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# Study of shallow donor level binding energies confined in a GaAs–Ga<sub>1–x</sub>Al<sub>x</sub>As spherical quantum dot

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## Abstract

We study the level structure of a Coulombic donor impurity that binds an electron that is confined within a spherical quantum dot in the GaAs–Ga<sub>1–x</sub>Al<sub>x</sub>As system. Initially, the electron is considered to be moving in a spherically symmetric rectangular potential well and then the effects of a hydrogenic donor with effective charge  $Z_D$  taken at the centre of the well are considered as a strong perturbation within the effective mass approximation. The perturbation calculations are carried out using the Jiang approach (Jiang 1987 *Phys. Rev. B* **35** 9287). We calculate the binding energies of the ground and a few higher excited states for both infinite and finite potential wells as a function of well width and barrier height. The results are compared with those obtained by other techniques such as the variational and direct numerical methods. It is found that the agreement among all these methods is excellent, and this would open the way for more investigations using our direct and relatively easy perturbation treatment, especially in more complicated cases in similar systems.

## 1. Introduction

In recent years, there has been a considerable amount of work devoted to the study of semiconductor confined structures due to their applicability in electronics and optoelectronics devices. Since the electronic movement in nanostructures with a quantum dot is confined in all three directions, it is expected that there will appear more obvious quantum size effects. For example, the energy levels will be strongly dependent on the size of such structures. A very interesting problem in quantum low-dimensional structures is to understand how an atom, i.e. an impurity, modifies the energy spectrum of the system. It is expected that the binding energy of the donor atom is increasing continuously as the well size is reduced [2, 3]. The most representative example of this configuration is the regions of GaAs which act as a well of conduction electrons separated by regions of GaAs–Ga<sub>1–x</sub>Al<sub>x</sub>As as barriers. The optical and electronic properties of these zero-dimensional structures have been the subject of both theoretical [1–9] and experimental [10–13] investigations.

Up to now, the study of energy levels of donor atoms confined in a quantum well has been performed mainly by the variational method [14] and numerical methods [15–18]. The difficulty arising in this problem is in accurately representing the actual state, which is partly due to the donor atom and partly due to the potential well. Hence, a very flexible trial function is needed, which accounts for both parts simultaneously. Villalba *et al* [18] used an alternative approach called the  $(1/N)$  method [19] along with the linear variational technique with reasonable success. In this work an attempt to use the perturbation method first proposed by Jiang [1] has been achieved. This approach treats strong perturbation in a very simple and direct way, in which we avoid the restrictions usually imposed by the traditional Schrödinger perturbation method. In this way, one can give an accurate account of the Coulombic part due to the donor atom, which is crucial for determining binding energies. In this paper, we report an almost exact quantum level structure for confined electron and hydrogenic donor states in a spherical quantum dot (SQD).

A closely related problem to our analysis consisting of an off centre donor in a confined geometry with dielectric mismatch at the boundary has been studied by Ferryra and Proetto [9] and elaborated by Bolcatto and Proetto [24]. In [9], Ferryra and Pretto express the Hamiltonian in terms of a scaling parameter  $R/a_0^* = \lambda$  ( $R$  is the dot radius), so that they can treat the strong-confinement limit ( $\lambda \rightarrow 0$ ) by standard perturbation theory. It will be shown that their results at the centre of the dot are nearly identical to the present results for  $0 < r_0 \leq 1$ , but expected to be not valid for  $r_0 > 1$ .

The dependence of quantum levels and binding energies on the dimensions of the quantum well is treated extensively in section 2, where the method of calculations is outlined for confined electron and hydrogenic donor states in an SQD. Explicit formulae for energy perturbation corrections from the strong perturbation theory are derived. In section 3, the numerical results are discussed. Section 4 concludes the present method with a short summary and conclusion.

## 2. Method of calculation

### 2.1. Perturbation treatment

Consider the Hamiltonian

$$H = H_0 + H' \quad (1)$$

where

$$H_0 = -\nabla^2 + V(r). \quad (2)$$

Moreover,

$$H' = -\frac{2Z_D}{r}. \quad (3)$$

In the SQD,  $V(r)$  is assumed to be

$$V(r) = \begin{cases} V_0 & \text{if } r \geq r_0 \\ 0 & \text{if } r < r_0. \end{cases} \quad (4)$$

$H'$  is comparable to  $H_0$ , and therefore the conventional Schrödinger perturbation theory is not applicable for such strong perturbations. Following Jiang [1], we introduce a function ( $f = e^{-g}$ ) and plug it into  $\Psi = f \Phi$ , where  $\Phi$  is the unperturbed state given by

$$H_0 \Phi = E^0 \Phi \quad (5)$$

and the perturbed state satisfies

$$H \psi = E \psi. \quad (6)$$

Substituting  $\psi = f\Phi$  into equation (6), and following the Jiang approach, we arrive at

$$f(h_0 + h')\phi = Ef\phi \tag{7}$$

where

$$h_0 = H_0 - \frac{Z_D^2}{n^2} \tag{8}$$

and

$$h' = \frac{2Z_D}{n'} \frac{\partial}{\partial r} - \frac{2Z_D}{r} \left(1 - \frac{1}{n'}\right) \tag{9}$$

where  $n'$  stands for the principal quantum number of the hydrogenic donor atom of effective charge  $Z_D$ . Therefore,  $h'$  depends on the quantum number  $n'$  as an example for  $n' = 1$ , the 1s level, we have

$$h'_{1s} = 2Z_D \frac{\partial}{\partial r} \tag{10}$$

and for  $n' = 2, \ell = 1$ , the 2p level, we have

$$\begin{aligned} h'_{2p} &= Z_D \frac{\partial}{\partial r} - \frac{Z_D}{r} \\ &= Z_D \left( \frac{\partial}{\partial r} - \frac{1}{r} \right). \end{aligned} \tag{11}$$

The zero-order  $\psi$  takes the form

$$\psi_{n\ell}^{(0)} = N \Phi_{n\ell} e^{-Z_D r/n'} \tag{12}$$

and the energy corrected to first order is

$$E_{n\ell} \approx E_{n\ell}^{(0)} + E_{n\ell}^{(1)} \tag{13}$$

where  $n = n' - \ell$  as will be explained later and

$$E_{n\ell}^{(0)} = \int \Phi_{n\ell}^* H_0 \Phi_{n\ell} d\tau \tag{14}$$

$$\varepsilon_{n\ell}^{(1)} = -\frac{Z_D^2}{n^2} + \int \Psi_{n\ell}^{(0)*} h' \Psi_{n\ell}^{(0)} d\tau. \tag{15}$$

The second term may be denoted by  $E_{n\ell}^{(1)}$ , i.e.

$$E_{n\ell}^{(1)} = \int \psi_{n\ell}^* h' \psi_{n\ell}^{(0)} d\tau = N_{n\ell}^2 \int f^2 \Phi_{n\ell}^* (h' \Phi_{n\ell}) d\tau \tag{16}$$

$$N^{-2} = \int f^2 |\Phi_{n\ell}|^2 d\tau. \tag{17}$$

Using equation (12), we obtain

$$\begin{aligned} E_{n\ell}^{(1)} &= N^2 \int e^{-2Z_D r/n'} \Phi_{n\ell}^* h' \Phi_{n\ell} d\tau \\ &= N^2 \int e^{-2Z_D r/n'} \Phi_{n\ell}^* \left( \frac{2Z_D}{n'} \frac{\partial}{\partial r} - \frac{2Z_D}{r} \left(1 - \frac{1}{n'}\right) \right) \Phi_{n\ell} d\tau \end{aligned} \tag{18}$$

$$N^{-2} = \int e^{-2Z_D r/n'} |\Phi_{n\ell}|^2 d\tau. \tag{19}$$

Using equations (10) and (11), we get for the 1s level ( $n' = 1$ ) and  $Z_D = 1$  the following:

$$E_{1s}^{(1)} = N_{1s}^2 \int e^{-2Zr} \Phi_{1s}^* \left( 2 \frac{\partial \Phi_{1s}}{\partial r} \right) d\tau \quad (20)$$

where

$$N_{1s}^{-2} = \int e^{-2r} |\Phi_{1s}|^2 d\tau. \quad (21)$$

Similarly, for the 2p level ( $n' = 2$ ) we get

$$E_{1s}^{(1)} = N_{2p}^2 \int e^{-r} \Phi_{2p}^* \left( \frac{\partial}{\partial r} - \frac{1}{r} \right) \Phi_{2p} d\tau \quad (22)$$

where

$$N_{2p}^{-2} = \int e^{-r} |\Phi_{2p}|^2 d\tau. \quad (23)$$

It is evident from a quick look at equations (20)–(23) that the whole procedure depends on the exact zero-order eigenfunctions  $\Phi_{n\ell}$ . If  $\Phi_{n\ell}$  are not available, a trial function may be used and the problem can be treated variationally. As Jiang [1] pointed out, the set of functions  $f_1 \Phi_{n\ell}$  is not orthogonal despite the fact that the  $\Phi_{n\ell}$  are themselves orthogonal.  $f_2 \Phi_{2s}$ ,  $f_2 \Phi_{3s} \dots$  etc, are not orthogonal to  $f_1 \Phi_{1s}$ , but  $f_1 \Phi_{1s}$  is orthogonal to  $f_2 \Phi_{2p}$  by the angular parts, namely  $Y_0^0$ ,  $Y_1^m(\vartheta, \varphi)$ . The above calculation can, of course, be extended to higher order in perturbation if necessary, but, as will be seen, good accuracy with first order alone may be achieved. We will apply the theory for 1s and 2p states at the present stage and of 2s and 3s for future work, since 2s and 3s are more involved and need to be Schmidt orthogonalized on the 1s state before they can be incorporated in such calculations.

## 2.2. Calculation of $\Phi_{n\ell}$ , $E_{n\ell}^{(0)}$

The hydrogenic effective mass theory (EMT) is normally well suited for slowly varying fields of screened impurities, i.e. it is reliable for weakly bound states or shallow energy levels. In the case of the GaAs·Ga<sub>1-x</sub>Al<sub>x</sub>As superlattice, the gap of GaAs is 1.4 eV, while  $Ry^* = 5.3$  meV, which means that the binding energy is well within the applicability of the EMT even if it is doubled 100 times. The expected enhancement of the binding energy in the cases that will be considered here does not exceed the above limit, so that the theory is still reliable for the bound states in the SQD of GaAs·Ga<sub>1-x</sub>Al<sub>x</sub>As.

According to the EMT, the Hamiltonian for the donor in the SQD is given by

$$H = -\nabla^2 - \frac{2Z_D}{r} + V(r) \quad (24)$$

where  $V(r)$  is defined by equation (4). The unit of energy is the effective Rydberg  $R^* = \frac{m^* e^4}{2\hbar^2 k}$ , where  $k$  is the dielectric constant of GaAs,  $m^*$  is the electronic effective mass and the distance is measured by the effective Bohr unit  $a^* = \frac{\hbar^2 k}{m^* e^2}$ . Since the total potential energy is still of radial symmetry, the solutions of  $H \Psi = E \Psi$  are, as usual, defined by two quantum numbers ( $n\ell$ ), but the exact solutions  $\Psi_{n\ell}$  cannot be expressed in closed form in terms of known special functions except the angular part, which remains unaffected (i.e.  $Y_{\ell m}(\vartheta, \varphi)$ ).

A number of methods may be used to deal with equation (24) as mentioned earlier, but we prefer to use the strong perturbation theory to treat the donor part of the potential. The remaining unperturbed problem simply consists of an electron that is moving in a spherically

symmetric potential well as defined by equation (4). The solution of  $H_0\Phi = E^0\Phi$  has the form [21];

$$\Phi_{n\ell}(r, \vartheta, \varphi) = \begin{Bmatrix} A j_\ell(k_{n\ell} r) \\ B h_\ell^{(1)}(i\alpha_{n\ell} r) \end{Bmatrix} Y_{\ell m}(\vartheta, \varphi) \quad (25a)$$

where

$$\begin{aligned} k_{n\ell} &= \sqrt{E_{n\ell}^{(0)}} \\ \alpha_{n\ell} &= \sqrt{V_0 - E_{n\ell}^{(0)}} \end{aligned} \quad (25b)$$

and they satisfy

$$ik_{n\ell} h_\ell^{(1)}(i\alpha_{n\ell} r_0) j_{\ell-1}(k_{n\ell} r_0) + \alpha_{n\ell} h_{\ell-1}^{(1)}(i\alpha_{n\ell} r_0) j_\ell(k_{n\ell} r_0) = 0. \quad (26)$$

For  $\ell \geq 1$  and for  $\ell = 0$ , we have

$$k_{n0} + \alpha_{n0} \tan(k_{n0} r_0) = 0. \quad (27)$$

To obtain the zero-order eigenvalues  $E_{n\ell}^{(0)}$  the above transcendental relations have to be solved numerically. If  $V_0 \rightarrow \infty$ , then these solutions are simplified to  $\Phi_{n\ell} = Y_{\ell m} j_\ell(k_{n\ell} r)$ ,  $r \leq r_0$  and  $E_{n\ell}^{(0)} = (x_{n\ell}/r_0)^2$ , where  $x_{n\ell}$  is the  $n$ th root of the  $\ell$ th-order spherical Bessel's function, where  $n = n' - \ell$ . The full zero-order eigenfunctions are then given by

$$\Phi_{n\ell}(r, \vartheta, \varphi) = A Y_{\ell m}(\vartheta, \varphi) \begin{cases} j_\ell(k_{n\ell} r) & r \leq r_0 \\ \frac{j_\ell(k_{n\ell} r_0)}{h_\ell^{(1)}(i\alpha_{n\ell} r_0)} h_\ell^{(1)}(i\alpha_{n\ell} r) & r > r_0 \end{cases} \quad (28)$$

where

$$|A|^{-2} = \int_0^{r_0} j_\ell^2(k_{n\ell} r) r^2 dr + \left| \frac{j_\ell(k_{n\ell} r_0)}{h_\ell^{(1)}(i\alpha_{n\ell} r_0)} \right|^2 \int_{r_0}^\infty |h_\ell^{(1)}(i\alpha_{n\ell} r)|^2 r^2 dr. \quad (29)$$

### 2.3. First-order energy corrections

(i) For  $V_0 \rightarrow \infty$ .

Considering the impurity atom as the source of the perturbing term in an infinite potential well, the first-order energy corrections can be calculated by using relations (20) and (21) for the 1s state and the relations (22) and (23) for the 2p-like state, as follows:

$$\begin{aligned} E_{1s}^{(1)} &= \frac{2N_{1s}^2}{X_{10}^2 j_1^2(x_{10})} \int_0^{X_{10}} e^{-\left(\frac{2r_0}{x_{10}}\right)\rho} j_0(\rho) \frac{\partial j_0}{\partial \rho} \rho^2 d\rho \\ &= -\frac{2N_{1s}^2}{X_{10}^2 j_1^2(x_{10})} \int_0^{X_{10}} e^{-\left(\frac{2r_0}{x_{10}}\right)\rho} j_0(\rho) j_1(\rho)^2 d\rho \end{aligned} \quad (30)$$

and

$$N_{1s}^{-2} = \frac{2r_0}{X_{10}^3 j_1^2(x_{10})} \int_0^{X_{10}} e^{-\left(\frac{2r_0}{x_{10}}\right)\rho} j_0^2(\rho) \rho^2 d\rho \quad (31)$$

and

$$\begin{aligned} E_{2p}^{(1)} &= N_{2p}^2 \frac{2}{X_{11}^2 j_2^2(x_{11})} \int_0^{X_{11}} e^{-\left(\frac{r_0}{x_{11}}\right)\rho} j_1(\rho) \left( \frac{\partial}{\partial \rho} - \frac{1}{\rho} \right) j_1(\rho) \rho^2 d\rho \\ &= \frac{2N_{2p}^2}{X_{11}^2 j_2^2(x_{11})} \int_0^{X_{11}} e^{-\left(\frac{r_0}{x_{11}}\right)\rho} j_1(\rho) \left( j_0(\rho) - \frac{3}{\rho} j_1(\rho) \right) \rho^2 d\rho \end{aligned} \quad (32)$$

where

$$N_{2p}^{-2} = \frac{2r_0}{X_{11}^3 j_2^2(x_{11})} \int_0^{X_{11}} e^{-\left(\frac{r_0}{x_{11}}\right)^p} j_1^2(\rho) \rho^2 d\rho. \quad (33)$$

(ii) For finite  $V_0$ .

In the case where  $n' = 1$  and  $\ell = 0$  (i.e. the 1s state) and using equations (20) and (21) we obtain the following:

$$\begin{aligned} E_{1s}^{(1)} &= 2N_{1s}^2 \left[ \int_0^{r_0} e^{-2r} j_0(k_{10}r) \frac{\partial j_0(k_{10}r)}{\partial r} r^2 dr + \left| \frac{j_0(k_{10}r)}{h_1^{(1)}(i\alpha_{10}r_0)} \right|^2 \right. \\ &\quad \left. \times \int_{r_0}^{\infty} e^{-2r} h_0^{*(1)}(i\alpha_{10}r) \frac{\partial h_0^{(1)}(i\alpha_{10}r)}{\partial r} r^2 dr \right] \\ &= 2N_{1s}^2 \left\{ \frac{1}{k_{10}^2} \int_0^{k_{10}r_0} e^{-2\left(\frac{\rho}{k_{10}}\right)} j_1(\rho) j_0(\rho) \rho^2 d\rho + \frac{1}{\alpha_{10}^2} \left| \frac{j_0(k_{10}r)}{h_1^{(1)}(i\alpha_{10}r_0)} \right|^2 \right. \\ &\quad \left. \times \int_{\alpha_{10}r_0}^{\infty} e^{-2\left(\frac{\sigma}{\alpha_{10}}\right)} i h_0^{(1)*}(i\sigma) h_1^{(1)}(i\sigma) \sigma^2 d\sigma \right\} \end{aligned} \quad (34)$$

where

$$\begin{aligned} N_{1s}^{-2} &= \frac{1}{k_{10}^3} \int_0^{k_{10}r_0} e^{-2\left(\frac{\rho}{\alpha_{10}}\right)} j_0^2(\rho) \rho^2 d\rho + \frac{1}{\alpha_{10}^2} \left| \frac{j_0(k_{10}r)}{h_1^{(1)}(i\alpha_{10}r_0)} \right|^2 \\ &\quad \times \int_{\alpha_{10}r_0}^{\infty} e^{-2\left(\frac{\sigma}{\alpha_{10}}\right)} |h_0^{(1)*}(i\sigma)|^2 \sigma^2 d\sigma. \end{aligned} \quad (35)$$

Following similar steps and using equation (28) in equations (22) and (23) for the 2p level, we obtain

$$\begin{aligned} E_{2p}^{(1)} &= N_{2p}^2 \left\{ \int_0^{r_0} e^{-r} j_1(k_{11}r) \left( \frac{\partial}{\partial r} - \frac{1}{r} \right) j_1(k_{11}r) r^2 dr + \left| \frac{j_0(k_{10}r)}{h_1^{(1)}(i\alpha_{10}r_0)} \right|^2 \right. \\ &\quad \left. \times \int_{\alpha_{10}r_0}^{\infty} e^{-r} h_1^{(1)*}(i\alpha_{11}r) \left( \frac{\partial}{\partial r} - \frac{1}{r} \right) h_1^{(1)}(i\alpha_{11}r) r^2 dr \right\}. \end{aligned} \quad (36)$$

Using the relation

$$\begin{aligned} \frac{\partial j_1(k_{11}r)}{\partial r} &= k_{11} j_0(k_{11}r) - \frac{2}{r} j_1^{(1)}(k_{11}r) \\ \frac{\partial h_1^{(1)}(i\alpha_{11}r)}{\partial r} &= i\alpha_{11} h_0^{(1)}(i\alpha_{11}r) - \frac{2}{r} h_1^{(1)}(i\alpha_{11}r) \end{aligned} \quad (37)$$

in equation (36) we get

$$\begin{aligned} E_{2p}^{(1)} &= N_{2p}^2 \left\{ \frac{1}{k_{11}^2} \int_0^{k_{11}r_0} e^{-\rho/k_{11}} j_1(\rho) \left[ j_0(\rho) - \frac{3}{\rho} j_1(\rho) \right] \rho^2 d\rho + \frac{1}{\alpha_{11}^2} \left| \frac{j_1(k_{10}r)}{h_1^{(1)}(i\alpha_{10}r_0)} \right|^2 \right. \\ &\quad \left. \times \int_{\alpha_{11}r_0}^{\infty} e^{-\sigma/\alpha_{11}} \left[ i h_0^{(1)}(i\sigma) - \frac{3}{\sigma} h_1^{(1)}(i\sigma) \right] h_1^{(1)*}(i\sigma) \sigma^2 d\sigma \right\} \end{aligned} \quad (38)$$

where

$$N_{2p}^{-2} = \frac{1}{k_{11}^3} \int_0^{k_{11}r_0} e^{-\rho/k_{11}} j_1^2(\rho) \rho^2 d\rho + \frac{1}{\alpha_{11}^3} \left| \frac{j_0(k_{10}r)}{h_1^{(1)}(i\alpha_{10}r_0)} \right|^2 \int_{\alpha_{11}r_0}^{\infty} e^{-\sigma/\alpha_{11}} |h_1^{(1)}(i\sigma)|^2 \sigma^2 d\sigma. \quad (39)$$

**Table 1.** Energy levels in the SQD of GaAs–Ga<sub>1-x</sub>Al<sub>x</sub>As in the absence of a donor atom, for various values of well width  $r_0$  and barrier height  $V_0$ . Effective atomic units are used (Ry\* for energy and  $a^*$  for distance) (dashes mean no solutions).

$r_0$	$V_0$	$E_{n\ell}^{(0)}$			
		1s	2s	3s	1p
0.8	$\infty$	15.422	61.740	138.924	31.542
	90	11.967	46.865	88.352	24.350
	50	10.990	41.314	—	22.214
	30	9.968	29.269	—	19.833
1.6	$\infty$	3.856	15.435	34.726	7.886
	90	3.389	13.527	30.287	6.929
	50	3.246	12.913	28.660	6.632
	30	3.092	12.209	26.355	6.305
3.2	$\infty$	0.964	3.859	8.682	1.971
	90	0.903	3.611	8.121	1.847
	50	0.883	3.920	7.936	1.807
	30	0.857	3.442	7.721	1.762

To compute the integrals (34), (35), (38) and (39), we have to solve equations (26) and (27) first to obtain  $k_{10}$ ,  $k_{11}$ ,  $\alpha_{10}$ , and  $\alpha_{11}$  and then evaluate  $E_{1s}^{(1)}$  and  $E_{2p}^{(1)}$ . The electronic binding energy in a given state may be taken as the difference in energy between eigenvalues in that particular state in the absence of the donor atom ( $Z_D = 0$ ) and that in its presence ( $Z_D = 1$ )

$$E_B(\ell) = E_{n\ell}(Z_D = 0) - E_{n\ell}(Z_D = 1). \quad (40)$$

For the p state for example, we obtain

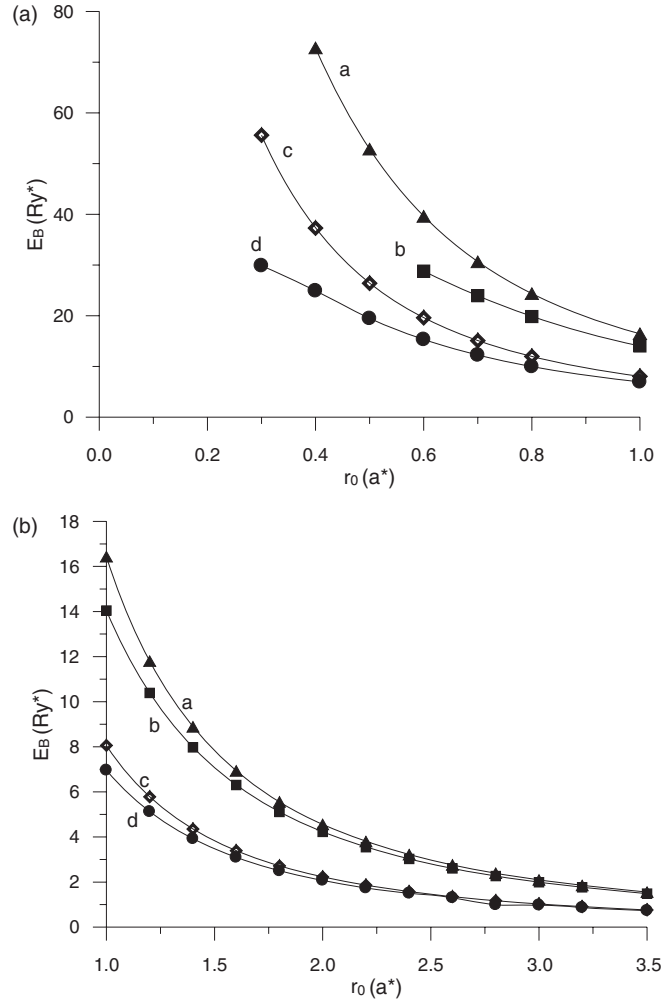
$$\begin{aligned} E_B(\ell = 1) &= E_{1p}(Z_D = 0) - E_{1p}(Z_D = 1) \\ E_B(\ell = 1) &= 0.25 - E_{2p}^{(1)}. \end{aligned} \quad (41)$$

### 3. Numerical results

#### 3.1. The zero-order problem ( $Z_D = 0$ )

A numerical calculation for the GaAs–Ga<sub>1-x</sub>Al<sub>x</sub>As spherical quantum dot of radius  $r_0$  ranging between  $0.1a^*$  and  $4a^*$ , with  $V_0$  from 30 Ry\* up to 90 Ry\*, has been carried out. In table 1 we have shown some selective values for quick reference. Detailed behaviour of  $E_{n\ell}^{(0)}$  for full ranges are shown in figure 1. The levels  $E_{n\ell}^{(0)}$  are designated by two quantum numbers:  $n$ , indicating the  $n$ th root of equation (27) for  $\ell = 0$  and of equation (26) for  $\ell \geq 1$  in order of increasing magnitude i.e.  $n = 1, 2, 3, \dots$ , and  $\ell$ , the usual orbital quantum number. Thus, we have for example  $n\ell$  1s, 1p, 1d, 2s, 1f, etc in order of increasing energy. If one retains the usual principal quantum number of hydrogenic atom  $n'$ , which in the present case is related to  $n$  by  $n' = n + \ell$  then, we have the corresponding notations  $n'\ell$ ; 1s, 2p, 3d, 2s, 4f, ... etc. When  $V_0 \rightarrow \infty$ ,  $E_{n\ell}^{(1)}$  takes the simple form given by  $E_{n\ell}^{(1)} = (x_{n\ell}/r_0)^2$ , where  $x_{n\ell}$  is the  $n$ th root of the  $\ell$ th order spherical Bessel's function. The levels of energy are, however, different between infinite and finite  $V_0$ . The values of the infinite  $V_0$  are becoming higher and higher as  $r_0$  decrease as shown in table 2, while the SQD can hold a finite number of bound states governed by the condition  $r_0 < 0.5\pi/V_0^{1/2}$ . There is no limit on such a number in the infinite  $V_0$  case. However, the order of  $E_{n\ell}^{(1)}$  is the same in both cases, but differs from the hydrogenic sequence





**Figure 1.** (a) Ground  $E$  (1s) and excited state  $E$  (1p) energy levels of an electron bounded inside a spherical potential well of width  $r_0$  and height  $V_0$ . (a), (b) denote  $V_0 = 90 \text{ Ry}^*$  and (c), (d) denote  $V_0 = 30 \text{ Ry}^*$ , with well width in the range of  $0-1a^*$ . (b) Energy levels  $E_B$  (1s) and  $E_B$  (1p) for an electron confined within a potential well of width  $r_0$  in the range of  $1a^*-3.5a^*$  for barrier height  $V_0 = 90 \text{ Ry}^*$  indicated by (a), (b) and for barrier height  $V_0 = 30 \text{ Ry}^*$  by (c), (d).

(1s, 2s, 2p, 3s, 3p, 3d, . . . etc) compared with 1s, 1p(2p), 1d(3d), 2s(2s), 1f(4f), 2p(3p) and so on. We notice also that the level of degeneracy is reduced from  $n^2$  (excluding spin degeneracy) in the hydrogen case to  $(2\ell + 1)$  in the SQD case. This means that in the SQD the degeneracy is governed by the different values of the magnetic quantum number  $m$  for a given  $\ell$ , but  $E_{n\ell}^{(0)}$  is different for different  $\ell$  values even with the same  $n$  value. This difference in degeneracy in the SQD as compared with the Coulomb field is a distinguishing feature in the SQD, which might cause new phenomena in this type of GaAs-Ga<sub>1-x</sub>Al<sub>x</sub>As structure. In figure 1, we have plotted 1s and 1p as a function of  $r_0$  for  $V_0 = 90 \text{ Ry}^*$  and  $30 \text{ Ry}^*$ . The differences of energy levels along these states increase as the value of  $r_0$  decreases. It is also shown that there are no bound states for an SQD with a finite  $V_0$  if  $r_0 < 0.5\pi/V_0^{1/2}$ . But for  $V_0 \rightarrow \infty, r_0 \rightarrow 0$  the situation resembles that of the  $\delta$ -function potential problem.

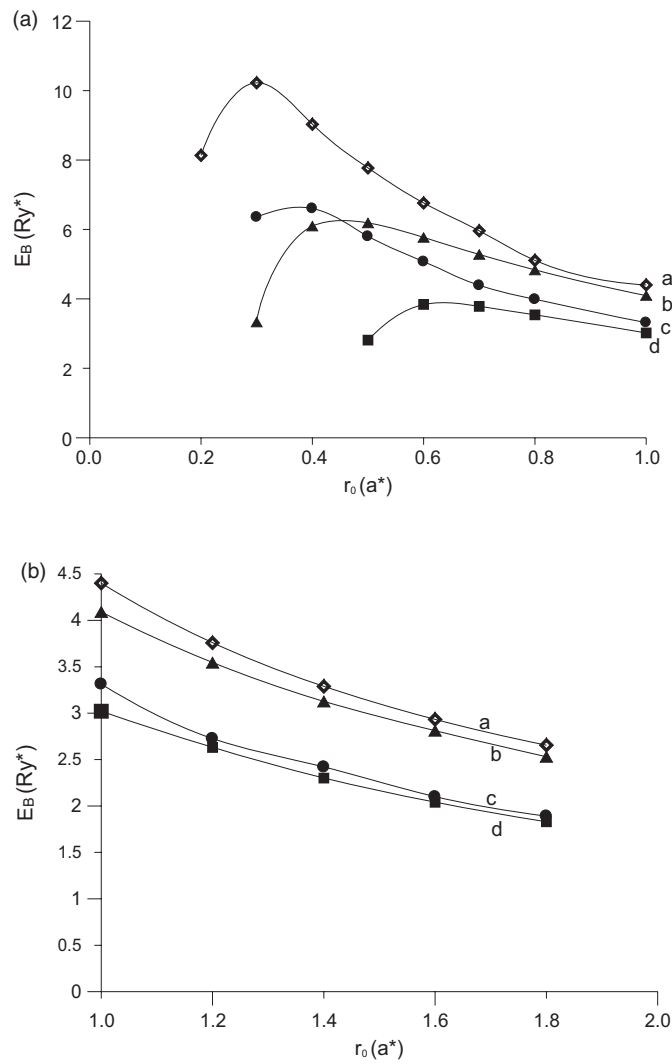
**Table 2.** Binding energy of the ground state  $E_B$  (1s) and excited state  $E_B$  (1p) of a donor in an SQD versus the well radius  $r_0$  for barrier heights  $V_0 = \infty$  and  $V_0 = 50 \text{ Ry}^*$  (blanks mean no solutions).

$r_0$	$V_0 = \infty$		$V_0 = 50 \text{ Ry}^*$	
	$E_B$ (1s) (Ry*)	$E_B$ (1p) (Ry*)	$E_B$ (1s) (Ry*)	$E_B$ (1p) (Ry*)
0.1	48.646	—	—	—
0.2	24.279	—	—	—
0.3	16.164	12.281	7.435	—
0.4	12.113	9.190	7.768	4.871
0.5	9.687	7.348	7.063	5.016
0.6	8.074	6.115	6.308	4.700
0.7	6.925	5.235	5.648	4.190
0.8	6.066	4.575	5.100	3.799
1.0	4.470	3.652	4.249	3.160
1.2	4.081	3.317	3.653	2.606
1.4	3.524	2.600	3.211	2.370
1.6	3.111	2.271	2.875	2.087
1.8	2.795	2.016	2.609	1.881
2.0	2.547	1.909	2.400	1.694
2.2	2.346	1.647	2.226	1.510
2.4	2.183	1.509	2.150	1.426
2.6	2.047	1.393	1.964	1.322
2.8	1.933	1.293	1.830	1.232
3.0	1.837	1.207	1.776	1.154
3.2	1.754	1.076	1.702	1.085
3.4	1.701	1.037	1.606	0.998

### 3.2. Binding energies in SQD

To calculate binding energies of the ground state (1s) we have started with equations (34) and (35), and for the first excited state (1p) we used equations (38) and (39). These results are further simplified in the appendix, where we reach final analytical results for the integrals involving  $h_\ell^{(1)}$ . Using equation (40), we have evaluated  $E_B$  (1s) and  $E_B$  (1p) as a function of  $r_0$ . In figure 2 we have shown  $E_B$  (1s) and  $E_B$  (1p) of a donor in an SQD for  $V_0 = 90$ , and  $30 \text{ Ry}^*$ . As  $r_0$  decreases, all binding energies increase continuously, being more for the 1s level, which passes through a maximum at low  $r_0$  and then decreases sharply at even lower  $r_0$ , in complete agreement with other authors' results [2, 3]. The major property which these curves reveal is that the values of binding energies can be much larger than those in the quantum wire and two dimensional quantum well as  $r_0$  is smaller. Figure 2 also shows that as  $r_0$  decreases the binding energy and consequently the confining effects with respect to different states of a donor in an SQD increase until they reach their maxima. It seems that the confinement effects are dominant in the allowed range of  $r_0$  with much larger binding energies compared with the two dimensional quantum well and quantum wire. On the other hand, the level sequential order resembles that of a three-dimensional hydrogen donor if  $r_0$  is much larger in value and quantum confinement due to the SQU becomes weaker to a larger extent.

In table 3, the maximum binding energies for the states 1s, 1p are shown against barrier height  $V_0$ . It is clear that the enhancement of the maximum is greater in an SQD, which may be considered as almost zero dimensional, than in the corresponding quantum wire and two-dimensional quantum well, as  $V_0$  is increased. This can be attributed to the fact that in our case (SQD) the enhancement of the electron confinement is effected in three dimensions compared to the one and two dimensions in the above stated cases.



**Figure 2.** (a) Binding energy of a donor atom in an SQD versus the well radius  $r_0$ . The curves (a), (b) represent  $E_B$  (1s) of the well of  $V_0 = 90, 30 Ry^*$ , and the curves (c), (d) represent  $E_B$  (1p) for  $V_0 = 90, 30 Ry^*$ , in the range of  $(0, a^*)$  for  $r_0$ . (b) The same as in (a) but the  $r_0$  range is extended to  $2 a^*$ .

**Table 3.** Maximum binding energies for 1s and 1p states versus barrier height (all values are in  $Ry^*$  units).

$V_0$	$E_{\max}$ (1s)	$E_{\max}$ (1p)
30	6.193	3.840
50	7.768	6.05
90	10.223	6.62

In table 4 we list our results for the range of  $0 < r_0 < 1$  (which defines the strong confinement region, where the dot dimension is smaller than the effective Bohr radius) along with the results that are extracted from figures 1 and 2 of [9]. It seems that the agreement

**Table 4.** Binding energies of  $E_B$  (1s) and  $E_B$  (1p) states of a hydrogenic donor centred in an SQD compared with the corresponding results of the strong confinement limit ( $V_0 \rightarrow \infty, r_0 < 1$ , where the dot radius is much smaller than the effective Bohr radius  $a^*$ ) of [9] indicated by (FP). Our  $r_0$  correspond to  $\lambda$  and the numerical values shown in table are extracted from  $E_c^{(1)}(r_i = 0)$  of figures 1 and 2 for the case of  $\varepsilon_1 = \varepsilon_2$ , which maybe applied to GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>.

$r_0$	$E_B$ (1s) (Ry*)		$E_B$ (1p) (Ry*)	
	Present	(FP)	Present	(FP)
0.1	48.646	48.333	—	—
0.2	24.279	24.167	—	—
0.3	16.164	16.111	12.281	12.381
0.4	12.113	12.083	9.190	9.286
0.5	9.687	9.667	7.348	7.429
0.6	8.074	8.056	6.115	6.191
0.7	6.925	6.905	5.235	5.306
0.8	6.066	6.042	4.575	4.643
1.0	4.470	4.833	3.652	3.714

between the two approaches is complete. This is expected since both approaches; the weak and strong perturbations, become identical in this region. As  $r_0$  (or  $\lambda$ ) increases and  $V_0$  decreases, the weak perturbation is no longer valid because  $\lambda$  becomes large ( $r_0 \gg 1$ ). However, it remains to extend our calculations for the off-centre case to see how the method works. This will be treated in a future publication.

#### 4. Summary

We have studied the problem of the SQD by using the strong perturbation method. The source of perturbation is taken to be due to the presence of the donor atom at the centre of the spherical dot. To the best of our knowledge, this is the first time this approach has been employed in such a problem. The zero-order problem simply consists of an electron moving in a spherical rectangular potential box, and treated by solving appropriate transcendental relations. The quantum levels and binding energies of the donor in the SQD are calculated to the first order. Previous experience [1] shows that the first order strong perturbation yields accurate results for non-degenerate states. The numerical results that we have obtained show a very close connection between binding energies and barrier height  $V_0$ , and sphere radius  $r_0$  of the SQD. In comparison to the  $V_0 \rightarrow 0$  case and  $r_0 \rightarrow 0$ , the binding energy passes through a maximum value, indicating optimum confinement effects. On the basis of the numerical values that have been obtained, one can demonstrate the cross-over from three-dimensional to zero-dimensional behaviour of the donor states in an SQD as the radius  $r_0$  of the SQD is reduced to very small values.

The binding energy of a hydrogen donor state in the well of GaAs<sub>1-x</sub>Al<sub>x</sub>As and its maximum are strongly dependent on the well extent and barrier height. Also there is a larger confinement and binding energy of a donor state in an SQD than in a quantum well and quantum wire. This is clearly demonstrated in the strong confinement limit and is indicated in [9]. In conclusion, the perturbative approach that has been employed is very useful if the two Hamiltonian terms are comparable, a case which one encounters in a reduced dimensional problem such as the one we were dealing with. To extend these calculations, one might attempt to deal with degenerate excited states and also extend the calculation to higher orders. It is also of interest to attempt the off-centre case with dielectric mismatch in and out of the spherical dot in the spirit of [9].

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**Appendix**

Equations (34) and (35) involve the following integrals:

$$I_1 = \int_{\alpha_{10}r_0}^{\infty} e^{-\left(\frac{\sigma}{\alpha_{10}}\right)} ih_0^{(1)*}(\i\sigma)h_1^{(1)}(\i\sigma)\sigma^2 d\sigma$$

$$I_2 = \int_{\alpha_{10}r_0}^{\infty} e^{-\left(\frac{\sigma}{\alpha_{10}}\right)} |h_0^{(1)}(\i\sigma)|^2\sigma^2 d\sigma.$$
(A.1)

Using the definitions

$$h_0^{*(1)}(\i\sigma) = -\frac{e^{-\sigma}}{\sigma} \quad \text{and} \quad ih_1^{(1)} = -\left[\frac{1}{\sigma} + \frac{1}{\sigma^2}\right]e^{-\sigma}$$
(A.2)

we get

$$ih_0^{*(1)}(\i\sigma)h_1^{(1)}(\i\sigma)\sigma^2 = \left(1 + \frac{1}{\sigma}\right)e^{-2\sigma}$$
(A.3)

$$|h_0^{(1)}(\i\sigma)|^2\sigma^2 = e^{-2\sigma}.$$
(A.4)

Substitute (A.3) in (A.1) and (A.4) in (A.2), we obtain

$$I_1 = \int_{\alpha_{10}r_0}^{\infty} \left(1 - \frac{1}{\sigma}\right) e^{-2\left(1+\frac{\sigma}{\alpha_{10}}\right)\sigma} d\sigma$$
(A.5)

$$I_1 = \int_{\alpha_{10}r_0}^{\infty} e^{-2\left(1+\frac{\sigma}{\alpha_{10}}\right)\sigma} d\sigma.$$
(A.6a)

Using

$$\int_{\vartheta}^{\infty} \frac{e^{-x}}{x} dx = E_1(\vartheta) = -\gamma - \ln \vartheta - \sum_{n=1}^{\infty} \frac{(-1)^n \vartheta^n}{n n!}$$
(A.6b)

where  $\gamma$  is the Euler–Mascheroni constant ( $\gamma = 0.577\ 2160$ ) and

$$\frac{1}{\alpha_{10}^2} \left| \frac{j_0(k_{10}r_0)}{h^{(1)}(\i\alpha_{10}r_0)} \right|^2 = \frac{1}{k_{10}^2} \sin^2(k_{10}r_0)e^{2\alpha_{10}r_0}$$
(A.7)

we get

$$I_1 = \frac{\alpha_{10}e^{-2(\alpha_{10}+1)r_0}}{2(1 + \alpha_{10})} + E_1(2(1 + \alpha_{10})r_0).$$
(A.8)

Therefore,

$$E_{1s}^{(1)} = -2N_{1s}^2 \left[ \frac{1}{k_{11}^2} \int_0^{k_{11}r_0} e^{-2\rho/k_{10}} j_0(\rho)j_1(\rho)\rho^2 d\rho + \frac{\alpha_{10} \sin^2(k_{10}r_0)}{2k_{10}(1 + \alpha_{10})} e^{-2r_0} + \frac{\sin^2(k_{10}r_0)}{2k_{10}^2} e^{2\alpha_{10}r_0} E_1(2(1 + \alpha_{10})r_0) \right]$$
(A.9)

$$N_{12}^{-2} = \frac{1}{k_{10}^3} \int_0^{k_{11}r_0} e^{-\rho/k_{10}} j_0^2(\rho)(\rho)^2 d\rho + \frac{\sin^2(k_{10}r_0)}{2k_{10}^2(1 + \alpha_{10})} e^{-2r_0}.$$
(A.10)

The remaining integrals in (A.9) and (A.10) are evaluated numerically.

Equations (38) and (39) for  $E_{2p}^{(1)}$  and  $N_{2p}^{-2}$  respectively involve the following integrals:

$$I_3 = \int_{\alpha_{11}r_0}^{\infty} e^{-\sigma/\alpha_{11}} \left[ ih_0^{(1)}(i\sigma) - \frac{3}{\sigma} h_1^{(1)}(i\sigma) \right] h_1^{(1)*}(i\sigma) \sigma^2 d\sigma \tag{A.11}$$

and

$$I_4 = \int_{\alpha_{11}r_0}^{\infty} e^{-\sigma/\alpha_{11}} |h_1^{(1)}(i\sigma)|^2 \sigma^2 d\sigma. \tag{A.12}$$

Using the definition of  $h_1^{(1)}(i\sigma)$ , we get

$$|h_1^{(1)}(i\sigma)|^2 \sigma^2 = \left( 1 + \frac{2}{\sigma} + \frac{1}{\sigma^2} \right) e^{-2\sigma} \tag{A.13}$$

$$h_1^{*(1)} \left\{ ih_0^{(1)}(i\sigma) - \frac{3}{\sigma} h_1^{(1)}(i\sigma) \right\} \sigma^2 = - \left\{ 1 + \frac{4}{\sigma} + \frac{6}{\sigma^2} + \frac{3}{\sigma^3} \right\} e^{-2\sigma} \tag{A.14}$$

and using the definitions

$$E_n(x) = \int_1^{\infty} \frac{e^{-xt}}{t^n} dt \tag{A.15}$$

and the recurrence relation

$$E_{n+1}(x) = \frac{1}{n} e^{-x} - \frac{x}{n} E_n(x) \tag{A.16}$$

we obtain

$$E_2 = e^{-x} - x E_1(x) \tag{A.17}$$

$$E_3 = \frac{1}{2} (1 - x) e^{-x} + \frac{x^2}{2} E_1(x). \tag{A.18}$$

Therefore,

$$I_3 = \int_{\alpha_{11}r_0}^{\infty} e^{-(\frac{2}{\alpha_{11}})\sigma} \left\{ 1 + \frac{4}{\sigma} + \frac{6}{\sigma^2} + \frac{3}{\sigma^3} \right\} d\sigma \tag{A.19}$$

$$= \frac{\alpha_{11}}{(2\alpha_{11} + 1)} e^{-(2\alpha_{11}+1)r_0} + 4E_1(r_0(2\alpha_{11} + 1)) + \frac{6}{(\alpha_{11}r_0)} E_2(r_0(2\alpha_{11} + 1)) + \frac{3}{(\alpha_{11}r_0)} E_3(r_0(2\alpha_{11} + 1)) \tag{A.20}$$

and

$$I_4 = \frac{\alpha_{11}}{(2\alpha_{11} + 1)} e^{-(2+\frac{1}{\alpha_{11}})\alpha_{11}r_0} + 2E_1(r_0(2\alpha_{11} + 1)) + \frac{6}{(\alpha_{11}r_0)} E_2(r_0(2\alpha_{11} + 1)). \tag{A.21}$$

By employing (A.17) and (A.18) we get

$$I_3 = - \left\{ \left[ \frac{\alpha_{11}}{(2\alpha_{11} + 1)} + \frac{2}{\alpha_{11}r_0} + \frac{3(1 - r_0(2\alpha_{11} + 1))}{2(\alpha_{11}r_0)^2} \right] e^{-(2\alpha_{11}+1)r_0} + \left[ 4 - \frac{6(2\alpha_{11} + 1)}{\alpha_{11}} + \frac{6(2\alpha_{11} + 1)^2}{2\alpha_{11}^2} \right] E_1 \right\} \tag{A.22}$$

$$I_4 = \left\{ \frac{\alpha_{11}}{(2\alpha_{11} + 1)} + \frac{1}{\alpha_{11}r_0} \right\} e^{-(2\alpha_{11}+1)r_0} + \left\{ 2 - \frac{(2\alpha_{11} + 1)}{\alpha_{11}} \right\} E_1. \tag{A.23}$$

Equations (38) and (39) can be reduced to

$$E_{2p}^{(1)} = N_{2p}^2 \left\{ \frac{1}{k_{11}^2} \int_0^{k_{11}r_0} e^{-\rho/k_{11}} j_0(\rho) j_0(\rho) - \frac{3}{\rho} j_1(\rho) \rho^2 d\rho \right. \\ \left. - \frac{1}{\alpha_{11}^2} \left| \frac{j_1(k_{11}r_0)}{h(i\alpha_{11}r_0)} \right|^2 \left[ \left( \frac{\alpha_{11}}{(2\alpha_{11} + 1)} + \frac{6}{(r_0\alpha_{11})} \right) \right. \right. \\ \left. \left. + \frac{3(1 - (2\alpha_{11} + 1)r_0)}{(r_0\alpha_{11})^2} \right) e^{-(2\alpha_{11} + 1)r_0} \right. \\ \left. \left. + \left( 4 - \frac{6(2\alpha_{11} + 1)}{\alpha_{11}} + \frac{3(2\alpha_{11} + 1)^2}{2\alpha_{11}^2} \right) E_1 \right] \right\} \quad (\text{A.24})$$

where

$$N_{2p}^{-2} = \frac{1}{k_{11}^2} \int_0^{k_{11}r_0} e^{-\rho/k_{11}} j_1^2(\rho) (\rho)^2 d\rho + \frac{1}{\alpha_{11}^3} \left| \frac{j_1(k_{11}r_0)}{h_1^{(1)}(i\alpha_{11}r_0)} \right|^2 \\ \times \left[ \left( \frac{\alpha_{11}}{(2\alpha_{11} + 1)} + \frac{1}{\alpha_{11}r_0} \right) e^{-(2\alpha_{11} + 1)r_0} \right. \\ \left. + \left( 2 - \frac{(2\alpha_{11} + 1)}{\alpha_{11}} \right) E_1 \right]. \quad (\text{A.25})$$

The values of  $E_1$  are either taken from the tables for large argument, or by using equation (A.6). As one notice that (A.24), (A.25) involve  $\alpha_{11}$  and  $k_{11}$ , which depends on  $V_0$  and  $E_{2p}$  as given in the text in addition to  $r_0$ , i.e. solving the transcendental relation is a prerequisite to evaluate the above integrals.

## References

- [1] Jiang H X 1987 *Phys. Rev. B* **35** 9287
- [2] Zhu J L 1989 *Phys. Rev. B* **39** 8780
- [3] Zhu J L, Xiong J J and Gu B L 1990 *Phys. Rev. B* **41** 6001
- [4] Ribeiro F J and Latgé A 1994 *Phys. Rev. B* **50** 4913
- [5] Paredes-Gutierrez H, Cuero-Yopez J C and Porras-Montenegro J 1994 *J. Appl. Phys.* **75** 5150
- [6] Corella-Madueña A, Rosas R, Martín J L and Reira R 2001 *J. Appl. Phys.* **90** 2333
- [7] Kosciak P *et al* 2005 *J. Phys. A: Math. Gen.* **38** 7743
- [8] Movilla J L and Planelles J 2005 *Phys. Rev. B* **71** 7539
- [9] Ferreya J M and Proetto C R 1995 *Phys. Rev. B* **52** R2309
- [10] Reed M A, Bate R T, Bradshaw K, Duncan W M, Frenslay W R, Lee J W and Shin H D 1986 *J. Vac. Sci. Technol. B* **4** 358
- [11] Bimberg D, Grudmann M and Ledenstov N N 2001 *Quantum Dot, Heterostructures* (Chichester: Wiley)
- [12] Mason N, Beircuk M J and Marcus C M 2004 *Science* **303** 635
- [13] Jiang Y W, Zhu K D, Wu Z J, Yuan X Z and Yao M 2006 *J. Phys. B: At. Mol. Phys.* **39** 2621
- [14] Green C and Bajaj K 1985 *Phys. Rev. B* **31** 913
- [15] Villalba V M and Oino K 2002 *Physica B* **315** 289
- [16] Zhu J L, Wu J, Fu R T and Kawazoe Y 1997 *Phys. Rev. B* **55** 1673
- [17] Stopa M and DasSarma S 1981 *Phys. Rev. B* **40** 8466
- [18] Villalba V M and Pino R 2003 *Mod. Phys. Lett. B* **17** 1331
- [19] Lmbo T and Sukhatme U 1985 *Phys. Rev. D* **31** 2655
- [20] Pokutyi S I and Efremov N A 1991 *Phys. Status Solidi a* **165** 109
- [21] Schiff L I 1968 *Quantum Mechanics* 3rd edn (New York: Mc-Graw-Hill)
- [22] Zrenner A, Butov L V, Hagn M, Abstreiter G, Bohm G and Weiman G 1994 *Phys. Rev. Lett.* **72** 3382
- [23] Barticevic Z, Pacheco M, Duque C A and Oliveira L E 2003 *Phys. Rev. B* **68** 3312
- [24] Bolcatto P G and Proetto C R 1999 *J. Phys.: Condens. Matter* **11** 1–11