PHYSICAL REVIEW B VOLUME 43, NUMBER 6 15 FEBRUARY 1991-II

Electron-phonon interaction in a quantum well

Xi-Xia Liang
Center of Theoretical Physics, Chinese Center of Advanced Science and Technology (World Laboratory), Beijing, People's Republic of China
and Laboratory of Solid State Physics, Department of Physics, Neimenggu University, Hohhot, Neimenggu 010 021, People's Republic of China

Xu Wang
Laboratory of Solid State Physics, Department of Physics, Neimenggu University, Hohhot, Neimenggu 010 021, People's Republic of China

(Received 7 June 1990)

Within the framework of the continuum model, optical polarization modes of lattice vibrations and a Fröhlich-like Hamiltonian of the interaction between an electron and optical phonons are derived. It is found that there are four branches of interface optical modes besides the usual transverse-optical and longitudinal-optical modes. The frequencies of these modes and coupling functions of an electron with the optical phonons are discussed.

The electron-phonon interaction plays an important role in the properties of quantum wells and superlattices. Previous authors[1-4] have used a three-dimensional (3D) or purely 2D Fröhlich Hamiltonian or an effective model Hamiltonian for the electron-phonon interaction in a quantum well. These Hamiltonians can partly describe the interaction, but a more complete Hamiltonian is needed. In this work the interaction between an electron and optical phonons in a quantum well has been considered in more detail and a Fröhlich-like Hamiltonian has been developed. In our discussion a method analogous to those of Fuchs and Kliewer[5] (FK) and of Lucas, Kartheuser, and Badro[6] (LKB) are used that had been used by Licari and Evrard[9] and by Wendler *et al.*[10] to develop the electron-phonon interaction Hamiltonian for a dielectric slab or a bilayer system.

We consider a quantum well for which the polar dielectric region, labeled as 1, is $-d \leq z \leq d$ and region 2 is $|z| > d$. Thus the space can be divided into three zones: zone I ($|z| \leq d$), zone II ($z > d$), and zone III ($z < -d$). Denoting the relative displacement of the ion pair in zone λ (λ=I, II, or III) as $\mathbf{u}_\lambda(\mathbf{r},t)=\mathbf{u}_{\lambda+}(\mathbf{r},t)-\mathbf{u}_{\lambda-}(\mathbf{r},t)$ the corresponding polarization field $\mathbf{p}(\mathbf{r},t)$ in zone λ produced by the ion vibration can be written as

$$\mathbf{p}^\lambda(r,t)=n_\lambda e_\lambda \mathbf{u}_\lambda(\mathbf{r},t)+n_\lambda \alpha_\lambda \mathbf{E}^{l\lambda}(\mathbf{r},t) \ . \tag{1}$$

In the above equation, n_λ, e_λ, and α_λ are the number of Wigner-Seitz cells per unit volume, the effective charge of the ions, and the electric polarizability per cell in zone λ, respectively. $E^l_\lambda(\mathbf{r},t)$ is the local electric field associated with the optical modes in the zone λ. Following LKB and LE,[6,9] we have a system of nine coupled integral equations,

$$\gamma_i^\lambda P_i^\lambda(\mathbf{r},t)=\sum_{\lambda'}\int_{(\lambda')} T_{ij}(\mathbf{r}-\mathbf{r}')P_j^{\lambda'}(\mathbf{r}',t)d\mathbf{r}' \ , \tag{2}$$

where the subscripts i and j stand for the coordinate components x, y, or z and T_{ij} is the dipolar tensor.[6,9] In Eq. (2), γ_i^λ are given as follows:

$$\gamma_x^\lambda=\gamma_y^\lambda=\gamma_k^\lambda=\frac{(\omega_{0\lambda}^2-\omega^2)(1-\frac{4}{3}\pi n_\lambda\alpha_\lambda)-\omega_{p\lambda}^2/3}{n_\lambda\alpha_\lambda(\omega_{0\lambda}^2-\omega^2)+\omega_{p\lambda}^2/4\pi} \ , \tag{3}$$

$$\gamma_z^\lambda=\frac{(\omega_{0\lambda}^2-\omega^2)(1+\frac{8}{3}\pi n_\lambda\alpha_\lambda)+2\omega_{p\lambda}^2/3}{n_\lambda\alpha_\lambda(\omega_{0\lambda}^2-\omega^2)+\omega_{p\lambda}^2/4\pi} \ , \tag{4}$$

where $\omega_{0\lambda}$ is the frequency associated with the short-range force between the ions and $\omega_{p\lambda}$ is the ion plasma frequency. Here we have chosen $\mathbf{P}(\mathbf{r},t)$ as the form

$$\mathbf{P}(\mathbf{r},t)=\mathbf{P}(\mathbf{r})e^{-i\omega t} \ . \tag{5}$$

After carrying out a two-dimensional Fourier transformation

$$\mathbf{P}(\mathbf{r})=\frac{S}{4\pi^2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\boldsymbol{\rho}}\mathbf{P}(\mathbf{k},z) \ , \tag{6}$$

we get another system of coupled integral equations,

$$\gamma_k^\lambda P_y^\lambda(\mathbf{k},z)=0 \ , \tag{7a}$$

$$\gamma_k^\lambda P_k^\lambda(\mathbf{k},z)=-2\pi k\int_{-\infty}^{+\infty}dz'\, e^{-k|z-z'|}[P_k(\mathbf{k},z')+i\theta(z-z')P_z(\mathbf{k},z')] \ , \tag{7b}$$

$$\gamma_z^\lambda P_z^\lambda(\mathbf{k},z)=-2\pi k\int_{-\infty}^{+\infty}dz'\, e^{-k|z-z'|}[i\theta(z-z')P_k(\mathbf{k},z')-P_z(\mathbf{k},z')] \ , \tag{7c}$$

where $\theta(z)$ is the step function

$$\theta(z)=\begin{cases}1, & z>0\\ -1, & z<0 \ ,\end{cases}$$

$\mathbf{k}$ is the 2D wave vector in the x-y plane, and the x axis is chosen to lie along $\mathbf{k}$.

We obtain three kinds of polarization mode from this system of equations: TO, LO, and surfacelike optical (SO) modes.

When $\gamma_k^\lambda=0$, we get transverse-optical (TO) modes of frequency $\omega_{T\lambda}$. They are localized in zone λ and do not couple with the electron. We shall ignore them in the present work.

For the case of $\gamma_z^\lambda=0$, we have the longitudinal-optical (LO) modes of frequency $\omega_{L\lambda}$. If $\lambda=\mathrm{I}$, the modes have frequency ω_{L1} and are confined in zone I, i.e., in the quantum well. We obtain the same eigenvectors as did FK (Ref. 5) and omitted them here.

We focus our attention on the case in which both γ_k^λ and γ_z^λ are nonzero. For solving the system of equations (7b) to (7c), we differentiate Eqs. (7b) and (7c) twice and then get the following equations:

$$\gamma_k^\lambda \frac{d}{dz} P_k^\lambda(\mathbf{k},z) = -ik\gamma_k^\lambda P_z^\lambda(\mathbf{k},z) , \tag{8a}$$

$$\gamma_z^\lambda \frac{d}{dz} P_z^\lambda(\mathbf{k},z) = -ik\gamma_z^\lambda P_k^\lambda(\mathbf{k},z) , \tag{8b}$$

and

$$\gamma_i^\lambda \left[\frac{d^2}{dz^2} - k^2 \right] P_i^\lambda(k,z) = 0 \quad (i=k,z) . \tag{9}$$

On the basis of Eqs. (8) and (9) and the convergence of the solutions in zones II and III, we may assume the following forms for the solutions:

$$\phi_k^{\mathrm{I}}(\mathbf{k},z) = A^{\mathrm{L}} e^{kz} + B^{\mathrm{I}} e^{-kz} ,$$

$$\phi_z^{\mathrm{I}}(\mathbf{k},z) = -iA^{\mathrm{I}} e^{kz} + iB^{\mathrm{I}} e^{-kz}, \quad |z| \le d ; \tag{10a}$$

$$\phi_k^{\mathrm{II}}(\mathbf{k},z) = A^{\mathrm{II}} e^{-kz} ,$$

$$\phi_z^{\mathrm{II}}(\mathbf{k},z) = iA^{\mathrm{II}} e^{-kz}, \quad z > d ; \tag{10b}$$

$$\phi_k^{\mathrm{III}}(\mathbf{k},z) = A^{\mathrm{III}} e^{kz} ,$$

$$\phi_z^{\mathrm{III}}(\mathbf{k},z) = -iA^{\mathrm{III}} e^{kz}, \quad z < -d . \tag{10c}$$

Inserting the solutions into Eqs. (7b) and (7c), one can obtain the following conditions between coefficients A and B:

$$\left[\frac{\epsilon_1+1}{\epsilon_1-1} + e^{-2kd} \right] (A^{\mathrm{I}} - B^{\mathrm{I}}) + e^{-2kd} (A^{\mathrm{II}} - A^{\mathrm{III}}) = 0 ,$$

$$(e^{2kd} - e^{-2kd})(A^{\mathrm{I}} + B^{\mathrm{I}}) + \left[\frac{\epsilon_2+1}{\epsilon_2-1} + e^{-2kd} \right] (A^{\mathrm{II}} + A^{\mathrm{III}}) = 0 , \tag{11}$$

$$\left[\frac{\epsilon_1+1}{\epsilon_1-1} + e^{-2kd} \right] (A^{\mathrm{I}} - B^{\mathrm{I}}) + e^{-2kd} (A^{\mathrm{II}} - A^{\mathrm{III}}) = 0 ,$$

$$(e^{2kd} - e^{-2kd})(A^{\mathrm{I}} - B^{\mathrm{I}}) + \left[\frac{\epsilon_2+1}{\epsilon_2-1} - e^{-2kd} \right] (A^{\mathrm{II}} - A^{\mathrm{III}}) = 0 .$$

The criterion for existence of the nonzero solutions of Eq. (14) is

$$\frac{\epsilon_1+\epsilon_2}{\epsilon_1+\epsilon_2} = \pm e^{-2kd} . \tag{12}$$

Using the relation between the dielectric function in the medium j and the frequency ω,

$$\epsilon_j(\omega) = \epsilon_{\infty j} \frac{\omega_{Lj}^2 - \omega^2}{\omega_{Tj}^2 - \omega^2} , \tag{13}$$

the frequency satisfying Eq. (12) can be given as follows:

$$\omega_{\pm p}^2 = \frac{B_p(k) \pm [B_p^2(k) - 4A_p(k)C_p(k)]^{1/2}}{2A_p(k)} , \tag{14}$$

where

$$A_p(k) = a_1^p + a_2^p ,$$

$$B_p(k) = a_1^p(\omega_{L1}^2 + \omega_{T2}^2) + a_2^p(\omega_{L2}^2 + \omega_{T1}^2) ,$$

$$C_p(k) = a_1^p \omega_{L1}^2 \omega_{T2}^2 + a_2^p \omega_{L2}^2 \omega_{T1}^2 ,$$

and p is the parity and can be chosen as $+$ or $-$. The corresponding a_j^p are given by the formulas

$$a_1^{\pm} = (1 \mp e^{-2kd}) \epsilon_{\infty 1} ,$$

$$a_2^{\pm} = (1 \pm e^{-2kd}) \epsilon_{\infty 2} ,$$

where $\epsilon_{\infty j}$ is the high-frequency dielectric constant for medium j.

We have the four branches of polarization modes $\omega_{\sigma p}$ for $\sigma = +$ or $-$ and $p = +$ or $-$. The normalized eigenvectors of the modes can be given by

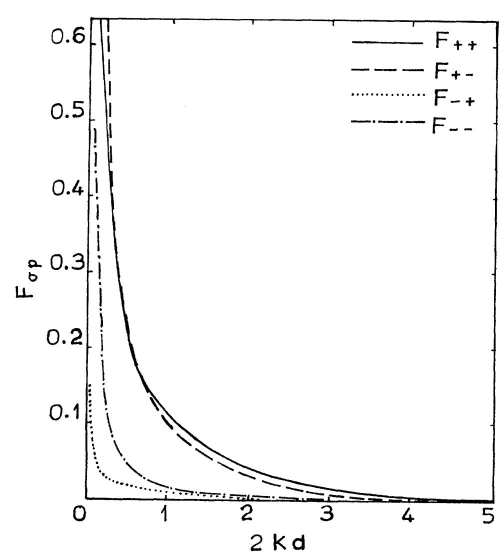

FIG. 1. Electron–SO-phonon coupling functions $F_{\sigma p}$ as functions of $2kd$ for a GaSb-InAs-GaSb quantum well. $F_{\sigma p}$ is measured in units of $(2\pi e^2 \hbar \omega_{T1}/S)^{1/2}$ and the length in units of $2d$. We have set the z-dependent factor in $F_{\sigma p}$ to 1.

$$\phi_{\sigma+}(\mathbf{k},z)=\begin{cases}2A_+(\cosh(kz),\ -i\sinh(kz)), & |z|\le d\\ \left[1-\frac{\epsilon_1+1}{\epsilon_1-1}e^{2kd}\right]A_+(e^{-kz},\ -ie^{-kz}), & z>d\\ \left[1-\frac{\epsilon_1+1}{\epsilon_1-1}e^{2kd}\right]A_+(e^{kz},\ -ie^{kz}), & z<-d\ ;\end{cases} \tag{15}$$

$$\phi_{\sigma-}(\mathbf{k},z)=\begin{cases}2A_-(\sinh(kz),\ -i\cosh(kz)), & |z|\le d\\ \left[1+\frac{\epsilon_1+1}{\epsilon_1-1}e^{2kd}\right]A_-(-e^{-kz},\ -ie^{-kz}), & z>d\\ \left[1+\frac{\epsilon_1+1}{\epsilon_1-1}e^{2kd}\right]A_-(e^{kz},\ -ie^{kz}), & z<-d\ ;\end{cases} \tag{16}$$

with

$$A_\pm=\left[\frac{k}{2\left[\left[\frac{\epsilon_1+1}{\epsilon_1-1}e^{2kd}\mp 1\right]^2 e^{-2kd}+2\sinh(2kd)\right]}\right]^{1/2}. \tag{17}$$

Now let us consider the electron-phonon interaction. We write the relative displacement $\mathbf{u}(r,t)$ as

$$\mathbf{u}(\mathbf{r},t)=\sum_{\mathbf{k},m,p}\mathbf{e}_{\mathbf{k}mp}(\mathbf{r})\left[\frac{\hbar}{2n\mu\omega_{mp}}\right]^{1/2}(a_{\mathbf{k}mp}-a^\dagger_{-\mathbf{k}mp})\ , \tag{18a}$$

and its conjugate momentum as

$$\pi(\mathbf{r},t)=-i\sum_{\mathbf{k},m,p}\mathbf{e}_{\mathbf{k}mp}(\mathbf{r})\left[\frac{\hbar n\mu\omega_{mp}}{2}\right]^{1/2}(a_{\mathbf{k}mp}+a^\dagger_{-\mathbf{k}mp})\ . \tag{18b}$$

In Eq. (18) $\mathbf{e}_{\mathbf{k}mp}(r)$ is given by

$$\mathbf{e}_{\mathbf{k}mp}(\mathbf{r})=\frac{1}{\sqrt{S}}e^{i\mathbf{k}\cdot\mathbf{p}}\boldsymbol{\phi}_{mp}(\mathbf{k},z)$$

and $a_{\mathbf{k}mp}$ is the annihilation operator of the phonon corresponding to the eigenvector $\boldsymbol{\phi}_{mp}(\mathbf{k},z)$. When m is a positive integer we have the LO mode. If m is σ we get the SO modes. We also have the commutation relations

$$[u_i(\mathbf{r},t),\ \pi_j(\mathbf{r}',t)]=i\hbar\delta_{ij}\delta(\mathbf{r}-\mathbf{r}')\ ,$$

$$[u_i(\mathbf{r},t),\ u_j(\mathbf{r}',t)]=[\pi_i(\mathbf{r},t),\ \pi_j(\mathbf{r}',t)]=0\ ,$$

and then

$$[a_{\mathbf{k}mp},a^\dagger_{\mathbf{k}'m'p'}]=\delta_{\mathbf{k}\mathbf{k}'}\delta_{mm'}\delta_{pp'}\ ,$$

$$[a_{\mathbf{k}mp},a_{\mathbf{k}'m'p'}]=[a^\dagger_{\mathbf{k}mp},a^\dagger_{\mathbf{k}'m'p'}]=0\ .$$

By the usual quantization procedure we obtain the Hamiltonian of the free-phonon field

$$H_{\rm ph}=\sum_{k,m,p}\hbar\omega_{mp}(a^\dagger_{\mathbf{k}mp}a_{\mathbf{k}mp}+\tfrac{1}{2})\ . \tag{19}$$

For the Hamiltonian of electron-phonon interaction, we have

$$H_{e\text{-ph}}=\int e\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|^3}\cdot\mathbf{P}(\mathbf{r}')d\mathbf{r}'\ , \tag{20}$$

where $\mathbf{r}$ is the position vector of the electron. On the other hand, one can easily find the following relations from Eqs. (1)–(4):

$$\mathbf{E}^\lambda(\mathbf{k},z)=(4\pi/3+\nu_k)\mathbf{P}^\lambda(\mathbf{k},z)\ , \tag{21a}$$

$$\mathbf{P}^\lambda(\mathbf{k},z)=\frac{n_\lambda e_\lambda}{1-n_\lambda\alpha_\lambda(4\pi/3+\nu_k^\lambda)}\mathbf{u}_\lambda(\mathbf{k},\mathbf{z})\ . \tag{21b}$$

Carrying out a 2D Fourier transform for Eq. (20), using (18a) and (21), we have finally obtained a Fröhlich-like Hamiltonian as follows:

$$H_{e\text{-ph}}=\sum_{k,m,p}F_{mp}(\mathbf{k},z)e^{i\mathbf{k}\cdot\mathbf{p}}(a_{\mathbf{k}mp}-a^\dagger_{-\mathbf{k}mp})\ , \tag{22}$$

where

$$F_{mp}(\mathbf{k},z)=\int dz'\left[\frac{\pi\hbar e^2\omega_p^2}{2S\omega_{mp}}\right]^{1/2}[1-n\alpha(\tfrac{4}{3}\pi+\nu_k)]^{-1}\times e^{-k|z'-z|}\frac{i\mathbf{K}}{k}\cdot\boldsymbol{\phi}^*_{mp}(\mathbf{k},z')\ . \tag{23}$$

For the electron–LO-phonon interaction, we have the following from (23):

$$H_{e\text{-}l}=\sum_{\mathbf{k}}i\left[\frac{4\pi e^2}{V}\hbar\omega_{\rm L1}\left[\frac{1}{\epsilon_{\infty 1}}-\frac{1}{\epsilon_{01}}\right]\right]^{1/2}e^{i\mathbf{k}\cdot p}\times\left[\sum_{m=1,3,\ldots}\frac{\cos\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}a_{\mathbf{k}m+}+\sum_{m=2,4,\ldots}\frac{\sin\left[\frac{m\pi}{2d}z\right]}{\left[k^2+\left[\frac{m\pi}{2d}\right]^2\right]^{1/2}}a_{\mathbf{k}m-}\right]+\text{H.c.} \tag{24}$$

This is the same result as Licari and Evrard (LE).[9] Here ϵ_{01} and $\epsilon_{\infty 1}$ are, respectively, the static and the high-frequency dielectric constants. ρ is the 2D component of the position vector of the electron on the x-y plane.

For the surfacelike optical phonons we have

$$H_{e\text{-SO}}=\sum_{\mathbf{k},\sigma,p} F_{\sigma p}(\mathbf{k},z)e^{i\mathbf{k}\cdot\rho}(a_{\mathbf{k}\sigma p}-a^{\dagger}_{-\mathbf{k}\sigma p}) \quad (25)$$

and

$$F_{\sigma+}(\mathbf{k},z)=i\left[\frac{2\pi\hbar e^2}{S\omega_{\sigma+}}\right]^{1/2}\frac{(\epsilon_2\Delta_1-\epsilon_1\Delta_2)}{(\epsilon_1-1)(\epsilon_2-\epsilon_1)}\left[\frac{2A_+}{k}\right]\cosh(kz)\,, \quad (26a)$$

$$F_{\sigma-}(\mathbf{k},z)=i\left[\frac{2\pi\hbar e^2}{S\omega_{\sigma-}}\right]^{1/2}\frac{(\epsilon_2\Delta_1-\epsilon_1\Delta_2)}{(\epsilon_1-1)(\epsilon_2-\epsilon_1)}\left[\frac{2A_-}{k}\right]\sinh(kz)\,, \quad (26b)$$

with

$$\Delta_j=\frac{\omega_{Tj}(\epsilon_{0j}-\epsilon_{\infty z})^{1/2}(\epsilon_j-1)^2}{\epsilon_j-\epsilon_{\infty j}} \quad (j=1,2)\,.$$

It is seen from our results that the SO modes in a quantum well are different from that in a film. For the case of quantum well we have four branches of the surfacelike optical modes and the electron-phonon coupling function relates to not only the wave vector $\mathbf{k}$, the thickness of the quantum well, and the position z, but also the parameters of the two kinds of medium, such as the dielectric constants and the frequencies of the optical phonons, etc.

It is easily found that eigenvectors and the electron-phonon coupling functions for the SO modes are localized near the interfaces. Their absolute values get maximum values at $z=\pm d$ and go down when they are far from the interfaces. This is why we call them surfacelike modes.

For understanding the properties of the electron–SO-phonon interaction in detail, we have numerically computed the coupling functions $F_{\sigma p}$ for the GaSb-InAs-GaSb quantum well. The parameters used for the computation are chosen as InAs: $\epsilon_{01}=14.61$, $\epsilon_{\infty 1}=11.80$, $\hbar\omega_{T1}=27.14$ meV, and $\hbar\omega_{L1}=30.20$ meV; GaSb: $\epsilon_{02}=15.69$, $\epsilon_{\infty 2}=14.44$, $\hbar\omega_{T2}=28.59$, and $\hbar\omega_{L2}=29.80$ from Ref. 11. We have plotted these coupling functions as functions of $2kd$ in Fig. 1. For simplicity, we set the factor depending upon z as 1 here. It is shown that the coupling functions $F_{\sigma p}$ attenuate with an increase of the wave vector k and the thickness $2d$. Only the phonons of longer wavelengths are important for the electron-phonon interaction. The two branches of higher frequencies are more important for the electron-phonon interaction than the other two in the four branches of SO modes. On the other hand, the thinner the quantum well, the stronger is the electron–SO-phonon interaction. For a sufficiently thick well the interaction between the electron and SO phonons can be neglected.

It is also found that when the thickness is large enough, we get the 3D Hamiltonian for the electron-phonon interaction from our Hamiltonian (22). If the electron is localized near an interface, the Hamiltonian then reduces to the ordinary Hamiltonian of the electron–interface-optical-phonon interaction. If the medium outside the quantum well is a nonpolar crystal—for instance, the vacuum—our results reduce to Licari and Evrard's.[9] We had used it to discuss the properties of polarons in a polar slab in previous work.[12]

To sum up, we have discussed the optical polarization modes of lattice vibration in a quantum well and developed a more complete Fröhlich-like Hamiltonian of electron–optical-phonon interaction in this work. Our results have demonstrated that the LO modes in a quantum well are the same as those in a thin film. However, the SO modes are quite different from those in a monolayer film. This new Hamiltonian is necessary for providing a more accurate description of the electron-phonon interaction in a quantum well.

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