The effect of electron-phonon interaction on the impurity binding energy in a quantum well

1999 J. Phys.: Condens. Matter 11 8185

(http://iopscience.iop.org/0953-8984/11/42/302)

J. Phys.: Condens. Matter **11** (1999) 8185–8196. Printed in the UK PII: S0953-8984(99)05051-1

The effect of electron–phonon interaction on the impurity binding energy in a quantum well

Yueh-Nan Chen, Der-San Chuu† and Yuh-Kae Lin

Department of Electrophysics, National Chiao Tung University, HsinChu 30050, Taiwan

E-mail: dschuu@cc.nctu.edu.tw

Received 7 July 1999, in final form 19 August 1999

Abstract. The effect of confined electron–optical phonon interaction on the hydrogenic impurity binding energy in a quantum well is studied. By using the Landau and Pekar variational method, the Hamiltonian is separated into two parts which contain phonon variables and electron variables. A perturbative–variational technique is then employed to construct the trial wave function for the electron part. The effects of electron–optical phonon interaction on the binding energies are calculated as functions of the well width. In the study of the polaron effects on the impurity binding energies in a quantum well, both confined bulk optical phonon and surface optical phonon effects are taken into account. It is found that the surface phonon effect prevails over the bulk phonon effect when the well width is small. The polaron effects on lower-lying excited states are also calculated. The line strengths of transitions from the ground state to lower-lying excited states are calculated as functions of the donor position and the well width.

1. Introduction

During recent decades the great progress in epitaxial crystal growth techniques has made it possible to fabricate quasi-two-dimensional (quantum well) or quasi-one-dimensional (quantum wire) [1–4] systems with controllable well width or wire radius. This has led to much intensive study of these low-dimensional systems because of their potential device applications. The physics of impurity states of a donor in a quantum well is very interesting, because specific properties can easily be achieved by varying the well width [5–9]. An electron bound to an donor impurity at the centre of the quantum well behaves like a bound three-dimensional electron when the boundary is far away. However, as the well width is reduced, the confinement due to the potential barrier becomes very important. Recently, many authors have studied the polaron effect on the binding energy of impurities or excitons in quantum wells [10–18]. In studying the polaron effect on the impurity binding energy, most of the previous works considered the interaction of the electron and bulk longitudinal optical (BO) phonon only. The polaron shifts in donor energy levels are found to be of the order of 10% in a weakly polar system.

Since the surface-to-volume ratio is significantly large for a narrower quantum well structure, an electron moving inside such quantum structures may be affected significantly by the surface (SO) phonon [19]. Besides this, the electron–phonon interaction Hamiltonians in many of the previous works were valid only for the bulk. Therefore, we will choose the

† Author to whom any correspondence should be addressed.

0953-8984/99/428185+12$30.00

Hamiltonian derived by Zheng, Ban, and Liang [20], who considered the confined phonon modes in a quantum well.

Conventionally, the previous workers usually exploited the variational method or perturbation method, and concentrated on the polaron effect on the ground state of an impurity in a quantum well. However, the construction of variational trial wave functions is based entirely on physical intuition, and the estimation of the accuracy of the results obtained from the variational approach is very difficult. Furthermore, the perturbation method only provides good access to those systems with very small perturbation in most cases. Therefore, it would be most desirable to have an alternative approach to the quantum well problem which is not only simple but also efficient.

In this work, we employ a simple approximation treatment which combines the spirit of the variational principle and the perturbational approach to study the confined phonon effects on the binding energy of a hydrogenic impurity located inside a quantum well. The electron–BO phonon and the electron–SO phonon interactions are both taken into account in our calculation. The image charge effects may be significant if there is a large dielectric discontinuity between the well and the surrounding medium. However, since the purpose of this work is to concentrate on the confined phonon effects on the impurity binding energies, the image effects are not taken into account in the present calculation.

2. Theory

We consider a quantum well consisting of well material in region 1, $-L/2 < z < L/2$, and barriers in region 2, $|z|\rangle L/2$. Within the framework of the effective-mass approximation, the total Hamiltonian of the electron interacting with the BO and SO phonons can be written as

$$H = H_e + H_{bp} + H_{sp} + H_{e-bp} + H_{e-sp}. \tag{1}$$

Here the first term, H_e, is the electronic part including the electronic energy and the confining potential experienced by the electron, and is given by

$$H_e = -\frac{\overline{h}^2}{2\mu}\nabla_e^2 - \frac{e^2}{\epsilon\sqrt{(x^2+y^2+(z-z_i)^2)}} + V(z) \tag{2}$$

with

$$V(z) = \begin{cases} 0 & \text{for } |z| \leqslant L/2 \\ \infty & \text{for } |z| > L/2 \end{cases} \tag{3}$$

where ε, μ, and z_i are the dielectric constant of the well, the effective mass of the electron, and the impurity nucleus position, respectively. The confined BO phonon Hamiltonian H_{bp} is given by

$$H_{bp} = \sum_{\vec{q}m} \overline{h}\omega_{\vec{q}m} b^\dagger_{\vec{q}m} b_{\vec{q}m} \tag{4}$$

where $b^\dagger_{\vec{q}m}$ ($b_{\vec{q}m}$) is the creation (annihilation) operator of a BO phonon with frequency $\omega_{\vec{q}m}$ and wave vector $(\vec{q}, k_m)$. m refers to the confined LO phonon in the well material with frequency ω_{L_1} and wave vector $k_m = m\pi/L$. Also, the confined SO phonon Hamiltonian H_{sp} is given by

$$H_{sp} = \sum_{\vec{q}\sigma p} \overline{h}\omega_{\vec{q}\sigma p} a^\dagger_{\vec{q}\sigma p} a_{\vec{q}\sigma p} \tag{5}$$

where $a^\dagger_{\vec{q}\sigma p}$ ($a_{\vec{q}\sigma p}$) is the creation (annihilation) operator of a SO phonon (indices $\sigma = +, -$ label the high and low branches of the modes, and $p = +, -$ denote symmetric and antisymmetric

modes, respectively) with frequency $\omega_{\vec{q}\sigma p}$ and wave vector $\vec{q}$. The dispersion relation for the frequency $\omega_{\vec{q}\sigma p}$ is given by

$$\omega^2_{\vec{q}\pm p} = \frac{B_p(\vec{q}) \pm [B_p^2(\vec{q}) - 4A_p(\vec{q})C_p(\vec{q})]^{1/2}}{2A_p(\vec{q})} \tag{6}$$

where A_p, B_p, C_p are

$$A_p(\vec{q}) = \epsilon_{p1} + \epsilon_{p2}$$
$$B_p(\vec{q}) = \epsilon_{p1}(\omega^2_{L_1} + \omega^2_{T_2}) + \epsilon_{p2}(\omega^2_{L_2} + \omega^2_{T_1})$$
$$C_p(\vec{q}) = \epsilon_{p1}\omega^2_{L_1}\omega^2_{T_2} + \epsilon_{p2}\omega^2_{L_2}\omega^2_{T_1}$$

with

$$\epsilon_{\pm\lambda} = [1 \pm (-1)^\lambda \mathrm{e}^{-qL}]\epsilon_{\infty\lambda} \qquad (\lambda = 1, 2). \tag{7}$$

ω_{L_1} (ω_{L_2}) and ω_{T_1} (ω_{T_2}) are the longitudinal and transverse optical phonon frequencies, respectively, for material 1 (2). $\epsilon_{\infty\lambda}$ ($\epsilon_{0\lambda}$) is the high-frequency (static) dielectric constant for the material labelled λ.

H_{e-bp} is the interaction between the electron and BO phonon, which can be expressed as

$$H_{e-bp} = \sum_{\vec{q}m}[V_{\vec{q}m}(z)b_{\vec{q}m}\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{\rho}} + \mathrm{h.c.}] \tag{8}$$

where $\vec{\rho}$ is the position vector of the electron in the xy-plane, and $V_{\vec{q}m}(z)$ is the electron–BO phonon interaction strength:

$$V_{\vec{q}m}(z) = \frac{\mathrm{i}B}{\sqrt{q^2 + k_m^2}}\,\mathrm{csn}(k_m z) \tag{9}$$

with

$$B = \left(\frac{8\pi\alpha_1}{SL}\right)^{1/2}\left(\frac{\hbar}{2m_0\omega_{L_1}}\right)^{1/4}\hbar\omega_{L_1}$$

and

$$\mathrm{csn}(k_m z) = \begin{cases} \cos(k_m z) & m = 1, 3, 5, \ldots \\ \sin(k_m z) & m = 2, 4, 6, \ldots \end{cases} \tag{10}$$

where S stands for the area of the interface, and the positive integer m is limited by the Brillouin-zone boundary. The coupling constant α_1 is defined as

$$\alpha_1 = \frac{e^2}{2\hbar\omega_{L_1}}\left(\frac{2\mu\omega_{L_1}}{\hbar}\right)^{1/2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right). \tag{11}$$

H_{e-sp} is the term for the electron interacting with the SO phonon, and can be written as

$$H_{e-sp} = \sum_{\vec{q}\sigma p}[\Gamma_{\vec{q}\sigma p}(z)\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{\rho}}a_{\vec{q}\sigma p} + \mathrm{h.c.}]. \tag{12}$$

$\Gamma_{\vec{q}\sigma p}(z)$ are the electron–SO phonon interaction strengths:

$$\Gamma_{\vec{q}\sigma+}(z) = -\mathrm{i}D_{\sigma+}\left(\frac{qL}{2}\right)\left(\frac{2\pi\hbar e^2}{Sq\omega_{\vec{q}\sigma+}}\right)^{1/2}\frac{\cosh(qz)}{\cosh(qL/2)} \tag{13}$$

$$\Gamma_{\vec{q}\sigma-}(z) = -\mathrm{i}D_{\sigma-}\left(\frac{qL}{2}\right)\left(\frac{2\pi\hbar e^2}{Sq\omega_{\vec{q}\sigma-}}\right)^{1/2}\frac{\sinh(qz)}{\sinh(qL/2)} \tag{14}$$

where the $D_{\sigma\pm}$ are defined as

$$D_{\sigma+}\left(\frac{qL}{2}\right) = \left[2\xi_{1\sigma+}^2 \tanh\left(\frac{qL}{2}\right) + 2\xi_{2\sigma+}^2\right]^{-1/2} \tag{15}$$

$$D_{\sigma-}\left(\frac{qL}{2}\right) = \left[2\xi_{1\sigma-}^2 \coth\left(\frac{qL}{2}\right) + 2\xi_{2\sigma-}^2\right]^{-1/2} \tag{16}$$

with

$$\xi_{\lambda\sigma\pm} = \frac{\epsilon_{\lambda\sigma\pm} - \epsilon_{\infty\lambda}}{\omega_{T_\lambda}(\epsilon_{0\lambda} - \epsilon_{\infty\lambda})^{1/2}} \qquad (\lambda = 1, 2) \tag{17}$$

$$\epsilon_{\lambda\sigma\pm} = \epsilon_{\infty\lambda}\frac{\omega_{L_\lambda}^2 - \omega_{\sigma\pm}^2}{\omega_{T_\lambda}^2 - \omega_{\sigma\pm}^2} \qquad (\lambda = 1, 2). \tag{18}$$

Following Landau and Pekar's variational approach [21], the trial wave function can be written as

$$|\Psi\rangle = \Phi(\vec{r})\mathbf{U}_b\mathbf{U}_s|0\rangle \tag{19}$$

where $\Phi(\vec{r})$ depends only on the electron coordinate $\vec{r} = (\vec{\rho}, z)$, $|0\rangle$ is the phonon vacuum state defined by $b_{\vec{q}}|0\rangle = 0$, $a_{\vec{q}}|0\rangle = 0$, and the $\mathbf{U}$s are the unitary transformations given by

$$\mathbf{U}_b = \exp\left[\sum_{\vec{q}}(b_{\vec{q}m}^\dagger f_{\vec{q}m} - b_{\vec{q}m} f_{\vec{q}m}^*)\right] \tag{20}$$

$$\mathbf{U}_s = \exp\left[\sum_{\vec{q}\sigma p}(a_{\vec{q}\sigma p}^\dagger g_{\vec{q}\sigma p} - a_{\vec{q}\sigma p} g_{\vec{q}\sigma p}^*)\right] \tag{21}$$

and $f_{\vec{q}}$ and $g_{\vec{q}}$ are the variational functions. The unitary operators $\mathbf{U}_b$ and $\mathbf{U}_s$ transform the BO phonon and SO phonon operators as follows:

$$\mathbf{U}_b^\dagger b_{\vec{q}m}^\dagger \mathbf{U}_b = b_{\vec{q}m}^\dagger + f_{\vec{q}m}^* \tag{22}$$

$$\mathbf{U}_b^\dagger b_{\vec{q}m} \mathbf{U}_b = b_{\vec{q}m} + f_{\vec{q}m} \tag{23}$$

$$\mathbf{U}_s^\dagger a_{\vec{q}\sigma p}^\dagger \mathbf{U}_s = a_{\vec{q}\sigma p}^\dagger + g_{\vec{q}\sigma p}^* \tag{24}$$

$$\mathbf{U}_s^\dagger a_{\vec{q}\sigma p} \mathbf{U}_s = a_{\vec{q}\sigma p} + g_{\vec{q}\sigma p}. \tag{25}$$

Thus the expectation value of the total Hamiltonian can be obtained as

$$\begin{aligned}\langle\Psi|H|\Psi\rangle &= \langle 0|\Phi^*(\vec{r})\mathbf{U}_b^\dagger\mathbf{U}_s^\dagger H\mathbf{U}_s\mathbf{U}_b\Phi(\vec{r})|0\rangle \\ &= \langle\Phi(\mathbf{r})|H_e|\Phi(\vec{r})\rangle + \sum_{\vec{q}m}\overline{h}\omega_{\vec{q}m}|f_{\vec{q}m}|^2 + \sum_{\vec{q}\sigma p}\overline{h}\omega_{\vec{q}\sigma p}|g_{\vec{q}\sigma p}|^2 \\ &\quad + \sum_{\vec{q}m}[f_{\vec{q}m}^*\langle\Phi(\vec{r})|V_{\vec{q}m}^*(z)\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{\rho}}|\Phi(\vec{r})\rangle + \text{h.c.}] \\ &\quad + \sum_{\vec{q}\sigma p}[g_{\vec{q}\sigma p}^*\langle\Phi(\vec{r})|\Gamma_{\vec{q}\sigma p}^*(z)\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{\rho}}|\Phi(\vec{r})\rangle + \text{h.c.}].\end{aligned} \tag{26}$$

The variational parameters $f_{\vec{q}}$, $f_{\vec{q}}^*$, $g_{\vec{q}}$, $g_{\vec{q}}^*$ can be obtained by minimizing $\langle H\rangle$ with respect to $f_{\vec{q}}$, $f_{\vec{q}}^*$, $g_{\vec{q}}$, $g_{\vec{q}}^*$. After substituting in the optimum value of the variational parameters, the expectation value $\langle H\rangle$ finally turns out to be

$$\begin{aligned}\langle H\rangle = \langle\Phi(\vec{r})|H_e|\Phi(\vec{r})\rangle &- \sum_{\vec{q}m}\frac{1}{\overline{h}\omega_{\vec{q}m}}\langle\Phi(\vec{r})|V_{\vec{q}m}^*(z)\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{\rho}}|\Phi(\vec{r})\rangle\,\langle\Phi(\vec{r})|V_{\vec{q}m}(z)\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{\rho}}|\Phi(\vec{r})\rangle \\ &- \sum_{\vec{q}\sigma p}\frac{1}{\overline{h}\omega_{\vec{q}\sigma p}}\langle\Phi(\vec{r})|\Gamma_{\vec{q}\sigma p}^*(z)\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{\rho}}|\Phi(\vec{r})\rangle\,\langle\Phi(\vec{r})|\Gamma_{\vec{q}\sigma p}(z)\mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{\rho}}|\Phi(\vec{r})\rangle.\end{aligned} \tag{27}$$

Now let us turn to the electronic part. Since the major contribution to the energies of an electron and phonon system comes from the Coulomb interaction with the positive ion situated at the centre of the well, realistic energies for the bulk polaron and the surface polaron states can be obtained only if the Coulomb part can be solved more accurately. To achieve this goal we shall use a perturbative–variational approach to obtain more accurate eigenenergies for H_e. The main idea of this approach is to introduce firstly a parameter λ into the electronic part H_e by adding and subtracting a term

$$\frac{\lambda e^2}{\varepsilon\sqrt{x^2+y^2}}$$

(which contains the parameter λ) into the original Hamiltonian H_e and then regrouping H_e into three groups:

$$H_e = H_0(\lambda) + H'(\lambda) = H_z + H_{xy} + H'(\lambda) \tag{28}$$

where

$$H_z = \frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + V(z) \tag{29}$$

$$H_{xy} = \frac{-\hbar^2}{2\mu}\left[\frac{\partial}{\rho\,\partial\rho}\left(\rho\,\frac{\partial}{\partial\rho}\right) + \frac{\partial^2}{\rho^2\,\partial\phi^2}\right] - \frac{\lambda e^2}{\varepsilon\rho} \tag{30}$$

$$H'(\lambda) = \frac{\lambda e^2}{\varepsilon\rho} - \frac{e^2}{\varepsilon_0\sqrt{\rho^2+(z-z_i)^2}}. \tag{31}$$

In the above equations, the first two Hamiltonians H_z and H_{xy} can be solved exactly, whereas the third Hamiltonian H' is treated as a perturbation. And H_0 is the unperturbed Hamiltonian. λ is treated as a variational parameter which can be varied to minimize the perturbation term $H'(\lambda)$. The geometry of the quantum well is chosen such that the xy-plane is parallel to the interface and the impurity is located at a distance z_i (along the z-axis). Now let us roughly estimate the magnitude of the term H' from the uncertainty relation:

$$\langle H'\rangle \sim \frac{e^2}{\varepsilon_0\rho}\left(\frac{z^2}{\rho^2}\right) \sim R_y^*\left(\frac{L}{a^*}\right)^2 \tag{32}$$

for a small well width $L \ll a^*$; here $a^* = \varepsilon\hbar^2/(\mu e^2)$ is the effective Bohr radius, and $R_y^* = \mu e^4/(2\varepsilon^2\hbar^2)$ is the effective Rydberg calculated with effective mass μ. Hence, as $(L/a^*)^2 \ll 1$, the term H' in H_e can be taken as a small perturbation. The introduction of the variational parameter λ ensures that the term H' can be made as small as possible.

The eigenfunctions of the unperturbed term H_0 can be solved exactly. The first part H_z in H_0 represents the motion of an electron along the z-direction in a one-dimensional square-well potential which can be solved exactly. The eigenfunction of the transverse part H_{xy} is just the two-dimensional hydrogen wave function. For illustration, the ground-state eigenvalues and eigenfunctions for H_z and H_{xy} are now listed:

$$E_0 = -4\lambda^2 R_y^* \tag{33}$$

$$\varphi(z) = \sqrt{\frac{2}{L}}\cos\left(\frac{\pi z}{L}\right) \tag{34}$$

$$\psi_{1s}(\rho,\phi) = \frac{1}{2\pi}\frac{4\lambda}{a}\mathrm{e}^{-2\rho\lambda/a}. \tag{35}$$

And for the $n = 2$ state, the eigenvalue and eigenfunction of H_{xy} are

$$E_{2s,2p_\pm} = -\frac{4}{9}\lambda^2 R_y^* \tag{36}$$

$$\psi_{2s}(\rho,\phi) \sim \left(1 - \frac{4\rho}{3}\lambda_{2s}\right)e^{-2\rho\lambda_{2s}/a} \tag{37}$$

$$\psi_{2p_\pm}(\rho,\phi) \sim \rho e^{-2\rho\lambda_{2p_\pm}/3a}. \tag{38}$$

The unperturbed wave function of the electron can be written as

$$\Phi(\rho,\phi,z) = \varphi(z)\psi(\rho,\phi) \tag{39}$$

and the first-order energy correction of the ground state is

$$\begin{aligned}\Delta E_g^{(1)}(\lambda) &= \int_{-L/2}^{L/2} dz \mid \varphi(z)|^2 \int\int H'(\lambda)|\psi(\rho,\phi)|^2 \rho \, d\rho \, d\phi \\ &= \frac{16\lambda^2 e^2}{a^2\varepsilon^2}\int_{-L/2}^{L/2} dz\, |\varphi(z)|^2 \left[\int_0^\infty \lambda e^{-(4\lambda/a)\rho}\, d\rho - \int_0^\infty \frac{\rho e^{-(4\lambda/a)\rho}}{\sqrt{\rho^2 + (z-z_i)^2}}\, d\rho\right] \\ &= \frac{16\lambda^2 e^2}{a^2\varepsilon^2}\int_{-L/2}^{L/2} dz\, |\varphi(z)|^2 \left\{\frac{a}{4} + |z-z_i| - \frac{\pi}{2}|z-z_i| \right. \\ &\quad \left. \times \left[\mathcal{H}_1\left(\frac{4\lambda|z-z_i|}{a}\right) - \mathcal{N}_1\left(\frac{4\lambda|z-z_i|}{a}\right)\right]\right\}\end{aligned} \tag{40}$$

where $\mathcal{H}_1(x)$ and $\mathcal{N}_1(x)$ are the Struve and Neumann functions of order 1. On the basis of the first-order perturbation energy, the fast-convergence condition requires $\Delta E_g^{(1)}(\lambda_0) = 0$, which yields the optimum value λ_0 for the variational parameter. Hence the ground-state binding energy is defined as $-E_0$ ($=4\lambda_0^2\ R_y^*$). In a similar treatment, one can obtain the binding energies of the $n = 2, 3, \ldots$ excited states.

3. Results and discussion

We have calculated the effect of the electron–phonon interaction on the hydrogenic impurity located in a quantum well. Both confined electron–bulk (BO) phonon and electron–surface (SO) phonon interactions are taken into account and both on-centre and off-centre impurities are considered. Figure 1 shows the variation of the ground-state binding energy of a hydrogenic impurity located at the centre of an infinite-potential GaAs quantum well as a function of the well width. The energy is expressed in terms of the effective Rydberg R_y^* (for GaAs, 1 $R_y^* \sim 5.8$ meV), and the well width is expressed in terms of the effective Bohr radius a^* (for GaAs, 1 $a^* \sim 100$ Å). The binding energy E_b of the hydrogenic impurity is defined as the energy difference between the ground-state energy of the quantum well system with and without the impurity; i.e.,

$$E_b = E_0 - E_g \tag{41}$$

where E_0 is the ground-state energy of the quantum well system without the impurity, while E_g is that of the quantum well system with the impurity located inside the well.

In figure 1, three curves are presented. The solid curve represents the binding energy of the impurity without considering the interactions between the electron and phonon. The dotted curve represents the binding energy of the impurity with only electron–SO phonon interaction taken into account. And the dashed curve is the binding energy of the impurity including both electron–BO phonon and electron–SO phonon interactions in the calculation. One can note

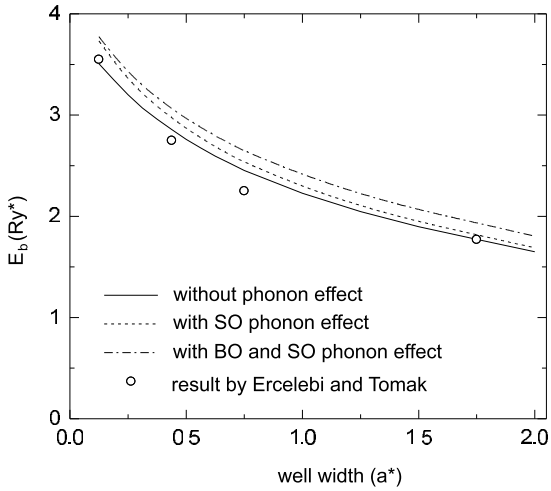


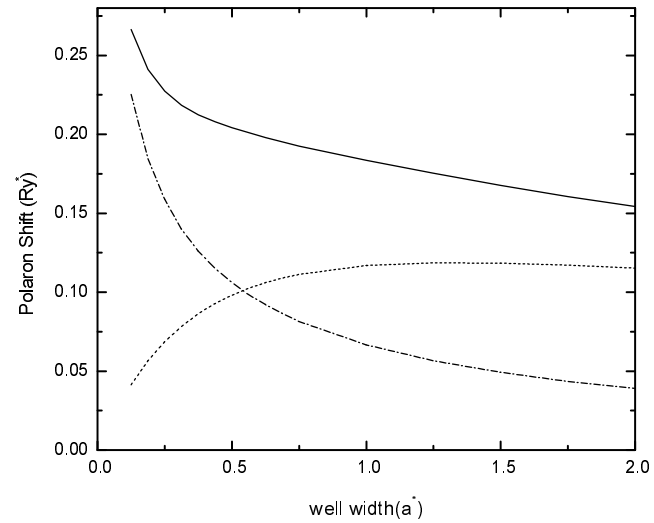
Figure 1. The variation of the ground-state binding energy of a hydrogenic impurity located at the centre of an infinite-potential GaAs quantum well as a function of the well width. The full circles are from reference [12].

from figure 1 that the binding energy of the impurity without the effect of the electron–phonon interaction included increases as the well width is reduced. This is because as the well width L is reduced, the electron wave function is compressed in the quantum well. This leads to increasing binding of the electron. One can also note that the binding energy E_b approaches 4 R^* as the well width L becomes extremely small; this is the ground-state binding energy of the 2D hydrogen atom. As the well width becomes larger and larger, the impurity binding energy approaches 1 R^*, which is just the ground-state binding energy of a 3D hydrogen atom. For comparison, we also present the results obtained by Erçelebi and Tomak [12]; one can note that our results agree nicely with theirs. In addition to this, our result also yields correct limits as the well width becomes very large or very small. Figure 1 also shows that the effect of the SO phonon on the ground-state binding energy becomes more important as the well width becomes smaller.

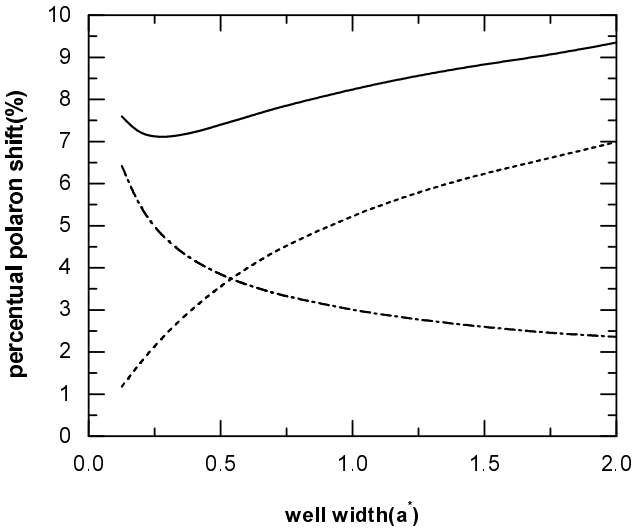
Figure 2 presents the polaron shift of the ground state as a function of the well width. One can note that the polaron shift is about 7.5% to 9.5% and thus cannot be neglected. When the well width decreases, the magnitude of the BO phonon effect approaches zero, while the SO phonon effect increases rapidly. The SO phonon effect plays the dominant role when the well width is less than 0.5 a^*. Our results are also in a good agreement with previous work [20].

Figure 3 presents the binding energies of the $n = 2$ and $n = 3$ lower-lying excited states as functions of the well width. For very small well width $L \to 0$, the binding energies of the $n = 2$ state approach $\frac{4}{9}\ R_y^*$ which is the limiting value of the $n = 2$ excited-state binding energy of the 2D hydrogen atom. Most of the previous works concentrated on the polaron effects on the ground-state binding energy only. To our knowledge, our calculation presents the first result for the polaron effects on the excited states.

Figures 4(a), 4(b), 4(c) display the polaron effects on the binding energies of the $n = 2$ and $n = 3$ lower-lying excited states as functions of the well width. It is found that for the $n = 2$ state, the SO phonon effect is more important when the well width is less than 1.5 a^*, and for $n = 3$ state, the corresponding value is about 3.5 a^*. This can be explained as follows: the higher the electron state energy, the larger the space over which the electron can distribute.



(a)



(b)

Figure 2. (a) The polaron shift of the ground state as a function of the well width. (b) The percentage polaron shift of the ground state as a function of the well width.

Therefore, the SO phonon effect on the higher-energy state is activated earlier when the well width is reduced on going from 3D to 2D.

Figure 5 shows the effect of the donor position on the impurity binding energies when the well width is 1 a^*. One can note that the ground-state binding energy depends sensitively on the donor position when the donor is located away from the centre of the well. In contrast, the excited-state binding energies are almost independent of the donor position. When the donor is located very close to the well boundary, the binding energy is decreased due to the repulsion of the barrier potential.

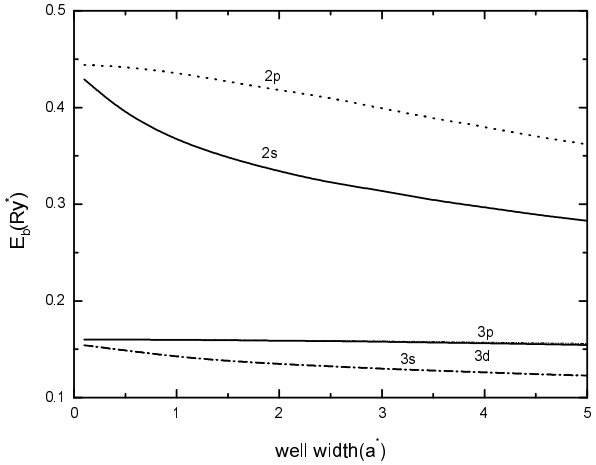


Figure 3. Binding energies of $n = 2$ and $n = 3$ lower-lying excited states as functions of the well width.

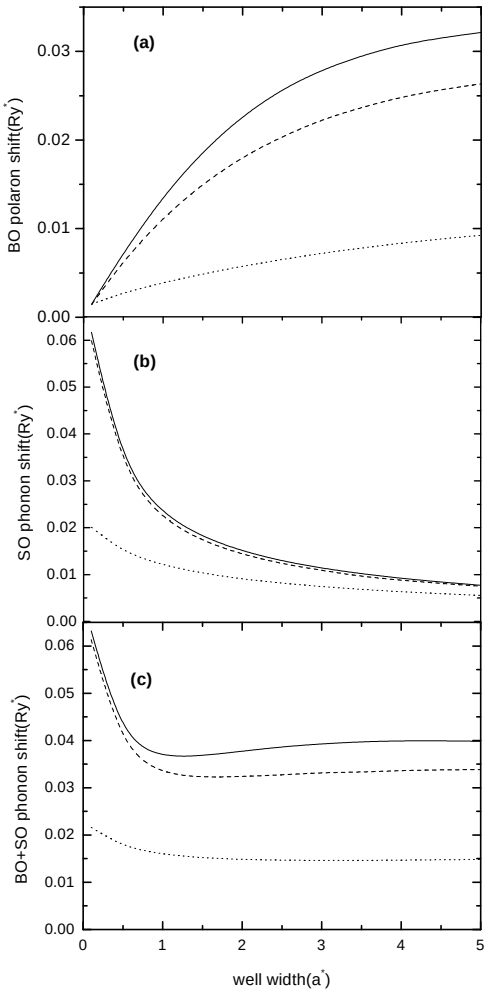


Figure 4. The polaron shifts of the binding energies of $n = 2$ and $n = 3$ lower-lying excited states as functions of the well width: the polaron shift due to the (a) BO and (b) SO phonons; and (c) the total polaron shift of the binding energies. The solid lines stand for $|2s\rangle$, the dashed lines stand for $|2p\rangle$, and the dotted lines stand for $n = 3$.

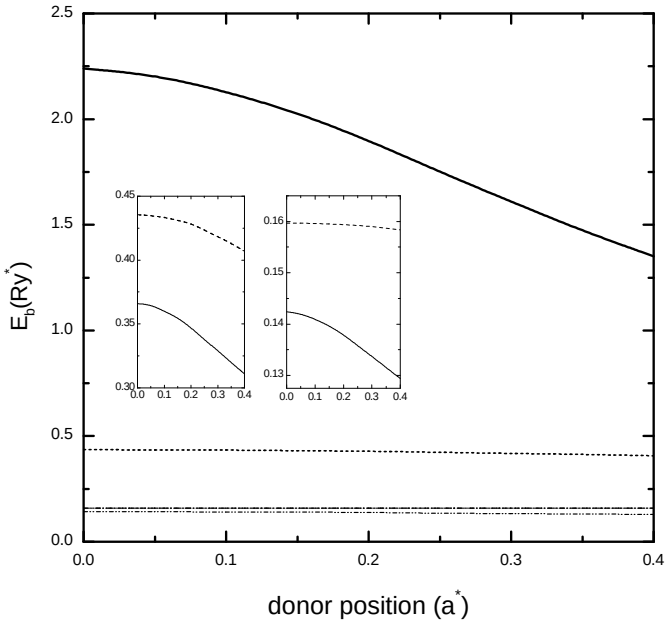


Figure 5. The effect of the donor position on the impurity binding energy. The well width is 1 a^*.

Figure 6 displays the oscillator strengths of transitions from the ground state $|1s\rangle$ to the excited states $|2p_{\pm}\rangle$ and $|3p_{m=1}\rangle$ for radiation polarized in the x-direction. Within the framework of the effective-mass approximation, the oscillator strength of the transition from an initial state $|i\rangle$ to a final state $|f\rangle$ is defined as

$$f_{i\to f} = \frac{2\mu E_{if}}{\hbar^2}|\langle f|x_j|i\rangle|^2 \tag{42}$$

where x_j represents x, y, or z, and E_{if} is the energy difference between the initial and final states involved in the transition. One can see from figure 6 that the oscillator strength $f_{1\to 3}$ increases more prominently with the donor position than $f_{1\to 2}$. For $f_{1\to 2p\pm}$, our result agrees very well with those obtained in previous works [22, 23]. Experimentally, a peak position located at 7.3 meV was observed for a GaAs quantum well with well width equal to 210 Å [24]; our result yields a value of 7.1 meV for this width. Although the well potential in the present work is assumed to be infinitely high (i.e. a hard wall; this seems to be far from reality), a reasonable result can still be obtained by perturbative–variational treatment. This is because the wave functions of the lower states have difficulty in spreading outside a quantum well with well width ∼200 Å. Therefore the binding energy for a moderate-potential quantum well is close to that for an infinite-potential quantum well.

4. Summary

In this work, an analytical solution for the confined phonon effects on the binding energy of an impurity located inside a quantum well is obtained by using a simple and efficient perturbative–variational method. We calculate both the BO and SO phonon effects on the ground and excited states of the impurity. Our results show that the SO phonon effect on the impurity binding

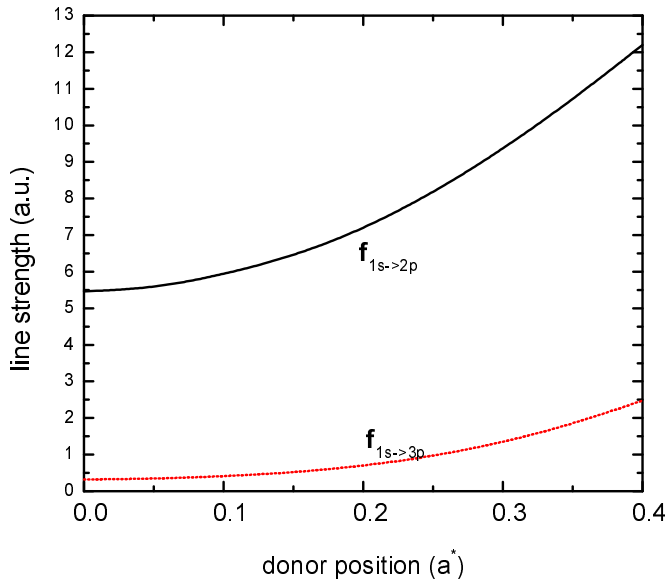


Figure 6. The oscillator strength f of an electric dipole transition from the ground state $|1s\rangle$ to the excited states $|2p_{\pm}\rangle$ and $|3p_{m=1}\rangle$ for radiation polarized in the x-direction. The upper line shows $f_{1s\rightarrow 2p\pm}$ and the lower line $f_{1s\rightarrow 3p}$; these are plotted as functions of the donor positions. The well width is 1 a^*.

energies is more prominent for a narrower quantum well. It is also found that the electric dipole transitions are enhanced by the polaron effect when the well width becomes smaller.

Acknowledgment

This work was supported partially under the grant number NSC 88-2112-M-009-004 by the National Science Council, Taiwan.

References

[1] Miller R C, Kleinman D A and Tsang W T 1981 *Phys. Rev.* B **24** 1134
[2] Fowler A B, Harstein A and Webb R A 1982 *Phys. Rev. Lett.* **48** 196
[3] Petroff P H, Gossard A C, Logan R A and Wiegman W 1985 *Appl. Phys. Lett.* **41** 635
[4] Plaut A S, Lage H, Grabow P, Heitmann D, von Klitzing K and Ploog K 1991 *Phys. Rev. Lett.* **67** 1642
[5] Bastard G 1981 *Phys. Rev.* B **24** 4714
[6] Mailhiot C, Chang Y C and McGill T C 1982 *Phys. Rev.* B **26** 4449
[7] Greene R L and Bajaj K K 1983 *Solid State Commun.* **45** 825
[8] Liu W M and Quinn J J 1985 *Phys. Rev.* B **35** 2348
[9] Sakai H 1980 *Japan. J. Appl. Phys.* **19** L735
[10] Degani M H and Hipólito O 1986 *Phys. Rev.* B **33** 4090
[11] Mason B A and Sarma S D 1986 *Phys. Rev.* B **33** 8379
[12] Erçelebi A and Tomak M 1985 *Solid State Commun.* **54** 883
[13] Shen Z J, Yuan X Z, Shen G T and Yang B C 1994 *Phys. Rev.* B **49** 11 053
[14] Thilagam A and Singh J 1994 *Phys. Rev.* B **49** 13 583
[15] Erçelebi A and Özdincer U 1986 *Solid State Commun.* **57** 441
[16] Degani M H and Hipólito O 1988 *Phys. Rev.* B **35** 4507
[17] Chuu D S, Won W L and Pei J H 1994 *Phys. Rev.* B **49** 14 554

[18] Zheng R S and Matsuura M 1998 *Phys. Rev.* **57** 1749
[19] Jiang T F and Chuu D S 1990 *Physica* B **164** 287 and references therein
[20] Zheng R S, Ban S L and Liang X X 1994 *Phys. Rev.* B **49** 1796
[21] Landau L D and Pekar S I 1946 *Zh. Eksp. Teor. Fiz.* **16** 341
[22] Greene R L and Lane P 1986 *Phys. Rev.* B **34** 8639
[23] Fraizzoli S, Bassani F and Buczko R 1990 *Phys. Rev.* B **41** 5096
[24] Jarosik N C, McCombe B D, Shanabrook B V, Comas J, Ralston J and Wicks G 1985 *Phys. Rev. Lett.* **54** 1283