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Electron and hole states in ultrathin quantum wells

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Abstract. Ultrathin quantum wells in semiconductor structures represent a short-range perturbation in the barrier material. In order to describe bound electronic states in such systems we adopt the concept of the zero-radius potential model, developed earlier in nuclear physics by Bethe and Peierls. Our one-dimensional version of this phenomenological model is applied to electrons, donors and holes.

1. Introduction

Presently there is a surge of activity in the experimental studies of semiconductor structures with ultrathin quantum wells of one or two monolayers [1]. The interest is stimulated by the possibility of fabricating heterostructures for optical and high-speed device applications but also by the fact that even materials with large lattice mismatch can be used for this purpose. The envelope-function approximation (EFA) [2] as the predominant concept to describe electron and hole states in quantum well heterostructures does not seem to apply here because the width of the well is of the order of the lattice constant.

From elementary quantum mechanics [3], it is known that a one-dimensional rectangular potential with finite barrier has always at least one (symmetrical) bound state. For a potential of given barrier height U_0 with decreasing width L we arrive at a situation where the space quantization energy for the lowest bound state becomes comparable to U_0, i.e. this state is only weakly bound by the potential. As the localization length of this state is large compared to the width L of the potential, its wavefunction is essentially determined by the barrier Hamiltonian. This situation is appropriately considered within the concept of zero-radius potential [4]. This model was introduced by Bethe and Peierls in their quantum theory of the deuteron [5]. In semiconductor physics this concept has been considered for deep defects [6–8] in the context of photoionization and multiphonon processes. In contrast to these three-dimensional problems ultrathin wells represent a one-dimensional zero-size potential problem.

To demonstrate the feasibility of this concept we consider electron and hole states in ultrathin quantum wells and calculate the dispersion of hole subbands and the binding energy of donor states with the impurity located in the ultrathin quantum well. Three phenomenological parameters will occur in this model which are related to the binding energies of electrons and heavy and light holes. These parameters have to be determined by fitting to experimental data.

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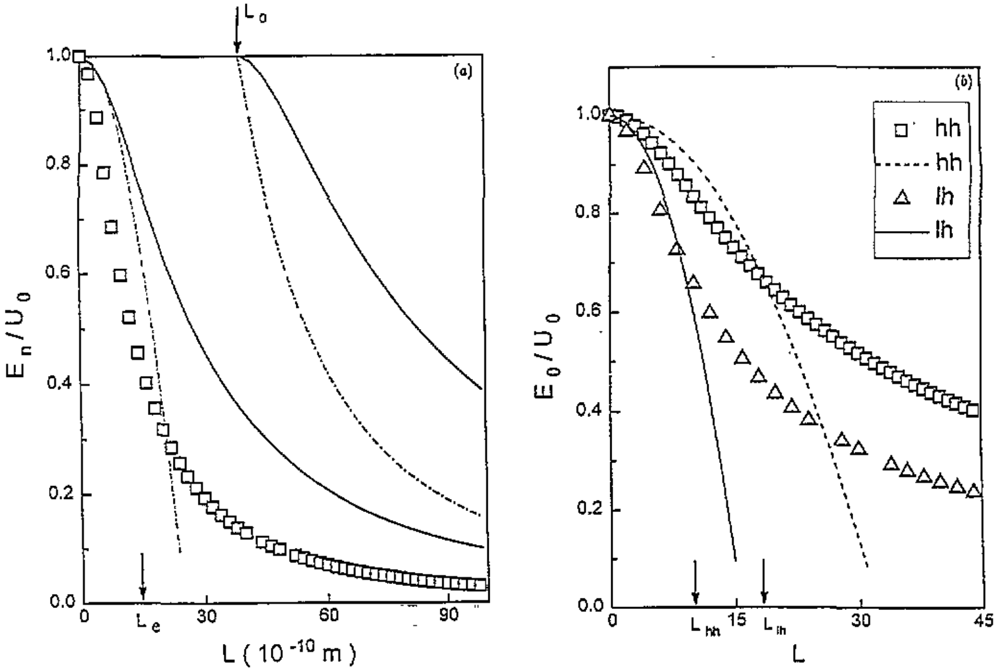

Figure 1. (a) Energy of lowest bound states in a quantum well with barrier height U_0 versus quantum well width L. Solid lines are effective-mass results assuming equal masses in well and barrier (solid lines); squares mark results obtained with different masses in well and barrier. Dash–dotted lines represent analytic results according to (1) and (2). Masses U_0 (given in the text) correspond to $Ga_{0.7}Al_{0.3}As/GaAs$. (b) Same as in (a) but for heavy holes (hh) and light holes (lh).

2. Range of validity of the model

Before we start to do calculations using the zero-size potential model, we want to demonstrate its range of validity. For this purpose we consider as an example $GaAs/Ga_{0.7}Al_{0.3}As$ quantum wells. Figure 1(a) shows the lowest subband states of electrons as functions of the width L of the quantum well obtained in the effective-mass approximation in comparison with the analytic expressions for the lowest bound state in the infinite-barrier model

$$E_0 = \frac{\hbar^2}{2m_e}\left(\frac{\pi}{L}\right)^2 \tag{1}$$

as the limiting case of large L, and for the ultrathin rectangular potential of infinite height U_0

$$E_0 = U_0 - \frac{m_e L^2}{2\hbar^2} U_0^2 \tag{2}$$

which is valid for $L \to 0$ [3]. The effective-mass data are obtained using equal masses in well and barrier (solid line) and taking the mass difference into account (squares). The parameters used are those for GaAs ($m_e = 0.0665 m_0$) and $Ga_{0.7}Al_{0.3}As$ ($m_e = 0.0887 m_0$) and an offset $U_0 = 343$ meV.

The quantum well width L_0 below which only a single state (E_0) is bound is related to the barrier height by [3]

$$L_0 = \pi\sqrt{\frac{\hbar^2}{2m_e U_0}}. \tag{3}$$

We may introduce the localization length κ^{-1} for a state with binding energy ϵ_b, which will be a parameter in the zero-size potential model (see section 3):

$$\epsilon_b(L) = U_0 - E_0(L) = \frac{\hbar^2\kappa(L)^2}{2m_e}. \tag{4}$$

Using equations (3) and (4) we obtain for $L = L_0$ (as indicated in figure 1) the relation

$$\kappa(L_0)L_0 = \pi\sqrt{\frac{\epsilon_b(L_0)}{U_0}}. \tag{5}$$

If the same mass is used in well and barrier (solid line in figure 1(a)) we find $\epsilon_b(L_0) \simeq 0.64U_0$ and for the right-hand side of equation (5) a value of about two.

The zero-size model requires the localization length κ^{-1} to be large compared to the width L of the potential, i.e. $\kappa L \ll 1$. This range is indeed reached when going to values L smaller than L_0, when $\epsilon_b(L)$ and thus $\kappa(L)$ get smaller at the same time. So the region of validity of the zero-size potential model is $L < L_e$, with L_e (indicated in figure 1(a)) defined by $\kappa(L_e)L_e = 1$. In this region we may also use the approximation of (4).

Similar considerations, though with different mass parameters, can be applied to heavy and light holes (see figure 1(b)). As the corresponding ultimate values for the validity of the zero-size model we introduce L_{hh} and L_{lh} for heavy and light holes, respectively.

3. Electron states and donors

We consider an isolated ultrathin quantum well grown in the $\langle 001\rangle$ direction embedded in the barrier material. It will be experienced by free electrons with effective mass m_e in the barrier material as a short-range potential, which in the framework of the zero-size potential model can be considered by the following Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{m_e}\kappa\delta(z)\right)\psi = \epsilon\psi. \tag{6}$$

Here the energy is counted from the bottom of the barrier-material conduction band. The only bound-state solution ($\epsilon < 0$) of equation (6) is

$$\psi = A\exp(-\kappa|z|) \tag{7a}$$

$$\epsilon = -\frac{\hbar^2\kappa^2}{2m_e} \tag{7b}$$

with the normalization constant

$$A = \sqrt{\kappa}. \tag{7c}$$

The solution of (6) can be given also in the k-representation:

$$\psi(z) = \int_{-\infty}^{\infty} c(k)e^{ikz}\frac{dk}{2\pi} \qquad c(k) = \sqrt{\frac{2}{\pi}}\frac{\sqrt{\kappa}}{k^2+\kappa^2}. \tag{8}$$

The case of donors with the impurity located in the centre of the ultrathin quantum well can be easily considered by adding the Coulomb potential thus dealing instead of equation (6) with the three-dimensional problem

$$\left(-\frac{\hbar^2}{2m_e}\Delta - \frac{e^2}{\epsilon_0 r} - \frac{\hbar^2}{m_e}\kappa\delta(z)\right)\Psi = E\Psi \tag{9}$$

where ϵ_0 is the dielectric constant, and $r = z\sqrt{x^2+y^2+z^2}$. The variational solution to (9) with the trial function [9]

$$\Psi_\lambda = \exp\left\{-\frac{\lambda r}{a_B} - \kappa|z|\right\} \tag{10}$$

leads to a simple equation for the variational parameter λ

$$\lambda = 1 + \frac{\kappa a_B}{(2\lambda + \kappa a_B)^2}. \tag{11}$$

Here $a_B = \hbar^2\epsilon_0/m_e e^2$ is the Bohr radius. The donor binding energy is equal to

$$E_D = 2E_B\left[\lambda_0\left(1+\sqrt{\lambda_0 - 1}\right) - \frac{\lambda_0^2}{2}\right] \tag{12}$$

where λ_0 is the root of (11) and $E_B = m_e e^4/2\hbar^2\epsilon_0^2$ the effective Rydberg constant. The dependence of E_D on the quantum-well parameter κ is presented in figure 2. For $\kappa = 0$ we recover the three-dimensional lowest bound donor state ($E_D = -E_B$). With increasing κ the binding to the quantum well increases as the electron is more and more localized around $z = 0$.

4. Dispersion of hole subbands

The hole states derive from the topmost fourfold Γ_8 valence-band state of the bulk band structure. Taking the growth direction of the quantum well as the quantization axis for the basis the effective-mass Hamiltonian is the 4×4 Luttinger matrix operator quadratic in $\boldsymbol{\kappa} = -i\nabla$ [10]:

$$\mathbf{H}_0 = \frac{\hbar^2}{m_0}\begin{pmatrix} a_+ & b & c & 0 \\ b^* & a_- & 0 & c \\ c^* & 0 & a_- & -b \\ 0 & c^* & -b^* & a_+ \end{pmatrix} \tag{13a}$$

where

$$a_\pm = -\tfrac{1}{2}(\gamma_1 \mp 2\gamma_2)\hat{k}_z^2 - \tfrac{1}{2}(\gamma_1 \pm \gamma_2)\left(\hat{k}_x^2 + \hat{k}_y^2\right) \tag{13b}$$

$$b - \sqrt{3}\gamma_3(\hat{k}_x - i\hat{k}_y)\hat{k}_z \tag{13c}$$

$$c = \frac{\sqrt{3}}{2}\bar{\gamma}(\hat{k}_x - i\hat{k}_y)^2 \qquad \bar{\gamma} = (\gamma_2 + \gamma_3)/2 \tag{13d}$$

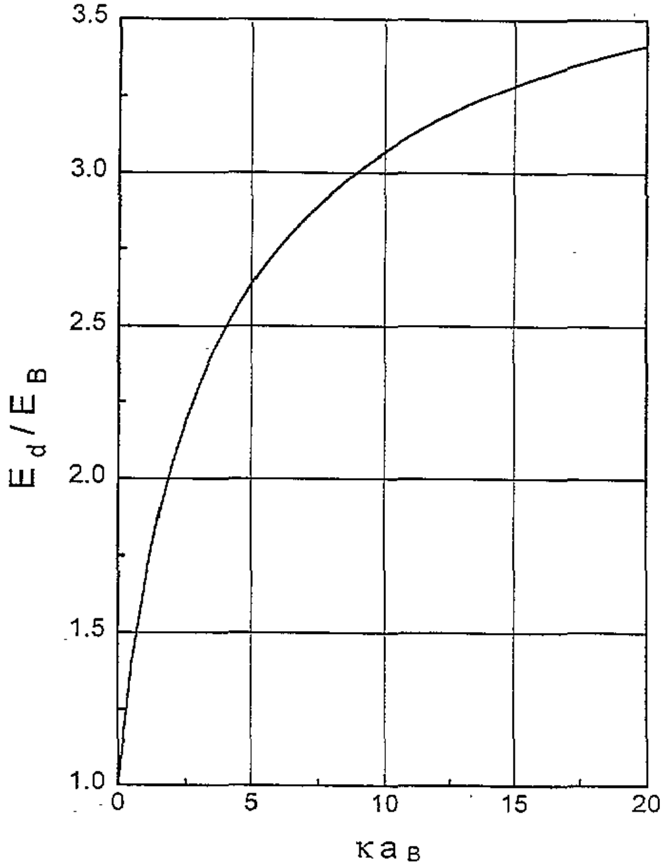

Figure 2. Binding energy of the lowest donor state in an ultrathin quantum well versus inverse localization length κ. Effective atomic units (E_B for energy, a_B for length) are used.

and γ_1 γ_2, γ_3 are the Luttinger parameters. Here we use the cylindrical approximation [11], by neglecting the warping of the valence band for motion along the quantum well, i.e. in the $(k_x,\ k_y)$ plane.

The effect of an ultrathin quantum well will be taken into account by introducing in analogy to equation (6) the potential matrix

$$\mathbf{V} = \frac{\hbar^2}{m_0}\begin{pmatrix} \bar{\kappa}_h(\gamma_1-2\gamma_2)\delta(z) & 0 & 0 & 0 \\ 0 & \bar{\kappa}_l(\gamma_1+2\gamma_2)\delta(z) & 0 & 0 \\ 0 & 0 & \bar{\kappa}_l(\gamma_1+2\gamma_2)\delta(z) & 0 \\ 0 & 0 & 0 & \bar{\kappa}_h(\gamma_1+2\gamma_2)\delta(z) \end{pmatrix}. \tag{14}$$

Here $\bar{\kappa}_h$ and $\bar{\kappa}_l$ will be considered as phenomenological parameters which are connected with the binding energy of confined holes by the relations (see equation (4))

$$\epsilon_{hh} = \frac{\hbar^2(\gamma_1-2\gamma_2)}{2m_0}\bar{\kappa}_h^2 \equiv \frac{\hbar^2\bar{\kappa}_h^2}{2m_{hh}} \tag{15a}$$

$$\epsilon_{lh} = \frac{\hbar^2(\gamma_1+2\gamma_2)}{2m_0}\bar{\kappa}_l^2 \equiv \frac{\hbar^2\bar{\kappa}_l^2}{2m_{lh}} \tag{15b}$$

m_{hh} and m_{lh} being the effective masses of heavy and light holes, respectively. These energies have to be different, because the quantum well breaks the cubic symmetry and removes the degeneracy of the bulk valence band Γ_8. We will look for the solution of the Schrödinger equation

$$(\mathbf{H}_0 + \mathbf{V})\Psi = \epsilon\Psi \tag{16}$$

following [11, 12].

The full Hamiltonian $\mathbf{H}_0 + \mathbf{V}$ has translational symmetry in the (x, y) plane, therefore, the in-plane momentum (k_x, k_y) is conserved. In the axial approximation of the Luttinger Hamiltonian we can deliberately choose $k_y = 0$ and call $k_x = q$.

Let us consider first the free Schrödinger equation $H_0\psi = \epsilon\psi$; however, for a bound state, i.e. ϵ is positive. As for travelling waves ($\epsilon < 0$) we obtain four pairwise degenerate solutions, which go to zero for $z \to \pm\infty$, for heavy and light holes η = h, l:

$$\psi_{\mu\eta} = \frac{1}{N} e^{iqx} e^{-\kappa_\eta |z|} \chi_{\mu\eta}(\kappa_\eta, q, \epsilon) \qquad \mu = 1, 2 \tag{17}$$

with

$$\chi_{1,\eta} = \begin{bmatrix} a_-(\kappa_\eta, q) - \epsilon \\ -b^*(\kappa_\eta, q) \\ -c^*(q) \\ 0 \end{bmatrix} \qquad \chi_{2,\eta} = \begin{bmatrix} 0 \\ -c(q) \\ b(\kappa_\eta, q) \\ a_-(\kappa_\eta, q) - \epsilon \end{bmatrix} \tag{18}$$

where $a_\pm(\kappa_\eta, q)$, $b(\kappa_\eta, q)$ and $c(q)$ are obtained by applying the operators of equations (13*a*–*d*) to the solution (17) of the free Schrödinger equation, i.e. replacing the vector operator $(\hat{k}_x, \hat{k}_y, \hat{k}_z)$ by $(q, 0, i\kappa_\eta \text{ sign } z)$. Here κ_η is connected with the energy ϵ by the relation

$$[a_+(\kappa_\eta, q) - \epsilon][a_-(\kappa_\eta, q) - \epsilon] - b^*(\kappa_\eta, q)b(\kappa_\eta, q) - c^*(q)c(q) = 0. \tag{19}$$

By solving this equation for κ_η, we obtain for η = l, h

$$\begin{aligned}\kappa_{\mathrm{h,l}}^2 = \frac{1}{\gamma_1^1 - 4\gamma_2^2}\Big\{ & 2\epsilon\gamma_1 + (\gamma_1^2 + 4\gamma_2^2 + 6\gamma_3^2)q^2 \\ & \pm [2\epsilon\gamma_1 + (\gamma_1^2 + 4\gamma_2^2 + 6\gamma_3^2)q^2]^2 - (\gamma_1^2 - 4\gamma_2^2)[(4\epsilon^2 + 4\epsilon\gamma_1 q^2) \\ & + (\gamma_1^2 - \gamma_2^2 - 3\bar{\gamma}^2)q^4]^{-1/2}\Big\}.\end{aligned} \tag{20}$$

In (20) the + sign (− sign) corresponds to heavy (light) holes.

The solution of (16) can now be represented as a superposition of the solutions obtained for the free Schrödinger equation with fixed in-plane momentum q and energy ϵ:

$$\Psi = \sum_{\mu\eta} \Psi_{\mu\eta} A_{\mu\eta}. \tag{21}$$

Note that $\Psi_{\mu\eta}$ solves the full Schrödinger equation already for $z \neq 0$. In order to find the determining equations for the expansion coefficients $A_{\mu\eta}$ we integrate the full Schrödinger

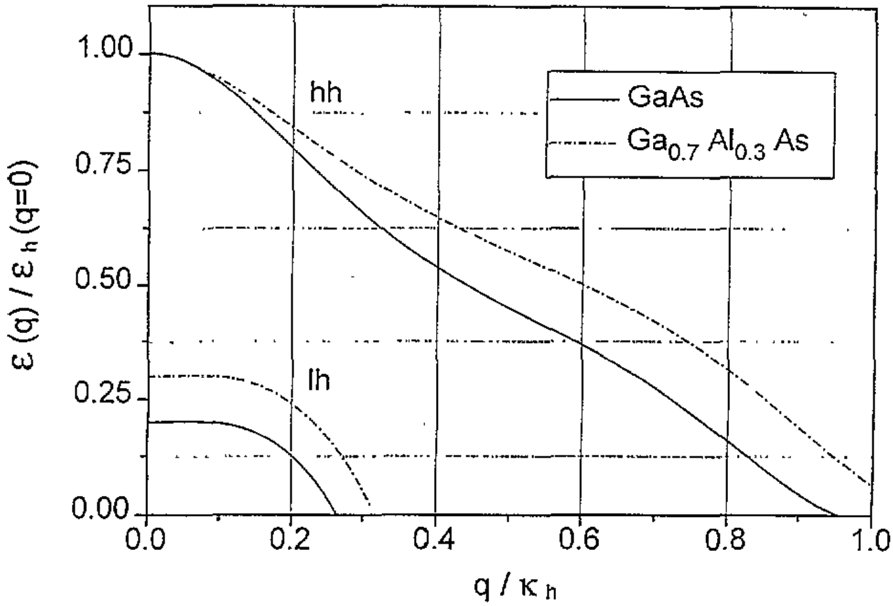

Figure 3. Dispersion of the heavy-hole (hh) and light-hole (lh) subband for an ultrathin quantum well in GaAs and $Ga_{0.7}Al_{0.3}As$. Energies are given in units of the heavy-hole energy ϵ_h at $q = 0$, and the in-plane wave vector q in units of the inverse localization length κ_h of the heavy hole.

equation over the small interval which includes the zero-size potential **V** and obtain

$$\begin{aligned}
&\sum_{\mu\eta}(\bar{\kappa}_h - \kappa_\eta)\chi^{(1)}_{\mu\eta}A_{\mu\eta} = 0\\
&\sum_{\mu\eta}(\bar{\kappa}_l - \kappa_\eta)\chi^{(2)}_{\mu\eta}A_{\mu\eta} = 0\\
&\sum_{\mu\eta}(\bar{\kappa}_l - \kappa_\eta)\chi^{(3)}_{\mu\eta}A_{\mu\eta} = 0\\
&\sum_{\mu\eta}(\bar{\kappa}_h - \kappa_\eta)\chi^{(4)}_{\mu\eta}A_{\mu\eta} = 0\\
&\mu = 1,\, 2 \qquad \eta = \mathrm{h},\ \mathrm{l}.
\end{aligned} \tag{22}$$

The upper index indicates the component of the spinor $\chi_{\mu\eta}$ counted from top to bottom (see (18)). The condition of solvability for these linear equations, which allows us to find the energy ϵ, reads

$$\begin{aligned}
&(\bar{\kappa}_h - \kappa_h)^2(\bar{\kappa}_l - \kappa_l)^2 A - 2(\bar{\kappa}_h - \kappa_h)(\bar{\kappa}_l - \kappa_l)(\bar{\kappa}_h - \kappa_l)(\bar{\kappa}_l - \kappa_h)B\\
&\qquad + (\bar{\kappa}_l - \kappa_h)^2(\bar{\kappa}_h - \kappa_l)^2 C = 0
\end{aligned} \tag{23a}$$

where

$$A = [a_+(\kappa_l, q) - \epsilon][a_-(\kappa_h, q) - \epsilon] \tag{23b}$$

$$B = b(\kappa_h, q)b^*(\kappa_l, q) + c(q)c^*(q) \tag{23c}$$

$$C = [a_+(\kappa_h, q) - \epsilon][a_-(\kappa_l, q) - \epsilon]. \tag{23d}$$

In order to find (23*a*–*d*) we have used also equation (19).

In view of application to special cases we present in figure 3 calculations for hole subband dispersions obtained for ultrathin quantum wells in $Ga_{0.7}Al_{0.3}As$ (the standard well material would be GaAs) or in GaAs (with e.g. InAs as well material). The materials determine the results (except for the Luttinger parameters) by the ration $\epsilon_{lh}/\epsilon_{hh}$ which was taken to be 0.3 in the former (solid line) and 0.2 in the latter case (dash–dotted line). The following Luttinger parameters have been used: $\gamma_1 = 6.85$ (5.308), $\gamma_2 = 2.10$ (1.434), $\gamma_3 =$ 2.90 (2.162) for GaAs ($Ga_{0.7}Al_{0.3}As$).

The corresponding coefficients $A_{\mu\eta}$ can be easily obtained from (22). Thus, the problem of hole states in the ultrathin quantum well is solved. However, the phenomenological parameters $\bar{\kappa}_h$ and $\bar{\kappa}_l$ should be found by fitting to experiments.

In conclusion, we have introduced the zero-size potential model to describe bound electronic states in ultrathin quantum wells. The model, which contains the binding energy (or the localization length of the bound state) as a phenomenological parameter, is applied to electrons, donors and holes. This model may serve in future applications to excitons and optical properties in systems with ultrathin quantum wells.

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