Electron-phonon effects on Stark shifts of a bound polaron in a quantum well

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The polaron effects on the quantum confined Stark effect of a bound polaron in a finite quantum well are investigated by means of the perturbation-variation technique. The presence of an ionized impurity is found to decrease the Stark shift and weaken the effect of finite barrier height. The electron-phonon effects contribute significant corrections to the energy shifts.

The study of the quantum confined Stark effect in a quantum well (QW) has received considerable attention in the past few years.[1-6] To date, most theoretical work has dealt with the calculation of a ground state, in which the infinite-well approximation is employed. Strictly speaking, for a very thin QW, the barrier penetration from a well cannot be neglected, so many techniques for the calculation of quasibound states in a finite QW have been proposed.[4-7] Among these methods, the variation approach has the advantage of not only providing analytical expressions for the eigenstate energies and the trial wave functions, but also giving numerical results with reasonable accuracy in the weak-field limit.[6-8]

The development of doped superlattice structures has greatly contributed to the understanding of the role of impurities in QW's. Recently, the presence of ionized impurities in QW's was suggested as one possible mechanism to explain the strong broadening of the excitonic peaks in the electronic absorption spectra with applied fields.[9] The early theoretical studies concluded that the electron–optical-phonon coupling would have a significant influence on the properties of the polaron in QW's.[10,11] However, only recently has the interaction of the electron with bulk longitudinal-optical (LO) phonons been considered in the Stark-shift calculation of a polaron in an infinite QW.[12]

In this paper, with both LO and surface-optical (SO) phonons included, we investigate the Stark shifts of a bound polaron in a finite QW by means of the perturbation-variation method.

Consider a QW of width L and under an electric field $\mathbf{F}$ perpendicular to the well layers (along the z direction). A shallow doped impurity is located at the center of the well ($z=0$). The effective-mass approximation is assumed to be valid and the barrier penetration effect is taken into account. The problem may approximately be considered as the motion of an electron with charge e and effective mass m^* in a thin finite QW of depth V_0 and subjected to a weak electric field. For the electron-phonon system, the Hamiltonian is

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

and the Hamiltonian of the shallow donor is given by

$$H_e=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}-\frac{\hbar^2}{2m^*}\nabla_\rho^2-\frac{e^2}{\epsilon_\infty r}+V(z)+|e|Fz\ , \tag{2}$$

where ρ is the electron position vector in the xy plane parallel to the well layer and $-e^2/\epsilon_\infty r$ is the Coulomb potential between the electron and the ionized impurity, in which ϵ_∞ is the optical dielectric constant and $r=(\rho^2+z^2)^{1/2}$. $V(z)$ is the potential for the electron along the z direction and suggested as

$$V(z)=\begin{cases} V_0, & |z|>L/2 \\ 0, & |z|<L/2. \end{cases} \tag{3}$$

For simplicity, in the well and in the barrier, the slight differences of m^* and of ϵ_∞ are neglected. To solve the eigenequation of H_e, we introduce the plane Coulomb potential with the parameter λ (Ref. 13) and rewrite H_e as

$$H_e=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}-\frac{\hbar^2}{2m^*}\nabla_\rho^2-\frac{\lambda e^2}{\epsilon_\infty \rho}+\frac{e^2}{\epsilon_\infty}\left[\frac{\lambda}{\rho}-\frac{1}{r}\right] +|e|Fz+V(z)\ . \tag{4}$$

In Eq. (1), $H_{\rm ph}=H_{\rm LO}+H_{\rm SO}$ and $H_{\rm int}=H_{e\text{-LO}}+H_{e\text{-SO}}$ represent the phonon field Hamiltonian and the interaction Hamiltonian operator, respectively. For a weak electric field, the particle wave function decays very fast outside the well,[7] i.e., electrons still will be confined in a very narrow area (width $\sim L$) near the well, though the penetration effect should be considered. Therefore, $H_{\rm int}$ may also be approximately taken to be the operators de-

duced by Licari and Evrard.[14]

For the sake of convenience, we give a further approximation of H. First, by carrying out two canonical transformations U_1 and U_2 as

$$U_1=\exp\left[-i\sum_{\mathbf{k},m,p}a^{\dagger}_{m,p}(\mathbf{k})a_{m,p}(\mathbf{k})\mathbf{k}\cdot\mathbf{p}\right.$$
$$\left.-i\sum_{\mathbf{q},p}b^{\dagger}_{p}(\mathbf{q})b_{p}(\mathbf{q})\mathbf{q}\cdot\mathbf{p}\right], \tag{5a}$$

$$U_2=\exp\left[\sum_{\mathbf{k},m,p}[a^{\dagger}_{m,p}(\mathbf{k})f_{m,p}(\mathbf{k})-a_{m,p}(\mathbf{k})f^{*}_{m,p}(\mathbf{k})]\right.$$
$$\left.+\sum_{\mathbf{q},p}[b^{\dagger}_{p}(\mathbf{q})g_{p}(\mathbf{q})-b_{p}(\mathbf{q})g^{*}_{p}(\mathbf{q})]\right], \tag{5b}$$

where the variables have their respective senses as illustrated in Ref. 15 and the parameters $f_{m,p}$, $f^{*}_{m,p}$, g_p, and g^{*}_{p} will be determined by minimizing the effective Hamiltonian; subsequently, we get the transformed Hamiltonian $\mathcal{H}=U_2^{-1}U_1^{-1}HU_1U_2$. Then, in the low-temperature limit, we take $|0,0\rangle$ as the wave function of the phonon system and set $Q=\langle 0,0|\mathcal{H}|0,0\rangle$. At last the variation minimum of Q is taken as the system effective Hamiltonian. After some straightforward algebraic manipulation, for a slow electron, we obtain

$$H_{\text{eff}}=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}-\frac{\hbar^2}{2m^*}\nabla^2_{\rho}-\frac{\lambda e^2}{\epsilon_{\infty}\rho}+\frac{e^2}{\epsilon_{\infty}}\left[\frac{\lambda}{\rho}-\frac{1}{r}\right]$$
$$+|e|Fz+V(z)+V_I^{(B)}(z)+V_I^{(S)}(z) \tag{6}$$

where $V_I^{(B)}(z)$ and $V_I^{(S)}(z)$ are the effective interaction potentials, respectively, from LO and SO mode effects, and are expressed by the equations obtained elsewhere by us.[15]

For exploring the trial wave function in our variational approach, we rewrite H_{eff} as

$$H_{\text{eff}}=H_0+H_1=(H_z+H_{2D})+H_1\ , \tag{7}$$

in which

$$H_z=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+V(z)+e|Fz+V_I^{(B)}(z)+V_I^{(S)}(z)\ , \tag{7a}$$

$$H_{2D}=-\frac{\hbar^2}{2m^*}\nabla^2_{\rho}-\frac{\lambda e^2}{\epsilon_{\infty}\rho}\ , \tag{7b}$$

$$H_1=\frac{e^2}{\epsilon_{\infty}}\left[\frac{\lambda}{\rho}-\frac{1}{r}\right]. \tag{7c}$$

H_1 is taken as a perturbation by choosing an applicable value of λ in the thin well and H_0 as the unperturbed Hamiltonian. From Eqs. (7a) and (7b), the wave function can be written as $|\Phi(z,\rho)\rangle=|\varphi(z)\rangle\,|\psi(\rho)\rangle$ and

$$H_0|\Phi(z,\rho)\rangle=E_{\text{tot}}|\Phi(z,\rho)\rangle\ . \tag{8}$$

Compared with the subband energy of the conduction electron, $V_I^{(B)}(z)$ and $V_I^{(S)}(z)$ can be neglected because of their small values. We approximately regard the electron moving in a finite square-well potential along the z direction and have

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+|e|Fz+V(z)\right]|\varphi(z)\rangle=E_z|\varphi(z)\rangle\ . \tag{9}$$

If the electric field is not excessively strong, the electron state with a long lifetime may be considered as a quasi-ground state described well by the wave function as[7]

$$\varphi(z)=\begin{cases}N(\beta)(1+\beta z/L)\cos(k_0z/L), & |z|<L/2\\ N(\beta)e^{q_0/2}\cos(k_0/2)(1+\beta z/L)e^{-q_0z/L}, & z>L/2\\ N(\beta)e^{q_0/2}\cos(k_0/2)(1+\beta z/L)e^{q_0z/L}, & z<-L/2\ ,\end{cases} \tag{10}$$

where β is the variational parameter and $N(\beta)$ is the normalization constant. q_0 and k_0 are the characteristic dimensionless wave vectors and $q_0=2m^*L^2(V_0-E_1)/\hbar^2$; $k_0=2m^*L^2E_1/\hbar^2$, in which E_1 is the zero-field ground-state energy. Solving Eq. (9), we obtain

$$E_z=E_1+\frac{L^2}{L^2+\beta^2\langle z^2\rangle_0}\left[\frac{2|e|F\beta\langle z^2\rangle_0}{L}+\frac{\hbar^2\beta^2}{2m^*L^2}\right], \tag{11}$$

where $\langle z^2\rangle_0=\langle\phi_0(z)|z^2|\phi_0(z)\rangle$ and $\phi_0(z)$ is the electron wave function in the zero-field ground state. Equation (7b) shows that the electron motion in the xy plane is a 2D hydrogenlike atom problem. Referring to the equation

$$H_{2D}|\psi(\rho)\rangle=E_{2D}|\psi(\rho)\rangle \tag{12}$$

we get the solution of its ground state,

$$\psi(\rho)=\frac{1}{\sqrt{2\pi}}\frac{4\lambda}{a_0}\exp\left[-\frac{2\lambda}{a_0}\rho\right]\quad(a_0=\epsilon_{\infty}\hbar^2/m^*e^2)\ , \tag{13a}$$

$$E_{2D}=-2\lambda^2m^*e^4/\epsilon^2_{\infty}\hbar^2\ . \tag{13b}$$

By solving Eq. (8), the total energy is obtained as

$$E_{\text{tot}}=E_z+E_{2D}+E_s^B+E_s^S\ , \tag{14}$$

where

$$E_s^B=\langle\varphi(z)|V_I^{(B)}(z)|\varphi(z)\rangle\ ,$$
$$E_s^S=\langle\varphi(z)|V_I^{(S)}(z)|\varphi(z)\rangle\ .$$

For simplicity, in the coefficients of E_s^B and E_s^S we neglect the slight differences between the characteristic parameters of different crystals. The parameters β and λ may be determined simultaneously from $\partial E_{\text{tot}}/\partial\beta=0$ and

$$\overline{H}_1(\lambda)=\langle\Phi(z,\rho)|H_1|\Phi(z,\rho)\rangle=0\ . \tag{15}$$

Finally we get the field-induced energy shift as

$$\Delta E=\frac{L^2}{L^2+\beta^2\langle z^2\rangle_0}\left[\frac{2|e|F\beta}{L}\langle z^2\rangle_0+\frac{\hbar^2\beta^2}{2m^*L^2}\right]$$
$$-\frac{2m^*e^4}{\epsilon_\infty^2\hbar^2}(\lambda^2-\lambda_0^2)+\Delta E_s^B+\Delta E_s^S \quad (16)$$

in which we set $\Delta E_s^B=E_s^B-(E_s^B)_0$ and $\Delta E_s^S=E_s^S-(E_s^S)_0$ to represent the corrections to the energy shifts due to the LO-mode and SO-mode effect, respectively. λ_0, $(E_s^B)_0$, and $(E_s^S)_0$ are the corresponding variables in the zero-field state.

In this paper, taking GaAs-$Ga_{1-x}Al_xAs$ as an example, we make the calculations of the Stark shifts in a finite QW with a barrier height $V_0=0.4$ eV. In Fig. 1, the comparison of two curves shows us that the presence of an ionized doped impurity obviously decreases the energy shift of the electron. Under a weak field ($\beta^2\langle z^2\rangle_0\ll L^2$) and neglecting the small self-energies, we obtain the difference of the energy shifts of the electron between with and without an impurity as

$$\Delta\simeq\frac{\hbar^2(\Delta\beta)^2}{2m^*L^2}+\frac{2m^*e^4}{\epsilon_\infty^2\hbar^2}(\lambda_0^2-\lambda^2)\,, \quad (17)$$

where $\Delta\beta$ is the change of β in the two cases. From Eq. (17), it is seen that the effect of a doped impurity is composed of two parts: the correction in the z direction and in the xy plane. Our calculation demonstrates that both of them decrease the energy shift and the correction in the xy plane plays the more important role. For instance, with $L=34$ Å and $F=150$ kV/cm, it is nine times larger

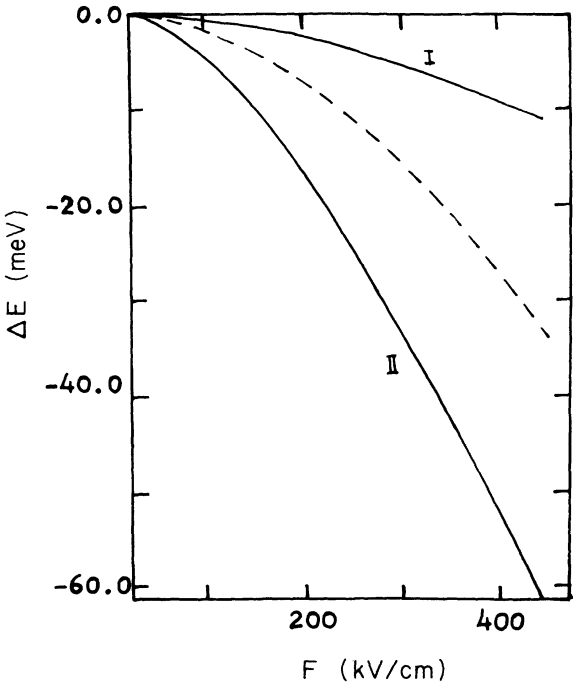

FIG. 2. Comparison of the energy shifts for the bound polaron in a finite QW and in an infinite QW. The solid lines show the results for a finite QW with $L=34$ Å (I) and $L=100$ Å (II). The dashed line shows results for an infinite QW with $L=100$ Å.

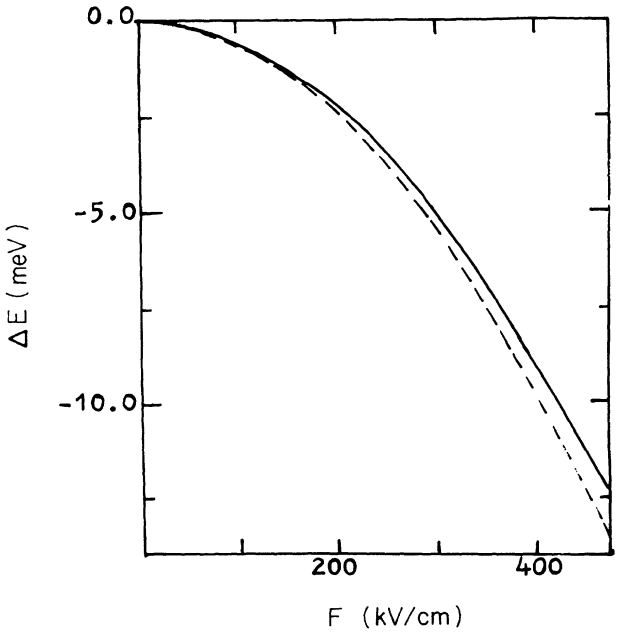

FIG. 1. The energy shifts vs the electric field for an electron in a finite QW with $L=34$ Å. The solid line represents results for the well with an on-center impurity and the dashed line those for the well without any impurity.

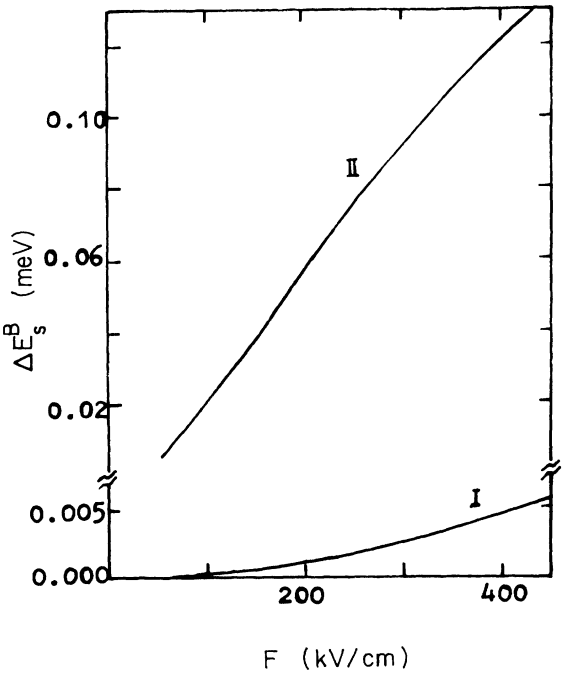

FIG. 3. The correction of LO-mode effect to the energy shift of the bound polaron vs the electric field in a finite QW with $L=34$ Å (I) and $L=100$ Å (II).

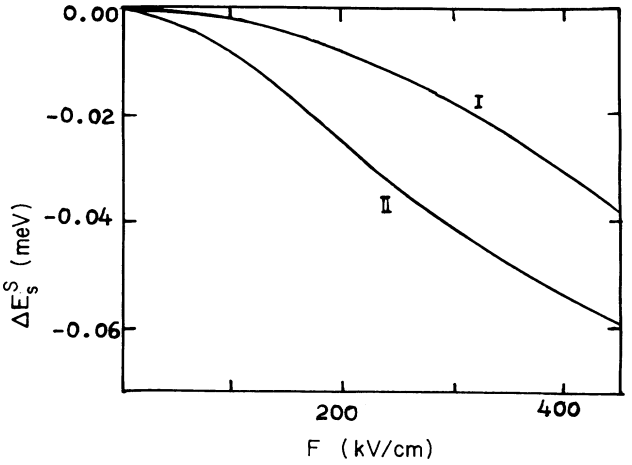

FIG. 4. The correction of SO-mode effect in the same case as in Fig. 3.

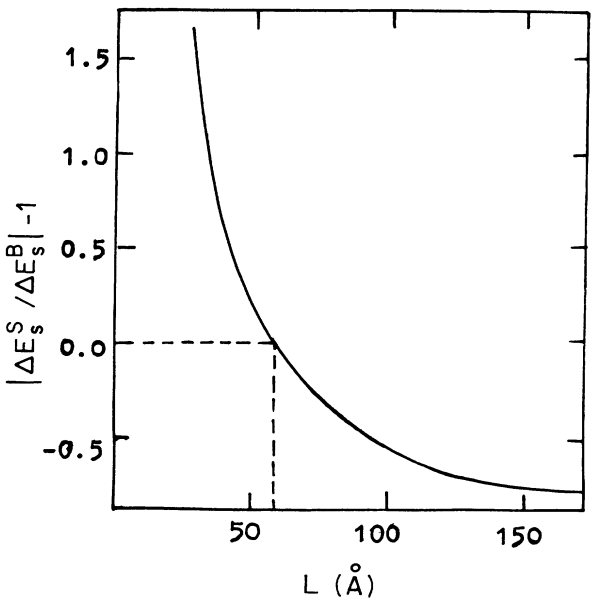

FIG. 5. Plot of the ratio $|\Delta E_s^S \Delta E_s^B|$ vs the well thickness.

than that in the z direction. Comparing our results with that of Ref. 15 in an infinite-well approximation, as shown in Fig. 2, we conclude that the effect of finite barrier height is also to enhance the Stark shift of a bound polaron. In particular, we find that such an effect becomes much weaker than that in Ref. 7 due to the presence of an on-center impurity. For instance, the shift of a bound polaron in a finite well of width $L=34$ Å is about 23 times larger than that in an infinite well, which is much smaller than 38 times that obtained in Ref. 7. It is because the attractive Coulomb action between the electron and the ionized impurity weakens the effect of the external electric field that we obtain the above considerations.

As shown in Figs. 3 and 4, both ΔE_s^B and ΔE_s^S give significant corrections to the energy shifts. In the presence of an 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 will increase ($\Delta E_s^S<0$) while the electron–LO-phonon interaction will decrease ($\Delta E_s^B>0$). So, their influences on the shifts are entirely contrary, i.e., the energy shift is enhanced by the SO-mode effect but weakened by the LO-mode effect. In our calculation, for a weak field ($\beta \ll 1$) both ΔE_s^B and ΔE_s^S are approximately proportional to β^2, so that the value of $|\Delta E_s^S/\Delta E_s^B|$ will only depend on the well thickness. In Fig. 5, one can see that for a very thin well ($L<60$ Å) the correction of the phonon effect is mainly attributed to the SO-mode contribution. With the thickness increasing, the LO-mode contribution rapidly becomes the dominate one. As $L \gg 60$ Å, the phonon effect on Stark shifts will depend only on the electron–LO-phonon interaction.

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