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The electron–phonon effect on the Stark shift in $GaAs–Ga_{1-x}Al_xAs$ quantum wells

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Abstract. With both longitudinal optical (LO) and surface optical (SO) modes included, the polaronic effects on the quantum-confined Stark effect in quantum wells is investigated by means of the variation technique. For an infinite and a finite well the significant corrections attributed to LO and SO modes are calculated. It is found that the Stark shift will be weakened by the LO-phonon effect and enhanced by the SO-phonon effect. It is also shown that the influence of electron–phonon interactions depends not only on the well width but also on the potential barrier.

1. Introduction

The quantum-confined Stark effect (QCSE) in a semiconductor quantum well (QW) has recently attracted a great deal of interest [1–8].

It is well known that, for QWs and other confined structures under an external electric field perpendicular to their layers, the behaviour of the electro-absorption is mainly determined by shifting the optical absorption peaks in the QCSE [1]. This electron-absorptive effect has already been applied to make a high-speed optical modulator, signal-processing devices and so on [9].

Initially the theoretical work has been confined to the calculations of the ground state in which the infinite-well approximation is employed. Because the band discontinuities in semiconductor heterostructures (e.g. $GaAs–Ga_{1-x}Al_xAs$) are of the order of a few hundred millielectronvolts, for a thin QW the possibility of tunnelling from the well should be taken into account. For a finite well subjected to an electric field, no exact ground states will exist. If the field is not excessively strong, the electron state can be considered as a quasi-ground state because of its long lifetime. Both for a ground state and for a quasi-ground state in a QW, in principle, the linear combinations of two dependent Airy functions are the exact solution of the eigenstates [10]. However, these solutions are too complicated to use in a real problem. So, many techniques of approaching the calculation have also been proposed [7, 11, 12].

As one of the calculation methods, in both the infinite well and the finite well, the variational technique is appropriate in the weak-field limit. It has the advantage of providing analytical expressions for the eigenstate energies and the field-dependent trial wavefunctions but also gives numerical results with reasonable accuracy over a wide range of moderate electric fields [13].

The early theoretical studies concluded that the electron–optical-phonon coupling would play an important role in determining the properties of polarons in QWs [14]. In the quasi-two-dimensional (2D) systems (ionic slabs, QWs and superlattices), the virtual coupling of a quasi-free electron with bulk longitudinal optical (LO) phonons has been investigated [15], in which the usual Fröhlich interaction for bulk materials was used. In fact, the effects of the confinement of phonons in the quasi-2D systems should be taken into account [16] and then the heterostructures would cause there to be 'bulk-like' phonon modes confined to the well layer and also would give rise to 'interface' (or 'surface') modes. With the surface optical (SO) phonons included, some studies have shown that the SO modes would also produce an obvious effect on the optical properties of the charge carriers in thin slabs and heterojunctions [17]. However, just recently the effect of only the LO modes was considered in the calculation of Stark shifts of an electron in an infinite QW by using the interaction Hamiltonian for bulk materials [18].

In this paper, the polaron effects coming from both the LO and the SO modes on the QCSE of an electron are investigated in an infinite and a finite GaAs–$Ga_{1-x}Al_xAs$ QW. The polaronic corrections to energy shifts are calculated using the variational method. It is found that the phonon effects give significant corrections to the Stark shifts and the different phonon modes make entirely contrary contributions, i.e. the LO effect weakens the Stark energy shift while the SO effect enhances it. We also find that, for a thin well in a weak field, the finite-barrier effect enhances the polaron corrections as it does the total energy shift.

2. The effective Hamiltonian

In the framework of the effective-mass approximation, consider an electron in a QW of width L and under an external electric field F perpendicular to well layers (along the z direction). The origins of distance and electrostatic potential are chosen to be at the centre of the well. Then, the Hamiltonian of the electron–phonon system is

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

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

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

where $\boldsymbol{K}_\rho$ and ρ are the wavevector and the position vector, respectively, of the electron in the x–y plane and m^* is the band mass of the electron. $V(z)$ is the potential for the electron along the z direction. The second term in (1) represents the phonon-field Hamiltonian

$$H_{ph} = H_{LO} + H_{SO} \tag{3a}$$

$$H_{LO} = \sum_{\boldsymbol{k},m,p} \hbar\omega_{LO} a^+_{m,p}(\boldsymbol{k}) a_{m,p}(\boldsymbol{k}) \tag{3b}$$

$$H_{SO} = \sum_{\boldsymbol{q},p} \hbar\omega_{S_p} b^+_p(\boldsymbol{q}) b_p(\boldsymbol{q}) \tag{3c}$$

where $a^+_{m,p}(\boldsymbol{k})$ and $a_{m,p}(\boldsymbol{k})$ are the creation and annihilation operators, respectively, for the LO phonon with frequency $\omega_{\rm LO}$ and $\boldsymbol{k}$ is the two-dimensional projection on the x–y plane of the wavevector, and $b^+_p(\boldsymbol{q})$ and $b_p(\boldsymbol{q})$ are the corresponding operators for the SO phonon with frequency $\omega_{{\rm S}_p}$ and wavevector $\boldsymbol{q}$. The phonon modes are specified by the 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 ($p = +$), m is odd and for odd parity ($p = -$), m is even. The phonon frequencies can be expressed in terms of the frequency $\omega_{\rm TO}$ of the transverse optical (TO) phonon by

$$\omega^2_{\rm LO} = (\epsilon_{01}/\epsilon_{\infty 1})\omega^2_{\rm TO} \tag{4a}$$

$$\omega^2_{\rm S\pm} = \frac{(\epsilon_{01} + \epsilon_{02}) \mp (\epsilon_{01} - \epsilon_{02})\exp(-qL)}{(\epsilon_{\infty 1} + \epsilon_{\infty 2}) \mp (\epsilon_{\infty 1} - \epsilon_{\infty 2})\exp(-qL)}\omega^2_{\rm TO} \tag{4b}$$

where ϵ_0 is the static dielectric constant, ϵ_∞ is the optical dielectric constant and the subscripts 1 and 2 represent the crystals in the areas with $|z| < L/2$ and $|z| > L/2$ respectively.

In equation (1), $H_{\rm int} = H_{\rm e-LO} + H_{\rm e-SO}$, which represents the sum of the interaction Hamiltonian operators from LO and SO modes, respectively. To our knowledge, the appropriate formulation for the polar interaction in QWs is currently unresolved. First the electron–LO-phonon interactions were derived by treating the lattice dynamics on the basis of the dielectric continuum model, in which the confined phonon modes were usually approximated by either slab modes [19, 20] or guided modes [21]. The two approximations are acceptable in the conditions $k \gg \pi/L$ and $k \ll \pi/L$ respectively [22]. Recently, a simple microscopic model has been advanced for the phonon modes of superlattices by Huang and Zhu [23], which is more appropriate for $k \simeq \pi/L$ [22]. The purpose of this paper is to discuss the contribution of the phonon effects to the energies. In the integral calculations, for a well width L = 10–150 Å, the LO self-energy is greatly dominated by the contribution of the LO effect in the region $k > \pi/L$. Then the slab modes provide a better approximation in the LO self-energy calculation than other methods do. On the other hand, the classification of phonons as bulk-like and interface (surface) modes is valid only in the dielectric continuum model [22]. It has already been shown [21] that in some respects the interface (surface) modes obtained from the dielectric continuum model give a reasonably good representation of the interface (surface) modes. So, in order to discuss and compare the influence of the phonon effects from LO and SO modes, the slab modes are used for a quantitative treatment of the phonon effect in the present paper. In addition, for the finite QW studied, although the penetration effect is considered, the electron wavefunction will decay very rapidly out of the well [12], i.e. the electron is still confined in a narrow region (of width about L). For simplicity, in both the infinite and the finite well the interaction operators deduced in [19] are employed.

$$H_{\rm e-LO} = \sum_{\boldsymbol{k}} \bigg[B^* \exp(-i\boldsymbol{k}\cdot\boldsymbol{\rho}) \bigg(\sum_{m=1,3,\dots}^{N/2} \frac{\cos(m\pi z/L)}{[k^2 + (m\pi/L)^2]^{1/2}} a^+_{m,+}(\boldsymbol{k}) + \sum_{m=2,4,\dots}^{N/2} \frac{\sin(m\pi z/L)}{[k^2 + (m\pi/L)^2]^{1/2}} a^+_{m,-}(\boldsymbol{k}) \bigg) + {\rm HC} \bigg] \tag{5a}$$

$$H_{e\text{-}SO} = \sum_{q} \left(\frac{\sinh(qL)}{q}\right)^{1/2} \exp\left(-\frac{qL}{2}\right) \times \{C^* \exp(-iq\cdot\rho)[G_+(q,z)b_+^+(q) + G_-(q,z)b_-^+(q)] + \mathrm{HC}\} \qquad (5b)$$

where

$$B^* = \mathrm{i}[(4\pi e^2/V)\hbar\omega_{\mathrm{LO}}(1/\epsilon_{\infty 1} - 1/\epsilon_{01})]^{1/2} \qquad (6a)$$

$$C^* = \mathrm{i}[(2\pi e^2/A)\hbar\omega_{\mathrm{TO}}(\epsilon_{01} - \epsilon_{\infty 1})]^{1/2} \qquad (6b)$$

$$G_+(q,z) = \begin{cases} [\cosh(qz)/\cosh(qL/2)]/[(\epsilon_{01}+\epsilon_{02}) - (\epsilon_{01}-\epsilon_{02})\exp(-qL)]^{1/4} \\ \times[(\epsilon_{\infty 1}+\epsilon_{\infty 2}) - (\epsilon_{\infty 1}-\epsilon_{\infty 2})\exp(-qL)]^{-3/4} \qquad (|z| < L/2) \\ [\exp(-q|z|)/\cosh(qL/2)]/[(\epsilon_{01}+\epsilon_{02}) - (\epsilon_{01}-\epsilon_{02})\exp(-qL)]^{1/4} \\ \times[(\epsilon_{\infty 1}+\epsilon_{\infty 2}) - (\epsilon_{\infty 1}-\epsilon_{\infty 2})\exp(-qL)]^{-3/4} \qquad (|z| > L/2) \end{cases} \qquad (6c)$$

$$G_-(q,z) = \begin{cases} [\sinh(qz)/\sinh(qL/2)]/\{(\epsilon_{01}+\epsilon_{02}) + (\epsilon_{01}-\epsilon_{02})\exp(-qL)]^{1/4} \\ \times[(\epsilon_{\infty 1}+\epsilon_{\infty 2}) + (\epsilon_{\infty 1}-\epsilon_{\infty 2})\exp(-qL)]^{3/4} \qquad (|z| < L/2) \\ [\exp(-q|z|)/\sinh(qL/2)]/[(\epsilon_{01}+\epsilon_{02}) + (\epsilon_{01}-\epsilon_{02})\exp(-qL)]^{1/4} \\ \times[(\epsilon_{\infty 1}+\epsilon_{\infty 2}) + (\epsilon_{\infty 1}-\epsilon_{\infty 2})\exp(-qL)]^{3/4} \qquad (|z| > L/2). \end{cases} \qquad (6d)$$

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

For convenience, we introduce two unitary transformations U_1 and U_2:

$$U_1 = \exp\left[-\mathrm{i}\left(\sum_{k,m,p} a_{m,p}^+(k)a_{m,p}(k)k\cdot\rho + \sum_{q,p} b_p^+(q)b_p(q)q\cdot\rho\right)\right] \qquad (7a)$$

$$U_2 = \exp\left(\sum_{k,m,p}[a_{m,p}^+(k)f_{m,p}(k) - a_{m,p}(k)f_{m,p}^*(k)] + \sum_{q,p}[b_p^+(q)g_p(q) - b_p(q)g_p^*(q)]\right) \qquad (7b)$$

where $f_{m,p}$, $f_{m,p}^*$, g_p and g_p^* are the variational parameters determined by minimizing the total energy.

In the low-temperature limit, no real phonons are proposed to be present in the phonon ground state. Hence, we take $|0,0\rangle$ as the wavefunction of the phonon system and set $a_{m,p}(k)|0,0\rangle = b_p(q)|0,0\rangle = 0$.

After some straightforward algebra, we directly obtained

$$
\begin{aligned}
Q = \langle 0,0|U_2^{-1}U_1^{-1}HU_1U_2|0,0\rangle &= -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} - \frac{\hbar^2|\boldsymbol{K}_\rho^2|}{2m^*} + V(z) + |e|Fz \\
&+ \frac{\hbar^2}{2m^*}\left(\left|\sum_{\boldsymbol{k},m,p}|f_{m,p}(\boldsymbol{k})|^2\boldsymbol{k}\right|^2 + \left|\sum_{\boldsymbol{q},p}|g_p(\boldsymbol{q})|^2\boldsymbol{q}\right|^2\right) \\
&+ \sum_{\boldsymbol{k},m,p}|f_{m,p}(\boldsymbol{k})|^2\left(\hbar\omega_{\mathrm{LO}} + \frac{\hbar^2|\boldsymbol{k}|^2}{2m^*} - \frac{\hbar^2}{m^*}\boldsymbol{K}_\rho\cdot\boldsymbol{k}\right) \\
&+ \sum_{\boldsymbol{q},p}|g_p(\boldsymbol{q})|^2\left(\hbar\omega_{\mathrm{S}p} + \frac{\hbar^2|\boldsymbol{q}|^2}{2m^*} - \frac{\hbar^2}{m^*}\boldsymbol{K}_\rho\cdot\boldsymbol{q}\right) \\
&+ \sum_{\boldsymbol{k}}\left[B\left(\sum_{m=1,3,\ldots}^{N/2}\frac{\cos(m\pi z/L)}{[k^2+(m\pi/L)^2]^{1/2}}f_{m,+}(\boldsymbol{k})\right.\right. \\
&+ \left.\left.\sum_{m=2,4,\ldots}^{N/2}\frac{\sin(m\pi z/L)}{[k^2+(m\pi/L)^2]^{1/2}}f_{m,-}(\boldsymbol{k})\right) + \mathrm{HC}\right] + \sum_{\boldsymbol{q}}\left[\left(\frac{\sinh(qL)}{q}\right)^{1/2}\right. \\
&\times \left.\exp(-qL/2)\{C[G_+g_+(\boldsymbol{q}) + G_-g_-(\boldsymbol{q})] + \mathrm{HC}\}\right].
\end{aligned} \tag{8}
$$

Because we are interested only in the slow electron, we approximately set $\boldsymbol{K}_\rho = \boldsymbol{0}$. By symmetry, we also have

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

Then from

$$
\partial Q/\partial f^* = \partial Q/\partial f = \partial Q/\partial g^* = \partial Q/\partial g = 0 \tag{9}
$$

we obtain

$$
f_{m,+}(\boldsymbol{k}) = -\{[B^*\cos(m\pi z/L)]/[k^2+(m\pi/L)^2]^{1/2}\}/[\hbar\omega_{\mathrm{LO}} + \hbar^2|k|^2/2m^*] \tag{10a}
$$

$$
f_{m,-}(\boldsymbol{k}) = -\{[B^*\sin(m\pi z/L)]/[k^2+(m\pi/L)^2]^{1/2}\}/[\hbar\omega_{\mathrm{LO}} + \hbar^2|k|^2/2m^*] \tag{10b}
$$

$$
g_+(\boldsymbol{q}) = -[\![C^*\{[\sinh(qL)]/q\}^{1/2}\exp(-qL/2)G_+]\!]/[\hbar\omega_{\mathrm{S}+} + \hbar^2|q|^2/2m^*] \tag{10c}
$$

$$
g_-(\boldsymbol{q}) = -[\![C^*\{[\sinh(qL)]/q\}^{1/2}\exp(-qL/2)\,G_-]\!]/[\hbar\omega_{\mathrm{S}-} + \hbar^2|q|^2/2m^*]. \tag{10d}
$$

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

Inserting equations (10*a*)–(10*d*) into equation (8), we take the variation minimum of Q as the effective Hamiltonian of the electron–phonon system:

$$
H_{\mathrm{eff}} = \min Q = -(\hbar^2/2m^*)(\partial^2/\partial z^2) + |e|Fz + V(z) + V_1^{(\mathrm{B})}(z) + V_1^{(\mathrm{S})}(z) \tag{11}
$$

where $V_{\rm I}^{(\rm B)}(z)$ and $V_{\rm I}^{(\rm S)}(z)$ are the effective potentials from the effects of LO and SO modes, respectively, and directly derived as

$$V_{\rm I}^{(\rm B)}(z) = -\alpha\hbar\omega_{\rm LO}4Lu_{\rm l}\left[\sum_{m=1,3,\ldots}^{N/2}\cos^2\left(\frac{m\pi z}{L}\right)\frac{\ln(m\pi/Lu_{\rm l})}{(m\pi)^2-(Lu_{\rm l})^2}\right.$$

$$\left.+\sum_{m=2,4,\ldots}^{N/2}\sin^2\left(\frac{m\pi z}{L}\right)\frac{\ln(m\pi/Lu_{\rm l})}{(m\pi)^2-(Lu_{\rm l})^2}\right] \qquad (12a)$$

$$V_{\rm I}^{(\rm S)}(z) = -\alpha\hbar\omega_{\rm LO}\epsilon_{\infty 1}^{3/2}\epsilon_{01}^{1/2}Lu_{\rm l}$$

$$\times\left[\int_0^{N\pi/2}[1-\exp(-2x)]\left(\frac{G_+^2}{(Lu_{\rm S+})^2+x^2}+\frac{G_-^2}{(Lu_{\rm S-})^2+x^2}\right)\mathrm{d}x\right] \qquad (12b)$$

where we define $x = Lq$, the dimensionless coupling constant α of the electron–LO-phonon interaction as

$$\alpha = (m^*e^2/\hbar^2u_{\rm l})(1/\epsilon_{\infty 1}-1/\epsilon_{01}) \qquad (13)$$

and the polaron wavevectors $u_{\rm l}$ and $u_{{\rm S}p}$ as

$$u_{\rm l}^2 = 2m^*\omega_{\rm LO}/\hbar \qquad u_{{\rm S}p}^2 = 2m^*\omega_{{\rm S}p}/\hbar. \qquad (14)$$

3. The wavefunction and energy shifts

Since it is exceedingly complicated to obtain an exact solution of the eigenequation associated with $H_{\rm eff}$, a trial wavefunction along the z direction should be found in our variational approach. Compared with the subband energy of the conduction electron, the effective interaction potentials $V_{\rm I}^{(\rm B)}(z)$ and $V_{\rm I}^{(\rm S)}(z)$ can be treated as perturbations owing to their small values. So, we approximately set the wavefunction to satisfy

$$[-(\hbar^2/2m^*)(\partial^2/\partial z^2)+V(z)+|e|Fz]|\phi(z)\rangle = Ez|\phi(z)\rangle. \qquad (15)$$

(i) In the infinite-well approximation, the electron can be considered to move in an infinite square well along the z direction. In the presence of an electric field, the conduction electron is pushed against the field direction and the charge distribution is concentrated near the well interface. Then such a physical situation can be described well by

$$\phi(z) = \begin{cases} N(\beta)\cos(\pi z/L)\exp[-\beta(z/L+\frac{1}{2})] & |z|\leqslant L/2 \\ 0 & |z|>L/2 \end{cases} \qquad (16)$$

where β is the variational parameter and $N(\beta)$ is the normalization constant. The corresponding eigenenergy in equation (15) is

$$E_z = E_1(1+\beta^2/\pi^2)+|e|FL[1/2\beta+\beta/(\beta^2+\pi^2)-\tfrac{1}{2}\coth\beta] \quad (17)$$

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

(ii) For a finite QW, we set the potential as

$$V(z) = \begin{cases} V_0 & |z| > L/2 \\ 0 & |z| < L/2 \end{cases} \tag{18}$$

where V_0 is the depth of the finite well. So, the electron can be suggested to be a quasi-particle moving in a finite square-well potential along the z direction. For a weak field, the trial wavefunction of the electron quasi-ground state in a finite well is taken as

$$\phi(z) = \begin{cases} N(\beta)(1+\beta z/L)\cos(k_0 z/L) & (|z| \leqslant L/2) \\ N(\beta)(1+\beta z/L)\cos(k_0/2)\exp[q_0(\frac{1}{2} - |z|/L)] & (|z| > L/2) \end{cases} \tag{19}$$

where k_0 and q_0 are the characteristic dimensionless wavevectors in the zero-field ground state and are given by

$$k_0 = 2m^* L^2 E_1/\hbar^2 \qquad q_0 = 2m^* L^2(V_0 - E_1)/\hbar^2.$$

β, $N(\beta)$ and E_1 are quantities corresponding to those in equations (16) and (17). For simplicity, we neglect the slight difference between the effective mass in the well and that in the barrier and then the eigenenergy can be approximately obtained as

$$E_z = E_1 + [L^2/(L^2 + \beta^2\langle z^2\rangle_0)]\{(2|e|F\beta\langle z^2\rangle_0/L + \hbar^2\beta^2/2m^* L^2)\} \tag{20}$$

where $\langle z^2\rangle_0$ is the expected value in the ground state at zero field:

$$\langle z^2\rangle_0 = (L^2/4)\{1 + (\sin k_0)/k_0 + [2\cos^2(k_0/2)]/q_0\}^{-1}[\tfrac{1}{3} + (\sin k_0)/k_0 + (2\cos k_0)/k_0^2 - (2\sin k_0)/k_0^3 + (2/q_0)(1 + 2/q_0 + 2/q_0^2)\cos^2(k_0/2)]. \tag{21}$$

The total energy of the polaron state in a QW is obtained as

$$E_{\mathrm{tot}} = \langle\phi(z)|H_{\mathrm{eff}}|\phi(z)\rangle = E_z + E_s^{\mathrm{B}} + E_s^{\mathrm{S}} \tag{22}$$

where E_s^{B} and E_s^{S} are the self-energies from the expected values of $V_{\mathrm{I}}^{(\mathrm{B})}(z)$ and $V_{\mathrm{I}}^{(\mathrm{S})}(z)$, respectively, i.e.

$$\begin{aligned} E_s^{\mathrm{B}} &= \langle\phi(z)|V_{\mathrm{I}}^{(\mathrm{B})}(z)|\phi(z)\rangle \\ E_s^{\mathrm{S}} &= \langle\phi(z)|V_{\mathrm{I}}^{(\mathrm{S})}(z)|\phi(z)\rangle. \end{aligned} \tag{23}$$

In the case of the finite QW, for simplicity, we neglect the slight differences between the characteristic parameters of the different media in calculating the coefficients of E_s^{B} and E_s^{S}. Inserting the value of β obtained from $\partial E_{\mathrm{tot}}/\partial\beta = 0$ into equation (22), we obtain the minimized energy E_{tot}. The field-induced energy shift is $\Delta E = E_{\mathrm{tot}} - E_1$; for the infinite well,

$$\Delta E = E_1\beta^2/\pi^2 + |e|FL[1/2\beta + \beta/(\beta^2 + \pi^2) - \tfrac{1}{2}\coth\beta] + \Delta E_s^{\mathrm{B}} + \Delta E_s^{\mathrm{S}} \tag{24a}$$

and, for the finite well,

$$\Delta E = [L^2/(L^2 + \beta^2\langle z^2\rangle_0)][(2|e|F\beta/L)\langle z^2\rangle_0 + \hbar^2\beta^2/2m^* L^2] + \Delta E_s^{\mathrm{B}} + \Delta E_s^{\mathrm{S}}. \tag{24b}$$

In both cases, we introduce $\Delta E_s^{\mathrm{B}} = E_s^{\mathrm{B}} - (E_s^{\mathrm{B}})_0$ and $\Delta E_s^{\mathrm{S}} = E_s^{\mathrm{S}} - (E_s^{\mathrm{S}})_0$ to represent the corrections to the energy shift due to the interaction of the electron with LO phonons and SO phonons, respectively. $(E_s^{\mathrm{B}})_0$ and $(E_s^{\mathrm{S}})_0$ are the corresponding quantities in their respective ground states with zero field.

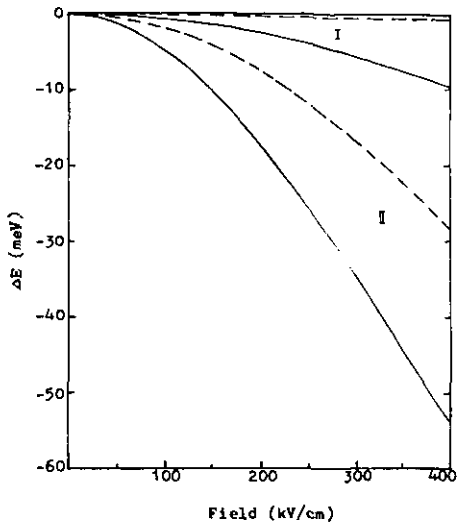

Figure 1. The energy shifts versus the electric field for a conduction electron in a GaAs–$Ga_{1-x}Al_xAs$ QW: ——, data for the finite well; - - - -, data for the infinite well. For curves I, $L = 34$ Å ($N = 6$) and, for curves II, $L = 100$ Å ($N = 18$).

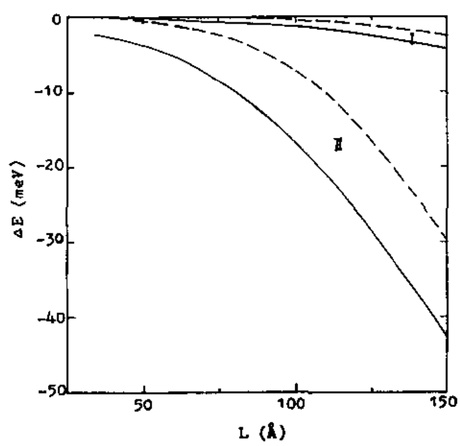

Figure 2. The energy shifts versus the well width for an electron in a GaAs–$Ga_{1-x}Al_xAs$ QW: ——, data for the finite well; - - - -, data for the infinite well. For curves I, $F = 50$ kV cm^{-1} and, for curves II, $F = 200$ kV cm^{-1}.

4. Results and discussion

Taking a GaAs–$Ga_{1-x}Al_xAs$ QW as an example, in the presence of an external electric field perpendicular to the well layers, we compute the energy shifts and the corrections attributed to the electron–phonon interaction. In this paper, we consider a slow electron ($\boldsymbol{K}_\rho = \mathbf{0}$) moving in a thin infinite QW and in a thin finite QW. For the finite well, we set the barrier height at $V_0 = 0.4$ eV. According to the variation method used in this paper, our study is confined to the thin QW subjected to a weak electric field.

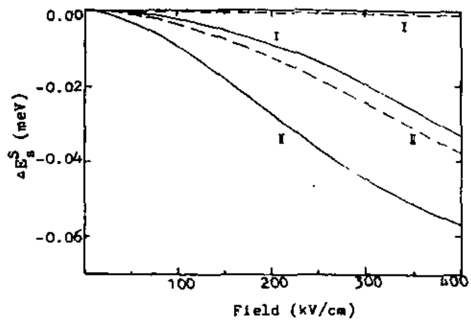

Figure 3. The SO-mode contribution to the energy shifts in a QW versus the electric field. The curves are represented in the same way as those in figure 1.

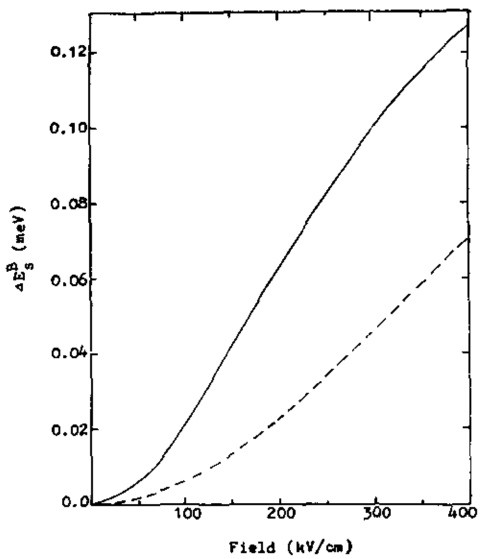

Figure 4. The LO-mode contribution to the energy shifts in a QW versus the electric field: ——, data for the finite well with $L = 100$ Å ($N = 18$); ----, data for the infinite well with $L = 100$ Å ($N = 18$).

In figures 1 and 2, it is shown that the Stark shifts depend not only on the field strength and the well width but also on the finite potential barrier. From comparison between the full and broken curves, we can see that the effect of a finite barrier height obviously enhances the field-induced energy shift. From our calculations, it is also found that the well width is the main factor in influencing the finite-barrier effect. For instance, for $F = 50$ kV cm^{-1}, when $L = 34$ Å ($N = 6$), the shift in a finite QW is 26 times larger than that in an infinite QW but, when $L = 100$ Å ($N = 18$), the specific value rapidly decreases to 2.5 times that in an infinite QW. The thicker the well, the smaller the possibility of barrier penetration from the well, and so the barrier height effect is greatly weakened with increasing well thickness. For a QW with a certain width, an increase in the field strength also weakens the finite-barrier effect. However, for a weak field such an influence is so weak that we

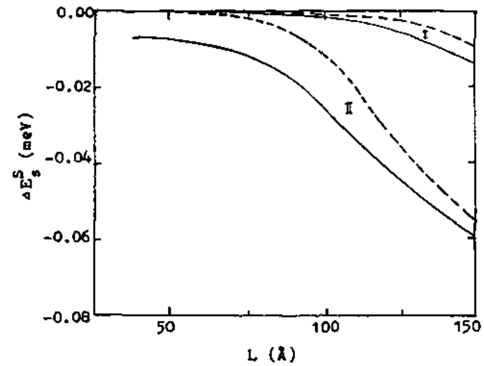

Figure 5. Variation in the SO-mode correction to the energy shifts with the well width. The curves are represented in the same way as in figure 2.

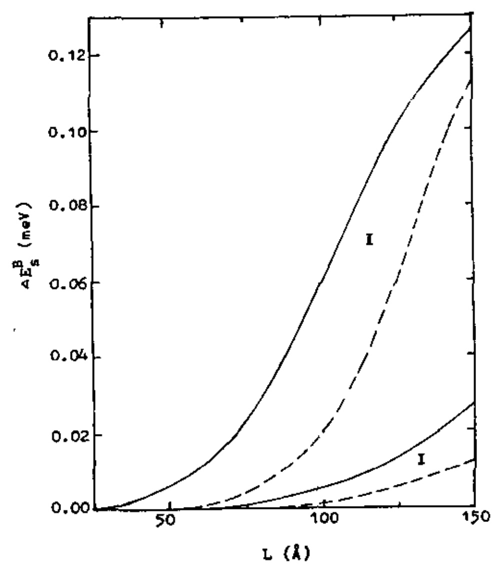

Figure 6. Variation in the LO-mode correction to the energy shifts with the well width. The curves are represented in the same way as in figure 2.

may approximately regard the ratio of the shift in an infinite well to that in a finite well as constant.

The effect of the electron–phonon interaction on the total energy shift contains two parts: ΔE_s^B and ΔE_s^S, which are due to the LO- and SO-phonon contributions, respectively. As shown in figures 3 and 4, both these contributions cause significant corrections to the energy shifts and drastically increase when the field becomes stronger. The value of the LO-mode correction ΔE_s^B obtained by us is not as large as that calculated in [18]. 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 QWs. As a result, the electron–SO-phonon interaction will increase (i.e. $\Delta E_s^S < 0$) while the electron–LO-phonon interaction will decrease (i.e. $\Delta E_s^B > 0$). So, the influences of the different modes are entirely contrary: the energy shift is enhanced by the

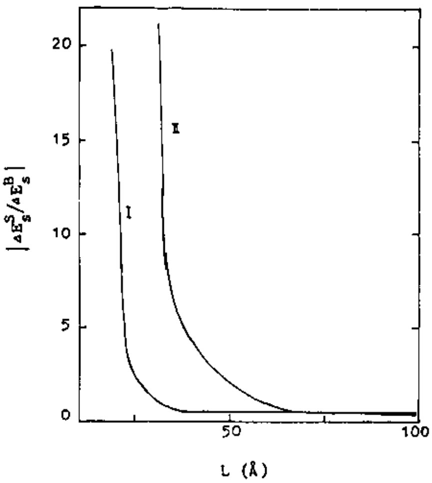

Figure 7. Plot of the ratio $|\Delta E_s^S/\Delta E_s^B|$ versus thickness of a QW. Curve I is for the infinite well and curve II for the finite well.

SO-mode effect and weakened by the LO-mode effect.

Figures 5 and 6 show us how to change the corrections with the well width. Irrespective of how the LO and SO self-energies change with the thickness, both their corrections to the shifts rapidly become large as the thickness increases. Comparing the full and broken curves in figures 3–6, we can conclude that the effect of the barrier height enhances the corrections from the phonon effects as it does the total energy shifts. It is also influenced mainly by the well width as shown in figures 5 and 6. The finite-barrier effect is so obviously weakened when the well becomes thicker that for a sufficiently thick ($L > 150$ Å) finite well the corrections will make the results close to those for an infinite well.

In our calculations, we find that for a weak field the value of $|\Delta E_s^S/\Delta E_s^B|$ will depend only on the well thickness. The change in $|\Delta E_s^S/\Delta E_s^B|$ as a function of the well thickness is plotted in figure 7 to compare the contributions due to the SO-mode and the LO-mode effects. It is obvious that for a very thin well the correction of the electron–phonon interaction to the energy shift will be mainly attributed to the SO-mode contribution. With increasing well thickness, the LO-mode contribution rapidly becomes dominant. In particular, as the well becomes sufficiently thick, the correction due to the phonon effect will mainly depend on the electron–bulk-LO-phonon interaction. As shown in figure 7, only for a very thin well is the influence of the finite-barrier effect on the ratio $|\Delta E_s^S/\Delta E_s^B|$ very strong and obvious.

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