Polarizability of a carrier in an isolated well of a quantum-well wire

B. Sukumar and K. Navaneethakrishnan
School of Physics, Madurai Kamaraj University, Madurai 625 021, India
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Polarizability (α_p) values are estimated for an electron confined to move within the well of a quasi-one-dimensional (Q1D) GaAs-$Ga_{1-x}Al_xAs$ superlattice system with a square cross section. The values of α_p obtained by two different methods, one using the expression for the dipole moment and the second from an estimate of the shift of the peak position of the wave function, are in good agreement with each other. The electron-lattice coupling leads to a uniform shift of the binding energies by an amount $-\alpha\hbar\omega$. While this result is different from that of a Q2D system, the values of α_p are of the same order for both Q1D and Q2D systems. Our results also show that α_p increases with well widths and depends on the direction of the electric field with reference to an axis defined parallel to an edge of the square cross section.

Partly due to their application in semiconductor devices and partly due to some novel phenomena such as the quantum Hall effect and universal conductance fluctuations exhibited by them, physics of low-dimensional systems is drawing considerable attention at present.[1–4] The problem of finding the binding energies of an electron in a quantum well of a quasi-two-dimensional (Q2D) GaAs-$Ga_{1-x}Al_xAs$ superlattice with[5,6] and without[7,8] impurities under external perturbations has also been pursued with great interest in the recent past. Impurity-limited mobility[9] and the calculation of thermoelectric power[10] in a semiconducting thin wire are other topics of interest.

Recently it has been shown that the polaron effects are also important in quasi-1D (Q1D) and Q2D semiconductor systems.[8,11,12] The polarizability of an electron confined to move within an infinite well of a Q2D system has been worked out recently.[13] In this report we present our calculations on a Q1D GaAs-$Ga_{1-x}Al_xAs$ semiconducting wire with a square cross section.

Let us consider a quantum wire extending along the z direction with a square cross section. The electron is thus confined to move within a square well in the x-y plane and free to move in the z direction. The well exists in the GaAs region of the superlattice. In what follows we shall assume a well of infinite strength. The Hamiltonian for the electron is given by

$$H=\frac{P^2}{2m^*}+V_w(x,y)+eF[x\cos\theta+y\sin\theta]\ , \tag{1}$$

where m^* is the effective mass of the electron in GaAs, $V_w(x,y)$ is the square-well potential given by

$$V_w(x,y)\begin{cases}\propto |x|\geq L/2 \ \text{ and/or } \ |y|\geq L/2\\ =0 \ \text{ elsewhere}\ ,\end{cases}$$

and F is the strength of the electric field applied along the direction making an angle θ with the x axis chosen parallel to an edge of the square cross section of the wire. The origin is chosen at the center of the cross section.

Using the variational ansatz

$$|\psi\rangle=N\cos\left[\frac{\pi x}{L}\right]\cos\left[\frac{\pi y}{L}\right]\times\exp\left[-\beta\left[\frac{x\cos\theta+y\sin\theta}{L}+\frac{1}{2}\right]\right]\ ,$$

where N is the normalization constant and β is the variational parameter (the factor $\frac{1}{2}$ in the wave function is chosen to account for the shift in the position of the electron in the presence of an electric field[7,13]), we obtain

$$\begin{aligned}H=&\frac{\hbar^2\beta^2}{2m^*L^2}-\frac{\hbar\pi^2}{m^*L^2}+\frac{N^2\hbar^2\pi^2}{m^*}\exp(-\beta)\sinh(\beta\cos\theta)\sinh(\beta\sin\theta)\\ &\times\left[\frac{1}{\beta^2\sin(2\theta)}+\frac{\beta^2\sin(2\theta)}{4(\beta^2\sin^2\theta+\pi^2)(\beta^2\cos^2\theta+\pi^2)}-\frac{\tan\theta}{2(\pi^2+\beta^2\sin^2\theta)}-\frac{\cot\theta}{2(\pi^2+\beta^2\cos^2\theta)}\right]\\ &+N^2eF\cos\theta\exp(-\beta)\left[\frac{L\sinh(\beta\sin\theta)}{4\beta\sin\theta}-\frac{L\beta\sin\theta\sinh(\beta\sin\theta)}{4(\beta^2\sin^2\theta+\pi^2)}\right](I_{SB1}+I_{SB2})\\ &+N^2eF\sin\theta\exp(-\beta)\left[\frac{L\sinh(\beta\cos\theta)}{4\beta\cos\theta}-\frac{L\beta\cos\theta\sinh(\beta\cos\theta)}{4(\beta^2\cos^2\theta+\pi^2)}\right](I_{SB3}+I_{SB4})\ ,\end{aligned}$$

where

$$I_{SB1}=\int_{-L/2}^{+L/2} x \exp\left[\frac{-2\beta x \cos\theta}{L}\right] dx \ ,$$

$$I_{SB2}=\int_{-L/2}^{+L/2} x \cos\frac{2\pi x}{L} \exp\left[\frac{-2\beta x \cos\theta}{L}\right] dx \ ,$$

$$I_{SB3}=\int_{-L/2}^{+L/2} y \exp\left[\frac{-2\beta y \sin\theta}{L}\right] dy \ ,$$

$$I_{SB4}=\int_{-L/2}^{+L/2} y \cos\frac{2\pi y}{L} \exp\left[\frac{-2\beta y \sin\theta}{L}\right] dy \ .$$

All these integrals can be evaluated in closed form. $\langle H\rangle_{\min}$ is obtained using a computer. The calculations were performed for $\theta=0°$, 30°, 45°, 60°, and 90°. The subband energy λ in the absence of the electric field is $\hbar^2\pi^2/m^*L^2$. We define the shift in the subband as

$$\Delta E=\lambda-\langle H\rangle_{\min} \ .$$

The results are presented in Figs. 1 and 2.

The polarizability of the charge carrier is computed as follows. The dipole moment is given by

$$P=\langle -e[x\cos\theta+y\sin\theta]\rangle_{F\neq 0} - \langle -e[x\cos\theta+y\sin\theta]\rangle_{F=0} \ .$$

In the above expression the zero-field term vanishes. Hence the polarizability becomes

$$\alpha_p=-e\langle (x\cos\theta+y\sin\theta)\rangle/F \ .$$

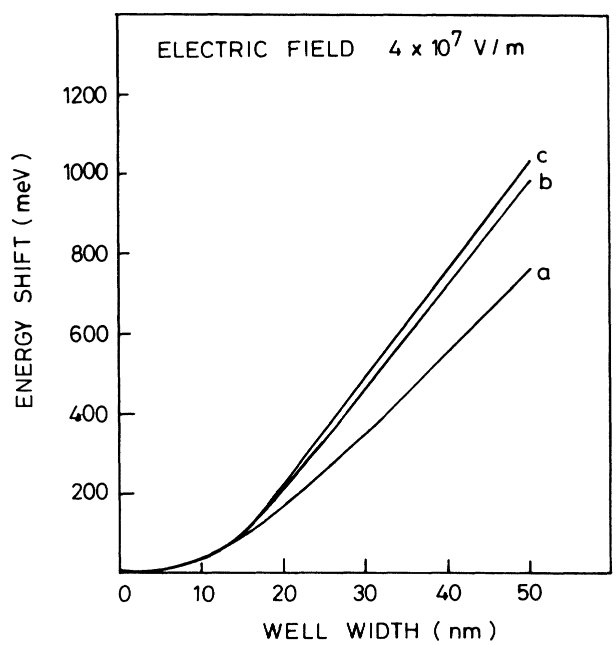

FIG. 1. Shift in the binding energy of a quantum confined electron in a Q1D system for different well widths in the presence of an electric field. a, b, and c refer to values for $\theta=0°$ (or 90°), 30° (or 60°), and 45°, respectively. θ is the angle between the electric field and the x axis parallel to an edge of the square cross section of the wire.

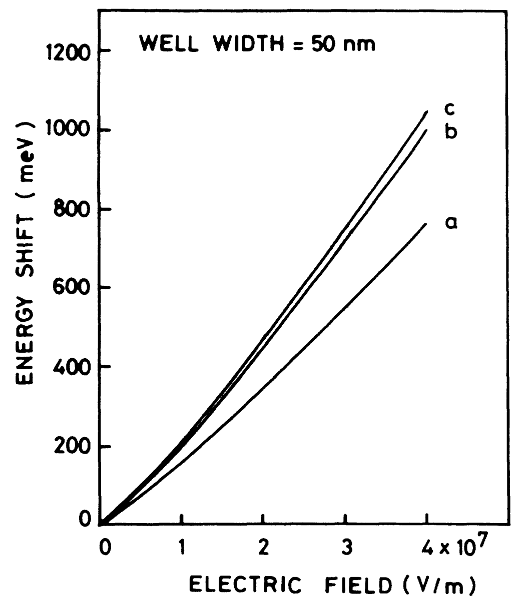

FIG. 2. Shift in the binding energy of a quantum confined electron in a Q1D system in the presence of different electric fields for a given well width. a, b, and c are as defined in Fig. 1.

The results obtained for different fields in the range of 10^7 V/m are given in Fig. 3.

One can also calculate the polarizability from a shift of the peak value of the wave function in the presence of the electric field. This value is obtained from

$$\alpha_w=\frac{e|\delta\bar{r}|}{F}=\frac{e[(\delta x)^2+(\delta y)^2]^{1/2}}{F} \ ,$$

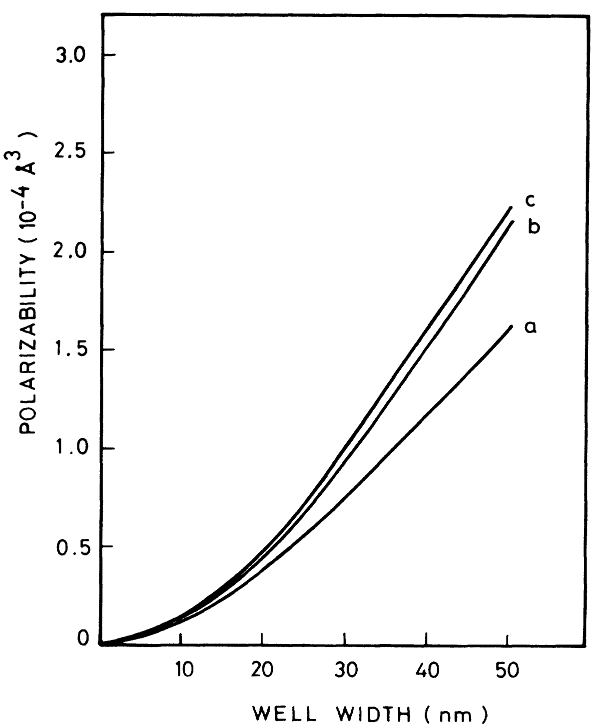

FIG. 3. Variation of polarizability with well width. a, b, and c refer to different directions of the electric field in the x-y plane as defined in Fig. 1.

TABLE I. Variational parameter (β), polarizability (α_p) obtained using Eq. (4), and polarizability (α_w) obtained using peak shift method for a well width of $L=50$ nm.

		F (10^7 V/m)			
θ	Quantity	1	2	3	4
0°,90°	β	11.3	14.5	16.7	18.4
	$\alpha_p^\dagger$(Å^3)	2.99×10^{-4}	1.60×10^{-4}	1.10×10^{-4}	0.84×10^{-4}
	$\alpha_w^\dagger$(Å^3)	3.31×10^{-4}	1.73×10^{-4}	1.18×10^{-4}	0.89×10^{-4}
30°,60°	β	13.7	17.8	20.7	22.9
	$\alpha_p^\dagger$(Å^3)	3.85×10^{-4}	2.09×10^{-4}	1.45×10^{-4}	1.11×10^{-4}
	$\alpha_w^\dagger$(Å^3)	4.43×10^{-4}	2.35×10^{-4}	1.61×10^{-4}	1.22×10^{-4}
45°	β	14.0	18.0	20.8	23.1
	$\alpha_p^\dagger$(Å^3)	4.05×10^{-4}	2.19×10^{-4}	1.51×10^{-4}	1.16×10^{-4}
	$\alpha_w^\dagger$(Å^3)	4.55×10^{-4}	2.39×10^{-4}	1.63×10^{-4}	1.24×10^{-4}

where δx and δy are the components of the shift $\delta\bar{r}$. The peak value of $|\psi\rangle$ is found out by solving the equations

$$\tan\left[\frac{\pi\delta x}{L}\right]=-\frac{\beta}{\pi}\cos\theta$$

and

$$\tan\left[\frac{\pi\delta y}{L}\right]=-\frac{\beta}{\pi}\sin\theta\ .$$

The values of α_p and α_w for different electric fields and for one well width are given in Table I.

To include the polaron effect we use the Fröhlich Hamiltonian

$$H_{e\text{-ph}}=\sum_k\frac{1}{k}[V_k\exp(i\bar{k}\cdot\bar{r})a_k+\text{H.c.}]\ ,$$

where

$$V_k=i\hbar\omega(\hbar/2m\omega)^{1/4}(4\pi\alpha/V)^{1/2}\ ,$$

ω is the zone-center LO-phonon frequency, and α is the electron-latttice (EL) coupling constant. This Hamiltonian is not correct for a strictly one-dimensional system.[14] However, for a Q1D system with well widths greater than 100 Å, this Hamiltonian is expected to yield reasonably good results. For smaller well widths even the use of the effective-mass approximation (EMA) adopted here breaks down. The use of the Fröhlich Hamiltonian for a Q2D system is well known.[7,11,13]

When this Hamiltonian is added to H given in Eq. (1) together with $H_p=\sum_k\hbar\omega a_k^\dagger a_k$, we get the total Hamiltonian for the electron interacting with LO phonons and the external electric field in the EMA. The shift in the ground-state energy due to the EL coupling following Ref. 7 is given by

$$\Delta E_{e\text{-ph}}=\sum_k\frac{-|V_k|^2}{(\hbar\omega+\hbar^2k^2/2m)k^2}\ .$$

Certain errors noticed in Ref. 7 have been corrected in Ref. 13. The other terms in Eq. (11) of Ref. 7 vanish for a Q1D system considered here. Replacing the summation by integration in the usual way, we obtain $\Delta E_{e\text{-ph}}=-\alpha\hbar\omega$. Hence we obtain an uniform shift of about 2.5 meV for GaAs using $\alpha=0.068$, and $\hbar\omega=36.7$ meV.

The results we obtain are as follows.

(i) From Fig. 1 as well width increases, the energy shift also increases for a given electric field. This result is similar to what one obtains in a Q2D system.[6,7]

(ii) From Fig. 2 it follows that, as the electric-field strength increases, the energy shift also increases for a given well width. This result is also similar to that of a Q2D system.[6,7]

(iii) The results for different angles for a given well width and electric field fall under three categories. The results for 0° and 90° are the same—similarly, the results for 30° and 60°. The results for $\theta=45°$ are different from the previous two categories. For small well widths and for the lowest electric field chosen (1×10^7 V/m), the subband shifts are 1.87, 1.86 and 1.86 meV, respectively, for these three categories of angles. Similarly, the polarizability values for these three cases are 6.25×10^{-6}, 6.26×10^{-6}, and 6.26×10^{-6} Å^3, respectively. The largest difference in ΔE and α_p values for these three categories arise for a well width of 50 nm and an electric field of 4×10^7 V/m. These values are $\Delta E=$ 763.50, 992.96, and 1038.25 meV, respectively. The corresponding α_p values are 8.41×10^{-5}, 11.13×10^{-5}, and 11.62×10^{-5} Å^3.

(iv) From Fig. 3, it follows that the α_p values increase with well width. This result is to be expected since the larger the well width, the weaker is the confinement. These values of polarizabilities for $\theta=0°$ or 90° are the same as for a Q2D system. Equation (3) leads to the same value for the polarizability if the corresponding wave function for a Q2D system is used, as can be easily verified.[13] Physically this means that when the electric field is applied along either the x axis or the y axis, the acceleration of the electron occurs along that direction only. The boundary condition along that direction alone is of importance. This situation is precisely the same as that in a Q2D system.

(v) Our results show a weak dependence of α_p on the electric field. For instance, for $L=10$ nm and $\theta=45°$, we get 6.26×10^{-6}, 5.71×10^{-6}, 5.49×10^{-6}, and 5.34×10^{-6} Å^3 as the values of α_p when F varies from 1×10^7 V/m to 4×10^7 V/m in steps of 10^7 V/m. The corresponding values for a 50-nm well are 4.1×10^{-4}, 2.19×10^{-4}, 1.51×10^{-4}, and 1.16×10^{-4} Å^3. This weak dependence is attributed to strong electric fields chosen in our study. At such large fields nonlinear terms seem to be important. However, when small electric fields in the order of 10^4 V/m are used, not appreciable shifts in the energy values and hence polarizabilities could be noticed. Also such strong fields are commonly employed in superlattice devices.[1,15,16]

(vi) The values obtained for polarizabilities by the two different methods are in good agreement, as can be seen from Table I.

The experimental values of the polarizability for Q1D and Q2D semiconductor systems do not seem to have been reported. However, the Stark shifts in an electric field have been shown to be in agreement with experiments for a Q2D system.[6,7] The measurements of polarizability will throw further light on the dynamics of carriers in 1D superlattice systems.

Our calculations can be extended along two lines. First, instead of an infinite potential well, a well of finite strength can be used. Except for very small well widths (less than 50 Å), the present results should not be very much different from those obtained using a well of finite strength—a result well known in a Q2D case.[5] Secondly, it is also interesting to work out the polarizability of a donor in such a quantum wire. Calculations are underway and the results will be published elsewhere.

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