf{q},p}^\dagger b_{\mathbf{q},p}(q^2+u_{\mathrm{SO}}^2) . \tag{29}$$

If the zero energy is neglected, the eigenenergy of the phonon field can be written as[17]

$$E_\parallel = \frac{\hbar^2}{2M}\sum_{\mathbf{k},m,p}(k^2+u_l^2)n_{\mathbf{k},m,p} + \frac{\hbar^2}{2M}\sum_{\mathbf{q},p}(q^2+u_{\mathrm{SO}}^2)n_{\mathbf{q},p} , \tag{30}$$

and its relevant eigenfunction is[17]

$$|\Psi_\parallel\rangle = |\{n_{\mathbf{k},m,p}\},\{n_{\mathbf{q},p}\}\rangle , \tag{31}$$

where $n_{\mathbf{k},m,p}$ and $n_{\mathbf{q},p}$ are the LO phonon number and SO phonon number, respectively, $n_{\mathbf{k},m,p}=0,1,2,\ldots$, $n_{\mathbf{q},p}=0,1,2,\ldots$; $\{n_{\mathbf{k},m,p}\}$ and $\{n_{\mathbf{q},p}\}$ are the abbreviations of $\{\ldots,n_{\mathbf{k},m,p},n_{\mathbf{k}',m',p'},\ldots\}$ and $\{\ldots,n_{\mathbf{q},p},n_{\mathbf{q}',p'},\ldots\}$, respectively.

Summarizing the above, we can write the eigenfunctions and eigenenergies of $\mathscr{H}_0$ as

$$|\Psi\rangle = |\phi_{n,l}(\rho,\lambda)\rangle\,|\phi_{l_1}(z_e)\phi_{l_2}(z_h)\rangle\,|\{n_{k,m,p}\},\{n_{q,p}\}\rangle , \tag{32}$$

$$\begin{aligned} E &= E(n)+E_{l_1 l_2}+E_\parallel \\ &= -e^2\lambda^2/2\epsilon_\infty a_0(n+\tfrac{1}{2})^2 + \frac{\pi^2\hbar^2 l_1^2}{8m_e d^2} + \frac{\pi^2\hbar^2 l_2^2}{8m_h d^2} \\ &\quad + \frac{\hbar^2}{2M}\sum_{\mathbf{k},m,p}(k^2+u_l^2)n_{\mathbf{k},m,p} + \frac{\hbar^2}{2M}\sum_{\mathbf{q},p}(q^2+u_{\mathrm{SO}}^2)n_{\mathbf{q},p} , \end{aligned} \tag{33}$$

where the range of the values for l_1, l_2, and m is

$$1 \le l_1,\ l_2 \le N ,$$

$$1 \le m \le N/2 ,$$

and

$$N = 2d/a ,$$

a is the lattice constant. This is because of the limits of the one-dimensional Brillouin zone.

IV. THE EFFECTIVE HAMILTONIAN

In this paper, we only study the behavior of the exciton at a low-temperature limit (at zero temperature). From the discussion in the last section, when no phonons are excited, the wave function of the $\mathscr{H}_0$ system can be written as

$$|\Psi_0\rangle = |\phi(\rho,\lambda)\rangle\,|\phi_{l_1}(z_e)\phi_{l_2}(z_h)\rangle\,|0,0\rangle , \tag{34}$$

where $|\phi(\rho,\lambda)\rangle$ is the normalized quasi-two-dimensional exciton internal wave function, and $|\phi_{l_1}(z_e)\phi_{l_2}(z_h)\rangle$ is the eigenfunction of the electron and the hole moving in the z direction. $|0,0\rangle$ expresses the unperturbed vacuum phonon state. Now the energy of the unperturbed exciton-phonon system can be written as

$$E_0 = \langle\Psi_0|\mathscr{H}_0|\Psi_0\rangle = \langle\phi(\rho,\lambda)|\mathscr{H}_{\mathrm{eff}}^{(0)}|\phi(\rho,\lambda)\rangle . \tag{35}$$

From Eq. (35), the effective Hamiltonian for the unperturbed exciton-phonon system is defined as

$$\begin{aligned} \mathscr{H}_{\mathrm{eff}}^{(0)} &= \langle 0,0|\,\langle\phi_{l_1}(z_e)\phi_{l_2}(z_h)|\mathscr{H}_0|\phi_{l_1}(z_e)\phi_{l_2}(z_h)\rangle\,|0,0\rangle \\ &= \frac{p^2}{2\mu} - \frac{\lambda e^2}{\epsilon_\infty \rho} + \frac{\pi^2\hbar^2 l_1^2}{8m_e d^2} + \frac{\pi^2\hbar^2 l_2^2}{8m_h d^2} . \end{aligned} \tag{36}$$

In order to obtain the perturbation to $\mathscr{H}_{\mathrm{eff}}^{(0)}$, now we analyze the contribution of $\mathscr{H}_1$ to the energy of the exciton-phonon systems. First, we analyze the first-order perturbation of $\mathscr{H}_1$ to the exciton-phonon system energy $\Delta E^{(1)}$,

$$\Delta E^{(1)} = \langle\Psi_0|\mathscr{H}_1|\Psi_0\rangle . \tag{37a}$$

From (22c) and (34), we can show that the contribution of all the terms in (22c), except the first one, to the energy of the exciton-phonon system are zero, so (37a) can be written as

$$\Delta E^{(1)}=\left\langle \phi_{l_1}(z_e)\phi_{l_2}(z_h)\phi(\rho,\lambda) \left| \frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{[\rho^2+(z_e-z_h)^2]^{1/2}}\right]\right| \phi_{l_1}(z_e)\phi_{l_2}(z_h)\phi(\rho,\lambda)\right\rangle . \tag{37b}$$

When the slab is not very thick, especially when the thickness of the slab compares with the effective Bohr radius of the exciton, the parameter λ in the equation can be obtained with the perturbative-variational method,[10], i.e., let the first-order contribution be zero,

$$\left\langle \phi_{l_1}(z_e)\phi_{l_2}(z_h)\phi(\rho,\lambda) \left| \frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{[\rho^2+(z_e-z_h)^2]^{1/2}}\right]\right| \phi_{l_1}(z_e)\phi_{l_2}(z_h)\phi(\rho,\lambda)\right\rangle =0 . \tag{38}$$

From Eq. (38), the relevant λ can be determined, and let it be expressed as $\lambda_{\min}$. Therefore the first-order contribution $\Delta E^{(1)}$ of the perturbing Hamiltonian $\mathscr{H}_1$ to the exciton-phonon system energy is zero.

In the following, we consider the second-order contribution $\Delta E^{(2)}$ of $\mathscr{H}_1$ to the exciton-phonon system:

$$\Delta E^{(2)}=\langle \phi(\rho,\lambda_{\min})\,|\,\mathscr{H}_{\rm eff}^{(2)}\,|\,\phi(\rho,\lambda_{\min})\rangle . \tag{39}$$

where $\Delta\mathscr{H}_{\rm eff}^{(2)}$ is the second-order correction of $\mathscr{H}_1$ to $\mathscr{H}_{\rm eff}^{(0)}$.

Using the perturbative method,[14] the second-order correction $\Delta\mathscr{H}_{\rm eff}^{(2)}$ of $\mathscr{H}_1$ to $\mathscr{H}_{\rm eff}^{(0)}$ can easily be divided into four parts,

$$\Delta\mathscr{H}_{\rm eff}^{(2)}=\Delta E_+^{(B)}+\Delta E_-^{(B)}+\Delta E_+^{(S)}+\Delta E_-^{(S)} , \tag{40a}$$

where

$$\Delta E_+^{(B)}=-\sum_{l_1',l_2',\mathbf{k},m}\frac{|(\mathscr{H}_1)_{(l_1,l_2 00)(l_1'l_2'k_+0)}|^2}{E_{l_1'l_2'k}-E_{l_1l_20}} , \quad m=1,3,5,\ldots,(l_1'-l_1),(l_2'-l_2)=0,\pm2,\pm4,\ldots \tag{40b}$$

$$\Delta E_-^{(B)}=-\sum_{l_1',l_2',\mathbf{k},m}\frac{|(\mathscr{H}_1)_{(l_1l_2 00)(l_1'l_2'k_-0)}|^2}{E_{l_1l_2'k}-E_{l_1l_20}}, \quad m=2,4,6,\ldots,(l_1'-l_1),(l_2'-l_2)=\pm1,\pm3,\ldots \tag{40c}$$

$$\Delta E_+^{(S)}=-\sum_{l_1',l_2',\mathbf{q}}\frac{|(\mathscr{H}_1)_{(l_1l_2 00)(l_1'l_2'q_+0)}|^2}{E_{l_1'l_2'q}-E_{l_1l_20}}, \quad (l_1'-l_1),(l_2'-l_2)=0,\pm2,\pm4,\ldots \tag{40d}$$

$$E_-^{(S)}=-\sum_{l_1',l_2',\mathbf{q}}\frac{|(\mathscr{H}_1)_{(l_1l_2 00)(l_1'l_2'q_-0)}|^2}{E_{l_1'l_2'q}-E_{l_1l_20}}, \quad (l_1'-l_1),(l_2'-l_2)=\pm1,\pm3,\pm5,\ldots . \tag{40e}$$

After a straightforward manipulation, we obtain

$$\Delta E_+^{(B)}=-\alpha\hbar\omega_{\rm LO}\frac{8Nau_l}{\pi^4}\left\{\sum_{l_1',m}\frac{s_1l_1^2\left[\frac{1}{(l_1'+m)^2-l_1^2}-\frac{1}{(l_1'-m)^2-l_1^2}\right]^2}{s_1m^2+l_1^2-l_1'^2-(Nau_{le}/\pi)^2}\ln\left|\frac{s_1m^2}{(l_1')^2-l_1^2+(Nau_{le}/\pi)^2}\right| + \sum_{l_2',m}\frac{s_2l_2^2\left[\frac{1}{(l_2'+m)^2-l_2}-\frac{1}{(l_2'-m)^2-l_2}\right]^2}{s_2m^2+l_2^2-(l_2')^2-(Nau_{lh}/\pi)^2}\ln\left|\frac{s_2m^2}{(l_2')^2-l_2^2+(Nau_{lh}/\pi)^2}\right|\right\}$$

$$+\alpha\hbar\omega_{\rm LO}\frac{8Nau_l}{\pi^4}\frac{2l_1l_2}{\pi}\left[\frac{\pi}{Na}\right]^2\sum_m\left[\frac{1}{(l_1+m)^2-l_1^2}-\frac{1}{(l_1-m)^2-l_1^2}\right] \times\left[\frac{1}{(l_2+m)^2-l_2^2}-\frac{1}{(l_2-m)^2-l_2^2}\right]\int_0^\infty\frac{2kJ_0(\rho k)dk}{[k^2+(m\pi/Na)^2](k^2+u_l^2)} , \tag{41a}$$

where $m=1,3,5,\ldots,N/2$, $(l_1'-1_1),(l_2'-l_2)=0,\pm2,\pm4,\ldots$, and $J_0(\rho k)$ is the zero-order Bessel function;

$$\Delta E_-^{(B)} = -\alpha\hbar\omega_{\rm LO}\frac{8Nau_l}{\pi^4}\left\{\sum_{l_1',m}\frac{s_1 l_1^2\left[\dfrac{1}{(l_1'+m)^2-l_1^2}-\dfrac{1}{(l_1'-m)^2-l_1^2}\right]^2}{s_1m^2+l_1^2-(l_1')^2-(Nau_{le}/\pi)^2}\ln\left|\frac{s_1m^2}{(l_1')^2-l_1^2+(Nau_{le}/\pi)^2}\right|\right.$$
$$\left.+\sum_{l_2',m}\frac{s_2 l_2^2\left[\dfrac{1}{(l_2'+m)^2-l_2^2}-\dfrac{1}{(l_2'-m)^2-l_2^2}\right]^2}{s_2m^2+l_2^2-(l_2')^2-(Nau_{lh}/\pi)^2}\ln\left|\frac{s_2m^2}{(l_2')^2-l_2^2+(Nau_{1h}/\pi)^2}\right|\right\}, \tag{41b}$$

where $m=2,4,6,\ldots,N/2$, $(l_1'-l_1)$, $(l_2'-l_2)=\pm1,\ \pm3,\pm5,\ldots$;

$$\Delta E_+^{(S)} = -\alpha\hbar\omega_{\rm LO}8Nau_l\epsilon_0^{1/2}\epsilon_\infty^{3/2}$$
$$\times\left\{\sum_{l_1'}\int_0^{N\pi/2}\left[s_1e^{-x}\sinh x(\tanh x/2)^2\left[\frac{x}{x^2+\pi^2(l_1'-l_1)^2}-\frac{x}{x^2+\pi^2(l_1'+l_1)^2}\right]^2dx\right]\right.$$
$$\times(\{s_1x^2+(Nau_{se+})^2+\pi^2[(l_2')^2-l_1^2]\}[(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}]^{3/2}[(\epsilon_0+1)-(\epsilon_0-1)e^{-x}]^{1/2})^{-1}$$
$$+\sum_{l_2'}\int_0^{N\pi/2}\left[s_2e^{-x}\sinh x(\tanh x/2)^2\left[\frac{x}{x^2+\pi^2(l_2'-l_2)^2}-\frac{x}{x^2+\pi^2(l_2'+l_2)^2}\right]^2dx\right]$$
$$\times(\{s_2x^2+(Nau_{sh+})^2+\pi^2[(l_2')^2-l_2^2]\}[(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}]^{3/2}$$
$$\left.\times[(\epsilon_0+1)-(\epsilon_0-1)e^{-x}]^{1/2})^{-1}\right\}$$
$$+\alpha\hbar\omega_{\rm LO}8Nau_l\epsilon_0^{1/2}\epsilon_\infty^{3/2}\int_0^{N\pi/2}\left[e^{-x}\sinh x\,(\tanh x/2)^2\left[\frac{1}{x}-\frac{x}{x^2+\pi^2(2l_1)^2}\right]\right.$$
$$\left.\times\left[\frac{1}{x}-\frac{x}{x^2+\pi^2(2l_2)^2}\right]J_0(\rho x/Na)dx\right]$$
$$\times\{[x^2+(Nau_{s+})^2][(\epsilon_\infty+1)-(\epsilon_\infty-1)e^{-x}]^{3/2}\,[(\epsilon_0+1)-(\epsilon_0-1)e^{-x}]^{1/2}\}^{-1}, \tag{41c}$$

where $(l_1'-l_1)$, $(l_2'-l_2)=0,\pm2,\pm4,\ldots$; and

$$\Delta E_-^{(S)} = -\alpha\hbar\omega_{\rm LO}8Nau_l\epsilon_0^{1/2}\epsilon_\infty^{3/2}$$
$$\times\left\{\sum_{l_1'}\int_0^{N\pi/2}\left[s_1e^{-x}\sinh x(\coth/2)^2\left[\frac{x}{x^2+\pi^2(l_1'-l_1)^2}-\frac{x}{x^2+\pi^2(l_1'+l_1)^2}\right]^2dx\right]\right.$$
$$\times(\{s_1x^2+(Nau_{se-})^2+\pi^2[(l_1')^2-l_1^2]\}[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^{3/2}$$
$$\times[(\epsilon_0+1)+(\epsilon_0-1)e^{-x}]^{1/2})^{-1}$$
$$+\sum_{l_2'}\int_0^{N\pi/2}\left[s_2e^{-x}\sinh x(\coth x/2)^2\left[\frac{x}{x^2+\pi^2(l_2'-l_2)^2}-\frac{x}{x^2+\pi^2(l_2'+l_2)^2}\right]^2dx\right]$$
$$\times(\{s_2x^2+(Nau_{sh-})^2+\pi^2[(l_2')^2-l_2^2]\}[(\epsilon_\infty+1)+(\epsilon_\infty-1)e^{-x}]^{3/2}$$
$$\left.\times[(\epsilon_0+1)+(\epsilon_0-1)e^{-x}]^{1/2})^{-1}\right\}, \tag{41d}$$

where $(l_1'-l_1)$, $(l_2'-l_2)=\pm 1, \pm 3 \pm 5, \ldots$.

In Eqs. (41a)–(41d), $\alpha=(Me^2/\hbar^2 u_l)(1/\epsilon_\infty - 1/\epsilon_0)$ is the coupling constant of the exciton-phonon interaction:

$$\frac{\hbar^2 u_{le}^2}{2m_e}=\hbar\omega_{\rm LO}, \quad \frac{\hbar^2 u_{lh}^2}{2m_h}=\hbar\omega_{\rm LO}, \quad \frac{\hbar^2 u_{sp}^2}{2M}=\hbar\omega_{\rm SO}\,,$$

$$\frac{\hbar^2 u_{sep}^2}{2m_e}=\hbar\omega_{\rm SO}, \quad \frac{\hbar^2 u_{shp}^2}{2m_h}=\hbar\omega_{\rm SO}\,.$$

where u_{le} is the wave number of an electron with a translation energy which equals the energy of the bulk longitudinal-optical phonon, and its reciprocal u_{le}^{-1} is the polaron radius. The physical meaning of other quantity can be understood in the same way.

Eventually, the effective Hamiltonian of the exciton-phonon system is obtained,

$$\mathcal{H}_{\rm eff}=\mathcal{H}_{\rm eff}^{(0)}+\Delta\mathcal{H}_{\rm eff}^{(2)} = \frac{p^2}{2\mu}-\frac{\lambda_{\min}}{\rho}+V_I(\rho)+\frac{\pi^2\hbar^2 l_1^2}{8m_e d^2}+\frac{\pi^2\hbar^2 l_2^2}{8m_h d^2}+E_s\,, \tag{42a}$$

$V_I(\rho)=$the last term of (41a)

+the last term of (41c) , (42b)

$$E_s=\Delta E^{(B)}+\Delta E^{(S)}\,, \tag{42c}$$

$$\Delta E^{(B)}= \text{ the first term of (41a) } + \Delta E_-^{(B)}\,, \tag{42d}$$

and

$$\Delta E^{(S)}= \text{ the first term of(41c) } + E_-^{(S)}\,. \tag{42e}$$

$V_I(\rho)$ is the effective potential between the electron and the hole. The potential is produced by the interaction of the electron (hole) with the phonons, and it is called "induced potential" for short. $\Delta E^{(B)}$ and $\Delta E^{(S)}$ are the self-energies produced by the longitudinal-optical phonons and the surface-optical phonons, respectively, and they make up the self-energy E_s of the exciton. From the effective Hamiltonian (42a), the energy E of the exciton in the polar crystal slab can be easily obtained.

$$E=E_{n,l}^{(2D)}+\frac{\pi^2\hbar^2 l_1^2}{8m_e d^2}+\frac{\pi^2\hbar^2 l_2^2}{8m_h d^2}+E_s\,, \tag{43}$$

where $E_{n,l}^{(2D)}$ is the eigenenergy of the quasi-two-dimension hydrogenlike atom Hamiltonian composed of the first three terms in (42a).

V. THE BEHAVIOR OF THE QUASI-TWO-DIMENSIONAL EXCITON

In the following, taking the exciton in GaAs as an example, we perform the numerical evaluation. In Table I, the data for GaAs are given.

Figure 2 shows the variation of the exciton self-energy $\Delta E^{(B)}$, produced by the interaction of the exciton with the bulk longitudinal-optical (LO) phonons, with the thickness N of the slab. Increasing the thickness N, we find the self-energy $\Delta E^{(B)}$ decreases monotonically. When the thickness of the slab is in the range of a few effective Bohr radii of the exciton, the change of $\Delta E^{(B)}$ is obvious. When N is very large, $\Delta E^{(B)}$ will decrease slowly to $-2\alpha\hbar\omega_{\rm LO}$, i.e., to the value of the exciton self-energy in the three-dimensional polar crystal (see the Appendix).

TABLE I. The data of GaAs. Energy is in meV, length in Å, and mass in the mass of the electron in the vacuum.

ϵ_0	12.83
ϵ_∞	10.9
$\hbar\omega_{\rm LO}$	36.7
m_e	0.0657
m_h	0.12
a	5.654
u_l	0.0422
u_{le}	0.0251
u_{lh}	0.0339
α	0.1145
α_e	0.0681
α_h	0.092

Figure 3 shows the variation of the exciton self-energy $\Delta E^{(S)}$, produced by the interaction of the exciton with the surface-optical (SO) phonons, with the thickness of the slab. Increasing the thickness of the polar-crystal slab, we find the self-energy $\Delta E^{(S)}$ increases monotonically, and $|\Delta E^{(S)}|$, the self-trapping energy produced by the interaction of the exciton with the surface-optical phonons, decreases monotonically. As the thickness of the slab N tends to ∞, $\Delta E^{(S)}$ will tend to zero.

Figure 4 shows the variation with ρ of the induced potential $V_I^{(B)}(\rho)$, produced by the interaction of the exciton with the bulk LO phonons. Under conditions of different thicknesses N of the slab, i.e., when $N=10$, 20, and 50, the relevant induced potentials $V_I^{(B)}(\rho)$ are shown in the figure. It is shown that for the Wannier exciton (its effective Bohr radius is about 20 times that of the lattice constant a), the thicker the slab, the larger the relevant induced potential $V_I^{(B)}(\rho)$.

Figure 5 shows the variation with ρ of the induced potential $V_I^{(S)}(\rho)$, produced by the interaction of the exciton with the SO phonons. Under conditions of different thicknesses N of the slab, i.e., when $N=10$, 20, and 50, the relevant induced potentials $V_I^{(S)}(\rho)$ are shown in the figure. It is shown that for the Wannier exciton, the

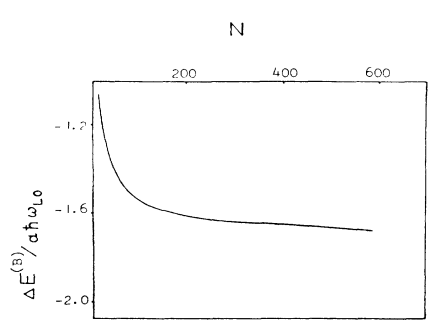

FIG. 2. Bulk LO self-energy vs slab thickness N (in the lattice constant a).

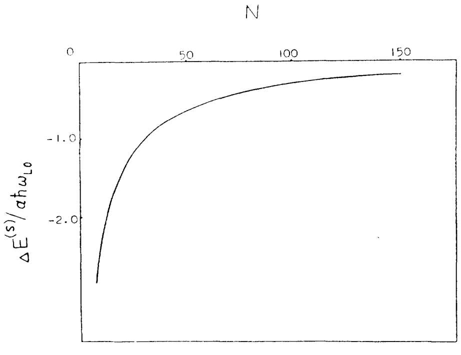

FIG. 3. SO self-energy vs slab thickness N (in the lattice constant a).

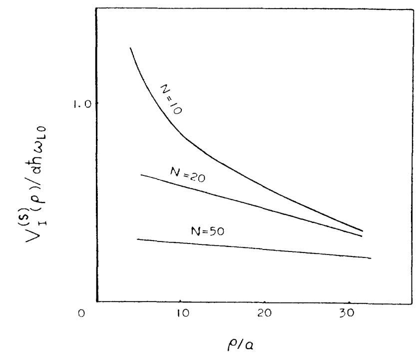

FIG. 5. SO-induced potential as a function of the relative position between the electron and the hole ρ.

thicker the slab, the smaller the relevant induced potential $V_I^{(S)}(\rho)$. This is because the surface-optical mode is a localized mode, and near the surface of the slab, the electron- (hole-) SO phonon coupling is very strong. Hence the smaller the thickness of the slab N, the larger the induced potential $V_I^{(S)}(\rho)$.

Figure 6 shows the variation of the induced potential $V_I(\rho)$, produced by the interaction of the exciton with the phonons, with ρ. The phonons include bulk LO phonons and SO phonons. Under conditions of different thicknesses N of the slab, i.e., when $N=10$, 20, and 50, the relevant induced potentials $V_I(\rho)$ are shown in the figure. After being fitted, the three curves in Fig. 6 can be expressed approximately by the following analytic function:

$$V_I(\rho)=\frac{D\alpha\hbar\omega_{\rm LO}}{\rho}(1-e^{-B\rho}) , \tag{44}$$

where D and B can be determined by fitting, and are given in the Table II. Equation (44) has the form of the induced potential in the three-dimensional polar crystal (see the Appendix).

In the following, the energy of the ground state and the first excited state of the internal motion in the x-y plane of the exciton in the polar slab (the quasi-two-dimensional exciton) are calculated with variational method.

Choosing properly a zero point of energy, and temporarily not considering the self-energy of the exciton, we obtain the Hamiltonian for the internal motion in the x-y plane of the exciton by Eq. (42). It can be written as

$$\mathcal{H}_{\rm eff}=\frac{p^2}{2\mu}-\frac{\lambda_{\min}e^2}{\epsilon_\infty\rho}+V_I(\rho) , \tag{45}$$

where

$$V_I(\rho)=\frac{D\alpha\hbar\omega_{\rm LO}}{\rho}(1-e^{-B\rho}) .$$

First we solve the ground-state problem of the exciton. Choose the ground-state trial function as

$$\phi_{0,0}(Z,\rho)=\frac{1}{\sqrt{2\pi}}\frac{4Z}{a_0'}e^{-2Z\rho/a_0'} , \tag{46}$$

where $a_0=a_0/\lambda_{\min}$, Z is a variational parameter.

From (30) the relevant $\lambda_{\min}$ in (45) or (22d) and (24) can be determined. The relevant quantum number for the ground state of the exciton is $l_1=1$, $l_2=1$, $n=0$, and $l=0$. The parameter $\lambda_{\min}$ can be written as $\lambda_{1,1,0,0}$, and it can be obtained from Eq. (47) with the "self-consistent method" (its value is given in Table III):

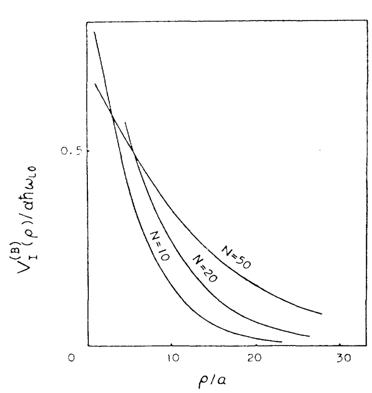

FIG. 4. Bulk LO-induced potential as a function of the relative position between the electron and the hole ρ.

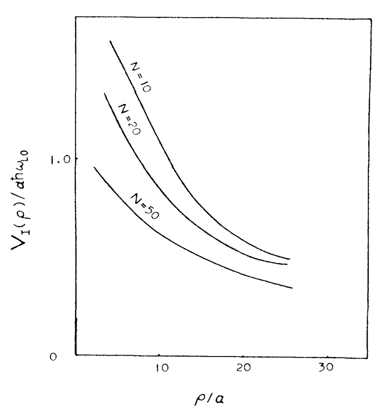

FIG. 6. Total induced potential as a function of the relative position between the electron and the hole ρ.

$$\lambda_{1,1,0,0}=\frac{4}{a_0'}\frac{1}{d^2}\int_0^\infty\int_{-d}^{d}\int_{-d}^{d}\frac{e^{-4\rho/a_0'}}{[\rho^2+(z_e-z_h)^2]^{1/2}}\sin^2\left[\frac{\pi}{2d}(z_e+d)\right]\sin^2\left[\frac{\pi}{2d}(z_h+d)\right]dz_e\,dz_h\,d\rho\ , \tag{47}$$

where $a_0'=a_0/\lambda_{1,1,0,0}$.

The expectation value of the Hamiltonian (45) for the trial function (46) is

$$\overline{\mathscr{H}}_{00}(Z)=\langle\phi_{00}(Z,\rho)\,|\,\mathscr{H}_{\rm eff}\,|\,\phi_{00}(Z,\rho)\rangle\ . \tag{48}$$

Let the derivative of the above equation with respect to Z be set equal to zero. Solve for Z, and substitute it into (48), then the energy $E_0^{(\rm ph)}$ of the ground state of the quasi-two-dimensional exciton is obtained. The relevant results for different thicknesses of the slab are listed in Table III.

Choose the first-excited-state trial function as

$$\phi_{1,\pm1}(Z,\rho)=\frac{2Z^2}{\sqrt{2\pi}}e^{\pm\varphi}\left[24\left[\frac{3a_0'}{4}\right]^2\right]^{-1/2}\times\left[\frac{4}{3a_0'}\right]e^{-2Z\rho/3a_0'}\ , \tag{49}$$

where $a_0'=a_0/\lambda_{\rm min}$, Z is variational parameter.

The first-excited-state energy $E_1^{(\rm ph)}$ of the exciton can also be obtained in the same way as in the ground-state problem. The results are also listed in Table III.

VI. RESULT AND ANALYSIS

In the above, having carried out a unitary transformation on the Hamiltonian, with the perturbative-variational[10] and the general perturbative method, we obtain the effective Hamiltonian (42) of the exciton in the polar-crystal slab. The effective Hamiltonian (42) can be divided into three parts: the energy of the internal motion in the x-y plane of the exciton composed of the first three terms; the energy in the z direction composed of the fourth and the fifth terms, which is what the energy of the free-moving electron and hole in a one-dimensional infinite square-well potential would have; and the self-energy comprised of the last term. The difference, between the effective Hamiltonian (42) of the exciton-phonon system in the slab obtained above and that of the exciton system in which the electron- (hole-) phonon coupling is not considered,[2] is very large. The main difference is that the self-energy and the induced potential exist in the former but not in the latter. Having taken the polar-crystal GaAs slab, the electron-phonon interaction in the crystal is weak. As an example, we give a numerical evaluation. In Table IV we list, for the different thicknesses ($N=10$, 20, and 50) of the slab, the slab exciton internal x-y plane motion energy that is obtained by not taking account of the electron (hole-) phonon interaction, the slab exciton internal x-y plane motion energy that is obtained by taking account of the electron (hole-) phonon interaction, the self-energys of the exciton in the slab, and the energy in the z direction.

In Table IV, we find that the ground-state energy for motion in x-y plane of the slab, E_0, obtained by not considering the electron-(hole-) phonon interaction relates to the thickness of the slab. With the decrease of the thickness of the slab, E_0 decreases. This is because the Hamiltonian (24) of the quasi-two-dimensional exciton is directly proportional to the square of λ. λ increases with the decrease of the thickness of the slab. As the thickness of the slab tends to zero, λ will tend to 1, i.e., the pure two-dimensional system. By taking account of the electron- (hole-) phonon coupling, the internal motion in the x-y plane Hamiltonian of the exciton in the slab has an induced repulsion potential produced by the electron- (hole-) phonon interaction beside the attractive Coulomb potential. Therefore $E_0^{(\rm ph)}$ ascends relative to E_0. $\Delta E^{(\rm ph)}=E_1^{(\rm ph)}-E_0^{(\rm ph)}$ also relates to the thickness of the slab. It increases with the decrease of the thickness of the slab. This just reflects the regularity of increasing the induced potential $V_I(\rho)$ with the decrease of the thickness of the slab in Fig. 6. The reason is that not only the electron- (hole-) SO-phonon interaction is stronger than the electron- (hole-) LO-phonon interaction, but also the former changes faster than the latter.

In Table IV, we can also find that $E_0^{(\rm ph)}$, $E_1^{(\rm ph)}$, $\Delta E^{(\rm ph)}$, and E_s all relate to the thickness of the slab. They change with the change of the thickness of the slab. The property that the energy spectrum changes with the change of the thickness of the slab should be especially noted. Utilizing this property, controlling the thickness of the slab, and by exciting the quasi-two-dimensional exciton system with external field, we shall obtain the artificial optical wavelength emitted from the system.

Figure 7 shows the ground- and the first-excited-state energy of the exciton internal moving in the x-y plane, i.e., $E_0^{(\rm ph)}$ and $E_1^{(\rm ph)}$ for different thicknesses of the slab. It is shown that the ground-state energy $E_0^{(\rm ph)}$ of the quasi-two-dimensional exciton decreases with the decrease of the thickness of the slab, as does the first-excited-state energy $E_1^{(\rm ph)}$ of the exciton, but the change of the latter is not as fast as the change of the former.

The energy of the exciton in the polar-crystal slab [see (43)] includes the energy of the exciton moving in the z direction $(\pi^2\hbar^2l_1^2/8m_ed^2+\pi^2\hbar^2l_2^2/8m_hd^2)$, the internal x-y plane motion (the mass center translational energy having been neglected) energy of the quasi-two-dimensional hydrogenlike exciton $E_{n,l}^{(\rm 2D)}$, and the self-

TABLE II. The value of D and B for different thicknesses N of the slab.

N	D (Å)	B (Å^{-1})
10	56.5	0.048
20	65.1	0.024
50	66.5	0.015

TABLE III. The ground-state energy $E_0^{(\mathrm{ph})}$ (or expressed as E_{1100}) and the first-excited-state energy $E_1^{(\mathrm{ph})}$ (or expressed as $E_{111\pm1}$) of the exciton in the polar-crystal slab.

N	$\lambda_{1,1,0,0}$	Z_{1100}	E_{1100} (meV)	$\lambda_{1,1,1,\pm1}$	$Z_{111\mp1}$	$E_{111\mp1}$ (meV)
10	0.980	0.8431	−5.236	0.998	0.6945	−0.521
20	0.942	0.8869	−5.053	0.993	0.6515	−0.413
50	0.797	0.9000	−3.519	0.959	0.6425	−0.351

energy E_s produced by the electron- (hole-) phonon interaction. Generally (see the value in Table IV), the energy and the energy difference between the energy levels of the electron and the hole in the z direction are very large when the slab is very thin, so to excite the z directional motion of the electron and the hole is very difficult at very low temperatures. The exciton in the slab can be considered as a quasi-two-dimensional system.

In Fig. 8, we show the energy levels of the exciton in the polar-crystal slab when $N=50$. If only the energy of the electron and the hole moving in the z direction is considered, the energy $E_{11}=10.84$ meV. The self-energy $E_s=-8.512$ meV induced by the electron- (hole-) phonon interaction reduces the energy of the exciton further, so the dotted line shown in Fig. 8 is the energy level $E_{11}+E_s=2.328$ meV. If the internal motion in the x-y plane of the exciton is considered, the energy of the exciton will decrease once again. The decrease in energy is $E_{n,l}^{(2\mathrm{D})}$. If in the state $n=0$, $l=0$, i.e., in the ground state, the decrease in energy is 3.519 meV. If in the state $n=1$, $l=\pm1$, i.e., in the first excited state, the decrease in energy is 0.351 meV. Therefore E_{1100} and $E_{111\pm1}$ shown in Fig. 8 express the energy levels of the exciton in the polar-crystal slab in the state $l_1=1$, $l_2=1$, $n=0$, and $l=0$, i.e., in the ground state and in the state $l_1=1$, $1_2=1$, $n=1$, and $l=\pm1$, i.e., in the first excited state, respectively.

From the data listed in Table IV, we can further see that the energy difference between the energy levels of the electron and the hole in the z direction is much larger than that between the x-y plane energy levels of the exciton when the slab is thin, so the motion of the exciton in the z direction is nearly isolated from the motion of the exciton in the x-y plane and the energy resonance transformation between the z direction motion and the x-y plane motion cannot occur. When the slab is thick, the energy difference between the z direction energy levels ($E_{12}-E_{11}$) equals that between the x-y plane interval energy levels ($E_{1\pm1}^{(\mathrm{ph})}-E_{00}^{(\mathrm{ph})}$), and the energy resonance transformation can take place. Thus it can be seen that under the generally discussed condition in which the thickness of the slab can be compared with the effective Bohr radius of the exciton, the energy transformation between the z direction and the x-y plane energy cannot occur. Therefore the exciton in the polar-crystal slab can be considered as a quasi-two-dimensional system.

With the energy spectrum of the exciton in the polar-crystal slab obtained, many optical, electrical, and other physical properties of the polar-crystal slab can be obtained. The results found are very useful in the further investigation of the transport and optical properties of the superlattice.

APPENDIX: THE WANNIER EXCITON IN THE THREE-DIMENSIONAL POLAR CRYSTAL

In the following, the Wannier exciton in three-dimensional polar crystal will be studied with the method used in the main body of this paper. The Hamiltonian of the exciton-phonon system in the three-dimensional polar

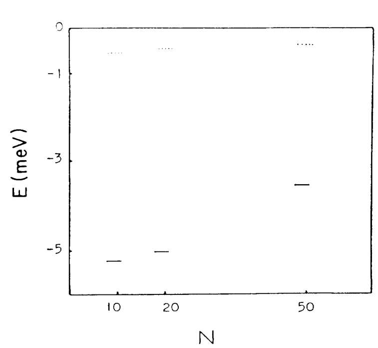

FIG. 7. The ground- and the first-excited-state energy levels of the exciton-phonon system for different thicknesses of the slab. · · · · for the first-excited-state energy; —— for the ground-state energy.

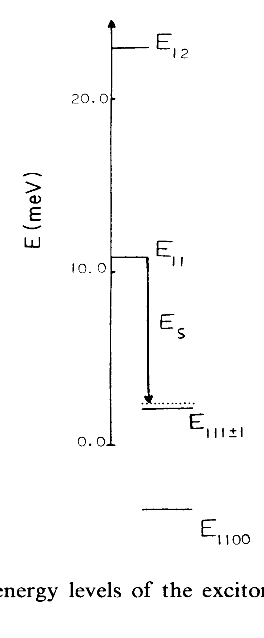

FIG. 8. The energy levels of the exciton-phonon system (as $N=50$).

TABLE IV. The energy of the exciton (in meV). E_0, E_1, $E_0^{(\mathrm{ph})}$, and $E_1^{(\mathrm{ph})}$ are the ground- and the first-excited-state energies for the exciton moving in x-y plane of the slab that are obtained by not taking and taking account of the electron- (hole-) phonon interaction, respectively; E_s is the self-energy; $E_{l_1 l_2}$ the energy of the exciton in the z direction; and $\Delta E = E_1 - E_0$, $\Delta E^{(\mathrm{ph})} = E_1^{(\mathrm{ph})} - E_0^{(\mathrm{ph})}$.

N	E_0	$E_0^{(\mathrm{ph})}$	E_1	$E_1^{(\mathrm{ph})}$	ΔE	$\Delta E^{(\mathrm{ph})}$	E_s	E_{11}	E_{12}
10	−8.768	−5.236	−1.010	−0.521	7.758	4.715	−14.26	276.4	570.5
20	−8.101	−5.053	−1.000	−0.413	7.101	4.640	−11.06	69.10	142.6
50	−5.799	−3.519	−0.933	−0.351	4.866	3.168	−8.512	10.84	22.80

crystal is

$$H = -\frac{\hbar^2}{2\mu_1}\nabla_1^2 - \frac{\hbar^2}{2\mu_2}\nabla_2^2 - \frac{e^2}{\epsilon_\infty |r_1 - r_2|} + \sum_{\mathbf{w}} \hbar\omega a_{\mathbf{w}}^\dagger a_{\mathbf{w}} + \sum_{\mathbf{w}} [V_w a_{\mathbf{w}} (e^{i\mathbf{w}\cdot\mathbf{r}_2} - e^{i\mathbf{w}\cdot\mathbf{r}_1}) + \mathrm{H.c.}] , \tag{A1}$$

$$V_w = \frac{4ie}{V^{1/2}} \left[\frac{F\hbar\omega}{8\pi w^2} \right]^{1/2}, \quad F = \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} ,$$

where μ_1, μ_2, $\mathbf{r}_1$, and $\mathbf{r}_2$ are the band mass and the position vectors of the electron and the hole, respectively. ϵ_∞ and ϵ_0 are the optical dielectric constant and static dielectric constant, respectively; $a_{\mathbf{w}}^\dagger$ ($a_{\mathbf{w}}$) is the creation (annihilation) operator of the phonons, and ω is the optical frequency of the phonons.

Introducing the center-of-mass coordinates of the exciton:

$$\mathbf{R} = s_1\mathbf{r}_1 + s_2\mathbf{r}_2, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad M = \mu_1 + \mu_2 , \quad \mu = \mu_1\mu_2/M, \quad s_1 = \mu_1/M, \quad s_2 = \mu_2/M . \tag{A2}$$

We rewrite (A1) as

$$H = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{\epsilon_\infty r} + \sum_{\mathbf{w}} \hbar\omega a_{\mathbf{w}}^\dagger a_{\mathbf{w}} + \sum_{\mathbf{w}} [V_w a_{\mathbf{w}} e^{i\mathbf{w}\cdot\mathbf{R}} (e^{-is_1\mathbf{w}\cdot\mathbf{r}} - e^{is_2\mathbf{w}\cdot\mathbf{r}}) + \mathrm{H.c.}] . \tag{A3}$$

Because the total momentum of the exciton-phonon system $\hbar\mathbf{K}$,

$$\hbar\mathbf{K} = \mathbf{P} + \sum_{\mathbf{w}} a_{\mathbf{w}}^\dagger a_{\mathbf{w}} \hbar\mathbf{w}$$

commutes with the Hamiltonian H, hence $\mathbf{K}$ is a constant of the motion, we can introduce a unitary transformation to eliminate the position vector R of the exciton mass center:[13]

$$U = \exp\left[i\mathbf{K}\cdot\mathbf{R} - i \sum_{\mathbf{w}} a_w^\dagger a_{\mathbf{w}} \mathbf{w}\cdot\mathbf{R} \right] . \tag{A4}$$

Applying the unitary transformation to (A3), we get

$$\mathscr{H} = U^{-1}HU = \mathscr{H}_0 + \mathscr{H}_1 , \tag{A5}$$

$$\mathscr{H}_0 = \frac{p^2}{2\mu} - \frac{e^2}{\epsilon_\infty r} + \frac{\hbar^2}{2M} \sum_{\mathbf{w}} a_{\mathbf{w}}^\dagger a_{\mathbf{w}} (u^2 + w^2) + \frac{\hbar^2 K^2}{2M} , \tag{A6}$$

$$\mathscr{H}_1 = \sum_{\mathbf{w}} [V_w a_{\mathbf{w}} (e^{-is_1\mathbf{w}\cdot\mathbf{r}} - e^{is_2\mathbf{w}\cdot\mathbf{r}}) + \mathrm{H.c.}] - \frac{\hbar^2}{M} \sum_{\mathbf{w}} a_{\mathbf{w}}^\dagger a_{\mathbf{w}} \mathbf{K}\cdot\mathbf{w} + \frac{\hbar^2}{2M} \sum_{\mathbf{w}\neq\mathbf{w}'} a_{\mathbf{w}}^\dagger a_{\mathbf{w}'}^\dagger a_{\mathbf{w}} a_{\mathbf{w}'} \mathbf{w}\cdot\mathbf{w}' , \tag{A7}$$

where $\hbar^2 u^2/2M = \hbar\omega$.

Only at the low-temperature limit (zero temperature), i.e., in the nonphonon state of the system $\mathscr{H}_0$ for the effective Hamiltonian of the exciton will be derived. In the following, take $\mathscr{H}_1$ as a perturbation.[14] With the perturbation method, the effective Hamiltonian of the exciton is

$$\mathscr{H}_{\mathrm{eff}} = \frac{\hbar^2 K^2}{2M} + \frac{p^2}{2\mu} - \frac{e^2}{\epsilon_\infty r} + \Delta E , \tag{A8}$$

$$\Delta E = -\sum_{\mathbf{w}} \frac{|\langle 0 | \mathscr{H}_1 a_w^\dagger | 0 \rangle|^2}{\frac{\hbar^2}{2M}(u^2 + w^2)} = -2\alpha\hbar\omega + \frac{Fe^2}{r}(1 - e^{-ur}) , \tag{A9}$$

where $\alpha = Fe^2 M/\hbar^2 u$.

Thus we know that the self-energy of the exciton is $-2\alpha\hbar\omega$, and the induced potential between the electron and the hole is

$$V_I(r) = \frac{Fe^2}{r}(1 - e^{-ur}) . \tag{A10}$$

In the above equation, only one unitary transformation to H has been taken. The results are only suitable for weak exciton-phonon coupling. One of the authors (S.W.G.),[18] in his study of the influence of the lattice vibration on the motion of the exciton, applied a two-time unitary transformation to H, and obtained the effective Hamiltonian as

$$H = \frac{\hbar^2 K^2}{2M^*} - \frac{\hbar^2 \nabla_r^2}{2\mu^*} + \alpha\hbar\omega \left[-2 + \frac{s_1^2 + s_2^2}{2s_1 s_2} \right] - \frac{e^2}{\epsilon_0 r} - \left[\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right] \frac{e^2}{r} e^{-ur} + \alpha\hbar\omega e^{-ur} , \tag{A11}$$

where

$$M^* = M/(1-\alpha/6)\ , \quad \mu^* = \mu \Bigg/ \left[1+\alpha/3\frac{s_1^2+s_2^2}{2s_1s_2} \right] .$$

The effective Hamiltonian (A9) is different from the Hamiltonian (A11). The main difference in the effective Hamiltonian (A11) is the mass M and μ are renormalized as M^* and μ^*, the self-energy increased by $(s_1^2+s_2^2)\alpha\hbar\omega/(2s_1s_2)$, and the induced potential increased by $\alpha\hbar\omega e^{-ur}$. The Hamiltonian (A11) is better than the Hamiltonian (A9), the former reveals more properties of the exciton-phonon system than the latter. The amount of calculation in the one-time unitary transformation to H is much less than that in the two-time unitary transformation. The Hamiltonian of the exciton-phonon system in a polar-crystal slab is very complex, so in this paper we only apply the one-time unitary transformation to the Hamiltonian of the exciton-phonon system in a polar-crystal slab.

ACKNOWLEDGMENTS

The authors acknowledge support from the Science Foundation of the Chinese Academy of Sciences. One of the authors (M.Y.S.) wishes to thank Mr. S. L. Ban sincerely for his help.

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