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The properties of a polaron in a polar-crystal slab

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Abstract. In this paper, using the effective-mass approximation and the variational method the ground-state and the first-excited-state energy shifts of a polaron in a polar-crystal slab, due to the interactions of the electron with the BO and SO phonons, are calculated self-consistently. Our results are different from the results obtained by Gu *et al*.

1. Introduction

There has been a considerable amount of work [2–10] on the properties of the electron in a quantum well in recent years. Licari and Evrard [1] derived a Hamiltonian for the electron–phonon interaction in a slab, which included the interactions of electron with confined bulk longitudinal optical (BO) phonons and with surface longitudinal optical (SO) phonons. Gu *et al* [2] applied the Hamiltonian of Licari and Evrard and the variational method to calculate the ground-state and the first-excited-state energy shifts of a polaron in a slab due to the interactions of the electron with the BO and SO phonons. However, Gu *et al* diagonalized approximately the polaron Hamiltonian instead of minimizing the energy to determine the variation parameters. Thus the variation parameters obtained by them are dependent on the electron space coordinate Z. In this paper, using a similar method to that of Gu *et al* [2] and minimizing the energies to determine the variation parameters we calculate self-consistently the ground-state and the first-excited-state energy shifts due to the interactions of the electron with the BO and SO phonons. Our results are different from their results. We point out that setting the linear term of the phonon operators in the effective Hamiltonian to zero, i.e. diagonalizing approximately the polaron Hamiltonian to determine the variation parameters as applied by Gu *et al* [2], is not suitable for the quasi-two-dimensional quantum well system.

2. The Hamiltonian

We assume that a slab with thickness $2d$ is made of a polar crystal and is surrounded by a vacuum (figure 1). The linear scale of the surface of the slab is taken to be much larger than $2d$. If the isotropic effective-mass approximation is adopted, the Hamiltonian of the system, consisting of an electron, the confined BO phonons and the SO phonons, may be written as [2]

$$H = H_e + H_{ph} + H_{e\text{-BO}} + H_{e\text{-SO}} \tag{1a}$$

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where

$$H_e = -(\hbar^2/2m^*)(\partial^2/\partial z^2 + \nabla_\rho^2) + v \tag{1b}$$

$$v = \begin{cases} 0 & |z| \leqslant d \\ \infty & |z| > d \end{cases} \tag{1c}$$

$$H_{ph} = H_{BO} + H_{SO} \tag{1d}$$

$$H_{BO} = \sum_{k,m,p} \hbar\omega_{LO} a^+_{m,p}(k) a_{m,p}(k) \tag{1e}$$

$$H_{SO} = \sum_{q,p} \hbar\omega_{so,p} b^+_p(q) b_p(q). \tag{1f}$$

In the above equations, ρ is the position vector of the electron on the X–Y plane and m^* is the band mass of the electron; H_{BO} and H_{SO} are the Hamiltonians of the BO phonons and the SO phonons, respectively; $a^+_{m,p}(k)$ and $a_{m,p}(k)$ are the creation and annihilation operators, respectively, of the BO phonons with the frequency ω_{LO} and the wavevector $(k, m\pi/2d)$ (k is the projection on the X–Y plane of the wavevector); $b^+_p(q)$ and $b_p(q)$ are the creation and annihilation operators, respectively, of the SO phonons with the frequency $\omega_{so,p}$ and the wavevector q. The subscript p is the parity with respect to the mirror symmetry of the plane for $Z = 0$, and m is the quantum number of the wavevector of the BO phonons in the Z direction. For even parity (represented by the + sign), m is odd while, for odd parity (represented by the − sign), m is even. We take N as the slab thickness in units of the lattice constant a, namely $Na = 2d$. Being limited by the Brillouin-zone boundary, m may be any integer within the range $1 \leqslant m \leqslant N/2$.

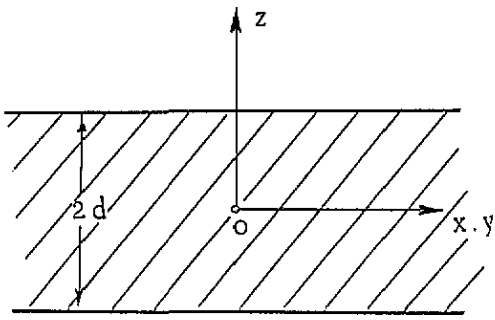

Figure 1. Geometry of the polar-crystal slab.

The phonon frequencies ω_{LO} and $\omega_{so,p}$ can be expressed in terms of the transverse-optical (TO)-phonon frequency ω_{TO} by

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

$$\omega^2_{so,\pm} = \omega^2_{TO}\{[(\epsilon_0 + 1) \mp (\epsilon_0 - 1)\exp(-2qd)]/[(\epsilon_\infty + 1) \mp (\epsilon_\infty - 1)\exp(-2qd)]\} \tag{2b}$$

where ϵ_0 and ϵ_∞ are the static and the optical dielectric constants, respectively.

$H_{e\text{-BO}}$ and $H_{e\text{-SO}}$ in equation (1) are the interaction Hamiltonians of the electron with the BO phonons and with the SO phonons, respectively and they are taken directly from [1]:

$$H_{e\text{-BO}} = \sum_{k}\left[B^* \exp(-i\boldsymbol{k}\cdot\boldsymbol{\rho})\left(\sum_{m=1,3,\ldots}\frac{\cos(m\pi z/2d)}{[k^2+(m\pi/2d)^2]^{1/2}}a^+_{m,+}(\boldsymbol{k}) + \sum_{m=2,4,\ldots}\frac{\sin(m\pi z/2d)}{[k^2+(m\pi/2d)^2]^{1/2}}a^+_{m,-}(\boldsymbol{k})\right) + \text{HC}\right] \tag{3a}$$

$$H_{e\text{-SO}} = \sum_{q}\left(\frac{\sinh(2qd)}{q}\right)^{1/2}\exp(-qd)\{C^*\exp(-i\boldsymbol{q}\cdot\boldsymbol{\rho}) \times [G_+(q,z)b^+_+(\boldsymbol{q}) + G_-(q,z)b^+_-(\boldsymbol{q})] + \text{HC}\} \tag{3b}$$

where A and V are the area and the volume, respectively, of the slab, and

$$B^* = i[(4\pi e^2/V)\hbar\omega_{LO}(1/\epsilon_\infty - 1/\epsilon_0)]^{1/2} \tag{3c}$$

$$C^* = i[(2\pi e^2/A)\hbar\omega_{TO}(\epsilon_0 - \epsilon_\infty)]^{1/2} \tag{3d}$$

$$G_+(q,z) = \{[\cosh(qz)/\cosh(qd)]/[(\epsilon_\infty+1) - (\epsilon_\infty - 1)\exp(-2qd)]\} \times \{[(\epsilon_\infty+1) - (\epsilon_\infty-1)\exp(-2qd)]/[(\epsilon_0+1) - (\epsilon_0-1)\exp(-2qd)]\}^{1/4} \tag{3e}$$

$$G_-(q,z) = \{[\sinh(qz)/\sinh(qd)]/[(\epsilon_\infty+1) + (\epsilon_\infty-1)\exp(-2qd)]\} \times \{[(\epsilon_\infty+1) + (\epsilon_\infty-1)\exp(-2qd)]/[(\epsilon_0+1) + (\epsilon_0-1)\exp(-2qd)]\}^{1/4}. \tag{3f}$$

Now we introduce the following two unitary transformations:

$$U_1 = \exp\left[-i\boldsymbol{\rho}\cdot\left(\sum_{k,m,p}\boldsymbol{k}\,a^+_{m,p}(\boldsymbol{k})a_{m,p}(\boldsymbol{k}) + \sum_{q,p}\boldsymbol{q}\,b^+_p(\boldsymbol{q})b_p(\boldsymbol{q})\right)\right] \tag{4a}$$

$$U_2 = \exp\left(\sum_{k,m,p}[a^+_{m,p}(\boldsymbol{k})f_{m,p}(\boldsymbol{k}) - a_{m,p}(\boldsymbol{k})f^*_{m,p}(\boldsymbol{k})] + \sum_{q,p}[b^+_p(\boldsymbol{q})g_p(\boldsymbol{q}) - b_p(\boldsymbol{q})g^*_p(\boldsymbol{q})]\right) \tag{4b}$$

where $f_{m,p}(\boldsymbol{k})$ and $g_p(\boldsymbol{q})$ and their conjugate terms $f^*_{m,p}(\boldsymbol{k})$ and $g^*_p(\boldsymbol{q})$ are the variation parameters which will subsequently be determined by minimizing the energy. Then H in equation (1) can be transformed into

$$\mathcal{H} = U_2^{-1}U_1^{-1}HU_1U_2 = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \frac{\hbar^2K_\parallel^2}{2m^*} + \frac{\hbar^2}{2m^*}\left(\sum_{k,m,p}u_1^2[a^+_{m,p}(\boldsymbol{k}) + f^*_{m,p}(\boldsymbol{k})] \times [a_{m,p}(\boldsymbol{k}) + f_{m,p}(\boldsymbol{k})] + \sum_{q,p}u^2_{s,p}[b^+_p(\boldsymbol{q}) + g^*_p(\boldsymbol{q})][b_p(\boldsymbol{q}) + g_p(\boldsymbol{q})]\right)$$

$$+\sum_k\left[B^*\left(\sum_{m=1,3,\ldots}\frac{\cos(m\pi z/2d)}{[k^2+(m\pi/2d)^2]^{1/2}}[a^+_{m,+}(k)+f^*_{m,+}(k)]\right.\right.$$

$$\left.\left.+\sum_{m=2,4,\ldots}\frac{\sin(m\pi z/2d)}{[k^2+(m\pi/2d)^2]^{1/2}}[a^+_{m,-}(k)+f^*_{m,-}(k)]\right)+\text{HC}\right]$$

$$+\sum_q\left(\frac{\sinh(2qd)}{q}\right)^{1/2}\exp(-qd)[[C^*\{G_+(q,z)[b^+_+(q)$$

$$+g^*_+(q)]+G_-(q,z)[b^+_-(q)+g^*_-(q)]\}+\text{HC}]]$$

$$+\frac{\hbar^2}{2m^*}\left|\sum_{k,m,p}k[a^+_{m,p}(k)+f^*_{m,p}(k)][a_{m,p}(k)+f_{m,p}(k)]\right|^2$$

$$+\frac{\hbar^2}{2m^*}\left|\sum_{q,p}q[b^+_p(q)+g^*_p(q)][b_p(q)+g_p(q)]\right|^2$$

$$-\frac{\hbar^2}{m^*}\sum_{k,m,p}\boldsymbol{K}_\parallel\cdot k[a^+_{m,p}(k)+f^*_{m,p}(k)][a_{m,p}(k)+f_{m,p}(k)]$$

$$-\frac{\hbar^2}{m^*}\sum_{q,p}\boldsymbol{K}_\parallel\cdot q[b^+_p(q)+g^*_p(q)][b_p(q)+g_p(q)]$$

$$+\frac{\hbar^2}{m^*}\sum_{k,m,p}k[a^+_{m,p}(k)+f^*_{m,p}(k)][a_{m,p}(k)+f_{m,p}(k)]$$

$$\cdot\sum_{q,p}q[b^+_p(q)+g^*_p(q)][b_p(q)+g_p(q)] \tag{5}$$

where $\boldsymbol{K}_\parallel$ is the projection of the momentum of the polaron on the X–Y plane and is a conservation quantity. u_l and $u_{s,p}$, respectively, are defined by the following equations:

$$\hbar^2u_l^2/2m^*=\hbar\omega_{LO}\qquad\hbar^2u_{s,p}^2/2m^*=\hbar\omega_{so,p}.$$

In the derivation of equation (5) we always keep the variation parameters independent of the electron space coordinate.

3. The energies

It is necessary to point out that we are interested only in the slow electron, i.e. we can set $\boldsymbol{K}_\parallel=0$. Here we pay attention only to the low-temperature limitation state where there are no real phonons in the system. For $\mathcal{H}$ represented by equation (5) the trial wavefunction of a polaron ($\boldsymbol{K}_\parallel=\boldsymbol{0}$) in the slab may be chosen as

$$|\psi_l\rangle=\begin{cases}(1/\sqrt{d})\sin[(l\pi/2d)(z+d)]|0\rangle & |z|\leqslant d\\ 0 & |z|>d\end{cases} \tag{6}$$

where l is a positive integer ($1\leqslant l\leqslant N=2d/a$); $|0\rangle$ is the vacuum state of the phonons, i.e.,

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

Considering the symmetry and the slow electron (setting $K_{\parallel} = 0$) we have [2]

$$\sum_{k,m,p} k\,|f_{m,p}(k)|^2 = 0$$

$$\sum_{q,p} q\,|g_p(q)|^2 = 0.$$

According to the variation method, from

$$\delta\langle\psi_l|\mathcal{H}|\psi_l\rangle/\delta f^*_{m,p}(k) = \delta\langle\psi_l|\mathcal{H}|\psi_l\rangle/\delta f_{m,p}(k) = \delta\langle\psi_l|\mathcal{H}|\psi_l\rangle/\delta g^*_p(q)$$
$$= \delta\langle\psi_l|\mathcal{H}|\psi_l\rangle/\delta g_p(q) = 0 \tag{7}$$

and inserting equation (5) and equation (6) into equation (7), we can obtain

$$f_{m,+}(k) = -B^* W_{m,+}(k)/[(\hbar^2/2m^*)(k^2 + u_l^2)] \tag{8a}$$

$$f^*_{m,+}(k) = -B W_{m,+}(k)/[(\hbar^2/2m^*)(k^2 + u_l^2)] \tag{8b}$$

$$g_+(q) = -\left\{C^* V_+(q)[\sinh(2qd)/q]^{1/2}\exp(-qd)\right\}/[(\hbar^2/2m^*)(q^2 + u^2_{s,+})] \tag{8c}$$

$$g^*_+(q) = -\left\{C V_+(q)[\sinh(2qd)/q]^{1/2}\exp(-qd)\right\}/[(\hbar^2/2m^*)(q^2 + u^2_{s,+})] \tag{8d}$$

$$f_{m,-}(k) = f^*_{m,-}(k) = g_-(q) = g^*_-(q) = 0 \tag{8e}$$

where

$$W_{m,+}(k) = [8l^2/m(4l^2 - m^2)\pi]\sin(m\pi/2)[k^2 + (m\pi/2d)^2]^{-1/2} \tag{9a}$$

$$V_+(q) = \left\{[(l\pi/d)^2\tanh(qd)]/qd[q^2 + (l\pi/d)^2]\right\}\{1/[(\epsilon_\infty + 1) - (\epsilon_\infty - 1)\exp(-2qd)]\}$$
$$\times\{[(\epsilon_\infty + 1) - (\epsilon_\infty - 1)\exp(-2qd)]/[(\epsilon_0 + 1) - (\epsilon_0 - 1)\exp(-2qd)]\}^{1/4}. \tag{9b}$$

These variation parameters are independent of the Z coordinate of the electron. In [2] these parameters were determined by diagonalizing approximately the polaron Hamiltonian $\mathcal{H}$ and they are all functions of the Z coordinate of the electron. From the derivation of equation (5) it can be found that these parameters must be independent of the Z coordinate of the electron.

Using equations (5), (6) and (8*a*)–(8*e*) we can obtain the energy of a polaron in the slab:

$$E = E_l + \Delta E \tag{10a}$$

where E_l is the energy for the electron motion along the Z direction confined in an infinite square-well potential:

$$E_l = \pi^2\hbar^2 l^2/2m^*(Na)^2. \tag{10b}$$

ΔE is the total energy shift:

$$\Delta E = E_s^B + E_s^S. \tag{10c}$$

E_s^B is the energy shift of an electron due to the interaction of the electron with the confined BO phonons:

$$E_s^B = -4\alpha\hbar\omega_{LO}\sum_{m=1,3,\ldots}\frac{u_1}{Na}\left(\frac{8l^2}{m(4l^2-m^2)\pi}\right)^2\frac{\ln(m\pi/Nau_1)}{(m\pi/Na)^2-u_1^2} \tag{10d}$$

where

$$\alpha = m^*e^2(1/\epsilon_\infty - 1/\epsilon_0)/\hbar^2u_1.$$

E_s^S is the energy shift of an electron due to the interaction of the electron with the SO phonons:

$$E_s^S = -2\alpha\hbar\omega_{LO}\epsilon_0^{1/2}\epsilon_\infty^{3/2}Nau_1I \tag{10e}$$

where

$$I = \int_0^{N\pi/2} dx\,\frac{\sinh(x)\exp(-x)}{x^2+(Nau_{s,+})^2}\left(\frac{8l^2\pi^2\tanh(x/2)}{x(x^2+4l^2\pi^2)}\right)^2\left(\frac{1}{(\epsilon_\infty+1)-(\epsilon_\infty-1)\exp(-x)}\right)^2$$
$$\times\left(\frac{(\epsilon_\infty+1)-(\epsilon_\infty-1)\exp(-x)}{(\epsilon_0+1)-(\epsilon_0-1)\exp(-x)}\right)^{1/2}. \tag{10f}$$

In equation (10*f*) we have set $x = 2qd$.

4. Results and discussion

We take a GaAs slab as an example to present our numerical results. The characteristic parameters in our numerical calculations are as follows: $\epsilon_0 = 12.83$, $\epsilon_\infty = 10.9$, $a = 0.5654$ nm, $\hbar\omega_{TO} = 33.83$ meV and $m^* = 0.0657m$.

Using equation (10*d*) we calculate the energy shift E_s^B due to the interaction of an electron with the BO phonons for the ground state ($l = 1$) and the first excited state ($l = 2$). Figure 2 shows the changes in E_s^B with the variation in the slab thickness N. For a very thin slab ($N < 22$), E_s^B rapidly decreases with increase in N. When $N = 22$, E_s^B is a minimum. When $N > 22$, E_s^B increases with increase in N. This result is different from that obtained by Gu *et al* [2].

Using equation (10*e*) we calculate the energy shift E_s^S due to the interaction of an electron with the SO phonons for the ground state ($l = 1$) and the first excited state ($l = 2$). Figure 3 shows the changes in E_s^S with the variation in the slab thickness N. For a thin slab the contribution of E_s^S is dominant compared with the total energy shift ΔE. When $N > 200$, E is very small compared with E_s^B. This result is also different from that obtained by Gu *et al* [2].

In three-dimensional polaron questions the variation parameters are determined by minimizing the energy. This method is consistent with the method diagonalizing approximately the polaron Hamiltonian, i.e. setting the linear term of the phonon operators in the effective Hamiltonian to zero since the variation parameters obtained by the two methods are the same and independent of the space coordinate of the electron [11]. In this paper we minimize the energies to determine the variation parameters (independent on the Z coordinate of the electron). This is a standard method [11]. Gu *et al* [2] did not

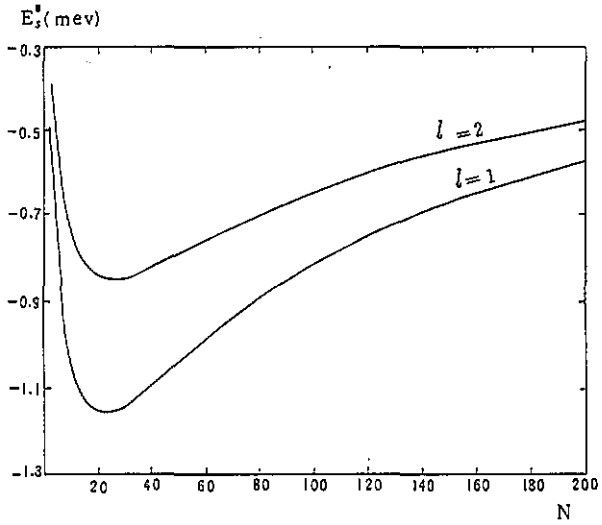

Figure 2. The energy shift E_s^B versus the slab thickness N.

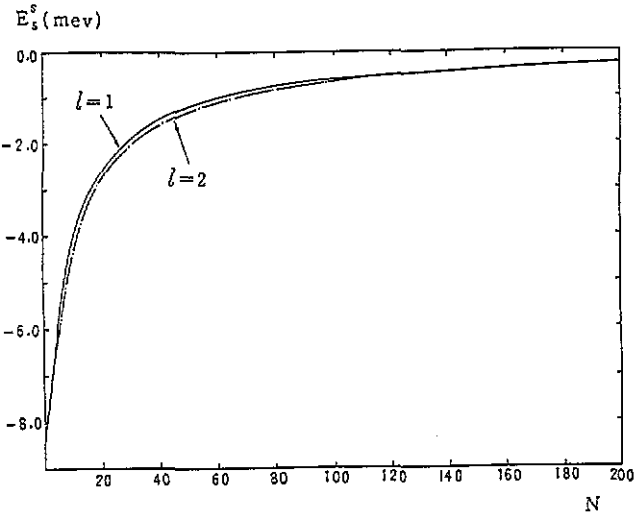

Figure 3. The energy shift E_s^S versus the slab thickness N.

fully take into account the difference between the quasi-two-dimensional system and the three-dimensional system. There is no translation symmetry in the Z direction (normal to the slab) for the quasi-two-dimensional quantum well system. The unitary transformation U_1 cannot be used to make the Hamiltonian in equation (1a) eliminate the Z coordinate of the electron. Taking note of the effective Hamiltonian in equation (5) which contains the Z coordinate of the electron and also the operator $\partial^2/\partial z^2$, we can understand that the variation parameters must be independent of the Z coordinate of the electron. In [2] the variation parameters obtained by Gu *et al* were functions of the Z coordinate of the electrons; thus their results are inaccurate. In this paper, by minimizing the energy to

determine the variation parameters (independent of the Z coordinate of the electron), we calculate the ground-state and the first-excited-state energy shifts of a polaron in a polar-crystal slab due to the interactions of the electron with BO and SO phonons. Our results are accurate compared with the results of [2]. This implies that the method employed in [2], i.e. diagonalizing approximately the polaron Hamiltonian to determine the variation parameters, is not suitable for the quasi-two-dimensional quantum well system.

References

[1] Licari J J and Evrard R 1977 *Phys. Rev.* B **15** 2254
[2] Gu S-W, Li Y-C and Zheng L-F 1989 *Phys. Rev.* B **39** 1346
[3] Sherman A V 1981 *Solid State Commun.* **39** 273
[4] Hawton M H and Paranjape V V 1983 *J. Phys. Soc. Japan* **49** 3563
[5] Das Sarma S 1983 *Phys. Rev.* B **27** 2590
[6] Larsen D M 1986 *Phys. Rev.* B **33** 799
[7] Gu S-W and Shen M-Y 1987 *Phys. Rev.* B **35** 9817
[8] Gu S-W, Kong X-J and Wei C-W 1988 *J. Phys. C: Solid State Phys.* **21** 1497
[9] Kong X-J, Wei C-W and Gu S-W 1989 *Phys. Rev.* B **39** 3230
[10] Wei B-H and Gu S-W 1990 *Phys. Rev.* B **43** 9190
[11] Lee T D, Low F E and Pines D 1953 *Phys. Rev.* **90** 297