Subband structure and excitonic binding of graded GaAs/Ga$_{1-x}$Al$_x$As quantum wells under an electric field

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The effects of an applied electric field on subband energies and excitonic binding for a graded GaAlAs quantum well are calculated variationally within the effective mass approximation. The very sensitive dependence of subband energies on the applied field is calculated using a model potential profile and exact electron and hole wavefunctions. Our calculations have revealed the dependence of the energy shifts of subbands, and excitonic binding on the field direction in the graded quantum well. This permits control over tunnelling which could be desirable for some applications.

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1. Introduction

The effects of an external electric field on the optical properties of graded or square quantum wells (QWs) are the subject of extensive studies [1–18]. This interest is partly due to the device possibilities in graded-gap structures such as sawtooth superlattices as first discussed by Coppaso et al. [15]. The electronic structures of the graded-gap systems without an applied electric field have been studied by several authors [10, 11]. There have been various studies on the effects of the external electric field applied along the growth axis—z on subband energies, carrier lifetimes [1–3], and exciton binding energies [18]. There are also some investigations on the corresponding superlattices [17,19–20].

The quantum-confined Stark effect (QCSE) is a shift of the excitonic absorption edge to lower energy with an electric field applied over a semiconductor quantum well. The QCSE offers tailororable optical response which can be used for devices such as high-speed optical modulators, self-electro-optic effect devices, and photodetectors. The previous studies have mostly concentrated on symmetric quantum wells but it is not certain that this is the best type of structure for devices. In recent studies on nonsquare quantum wells, it was shown that some quantum-well structures exhibited enhanced QCSE [21–24], therefore potential applications to optical devices can be actively studied [25–27]. Consequently by using a quantum well with a different shape one has a new freedom to achieve tailororable optical response and more sophisticated performance.
For optical devices based on excitonic binding the main problem is the short lifetime of excitons. In order to increase the lifetime one has to decrease the overlap between the electron and hole wavefunctions. This can be realized by gradually changing the Al concentration in GaAs/Ga\text{$_{1-x}$}Al\text{$_x$}As structures, since the spatially indirect exciton has a long lifetime due to the small overlap of the electron hole wavefunctions \cite{28}. In the graded quantum well the Stark shift depends on the direction of the applied field and the linear Stark shift can be modified by changing the direction of the field. This added degree of freedom may have applications in switching devices. Also recently, there has been considerable interest in quantum-well structures which reflect a parabolic spatial dependence on Al concentration in Ga\text{$_{1-x}$}Al\text{$_x$}As and GaAs superlattices.

In their study of the properties of electrons and excitons in graded quantum wells of Ga\text{$_{1-x}$}Al\text{$_x$}As in an electric field, Zhu \textit{et al.} \cite{18} used a novel method of series expansion and took the electric field term as a perturbation.

In this work, we attempt an exact solution in terms of Airy functions. Our calculations reveal the dependence of energy shifts of subbands, of exciton binding energy, and of the overlap between the electron and hole wave function on the field direction in the graded quantum well.

\section{2. Theory}

One can obtain the linearly changing valence and conduction band profile by changing the Al concentration $x$ in Ga\text{$_{1-x}$}Al\text{$_x$}As as shown in Fig. 1. The required change in $x$ to obtain the valence and conduction band profiles is also shown in the same figure. This linear variation can also be considered as obtainable by using an electric field $R$ applied in the $z$-direction in the region $|z| \leq L/2$. With this in mind, we can write the model potential in functional form as,

$$V(z) = \begin{cases} 
-q R (z + L/2), & |z| \leq L/2 \\
V_{0}^{(e,h)}, & |z| > L/2 
\end{cases}$$

(1)
where $V^{(e)}_0$ and $V^{(h)}_0$ are the energy discontinuities in the conduction and valence band, respectively, and the electric field $R$ needed to obtain the same profile should be given by

$$-qRL/2 = \frac{V^{(e,h)}_0}{4}. \quad (2)$$

The corresponding Hamiltonian for a particle with charge $q$ and the effective mass $m^*$, under an electric field $F$ in the $z$-direction, in terms of normalized parameters, is given by

$$H = \begin{cases} 
-\frac{1}{\pi^2} \frac{q^2}{\delta \xi^2} + \bar{V}^{(e,h)}_0 - \tilde{q} \bar{F} \tilde{z}, & |z| > L/2 \\
-\frac{1}{\pi^2} \frac{q^2}{\delta \xi^2} - \bar{q}(\tilde{R}(\tilde{z} + \frac{1}{2}) + \bar{F} \tilde{z}), & |z| \leq L/2 
\end{cases} \quad (3)$$

where the normalized parameters are defined as

$$\tilde{E} = \frac{E}{E_0}, \quad \tilde{F} = \frac{qFL}{E_0}, \quad \tilde{Z} = \frac{Z}{L}, \quad E_0 = \frac{\pi^2 \hbar^2}{2m^*L^2}$$

is the ground-state energy of an infinite quantum well with a width $L$ and the parameters $\tilde{q}$ with the values $-1(+1)$ representing electrons (holes). As the potential energy term in eqn (3) tends to be arbitrarily large and negative at large and negative (positive) distances for the electron (hole), the particle initially confined in a well can always lower its potential energy by tunnelling out of the well when the field is not zero. Although the true bound state of an isolated quantum well with an electric field is quasi-bound, it may be approximated by a bound state if the applied field is not too strong for the lifetime of the carrier in the well to be long enough [29–31]. In discussing the quasibound states, we use the following formal method which we have used in our previous study [32], we put infinite walls at $\tilde{z} = \pm \tilde{L}_B$ and in calculating the eigenstate energies we have ensured that the eigenvalues are independent of the choice of $L_B$ and that the wavefunctions are localized in the well region.

By introducing new variables

$$\tilde{z}_1 = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3}\left[(\tilde{E} - \bar{V}^{(e,h)}_0) + \tilde{q} \bar{F} \tilde{z}\right],$$
$$\tilde{z}_2 = -\left[\frac{\pi}{\tilde{F}}\right]^{2/3}\left[(\tilde{E} - \bar{V}^{(e,h)}_0) + \tilde{q}(\tilde{R}(\tilde{z} + \frac{1}{2}) + \bar{F} \tilde{z})\right],$$

the solutions of the Schrödinger equation,

$$H \psi(\tilde{z}) = \tilde{E} \psi(\tilde{z}) \quad (4)$$

may be written in terms of Airy functions $Ai(x)$ and $Bi(x)$ as follows

$$\psi_1(\tilde{z}_1) = C_1 Ai(\tilde{z}_1) + C_2 Bi(\tilde{z}_1)$$
$$\psi_2(\tilde{z}_2) = C_3 Ai(\tilde{z}_2) + C_4 Bi(\tilde{z}_2)$$
$$\psi_3(\tilde{z}_1) = C_5 Ai(\tilde{z}_1) + C_6 Bi(\tilde{z}_1) \quad (5)$$

where $C_1$, $C_2$, $C_3$, $C_4$, $C_5$ and $C_6$ are normalization constants. We employ the continuity conditions at $\tilde{z} = \pm \tilde{L}_B$ with $\psi(\tilde{L}_B) = 0$. The eigenvalues and eigenvectors can be calculated with these conditions.

We treat the degenerate valence bands of $Ga_1-xAl_x$ as ellipsoidal heavy- and light-hole bands for the Hamiltonian of excitons in a graded quantum well in the presence of an electric field. The form of the solution of the Schrödinger equation for the exciton is taken as

$$\psi(\mathbf{r}_e, \mathbf{r}_h) = N \psi_{l_e}(z_e) \psi_{l_h}(z_h) \exp\left[-\frac{\mathbf{L}^2}{\alpha} \right] \quad (6)$$
where $N$ is the normalization constant, $\rho$ is the relative coordinate for the bound electron and hole in the $(x-y)$ plane, $\alpha$ is treated as a variational parameter and $\psi_l(z_e)[\psi_h(z_h)]$ is the normalized $l$th electron ($l$th hole) subband wavefunction, and this is obtained using the method mentioned above. The motion of the exciton in the $(x-y)$ plane is described by the wavefunction of the ground state of a two-dimensional hydrogen-like atom.

Exciton energies are given by,

$$E_{ls}(l_e, l_h) = \min_\alpha \langle \psi | H | \psi \rangle$$

which can also be written as,

$$E_{ls}(l_e, l_h) = E_{l_e} + E_{l_h} - E_{ls}^B(l_e, l_h)$$

where $E_{ls}(l_e, l_h)$ is the binding energy of the electron–hole pair in the $l$th state, and $E_{l_e}$ and $E_{l_h}$ are energies of the electron and hole subbands. Finally, the electron–hole overlap function $F(0)$ given by

$$F(0) = \left| \int_{-\infty}^{\infty} dz \psi_{l_e}(z) \psi_{l_h}(z) \right|^2$$

is calculated.

3. Results and discussion

The subbands of the electron and hole have been calculated for the graded quantum well with different electric field values. For numerical calculations, we take $L = 120 \text{ Å}, V_{e0} = 228 \text{ meV}, V_{h0} = 176 \text{ meV},
Fig. 3. Amplitude of the normalized subband wavefunction of the hole A, $|\psi_1(\tilde{z})|^2$ and B, $|\psi_2(\tilde{z})|^2$ versus the normalized position $Z/L$. The electric field is taken to be A, $F = 0, -10, 10 \times 10^4$ V cm$^{-1}$ and B, $F = 0, -6, 6 \times 10^4$ V cm$^{-1}$.

$m_e^* = 0.067m_0$, and $m_h^* = 0.34m_0$ ($m_0$ is the free electron mass) for the electron and hole, respectively. These parameters are suitable for GaAs QWs. The variation of the electron and hole wavefunctions for the ground and first excited states under an electric field are shown in Figs 2 and 3. To find the equivalent electric field to produce the same graded QW profile, we use

$$R^{(e,h)} = \left[ \frac{V^{(e,h)}_0}{2L} \right] \times 10^4 \text{ V cm}^{-1}. \quad (10)$$

Whereas the wavefunctions in a square QW have symmetric and antisymmetric character, here the wavefunctions are asymmetric for $F = 0$. The electron and hole are localized in the left side of the well when there is no electric field. The electron (hole) moves in a $-z$ ($+z$) direction when an electric field is applied along the $z$-direction. Whereas the charge density $|\psi|^2$ in a square QW changes symmetrically with respect to the direction of electric field, this charge distribution varies in a different way in graded QWs, as shown in Figs 2 and 3. The variation of the graded QW is opposite for electrons and holes. For the electrons, the graded quantum well becomes sharper or flatter if the electric field is applied in a $z$ or $-z$ direction, respectively, and for holes the opposite occurs. A positive electric field affects the electron more than an electric field in the opposite direction, the opposite is true for a hole. The electron and hole subband energy variation under $+F$ and $-F$ fields are shown in Fig. 4. At a critical field the graded structure is completely levelled off and beyond this field, the ground subband energies decrease with increasing $F$. As seen in Fig. 4 this critical field is $\leq -10 \times 10^4$ V cm$^{-1}$ for the electron, and $\geq 8 \times 10^4$ V cm$^{-1}$ for the hole. The electron (hole) moves towards the right (left) under a $-F$ field. The first excited state of the electron does not satisfy the quasibound criterion, i.e. the eigenvalue is dependent of the choice of $L_B$ for fields greater than $F \cong 10 \times 10^4$ V cm$^{-1}$ in both the $\pm z$-directions. Although the ground state of the electron does not satisfy the quasibound criterion for
fields greater than $F \cong 14 \times 10^4 \text{ V cm}^{-1}$ in the $-z$-direction or for the electric field $F \cong 20 \times 10^4 \text{ V cm}^{-1}$ in the $z$-direction, the quasibound criterion is still valid. Furthermore, our results show that the ground state of the hole satisfies the quasibound criterion up to an electric field $F \cong 20 \times 10^4 \text{ V cm}^{-1}$ in both the $\pm z$-directions, but the first excited state of the hole does not satisfy the quasibound criterion for field values greater than $F \cong 16 \times 10^4 \text{ V cm}^{-1}$ in the $-z$-direction. The heavier hole is influenced more than the lighter electron; it reflects different changes in the wavefunctions under electric field. In Figs 2 and 3, it is easily seen that the change of the wavefunctions of the hole subbands is larger than that of the electron subbands for selected electric field values. Accordingly, the probability of tunnelling of carriers can be increased or decreased depending on the direction of the electric field. This control over tunnelling could be desirable for some applications.

The electric field dependence of the excitonic binding energy is given in Fig. 5. The electric field shifts the electron and hole subband energies and relative motion of the electron–hole pair. The excitonic binding at zero field ($F = 0$) can be thought of as the binding between two particles which may be considered in the same plane. When there is no electric field, the electron and hole are localized in the left side of the well, but the heavier hole wavefunction is more localized in the left side of the well than that of the electron. Due to this additional confinement, when the positive field is slightly increased, the electron and hole become close to each other and this behaviour gives an increment in the binding energy and the overlap functions $F(0)$, associated with an equal number of electron and hole subbands. However, after a critical field value ($F \geq 4 \times 10^4 \text{ V cm}^{-1}$) the binding energy, and the overlap functions, associated with an equal number of electron and hole subbands, begin to decrease (see Figs 5 and 6). This is resulting from the fact that, after the critical field value, the probability of finding the electron and hole in the same plane decreases with increasing $+F$ field value. On the other hand, the negative electric field puts the particles in different planes and thus establishes an electric dipole. The result is a reduction in the binding energy and the overlap functions,
Fig. 5. The dependence of the binding energy $E_{ls}^{R}(l, l)$ of the exciton on the field direction in a graded Ga$_{1-x}$Al$_x$As quantum well.

Fig. 6. The variations of the electron–hole overlap functions, associated with the $l_i$th electron and $l_h$th hole subbands, versus the electric field.

associated with the (1–1) and (2–2) electron–hole subbands. Also in Fig. 5 the binding energy $E_{ls}(l, l)$ for the square quantum well with the same parameters as a function of electric field is given. Despite the fact that the subband eigenvalues in the graded quantum well are higher than the subband eigenvalues in the square quantum well, due to the additional confinement, the exciton binding energy is greater in the graded well. The reason for this is the difference of the wavefunctions of the two models. For $+F$ field values in the square quantum well the reduction in the binding energy is almost linear but, in the graded quantum well, particularly for small field values, this behaviour is quite different.
In conclusion, the method used in this work is capable of describing the correct behaviour of electrons, holes and excitons in a graded QW under an external field. Calculated results reveal that this behaviour is quite different from that in a square quantum well, and strongly dependent on the field direction. We hope that this study will shed some light on developing new devices and their applications utilizing these properties of graded QWs.

References