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Stark shift of hydrogenic impurity states in a quantum well

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We present a variational calculation for the Stark shift of hydrogenic impurity states in an isolated quantum well under a constant electric field, due to the competition between the quantum-confined effect, impurity Coulomb potential, and electric field. The dependence of the ground impurity binding energy on the width of the well and the impurity position under different electronic fields is calculated. That the impurity at different positions causes different Stark shifts under an electric field is discussed. In a narrow well, the quantum-confined effect depresses the Stark effect.

The quantum-confined Stark effect in a quantum-well (QW) structure has attracted considerable attention recently, due to its interesting optical-absorption properties and electro-optical applications.[1,2] Up to now, most theoretical work has been devoted to the effects without impurities, e.g., the eigenstates of QW,[3] the exciton spectra,[4,5] and the quantum-confined Franz-Keldysh effect.[1]

In this paper we report the results of variational calculations for the Stark shift of the ground hydrogenic impurity state in an isolated GaAs/$Ga_{1-x}Al_xAs$ QW, under a constant electric field perpendicular to the layers defining the QW.

We ignore the tunneling between QW's, and take the single-well approximation. In the framework of the effective-mass approximation, the dimensionless Hamiltonian for an electron in an isolated infinite quantum-well structure is given by

$$H=-\nabla^2-2/r+V(z)+qz \ , \tag{1}$$

where

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

and

$$q=|e|Fa^*/\mathcal{R}^* \ ,$$

where F is the electric field applied along the direction of the well, z axes. (This direction is perpendicular to the interface plane.) In Eq. (1) all energies are expressed in units of the effective Rydberg $\mathcal{R}^*=m^*e^4/2\hbar^2\epsilon^2\sim 5.83$ meV, and all distances are expressed in units of the effective Bohr radius $a^*=\hbar^2\epsilon/m^*e^2\sim 98.7$ Å, where m^* and ϵ are the electronic effective mass and the dielectric constant, respectively, of GaAs. The position of the hydrogenic impurity as $(0,0,z_i)$, and the distance between the electron and the impurity is $r=[x^2+y^2+(z-z_i)^2]^{1/2}$. The origin of the coordinate system is chosen to be at the center of the well.

The square-well Hamiltonian under electric field without impurity is

$$H_0=-\frac{d^2}{dz^2}+V(z)+qz \ . \tag{2}$$

The trial wave function for the lowest eigenvalue of H_0 is

$$f(z)=N_0(\beta)\cos(\pi z/L)\exp(-\beta z/L), \quad |z|<L/2 \ . \tag{3}$$

The variational lowest eigenvalue of H_0 with respect to variational parameter β is given by

$$E_0=\min_f\{\langle f|H_0|f\rangle\} \ . \tag{4}$$

The normalization constant N_0 and the expectation value of H_0 are as follows:

$$N_0(\beta)=\{0.5[\tilde{F}_1(0)+\mathrm{Re}\tilde{F}_1(2\pi/L)]|_{z=-L/2}^{z=L/2}\}^{-1/2} \ , \tag{5}$$

$$\begin{aligned}\langle f|H_0|f\rangle=N_0^2\{&(\pi^2-\beta^2)/(2L^2)[\tilde{F}_1(0)+\mathrm{Re}\tilde{F}_1(2\pi/L)]\\&-(\pi\beta/L^2)\mathrm{Im}\tilde{F}_1(2\pi/L)\\&+0.5q[\tilde{F}_2(0)+\mathrm{Re}\tilde{F}_2(2\pi/L)]\}|_{z=-L/2}^{z=L/2} \ .\end{aligned} \tag{6}$$

The functions $\tilde{F}_1(\alpha)$, $\tilde{F}_2(\alpha)$, and others which will be used later are defined in the Appendix.

For the ground state of H in Eq. (1), we use the trial wave function containing variational parameter λ:

$$\psi(x,y,z)=N(\lambda)\cos(\pi z/L)\exp(-\beta z/L-r/\lambda) \ , \quad |z|<L/2 \ , \tag{7}$$

where the normalization constant

$$N(\lambda)=\{0.25\pi\lambda^2[P(\lambda)|_{z=-L/2}^{z=z_i}+P(-\lambda)|_{z=z_i}^{z=L/2}]\}^{-1/2} \ . \tag{8}$$

The variational binding energy E_b affecting an electron injected from the hydrogenic impurity is the difference between the lowest E_0 without the impurity potential and the variational minimum of the expectation of the Hamiltonian H:[6]

$$E_b = E_0 - \min_{\psi}\{\langle\psi|H|\psi\rangle\} \; . \tag{9}$$

The expectation values of H are as follows:

$$\begin{aligned}\langle\psi|H|\psi\rangle = {} & [\pi N^2/(2L^2)] \\ & \times\{T(\lambda)|_{z=-L/2}^{z=z_i} + T(-\lambda)|_{z=z_i}^{z=L/2}\} \\ & + (\pi N^2/L)\{S(\lambda)|_{z=-L/2}^{z=z_i} + S(-\lambda)|_{z=z_i}^{z=L/2}\} \; .\end{aligned} \tag{10}$$

Now, in the limit of infinite height barrier, $\langle\psi|H|\psi\rangle$ can easily be calculated from Eq. (10) and its minimization with respect to λ leads to the desired binding energy through Eq. (9). The electron density distribution in the layers of a QW can be shown as follows:

$$\begin{aligned}\Phi(z) = {} & \int d\rho\, 2\pi\rho|\psi(\rho,z)|^2 \\ & = (\pi\lambda^2N^2/4)[1+\cos(2/L)](1+2|z-z_i|/\lambda) \\ & \times\exp(-2|z-z_i|/\lambda - 2\beta z/L) \; .\end{aligned} \tag{11}$$

The results are displayed in the figures. Figure 1 shows the binding energy as a function of the position of the hydrogenic impurity with the electric field F as a parameter in different width QW's, $L = 70$, 100, 200, and 300 Å. $\alpha = z_i/L$ is the parameter of the impurity position in the QW. In the figure the dotted line is for $F = 500$ kV/cm, the dashed-dotted line is for $F = 200$ kV/cm, the dashed line is for $F = 50$ kV/cm, and the solid line is for $F = 0$. At zero field we obtain central symmetrical curves $E_b \sim \alpha$. Upon decreasing the well width L, E_b increases and the Stark shift decreases for all α, due to increase of the quantum-confined effect. The electron is mostly around the center of the QW for all α, due to the competition between the quantum-confined effect and the impurity Coulomb potential. For example, when the impurity shifts from the left edge to the right edge of the 300-Å-width QW, the maximum of the electron layer density distribution $\Phi(z)$ shifts from -30 to 30 Å. So the impurity binding energy has a maximum around the QW center for all L, when the electric field is not applied. When the applied electric field F is turned on, it drives the maximum region of $\Phi(z)$ to the $-z$ direction, and narrows it. For example, in the 300-Å QW the maximum region of $\Phi(z)$ for all α is ~ -90 to -75 Å for $F = 50$ kV/cm, ~ -112 to -105 Å for $F = 200$ kV/cm, and ~ -126 to -123 Å for $F = 500$ kV/cm. The binding energy is the result of competition between the quantum-confined effect, the electric field, and the impurity Coulomb potential. When the position of the maximum of $\Phi(z)$, which is dependent on the impurity position z_i, coincides with z_i itself, the binding energy of the impurity has a peak. When z_i increases from the left of the peak then the decrease of $\langle H_I\rangle$ is sharper than the increase of $\langle H_W\rangle[H_W = -\nabla^2 + V(z)]$ while $\langle H_F\rangle$ varies smoothly, causing a peak of E_b, and in this region the stronger electric field drives E_b to higher value. Similar to the case of $\Phi(z)$, the peak of curve $E_b \sim \alpha$ is driven by the applied electric field F to the $-z$ direction, and is narrowed by F.

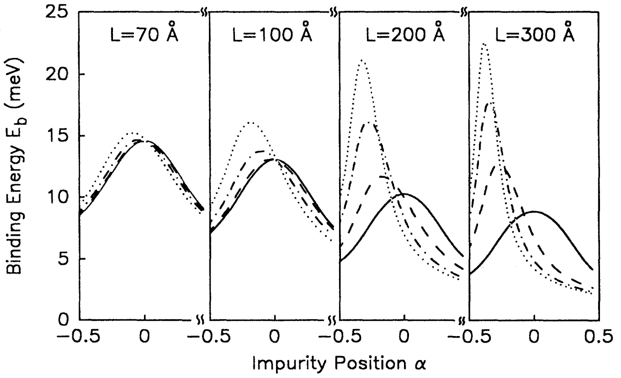

FIG. 1. Binding energy E_b vs impurity position α in different width QW for four values of the longitudinal electric field F: ——, $F = 0$; — — —, $F = 50$ kV/cm; —·—·—·, $F = 200$ kV/cm; and · · ·, $F = 500$ kV/cm.

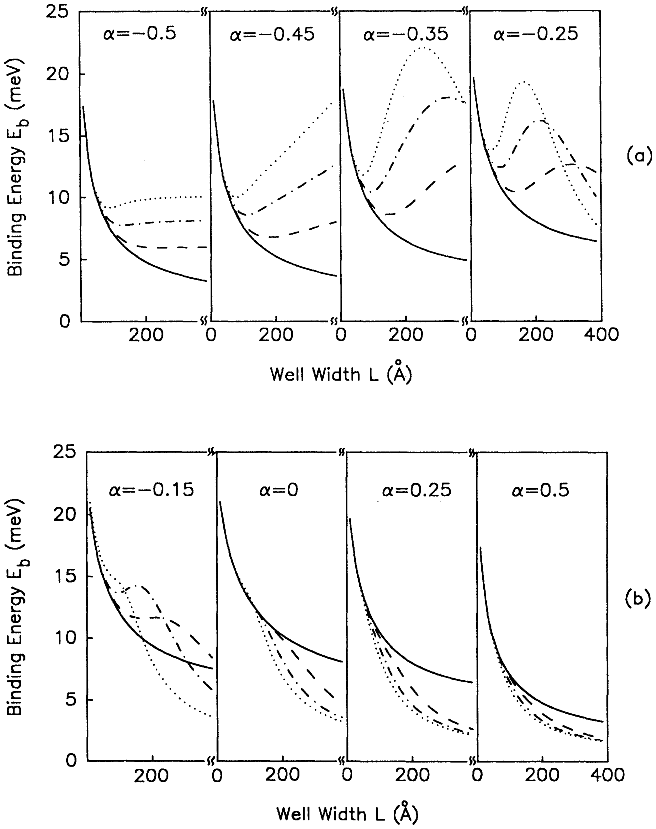

FIG. 2. Binding energy E_b vs well width L for four values of the longitudinal electric field F (the legend is the same as Fig. 1) for different position impurity doping.

On the other hand, when z_i increases in the right half of the QW, that smooth increase of $\langle H_I \rangle$ is a little faster than the decrease of $\langle H_W \rangle$ and $\langle H_F \rangle$ causes E_b to decrease, and in this region the stronger electric field drives E_b to lower value. Between them, there is a transformation region where the behavior of E_b under electric field is complicated. Both of the two kinds of Stark shift are depressed by the quantum-confined effect in the narrow QW.

Figure 2 shows the binding energy as a function of the well width with the electric field F as a parameter for the different position of the hydrogenic impurity in the QW. When the impurity is in the right half of the QW, $\alpha > 0$, the stronger electric field drives the impurity binding energy down. When the impurity is at the center of the QW, $\alpha = 0$, the situation is mostly like one where $\alpha > 0$, except for the QW with $50 < L < 110$ Å, where E_b has a small opposite shift under electric field. When the impurity is doped in the left side of the QW with $\alpha < -0.35$, E_b has the opposite Stark shift under electric field for the QW with $L < 400$ Å. When α is around -0.3, the strong electric field causes E_b to have a maximum. When the impurity is doped near the QW center with $z_i < 0$, the electric field causes E_b to have a complicated behavior. For any positions of impurity doped in a narrow QW the Stark shift becomes indistinguishable in the figure, due to the strong quantum-confined effect.

Figure 3 shows the binding energy as a function of electric field for well width $L = 100$ Å. In the figure the solid line represents the central impurity, and the dashed line, the dotted line, the dashed-dotted line, and the dashed-dotted-dotted line represent impurity position $Z_i = -50$, -25, 25, and 50 Å, respectively. For the negative-region doping the impurity binding energy E_b as a function of electric field has a positive slope. On the contrary, for the positive-region doping the E_b curve has a negative slope.

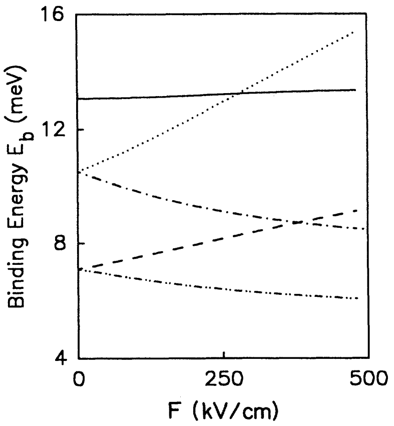

FIG. 3. Binding energy E_b vs electric field with $L = 100$ Å for different impurity positions α: — — —, $\alpha = -0.5$; $\cdots$, $\alpha = -0.25$; ——, $\alpha = 0$; –·–, $\alpha = 0.25$; and –··–, $\alpha = 0.5$.

In summary the effect of the hydrogenic impurity state on the Stark shift in a QW is studied in terms of variational calculation. The competition among the quantum-confined effect, the impurity Coulomb potential, and the constant electric field causes different Stark shift of the impurity binding energy. The strong quantum-confined effect depresses the Stark shift under electric field for a narrow QW.

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APPENDIX

$$F_1(\alpha) = \exp(Kz)/K, \quad K = 2/\lambda - 2\beta/L + i\alpha\ ,$$

$$F_2(\alpha) = F_1(\alpha)(z - 1/K)\ ,$$

$$F_3(\alpha) = F_1(\alpha)(z^2 - 2z/K + 2/K^2)\ ,$$

$$\tilde{F}_1(\alpha) = \exp(\tilde{K}z)/\tilde{K}, \quad \tilde{K} = -2\beta/L + i\alpha\ ,$$

$$\tilde{F}_2(\alpha) = \tilde{F}_1(\alpha)(z - 1/\tilde{K})\ ,$$

$$P(\lambda) = \{(1 + 2z_i/\lambda)[F_1(0) + \mathrm{Re}F_1(2\pi/L)] - (2/\lambda)[F_2(0) + \mathrm{Re}F_2(2\pi/L)]\}\exp(-2z_i/\lambda)\ ,$$

$$\begin{aligned} T(\lambda) = {} & (1 + 2z_i/\lambda)\exp(-2z_i/\lambda)\{A_1[F_1(0) + \mathrm{Re}F_1(2\pi/L)] + A_2[F_2(0) + \mathrm{Re}F_2(2\pi/L)] + A_3\mathrm{Im}F_1(2\pi/L)\} \\ & - (2/\lambda)\exp(-2z_i\lambda)\{A_1[F_2(0) + \mathrm{Re}F_2(2\pi/L)] + A_2[F_3(0) + \mathrm{Re}F_3(2\pi/L)] + A_3\mathrm{Im}F_2(2\pi/L)\}\ , \end{aligned}$$

$$S(\lambda) = \exp(-2z_i/\lambda)\{A_4[F_1(0) + \mathrm{Re}F_1(2\pi/L)] - \beta[F_2(0) + \mathrm{Re}F_2(2\pi/L)] + \pi z_i \mathrm{Im}F_1(2\pi/L) - \pi\,\mathrm{Im}F_2(2\pi/L)\}\ ,$$

where

$$A_1 = 0.5[(\pi^2 - \beta^2)\lambda^2 - L^2], \quad A_2 = 0.5q\lambda^2 L^2\ ,$$

$$A_3 = -\pi\beta\lambda^2, \quad A_4 = (1 - |\lambda|)L + \beta z_i\ .$$

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