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Polaron effects on the Stark shift of a bound polaron in infinite quantum wells†

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Abstract. With both longitudinal optical (LO) and surface optical (SO) modes included, the influence of electron–phonon interactions on the quantum confined Stark effect in quantum wells is investigated by means of the variational technique. For an infinite GaAs–GaAlAs quantum well with a shallow donor located at its centre and subjected to an external electric field, the energy shifts of a conduction electron are calculated approximately. It is found that the presence of an ionized impurity decreases the energy shift. The LO mode and SO mode effect will give significant corrections to the Stark energy shift individually and their influences on the shift are just opposed.

1. Introduction

Recently, the study of the electronic and optical properties of the quantum-well (QW) structure in the presence of an electric field has attracted a great deal of interest [1–7].

It is well known that, for QW and other confined structures subjected to an electric field perpendicular to the well layers, the quantum confined Stark effect (QCSE) determines the behaviour of the electron absorption by shifting the optical absorption peaks. The electron absorptive effect has already been applied to make small, high-speed optical modulators, and optical switching and signal processing devices [8]. So, studies of these areas are important from both a fundamental and a practical point of view.

Most theoretical work has been confined to the calculations of the ground state in which the possibility of tunnelling out of the well was neglected and the infinite-well approximation was employed. In principle, the linear combinations of two dependent Airy functions are an exact solution of the eigenstates in an infinite QW under a constant electric field [3]. However, these solutions are too complicated to use in a real problem. So sometimes, other approximation methods based on the Green function [9], perturbational treatment [10] and variational technique [11] are used.

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In the calculations for studying QCSE in the infinite-well approximation, the variational approach not only has the advantage of providing analytical expressions for the eigenstate energies and the field-dependent trial wavefunctions but gives numerical results with reasonable accuracy. It was found that its results agreed very well with that of other methods over a wide range of moderate electric fields [12].

On the other hand, with the development of the epitaxial growth technique and the applications of doped superlattice structures, in which electronic transport properties were shown to be significant, a lot of theoretical papers have discussed the binding energy and wavefunction of a hydrogenic donor in polar crystal slabs and semiconductor QW [13–16]. Recently, the presence of ionized impurities in the QW region has been suggested as one possible mechanism to explain the strong broadening of the excitonic peaks in the electro-absorption spectra with fields [17]. It has thus become more important to understand the role of impurities in semiconductor QW and other confined structures.

The early theoretical studies concluded that the electron–optical phonon coupling would play an important role in determining the properties of a polaron in QW. Both in 3D and in 2D systems, the virtual coupling of a quasi-free electron with bulk longitudinal optical (LO) phonons has been investigated [18–20]. However, to the best of our knowledge, only more recently was the electron–LO phonon interaction taken into account in the calculation of Stark energy shifts in an infinite QW [21], in which the LO modes effect was approximately described by the operators in the bulk not in the slab.

The first deduction of the Hamiltonian operators of the Fröhlich polaron in a polar crystal slab with both the electron–LO phonon and the electron–surface optical (SO) phonon interaction included was made by Licari and Evrard [22]. In the zero-temperature limit, we and our collaborators [16] investigated the influence of the SO modes effect and concluded that, for a thin polar crystal slab, the electron–SO phonon interaction would make an obvious contribution to the optical properties of a bound polaron.

In this paper, we report a study of the effect of an external electric field on the electronic bound states associated with an infinite quantum well in which there is a shallow donor located at its centre (on-centre impurity). Taking GaAs–GaAlAs as an example, we calculate the energy shifts by means of the variational technique. With the consideration of the electron interaction with both LO and SO modes, in particular, the electron–phonon effect on QCSE is discussed in detail

It is found that the presence of ionized impurities will decrease the energy shift and for such a correction the energy change in the xy plane will play an important role. The effects of LO and SO phonons will give significant corrections to the energy shifts individually. But because of the opposite influence of SO mode effect, the total correction attributed mainly to LO mode effect is decreased.

2. The effective Hamiltonian

Let us consider an electron, with charge e and effective mass m^*, in a quantum well of width L and in the presence of an external electric field F along the z direction, i.e. perpendicular to the well layers. The origin of distance is chosen at the centre of the well, the space for $|z| < L/2$ is filled with polar crystal 1 (GaAs) and for $|z| > L/2$ with polar crystal 2 (GaAlAs). The shallow doped impurity is located at the centre of the well ($z = 0$). We assume that the effective-mass approximation is valid and electron

tunnelling can be neglected. Therefore, in the infinite-well approximation, the Hamiltonian of this problem is written as

$$H = H_e + H_{ph} + H_{int}. \tag{1}$$

The first term, the Hamiltonian of the shallow donor, is given by

$$H_e = -(\hbar^2/2m^*)\partial^2/\partial z^2 + \hbar^2 K_\rho^2/2m^* - e^2/\varepsilon_{\infty 1} r + |e|Fz \tag{2}$$

where K_ρ and ρ are the wavevector and the position vector of the electron in the xy plane, respectively, and m^* is the band mass of the electron. In (2) $-e^2/\varepsilon_{\infty 1} r$ is the Coulomb potential to describe the interaction between the electron and the ionized impurity, in which ε_∞ is the optical dielectric constant of crystals and $r = (\rho^2 + z^2)^{1/2}$.

In order to solve the energy eigenequation of H_e, we introduce the plane Coulomb potential with the parameter λ [23]. Then

$$H_e = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \left(\frac{\hbar^2 K_\rho^2}{2m^*} - \frac{\lambda e^2}{\varepsilon_{\infty 1}\rho}\right) + \frac{e^2}{\varepsilon_{\infty 1}}\left(\frac{\lambda}{\rho} - \frac{1}{r}\right) + |e|Fz \tag{3}$$

where the value of λ will be determined by the perturbation theory.

The second term in (1) represents the phonon–field Hamiltonian

$$H_{ph} = H_{LO} + H_{SO} \tag{4a}$$

$$H_{LO} = \sum_{k,m,p} \hbar\omega_{LO} a^+_{m,p}(k) a_{m,p}(k) \tag{4b}$$

$$H_{SO} = \sum_{q,p} \hbar\omega_{Sp} b^+_p(q) b_p(q) \tag{4c}$$

where $a^+_{m,p}(k)$ $(a_{m,p}(k))$ is the creation (annihilation) operator for the LO phonon with frequency ω_{LO} and k is the two-dimensional projection on the xy plane of the wavevector, $b^+_p(q)$ $(b_p(q))$ is the corresponding operator for the SO phonon with frequency ω_{Sp} and wavevector q. The phonon modes are specified by subscripts p and m. The parity index p, taking the value + and −, refers to the mirror symmetry with respect to the plane $z = 0$. The index m is the quantum number denoting the z component of the LO phonon wavevector. For even parity (p takes +) m is odd, and for odd parity (p takes −) m is even. The phonon frequencies can be expressed in terms of the transverse optical (TO) phonon frequency ω_{TO} by

$$\omega^2_{LO} = (\varepsilon_{01}/\varepsilon_{\infty 1})\omega^2_{TO} \tag{5a}$$

$$\omega^2_{S\pm} = \frac{(\varepsilon_{01} + \varepsilon_{02}) \pm (\varepsilon_{01} - \varepsilon_{02})\,e^{-qL}}{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) \mp (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})\,e^{-qL}}\,\omega^2_{TO} \tag{5b}$$

where ε_0 is the static dielectric constant.

In equation (1), $H_{int} = H_{e\text{-}LO} + H_{e\text{-}SO}$, which represents the sum of the interaction Hamiltonian operators respectively from LO and SO modes. According to the results deduced in [22], they are directly taken as

$$H_{e\text{-}LO} = \sum_k \Bigg[B^* e^{-ik\cdot\rho} \Bigg(\sum_{m=1,3,\ldots} \frac{\cos[(m\pi/L)z]}{[k^2 + (m\pi/L)^2]^{1/2}}\, a^+_{m,+}(k) + \sum_{m=2,4,\ldots} \frac{\sin[(m\pi/L)z]}{[k^2 + (m\pi/L)^2]^{1/2}}\, a^+_{m,-}(k) \Bigg) + \text{HC} \Bigg] \tag{6a}$$

$$H_{e\text{-}SO} = \sum_q \left(\frac{\sinh(qL)}{q}\right)^{1/2} e^{-qL/2}\{C^* e^{-iq\cdot\rho} \times [G_+(q,z)b_+^\dagger(q) + G_-(q,z)b_-^\dagger(q)] + HC\} \tag{6b}$$

where

$$B^* = i\left[\frac{4\pi e^2}{V}\hbar\omega_{LO}\left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}}\right)\right]^{1/2} \tag{7a}$$

$$C^* = i[(2\pi e^2/A)\hbar\omega_{TO}(\varepsilon_{01} - \varepsilon_{\infty 1})]^{1/2} \tag{7b}$$

$$G_+ = \frac{\cosh(qz)/\cosh(qL/2)}{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) - (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})e^{-qL}} \times \left(\frac{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) - (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})e^{-qL}}{(\varepsilon_{01} + \varepsilon_{02}) - (\varepsilon_{01} - \varepsilon_{02})e^{-qL}}\right)^{1/4} \qquad (|z| < L/2) \tag{7c}$$

$$G_- = \frac{\sinh(qz)/\sinh(qL/2)}{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) + (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})e^{-qL}} \times \left(\frac{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) + (\varepsilon_{\infty 1} - \varepsilon_{\infty 2})e^{-qL}}{(\varepsilon_{01} + \varepsilon_{02}) + (\varepsilon_{01} - \varepsilon_{02})e^{-qL}}\right)^{1/4} \qquad (|z| < L/2). \tag{7d}$$

In the above equations, A and V are the surface area and the volume of crystal 1 respectively. We take N as the well thickness in the unit of the lattice spacing constant a, namely, $Na = L$. According to the Brillouin-zone boundary limitation $m\pi/L \leqslant \pi/2a$, the quantum number m of z component can be any integer within the range $1 \leqslant m \leqslant N/2$.

For the sake of convenience, we first carry out the canonical transformations developed by Lee *et al* [24] to $H(1)$ with

$$U_1 = \exp\left(-i\sum_{k,m,p} a_{m,p}^+(k)a_{m,p}(k)k\cdot\rho - i\sum_{q,p} b_p^+(q)b_p(q)q\cdot\rho\right) \tag{8a}$$

and

$$U_2 = \exp\left(\sum_{k,m,p}[a_{m,p}^+(k)f_{m,p}(k) - a_{m,p}(k)f_{m,p}^*(k)] + \sum_{q,p}[b_p^+(q)g_p(q) - b_p(q)g_p^*(q)]\right) \tag{8b}$$

where $f_{m,p}, f_{m,p}^*, g_p$ and g_p^* are the variational parameters determined by minimizing the total energy subsequently. After some straightforward algebra, we directly get the transformed Hamiltonian

$$\mathcal{H} = U_2^{-1}U_1^{-1}HU_1U_2. \tag{9}$$

In the low-temperature limit, few phonons will be excited and then no real phonons

are proposed to be present in the phonon ground state. Hence, in our study, we take $|0, 0\rangle$ as the wavefunction of the phonon system and have

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

We set

$$\begin{aligned} Q = \langle 0,0|\mathcal{H}|0,0\rangle = & -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + \left(\frac{\hbar^2 K_\rho^2}{2m^*} - \frac{\lambda e^2}{\varepsilon_{\infty 1}\rho}\right) + \frac{e^2}{\varepsilon_{\infty 1}}\left(\frac{\lambda}{\rho} - \frac{1}{r}\right) + |e|Fz \\ & + \sum_k \left[B\left(\sum_{m=1,3,\ldots}^{N/2} \frac{\cos[(m\pi/L)z]}{[k^2 + (m\pi/L)^2]^{1/2}} f_{m,+}(\boldsymbol{k}) \right.\right. \\ & \left.\left. + \sum_{m=2,4,\ldots}^{N/2} \frac{\sin[(m\pi/L)z]}{[k^2 + (m\pi/L)^2]^{1/2}} f_{m,-}(\boldsymbol{k}) \right) + \text{HC} \right] \\ & + \sum_q \left[\left(\frac{\sinh(qL)}{q}\right)^{1/2} \mathrm{e}^{-qL/2} \{C[G_+ g_+(\boldsymbol{q}) + G_- g_-(\boldsymbol{q})] + \text{HC}\} \right] \\ & + \frac{\hbar^2}{2m^*}\left[\left(\sum_{k,m,p} |f_{m,p}(\boldsymbol{k})|^2 k \right)^2 + \left(\sum_{q,p} |g_p(\boldsymbol{q})|^2 q \right)^2 \right] \\ & + \sum_{k,m,p} |f_{m,p}(\boldsymbol{k})|^2 \left(\hbar\omega_{\text{LO}} + \frac{\hbar^2 k^2}{2m^*} - \frac{\hbar^2}{m^*} \boldsymbol{K}_\rho \cdot \boldsymbol{k} \right) \\ & + \sum_{q,p} |g_p(\boldsymbol{q})|^2 \left(\hbar\omega_{\text{Sp}} + \frac{\hbar^2 q^2}{2m^*} - \frac{\hbar^2}{m^*} \boldsymbol{K}_\rho \cdot \boldsymbol{q} \right). \end{aligned} \tag{10}$$

In the above expression, because we are only interested in the slow electron always observed in experiments we approximately set $\boldsymbol{K}_\rho = 0$. And by symmetry, we also have

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

Then from

$$\partial Q/\partial f = \partial Q/\partial f^* = \partial Q/\partial g = \partial Q/\partial g^* = 0 \tag{11}$$

we obtain

$$f_{m,+}(\boldsymbol{k}) = \frac{-B^* \cos[(m\pi/L)z]}{[k^2 + (m\pi/L)^2]^{1/2}} \left(\hbar\omega_{\text{LO}} + \frac{\hbar^2 k^2}{2m^*} \right)^{-1} \tag{12a}$$

$$f_{m,-}(\boldsymbol{k}) = \frac{-B^* \sin[(m\pi/L)z]}{[k^2 + (m\pi/L)^2]^{1/2}} \left(\hbar\omega_{\text{LO}} + \frac{\hbar^2 k^2}{2m^*} \right)^{-1} \tag{12b}$$

$$g_+(\boldsymbol{q}) = -C^* \left(\frac{\sinh(qL)}{q}\right)^{1/2} \mathrm{e}^{-qL/2}\, G_+ \left(\hbar\omega_{\text{Sp}} + \frac{\hbar^2 q^2}{2m^*} \right)^{-1} \tag{12c}$$

$$g_-(\boldsymbol{q}) = -C^* \left(\frac{\sinh(qL)}{q}\right)^{1/2} \mathrm{e}^{-qL/2}\, G_- \left(\hbar\omega_{\text{Sp}} + \frac{\hbar^2 q^2}{2m^*} \right)^{-1}. \tag{12d}$$

In addition, $f^*_{m,p}(\boldsymbol{k})$ and $g^*_p(\boldsymbol{q})$ are expressed as the conjugate formulae of above equations.

We take the variation minimum of Q as the effective Hamiltonian of the electron–phonon system, i.e.

$$H_{\text{eff}} = \min Q.$$

Inserting (12*a*)–(12*d*) into equation (10), we have

$$H_{\text{eff}} = \left(-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + |e|Fz\right) + \left(\frac{\hbar^2 K_\rho^2}{2m^*} - \frac{\lambda e^2}{\varepsilon_{\infty 1}\rho}\right) + V_l^{(\text{B})}(z) + V_l^{(\text{S})}(z) + \frac{e^2}{\varepsilon_{\infty 1}}\left(\frac{\lambda}{\rho} - \frac{1}{r}\right) \tag{13}$$

where $V_l^{(\text{B})}(z)$ and $V_l^{(\text{S})}(z)$ are the effective potentials respectively from LO and SO modes effect. By direct calculations, they are derived as

$$V_l^{(\text{B})}(z) = -\alpha\hbar\omega_{\text{LO}} 4Lu_l\left[\sum_{m=1,3,\ldots}^{N/2} \cos^2\left(\frac{m\pi}{L}z\right)\frac{\ln(m\pi/Lu_l)}{(m\pi)^2 - (Lu_l)^2} + \sum_{m=2,4,\ldots}^{N/2} \sin^2\left(\frac{m\pi}{L}z\right)\frac{\ln(m\pi/Lu_l)}{(m\pi)^2 - (Lu_l)^2}\right] \tag{14a}$$

and

$$V_l^{(\text{S})}(z) = -\alpha\hbar\omega_{\text{LO}}\varepsilon_\infty^{3/2}\varepsilon_{01}^{1/2}Lu_l \times\left[\int_0^{N\pi/2}(1 - \mathrm{e}^{-2x})\left(\frac{G_+^2}{(Lu_{S+})^2 + x^2} + \frac{G_-^2}{(Lu_{S-})^2 + x^2}\right)\mathrm{d}x\right] \tag{14b}$$

where we define the variable $x = Lq$ and the dimensionless coupling constant of the electron–LO phonon interaction as

$$\alpha = (m^* e^2/\hbar^2 u_l)(1/\varepsilon_{\infty 1} - 1/\varepsilon_{01}) \tag{15}$$

and the polaron wavevectors u_l and u_{Sp} as

$$u_l^2 = 2m^*\omega_{\text{LO}}/\hbar \qquad u_{Sp}^2 = 2m^*\omega_{Sp}/\hbar. \tag{16}$$

3. The wavefunction and energy shifts

Since it is exceedingly complicated to get an exact solution of the eigenequation associated with H_{eff} (13), a trial wavefunction should be found in our variational approach. First, the effective Hamiltonian is rewritten as

$$H_{\text{eff}} = H_z + H_{2\text{D}} + H_1 + V_l^{(\text{B})}(z) + V_l^{(\text{S})}(z) \tag{17}$$

in which

$$H_z = -(\hbar^2/2m^*)\,\partial^2/\partial z^2 + |e|Fz \tag{17a}$$

$$H_{2\text{D}} = \hbar^2 K_\rho^2/2m^* - \lambda e^2/\varepsilon_{\infty 1}\rho \tag{17b}$$

$$H_1 = (e^2/\varepsilon_{\infty 1})(\lambda/\rho - 1/r). \tag{17c}$$

For a thin slab, the difference between λ/ρ and $1/r$ can be made very small by choosing an applicable value of λ, so we treat H_1 as the perturbation and take

$$H_0 = H_z + H_{2D} + V_1^{(B)}(z) + V_1^{(S)}(z)$$

as the unperturbed Hamiltonian. According to equations (14*a–b*) and (17*a–b*), the wavefunction of the electron motion referring to the unperturbed H_0 can be written as

$$|\Phi(z, \rho)\rangle = |\varphi(z)\rangle|\psi(\rho)\rangle. \tag{18}$$

Compared with the sub-band energy of the conduction electron, the effective interaction potentials $V_1^{(B)}(z)$ and $V_1^{(S)}(z)$ can be neglected due to their small values. So, the electron can be approximately regarded as a quasi-particle moving in an infinite square-well potential along the z direction and the wavefunction $\varphi(z)$ should be required to satisfy the Schrödinger equation as

$$H_z|\varphi(z)\rangle = E_z|\varphi(z)\rangle. \tag{19}$$

In the presence of an external electric field the conduction electron is pushed against the field direction and the charge distribution is concentrated near the well interface. Such a physical situation can be well described by the trial wavefunction given by [11]:

$$\varphi(z) = \begin{cases} N(\beta)\exp[-\beta(z/L + 1/2)]\cos(\pi z/L) & (|z| < L/2) \\ 0 & (|z| \geqslant L/2) \end{cases} \tag{20}$$

where β is the variational parameter determined by minimizing the total energy and $N(\beta)$ is the normalization constant easily obtained as

$$N^2(\beta) = 4\beta(\beta^2 + \pi^2)\,[L\pi^2(1 - e^{-2\beta})]^{-1}. \tag{21}$$

The corresponding eigenenergy is given by

$$E_z = E_1(1 + \beta^2/\pi^2) + |e|FL\{1/2\beta + [\beta/(\beta^2 + \pi^2)] - \tfrac{1}{2}\coth\beta\} \tag{22}$$

where E_1 is the ground-state energy at zero field.

The term H_{2D} (17*b*) shows that the electron motion parallel to the xy plane is the same as the 2D hydrogen-like atom problem. For the following eigenequation

$$H_{2D}|\psi(\rho)\rangle = E_{2D}|\psi(\rho)\rangle$$

we have the same solutions for the wavefunction and the energy eigenvalue as that of the 2D hydrogen atom in [25]. For the ground state, they are

$$\psi(\rho) = \frac{1}{(2\pi)^{1/2}}\left(\frac{4\lambda}{a_0}\right)\exp\left(-\frac{2\lambda}{a_0}\rho\right) \qquad E_{2D} = -\frac{2\lambda^2 m^* e^4}{\varepsilon_{\infty 1}^2\hbar^2} \tag{23}$$

where $a_0 = \varepsilon_{\infty 1}\hbar^2/m^*e$.

According to the perturbation technique [23], the expectation value of the perturbation term H_1 (17*c*) referring to $\Phi(z, \rho)$ should be set to zero, i.e.

$$\bar{H}_1(\lambda) = \langle \Phi(z, \rho) | H_1 | \Phi(z, \rho) \rangle = 0.$$

So, the parameter λ can be obtained from

$$\lambda(\beta) = \left(\int_{-\infty}^{\infty} |\varphi(z)|^2 \, dz \int_0^{\infty} |\psi(\rho)|^2 (\rho^2 + z^2)^{-1/2} \rho \, d\rho \right) \Big/ \int_0^{\infty} |\psi(\rho)|^2 \, d\rho. \tag{24}$$

Eventually, by solving the eigenequation of H_0

$$H_0 | \Phi(z, \rho) \rangle = E_{\text{tot}} | \Phi(z, \rho) \rangle$$

the total energy of the impurity state in an infinite quantum well under an electric field is obtained as

$$\begin{aligned} E_{\text{tot}} &= \langle \Phi(z, \rho) | H_z + H_{2D} + V_{\}}^{(B)}(z) + V_{\}}^{(S)}(z) | \Phi(z, \rho) \rangle \\ &= E_1 \left(1 + \frac{\beta^2}{\pi^2} \right) + |e| FL \left(\frac{1}{2\beta} + \frac{\beta}{\beta^2 + \pi^2} - \tfrac{1}{2} \coth \beta \right) \\ &\quad - \frac{2\lambda^2 m^* e^4}{\varepsilon_{\infty 1}^2 \hbar^2} + E_s^B + E_s^S \end{aligned} \tag{25}$$

where E_s^B and E_s^S are the self-energies coming respectively from the expected values of $V_{\}}^{(B)}(z)$ and $V_{\}}^{(S)}(z)$:

$$\begin{aligned} E_s^B &= \langle \varphi(z) | V_{\}}^{(B)}(z) | \varphi(z) \rangle \\ &= -\alpha \hbar \omega_{LO} 2 L u_l \frac{\beta^2(\beta^2 + \pi^2)}{\pi^2} \sum_{m=1,2,\ldots}^{N/2} \left(\frac{1}{\beta^2} - \frac{1}{\pi^2 + \beta^2} - \frac{1}{m^2 \pi^2 + \beta^2} \right. \\ &\quad \left. + \frac{(1 + m^2)\pi^2 + \beta^2}{[(1 + m)^2 \pi^2 + \beta^2][(1 - m)^2 \pi^2 + \beta^2]} \right) \frac{\ln(m\pi / L u_l)}{(m\pi)^2 - (L u_l)^2} \end{aligned} \tag{26a}$$

$$\begin{aligned} E_s^S &= \langle \varphi(z) | V_{\}}^{(S)}(z) | \varphi(z) \rangle \\ &= -\alpha \hbar \omega_{LO} \varepsilon_{\infty 1}^{3/2} \varepsilon_{01}^{1/2} L u_l \int_0^{N\pi/2} \left(\frac{(\sinh x) \, e^{-x}}{(L u_{S+})^2 + x^2} \right. \\ &\quad \times \frac{[(\varepsilon_{01} + \varepsilon_{02}) - (\varepsilon_{01} - \varepsilon_{02}) e^{-x}]^{-1/2}}{[(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) - (\varepsilon_{\infty 1} - \varepsilon_{\infty 2}) e^{-x}]^{3/2}} \frac{P(x) + 1}{\cosh^2(x/2)} \\ &\quad + \frac{(\sinh x) \, e^{-x}}{(L u_{S-})^2 + x^2} \frac{[(\varepsilon_{01} + \varepsilon_{02}) + (\varepsilon_{01} - \varepsilon_{02}) e^{-x}]^{-1/2}}{[(\varepsilon_{\infty 1} + \varepsilon_{\infty 2}) + (\varepsilon_{\infty 1} - \varepsilon_{\infty 2}) e^{-x}]^{3/2}} \\ &\quad \left. \times \frac{P(x) - 1}{\sinh^2(x/2)} \right) dx. \end{aligned} \tag{26b}$$

Here

$$P(x) = \frac{\beta(\beta^2 + \pi^2)}{2 \sinh \beta} \left(\frac{\sinh(x - \beta)}{(x - \beta)[(x - \beta)^2 + \pi^2]} + \frac{\sinh(x + \beta)}{(x + \beta)[(x + \beta)^2 + \pi^2]} \right). \tag{27}$$

The parameter β may be obtained from

$$\partial E_{\text{tot}} / \partial \beta = 0. \tag{28}$$

By inserting the two parameters λ and β simultaneously determined from equations (24)

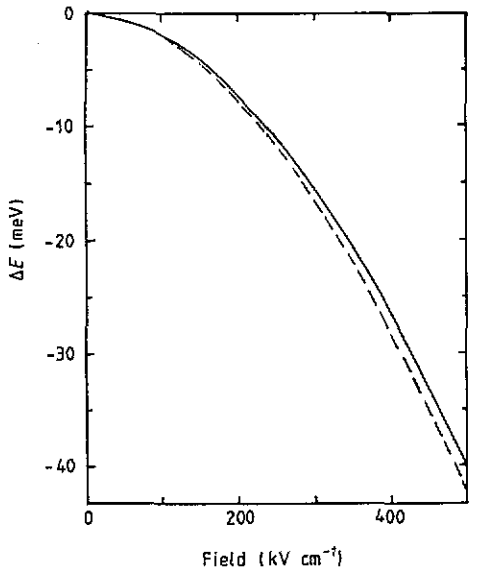

Figure 1. The energy shifts plotted against the electric field for a conduction electron in an infinite GaAs quantum well, $N = 18$ ($L \simeq 100$ Å). The full curve is the case with an on-centre impurity and the broken curve without any impurity.

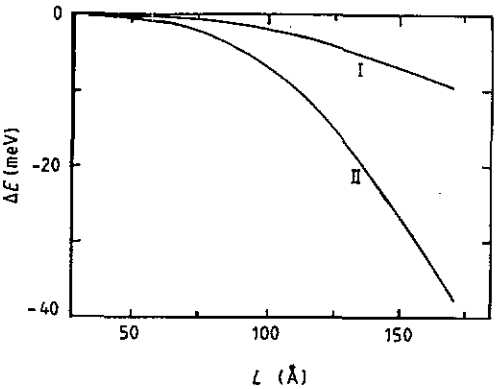

Figure 2. The energy shifts plotted against the well thickness for different electric fields: curve I, $F = 100$ kV cm^{-1}; curve II, $F = 200$ kV cm^{-1}.

and (28) into equation (25), we get the minimized energy E_{tot}. Then the field-induced energy shift is obtained as

$$\Delta E = E_1 \frac{\beta^2}{\pi^2} + |e|FL\left(\frac{1}{2\beta} + \frac{\beta}{\beta^2+\pi^2} - \tfrac{1}{2}\coth\beta\right) - \frac{2m^*e^4}{\varepsilon_{\infty 1}^2\hbar^2}(\lambda^2 - \lambda_0^2) + \Delta E_s^B + \Delta E_s^S \qquad (29)$$

in which we set

$$\Delta E_s^B = E_s^B - (E_s^B)_0 \qquad \Delta E_s^S = E_s^S - (E_s^S)_0$$

to represent the effects on the energy shift due to the electron–bulk LO phonon and the electron–SO phonon interaction, respectively. In (29), λ_0, $(E_s^B)_0$ and $(E_s^S)_0$ are the corresponding variables in the state with zero field; their expressions have been deduced by us in [16].

4. Results and discussion

Taking the GaAs–$Ga_{0.7}Al_{0.3}As$ quantum well as an example, we compute the total energy shift of a bound polaron induced by an external electric field perpendicular to the well layers. Particularly, we also make calculations of the correction of the electron–phonon effects on the Stark energy shift.

In the infinite-well approximation, we assume that the electron moves in an infinite QW under an external electric field and with a shallow impurity located at the centre of

the well. For the slow electron we are interested in, we set $K_\rho \simeq 0$, and treat the electron–phonon interaction by using the Hamiltonian operators deduced in [22].

Figure 1 describes the variation of the energy shifts with the field strength. It shows us that the energy shift of a bound polaron is smaller than that of the conduction electron in an infinite well without any impurity. This implies that the attractive action between the ionized donor and the electron will decrease the effect of the external electric field. In [11], by using the infinite-well approximation, the Stark energy shift without any impurity was obtained as

$$\Delta E = E_1(\beta^2/\pi^2) + |e|FL[1/2\beta + \beta/(\beta^2 + \pi^2) - \tfrac{1}{2}\coth\beta]. \tag{30a}$$

In this paper, neglecting the small terms proportional to $(\Delta\beta)^2$ and the small change of self-energies, we get the energy shift with on-centre impurity approximately as

$$\Delta E = E_1\frac{\beta^2}{\pi^2} + |e|FL\left(\frac{1}{2\beta} + \frac{\beta}{\beta^2+\pi^2} - \tfrac{1}{2}\coth\beta\right) - \frac{2m^*e^4}{\varepsilon_{\infty 1}^2\hbar^2}(\lambda^2 - \lambda_0^2)$$
$$+ \Delta\beta\left[E_1\frac{2\beta}{\pi^2} + |e|FL\left(-\frac{1}{2\beta^2}\frac{\pi^2-\beta^2}{(\beta^2+\pi^2)^2} + \frac{1}{2(\sinh\beta)^2}\right)\right] \tag{30b}$$

where $\Delta\beta$ is the change of variational parameter in the wavefunction, which is brought out due to the action of the doped impurity and $\Delta\beta \ll 1$. With a comparison between the two equations above, it is concluded that the correction to the energy shift due to the presence of the on-centre impurity is composed of two parts: the correction in the z direction (the fourth term in (30*b*)) and the energy shift in the xy plane (the third term in (30*b*)). Our calculations illustrate that both parts decrease the total shift, and the energy shift in the xy plane plays a more important role in the impurity correction. For instance, for $L = 100$ Å ($N = 18$) and $F = 200\ \mathrm{kV\ cm^{-1}}$, it is 11.6 times larger than the impurity correction in the z direction.

The dependence of the energy shift on the well thickness is depicted in figure 2. It is obvious that the energy shifts will rapidly become large with the thickness increasing. At the same time, the influence of an on-centre impurity on the energy shift will also become stronger.

The effect of the electron–phonon interaction on the total energy shift contains two parts, ΔE_s^B and ΔE_s^S, which are brought out respectively by LO and SO phonon contributions. As shown in figures 3 and 4, they give significant corrections to the Stark energy shift, individually. But their influences on the shifts are entirely opposed, i.e. the total energy shift will be enhanced by the SO mode effect ($\Delta E_s^S < 0$) and weakened by the LO mode effect ($\Delta E_s^B > 0$). In the presence of an external electric field, the electron is pushed against the direction of the field and close to the interface of the QW. As a result, the electron–SO phonon interaction must be enhanced and the SO self-energy will be lower; the electron–bulk LO phonon interaction must be weakened and the LO self-energy will be higher. So, we obtain $\Delta E_s^S < 0$ and $\Delta E_s^B > 0$, as described in figures 3 and 4. In these figures, we can also see that all the corrections will get rather large when the field becomes strong.

The sum of the two mode corrections, $\Delta E_s^B + \Delta E_s^S$, is plotted in figure 5, which illustrates that the phonon effect, mainly depending on LO mode contribution, will decrease the Stark shift. Owing to the opposite influence of SO mode effect, the LO mode effect is weakened. In our calculation, the total correction is much smaller than the LO mode correction obtained in [21].

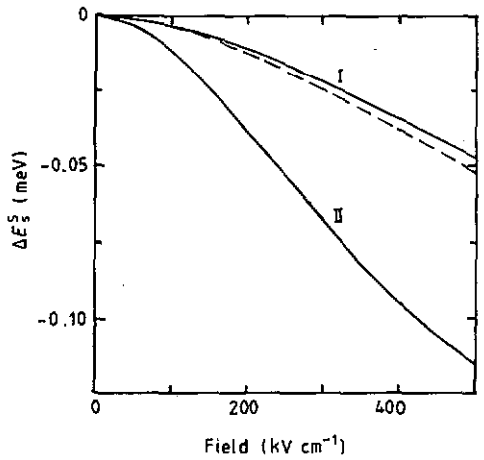

Figure 3. The correction of the SO modes contribution to the energy shift versus the electric field. The full curves are the results in an infinite QW with on-centre impurity: curve I, $L = 100$ Å ($N = 18$); curve II, $L = 135$ Å ($N = 24$). The broken curve is the result in the case without any impurity and $L = 100$ Å ($N = 18$).

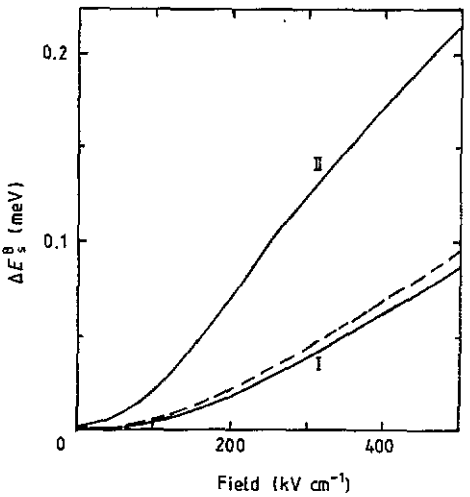

Figure 4. The correction of the bulk LO modes contribution to the energy shift versus the electric field. The curves are the same as in figure 3.

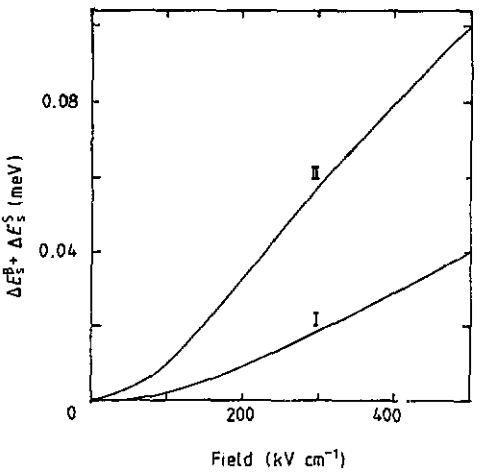

Figure 5. The total correction of phonon effect to the Stark shift, $(\Delta E_s^B + \Delta E_s^S)$, versus the field strength; $L \simeq 100$ Å ($N = 18$) for curve I and $L = 135$ Å ($N = 24$) for curve II.

For the electron–phonon system without any impurity, the total energy and its Stark shift can be easily deduced from equations (25) and (29) with $\lambda \to 0$

$$E_{tot} = E_1\left(1 + \frac{\beta^2}{\pi^2}\right) + |e|FL\left(\frac{1}{2\beta} + \frac{\beta}{\beta^2 + \pi^2} - \tfrac{1}{2}\coth\beta\right) + E_s^B + E_s^S \qquad (25a)$$

$$\Delta E = E_1\frac{\beta^2}{\pi^2} + |e|FL\left(\frac{1}{2\beta} + \frac{\beta}{\beta^2 + \pi^2} - \tfrac{1}{2}\coth\beta\right) + \Delta E_s^B + \Delta E_s^S. \qquad (29a)$$

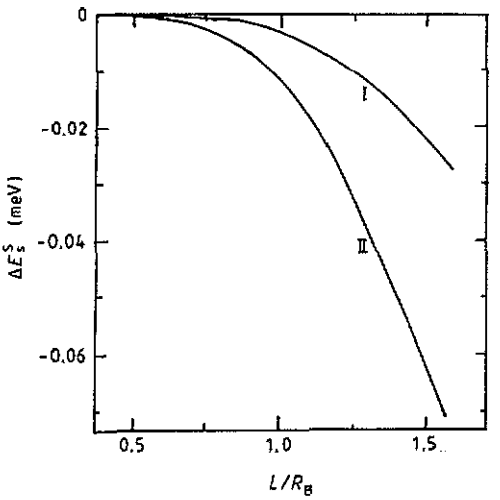

Figure 6. Variation of SO modes correction to the energy shifts with the well thickness: for curve I, $F = 150\ \mathrm{kV\ cm^{-1}}$; for curve II, $F = 300\ \mathrm{kV\ cm^{-1}}$. ($R_B$ is the effective Bohr radius of the shallow donor in GaAs.)

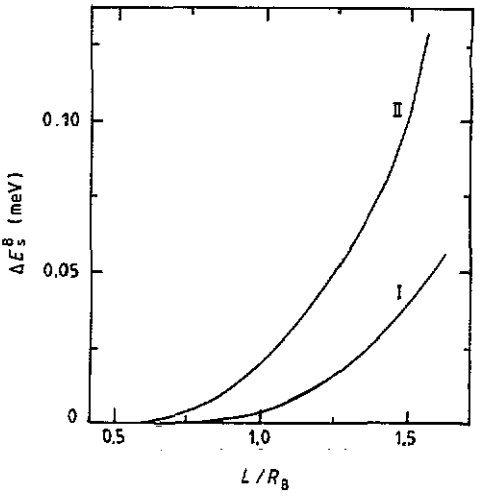

Figure 7. Variation of LO modes correction to the energy shifts with the well thickness: for curve I, $F = 150\ \mathrm{kV\ cm^{-1}}$; for curve II, $F = 300\ \mathrm{kV\ cm^{-1}}$. ($R_B$ is the effective Bohr radius of the shallow donor in GaAs.)

For $L = 100$ Å ($N = 18$) and without any impurity, the corrections of phonon effects are calculated by means of the same variational method. The results are plotted as the broken curves in figures 3 and 4. Comparing the full and broken curves in the two figures, it is seen that whether the correction is positive (ΔE_s^B) or negative (ΔE_s^S), the presence of an on-centre impurity will decrease the corrections from the phonon effects.

In figures 6 and 7, with the effective Bohr radius (R_B) as the unit of the well thickness, the variations of the phonon contributions with well thickness are described. No matter how large the field strength is, the phonon effects on the energy shift are very weak when R_B is much larger than the thickness ($L/R_B \ll 1$). With increasing well thickness, the phonon effects become stronger and stronger. When the effective Bohr radius of the donor approaches the well thickness ($L/R_B < 1$), the changes of the absolute values of the phonon self-energy shifts will be very smooth. And when R_B is relatively smaller than the well thickness ($L/R_B > 1$), the increase of phonon self-energy shifts becomes very drastic. The stronger the external field is, the more drastic will be the change of the phonon self-energy shift. Even though the LO and SO modes produce opposite influences on the Stark shift, both of them have the same characteristics in the change of their contributions with well thickness.

References

[1] Miller D A B, Chemla D S, Damen T C, Gossard A C, Wiegmann W, Wood T H and Burrus C A 1984 *Phys. Rev. Lett.* **53** 2173; 1985 *Phys. Rev.* B **32** 1043

[2] Chen Y J, Koteles E S, Elman B S and Armiento C A 1987 *Phys. Rev.* B **36** 4562

[3] Ahn D and Chuang S L 1986 *Phys. Rev.* B **34** 9034; 1987 *Phys. Rev.* B **35** 4149

[4] Collins R T, Vina L, Wang W I, Chang L L, Esaki L, Klitzing K V and Ploog K 1987 *Phys. Rev.* B **36** 1531

[5] Austin E J and Jaros M 1988 *Phys. Rev.* B **38** 6326
[6] Yu P W, Sander G D, Evans K R, Reynolds D C, Bajaj K K, Statz C E and Jones R L 1988 *Phys. Rev.* B **38** 7796
[7] Barrio D P, Glasser M L, Velasco V R and Garcia-Moliner F 1989 *J. Phys.: Condens. Matter* **1** 4339
[8] Taruch E and Okamoto H 1986 *Appl. Phys. Lett.* **48** 1
[9] Lukes T and Ringwood G A 1976 *Physica* A **84** 423
[10] Fernandez F M and Castro E A 1982 *Physica* A **11** 334
[11] Bastard G, Mendez E E, Chang L L and Esaki L 1983 *Phys. Rev.* B **28** 3241
[12] Austin E J and Jaros M 1985 *Phys. Rev.* B **31** 5569
[13] Bastard G 1981 *Phys. Rev.* B **24** 4714
[14] Mailhoit C, Chang Y C and McGill T C 1982 *Phys. Rev.* B **26** 4449
[15] Mason B A and Das Sarma S 1986 *Phys. Rev.* B **33** 8379
[16] Li Y C, Zheng L F and Gu S W 1988 *Phys. Rev.* B **38** 4096
[17] Bar-Joseph I, Kuo J M, Klingshirn C, Livescu G, Chang T Y, Miller D A B and Chemla D S 1987 *Phys. Rev. Lett.* **59** 1357
[18] Fröhlich H 1952 *Proc. R. Soc.* A **215** 291
[19] Low F E 1955 *Phys. Rev.* **97** 1392
Low F E and Pines D 1955 *Phys. Rev.* **98** 414
[20] Pekar S E 1952 *The Electronic Theory of the Crystals* (Moscow: Fizmatgiz) ch 2
[21] Wang X, Liang X X and Chang K 1988 *Solid State Commun.* **65** 83
[22] Licari J J and Evrard R 1977 *Phys. Rev.* B **15** 2254
[23] Lee Y C, Me W N and Liu K C 1982 *J. Phys. C: Solid State Phys.* **15** L469
[24] Lee T D, Low F E and Pines D 1953 *Phys. Rev.* **90** 297
[25] Schiff L I 1968 *Quantum Mechanics* 3rd edn (New York: McGraw-Hill) p 88