Renormalised perturbative series for the impurity levels in a quantum well

Augusto Gonzalez*,**, Ilia Mikhailov***

*Depto. de Fisica, Univ. Nacional de Colombia, Sede Medellin, AA 3840, Medellin, Colombia
**Instituto de Cibernetica, Matematica y Fisica, Calle E 309, Vedado, Habana 4, Cuba
***Escuela de Fisica, Universidad Industrial de Santander, AA 568, Bucaramanga, Colombia

Abstract

The energy levels of an impurity center in a deep quantum well of width $L$ and depth $g$ are studied analytically. Renormalised perturbative series are constructed in the regions $gL^2 \ll 1$ and $gL^2 \gg 1$. Maximal binding energy and wave function deformation to a quasi-twodimensional function are found to occur at a certain $L_c$ satisfying $\sqrt{g}L_c \sim 1$. Similar results may be obtained for the impurity in a quantum wire, in a dot or in a multiwell structure.
1 Introduction

The energy levels of donor and acceptor centers in quantum well, wires and dots have been widely studied recently in the literature [1].

In the present paper, we show that very simple analytic estimates to the energy levels may be obtained from perturbation theory. The perturbative series are renormalised to account for large orders corrections or, said in a different way, the renormalised series are forced to interpolate between the different expansions obtained in different regimes.

In a deep quantum well of depth $g$ and width $L$ (in effective atomic units), we construct renormalised series for $gL^2 \ll 1$, and $gL^2 >> 1$. The starting points are the perturbative expansions obtained in the following limits:

i) $gL^2 \ll 1, gL << 1$. Shallow level, three dimensional coulombic wave function.

ii) $gL^2 \ll 1, gL >> 1$. Shallow level, quasi two-dimensional wave function out of the well.

iii) $gL^2 >> 1, L << 1$. Deep level, quasi two-dimensional wave function inside the well.

iv) $gL^2 >> 1, L >> 1$. Deep level, three dimensional coulombic wave function.

At high values of $g$, the curve $E_b(L)$, i.e. the binding energy as a function of $L$, contains the four regimes i) – iv). Indeed, let us consider, for example, $g = 60$. Then, when $L < 1/60$ the conditions for i) are fulfilled. In the interval $1/60 < L < 1/\sqrt{60}$, we may use an approximation like ii). When $1/\sqrt{60} < L < 1$, the regime iii) holds and, finally, at $L > 1$, the wave function is certainly as indicated in iv).

The transition from ii) to iii) is found to occur at $\sqrt{g}L \sim 1$, and corresponds to a maximum of the binding energy.

2 Impurity in a quantum well

We start from the effective mass hamiltonian in effective atomic units
\[ H = -\frac{1}{2} \Delta - \frac{1}{r} + g\Theta(z), \]  
(1)

where the energy unit is \( me^4/(\hbar^2 \kappa^2) \), \( m \) is the electron effective mass, \( \kappa \) – the relative dielectric constant, \( g = V_0/\left[ \frac{me^4}{(\hbar^2 \kappa^2)} \right] \) is the well depth, and \( \Theta \) is the step function

\[ \Theta(z) = \begin{cases} 0, & z_1 < z < z_2, \quad z_2 - z_1 = L, \\ 1, & \text{outside}. \end{cases} \] 
(2)

Typically, \( g \geq 20 \). From the eigenvalue of \( H \), the binding energy is defined as

\[ E_b = E_w - E, \] 
(3)

where \( E_w \) is the threshold for the continuous spectrum in the well, i.e. the lowest eigenvalue of the one-dimensional hamiltonian

\[ H_w = -\frac{1}{2} \frac{d^2}{dz^2} + g\Theta(z). \] 
(4)

It is found from \( E_w = \frac{k^2}{2} \), where \( k \) is the smallest solution of

\[ \cos \left( \frac{kL}{2} \right) = \sqrt{\frac{2}{gL^2}} \left( \frac{kL}{2} \right). \] 
(5)

The asymptotic expressions for \( E_w \) are the following

\[ E_w = g \left\{ 1 - \frac{1}{2} gL^2 + \frac{1}{3} g^2 L^4 + \ldots \right\}, \quad gL^2 << 1 \] 
(6)

\[ E_w = \frac{\pi^2}{L^2} \left\{ \frac{1}{2} - \sqrt{\frac{2}{gL^2}} + \frac{3}{4} gL^2 - \left( 2 + \frac{\pi^2}{24} \right) \left( \frac{2}{gL^2} \right)^{3/2} + \ldots \right\}, \quad gL^2 >> 1. \] 
(7)

We shall obtain analytic estimates to \( E \) to compute the binding energy as a function of \( L \). The parameter \( g \) is assumed to be large.

The exact quantum number of the present problem is the \( z \)-projection of angular momentum, which will be called \( J \). Without loss of generality, we
may consider only positive values of $J$. To avoid using degenerate perturbation theory, we will study the first level with a given $J$. When $L \to 0$ or $L \to \infty$, we recover the unbounded (3D) coulomb problem, and the states we study have angular momentum equal to $J$.

3 The renormalised series for $gL^2 \ll 1$

When $gL^2 \ll 1$, the levels are shallow, i.e. located near the top of the barrier, and the wave function is mainly outside the well. The characteristic confinement distance along the $z$-direction is $l_z$, where $l_z^{-1} = \sqrt{2(g - E_w)} = gL + \ldots$. When $gL \ll 1$, the wave function is basically the 3D coulombic wave function, $\phi_{3D}$. On the other hand, when $gL >> 1$ (keeping $gL^2 \ll 1$, i.e. $l_z >> L$) the confinement length is much less than the Bohr radius (which in our units is one), and the wave function is written approximately as $\exp(-z/l_z)\phi_{2D}$, where $\phi_{2D}$ is the 2D coulombic wave function.

Accordingly, when $gL \ll 1$ we write

$$H = H_{3D} + g + V_1,$$

where $V_1 = -g\Theta^*(z)$, and the complementary step function is defined from $\Theta(z) + \Theta^*(z) = 1$. $V_1$ will be treated as perturbation. From first order perturbation theory, we obtain

$$E = g - \frac{1}{2(J+1)^2} - \frac{gL}{2^{J+1}J!(J+1)^{J+1}} + \frac{gL^3(z_1^2 + \zeta_1\zeta_2 + \zeta_2^2)}{J!(J+1)^{J+4}2^J} + O(L^5),$$

where we have written, $z_1 = \zeta_1 L$, $z_2 = \zeta_2 L$, $\zeta_2 - \zeta_1 = 1$, and without loss of generality, we will assume that $\zeta_1 < 0$, $\zeta_2 > 0$. The leading contribution of second order perturbation theory will be $-0.002 g^2L^2$ for the ground state ($J = 0$), and practically zero for $J > 0$.

Thus, grouping (6) and (9), we obtain for the binding energy at $gL \ll 1$,

$$E_b = a_0 + a_1(gL) + a_2(gL)^2 + a_3(gL)^3 + \ldots,$$
where $a_0 = 1/(2(J + 1)^2)$, $a_1 = 1/(2^{J+1}J!(J + 1)^{J+1})$, $a_2 = -0.498$ when $J = 0$ and $a_2 = -1/2$ when $J \geq 1$, $a_3 = -(\varsigma_2^2 + \varsigma_1\varsigma_2 + \varsigma_1^2)/(g^2J!(J + 1)^{J+2})$, etc.

Now, let us consider the opposite limit, $gL \gg 1$. The Hamiltonian will be written as

$$H = H_{2D} + H_w + V_2,$$

where $V_2 = 1/\rho - 1/\sqrt{\rho^2 + z^2}$ will be considered as perturbation. $\rho$ is the polar coordinate in the plane. In first order perturbation theory, we obtain

$$E = -\frac{1}{2(J + 1/2)^2} + E_w - \frac{b_k}{(gL)^k} + \ldots,$$

where the first correction is $b_1 = -8$ for the g.s. $(J = 0)$, and $b_2 = -2(2J - 2)!/(2J + 1)!/(J + 1/2)^3$ for the excited states $(J \geq 1)$. Consequently, for the binding energy, we obtain

$$E_b = \frac{b_k}{(gL)^k} + b_0 + \ldots,$$

where $b_0 = (J + 1/2)^{-2}/2$. Notice that Eq. (13) may be applied to the g.s. when $gL \geq 8$. If we recall that $gL^2 << 1$, then $g$ is forced to be greater than 64.

Note that the first three terms of (10) and the first two terms of (13) show that $E_b$ is, in certain approximation, “universal”, in the sense that it depends only on the variable $gL$. If we consider corrections such as the term $a_3(gL)^3$ of (10), this universality is lost. Notice also that the impurity position appears for the first time precisely in $a_3$.

Once we have the correct behaviour of $E_b$ for large values of $gL$, we may construct a “renormalised” series from (10) such that the large orders of this series will account for the correct asymptotics at $gL \gg 1$. We follow the idea of paper [2] in which the method was applied to the two-electron problem in a quantum dot.

For simplicity, we consider the g.s. of the centered impurity and include the first two terms of (10). We write $\beta = gL/(\alpha + gL)$. When $gL \to 0$, $\beta \to 0$, whereas when $gL \to \infty$, $\beta \to 1$. $\alpha$ is a free parameter which will be used to fit the numerical results. It gives an idea of where the transition
from “small” $gL$ to “large” $gL$ takes place. The renormalised series is looked for as a series in $\beta$

$$E_b = c_0 + c_1\beta + c_2\beta^2 + c_3\beta^3 + \ldots$$ (14)

The first coefficients $c_k$ are defined in such a way that when $\beta \to 0$ the first terms of (10) are reproduced. That is: $c_0 = 1/2$, $c_1 = \alpha/2$. On the other hand, $c_2$ and $c_3$ are chosen to reproduce the correct behaviour at $\beta \to 1$. We note that, as $\beta \to 1$

$$E_b = (c_0 + c_1 + c_2 + c_3) - (c_1 + 2c_2 + 3c_3)(1 - \beta) + \ldots,$$ (15)

that is, $c_3$ and $c_4$ are required to satisfy: $1/2 + \alpha/2 + c_2 + c_3 = 2$, $\alpha/2 + 2c_2 + 3c_3 = 8/\alpha$.

We show in Fig. 1 variational computations (points) for the g.s. of the centered impurity at $g = 60$, 100, 140 and 180. At each $g$, values of $L$ observing $L \leq 1/\sqrt{g}$ were included. A trial function with two nonlinear parameters was used in the computations [3]. The results show a very small dispersion of the points around a fixed curve, in accordance with the predicted universality. The curve is well fitted by the series (14) with $\alpha \approx 4$ (the solid line).

4 The renormalised series for $gL^2 >> 1$

Now, we consider the situation in which the level is deep inside the well, $gL^2 >> 1$. At large values of $g$, we have again two limiting situations: $L << 1 = a_B$, and $L >> 1$. The corresponding wave functions are approximately $\phi_{2D} \sin[\pi(z - z_1)/L]$, and $\phi_{3D}$.

When $L >> 1$, we take $V_3 = g\Theta(z)$ as a perturbation to $H_{3D}$. Assuming that $z_1$ and $z_2$ are both finite, we obtain

$$E = -\frac{1}{2(J + 1)^2} + \mathcal{O}\left(e^{-\varsigma L}\right),$$ (16)

where $\varsigma$ is the minimum between $|\varsigma_1|$ and $\varsigma_2$. The binding energy is thus

$$E_b = b_0' + \frac{b_1'}{L^2} + \frac{b_2'}{L^3} + \ldots,$$ (17)
where \( b'_0 = (J + 1)^{-2}/2 \), \( b'_2 = \pi^2/2 \), \( b'_3 = -\pi^2\sqrt{2/g} \), etc.

On the other hand, when \( L \ll 1 \) we write an expression like (11), and consider \( V_2 \) as a perturbation. To first order, we get

\[
E = -\frac{1}{2(J + 1/2)^2} + E_w - a'_kL^k + \ldots, \tag{18}
\]

where the first correction is

\[
a'_1 = -16(1/2 + \xi_1 + \xi_1^2 - (1 - \cos 2\xi_1)/(2\pi^2)) \text{ for the g.s. (} J = 0 \text{), and } a'_2 = -4(2J - 2)!((\xi_1^2 + \xi_1 + 1/3 - 1/2/\pi^2)/(2J + 1)!/(J + 1/2)^3 \text{ for the excited states (} J \geq 1 \text{). That is,}
\]

\[
E_b = a'_0 + a'_1L^k + \ldots, \tag{19}
\]

where \( a'_0 = 1/2/(J + 1/2)^2 \).

Notice that the series (17) and (19) suggest, again, a universal behaviour of \( E_b \) in the leading approximation. That is, \( E_b \) will not depend on \( g \) when \( gL^2 \gg 1 \).

For simplicity, we consider again the g.s. of the centered impurity and include terms up to \( 1/L^2 \) in (17). To construct the renormalised series for \( gL^2 \gg 1 \), we write \( \beta' = L/(\alpha' + L) \),

\[
E_b = c'_0 + c'_1(1 - \beta') + c'_2(1 - \beta')^2 + c'_3(1 - \beta')^3 + c'_4(1 - \beta')^4 + \ldots. \tag{20}
\]

The coefficients \( c'_0, c'_1 \) and \( c'_2 \) are obtained from (17), i.e. \( c'_0 = 1/2, c'_1 = 0, c'_2 = \pi^2/2/\alpha'^2 \). The coefficients \( c'_3 \) and \( c'_4 \) are required to satisfy the linear equations \( 1/2 + \pi^2/2/\alpha'^2 + c'_3 + c'_4 = 2, \pi^2/\alpha'^2 + 3c'_3 + 4c'_4 = \alpha'(4 - 16/\pi^2) \).

We show in Fig. 2 how close the behaviour of \( E_b(L) \) is to the universal behaviour when \( g = 60, 100, 140 \) and 180. Variational computations corresponding to values of \( L \) for which \( L \geq 2.6/\sqrt{g} \) are represented as points. The dispersion of the points is very small. The universal curve is fitted well by the series (20) when the parameter \( \alpha' \) is near to 1. The result of the fit is presented as a solid line.

5 The maximum of the curve \( E_b vs L \)

The conclusion of the previous analysis is the following. As \( L \) is increased from 0 to \( 1/\sqrt{g} \) the wave function changes from a tridimensional coulombic
wave function to a quasi-twodimensional function out of the well. The binding energy is a universal function of $gL$. On the other hand, as $L$ is decreased from infinity to $2.6/\sqrt{g}$ the wave function undergoes a change from the tridimensional coulombic wave function to a quasi-twodimensional function inside the well. The binding energy turns out to be a universal function of $L$. As a result of compressing the wave function, the binding energy increases. There is a critical value, $L_c$, at which the wave function is maximally compressed and $E_b$ is maximal. As indicated,

$$\frac{1}{\sqrt{g}} < L_c < \frac{2.6}{\sqrt{g}}$$ (21)

We may obtain a rough estimate to $L_c$ as the point at which the two series (13) and (19) coincide. For the g.s. of the centered impurity, we get

$$L_c \approx \frac{1.83}{\sqrt{g}}.$$ (22)

Numerical computations at $g \geq 60$ show that the product $\sqrt{gL_c}$ is almost constant, taking a value near 1.5 (Fig. 3).

We note that the dependence $L_c \sim 1/\sqrt{g}$ comes also from very simple reasonings based on the indeterminacy relations [4].

6 Concluding Remarks

We have shown that, at large values of $g$, the parameters $gL$ and $gL^2$ identify different regimes in the behaviour of the binding energy and the wave function of the impurity problem in a quantum well. In particular, the binding energy was shown to be a “universal” function in each of the regions $gL^2 << 1$ and $gL^2 >> 1$.

Our description is qualitatively valid in problems where $g = 20 - 60$. As $g$ is still decreased, regimes ii) and iii) become less applicable, and may be absent at all. In particular, at $g \approx 1$, we expect a transition directly from i) to iv) as $L$ goes from $L << 1$ to $L >> 1$.

We would like to stress that there are similarities between the results of our section 4 and paper [5], in which the $g \to \infty$ limit is studied. In that paper, a decomposition like (11) is choosen in the entire interval $0 < L < \infty$, and perturbation theory is applied. The failure of this decomposition at
$L \geq 1$ is corrected by introducing a scaling parameter and asking for the virial theorem to hold. Our approach is more qualitative but, at the same time, more exact, stressing what the actual wave function really is at any $L$.

A qualitative analysis of wave functions and energy curves for the impurity problem in dots, wires and multiwell structures is as simple as the analysis presented above. It may be a useful complement to the existing (or in progress) sophisticated numerical calculations.

7 Acknowledgments

One of the authors (A. G.) acknowledges financial support from the Colombian Institute for Science and Technology (COLCIENCIAS) under Project 1118-05-661-95, and from the Committee for Scientific Research at the Universidad Nacional (CINDEC). The authors are indebted to B. Rodriguez, J. Marin and J. Betancur for useful discussions.
References

[1] Bastard G 1988 Wave mechanics applied to semiconductor structures (Paris: Les Editions de Physique)

[2] Matulis A and Peeters F M 1994 J. Phys.: Cond. Matter 6 7751

[3] Betancur F J and Mikhailov I D 1995 Phys. Rev. B 51 4982

[4] Mikhailov I and Betancur F 1996 unpublished

[5] Debarge G, Erasme A and Toledo-Alvarez A 1996 Phys. Rev. B 53 3983
Figure Captions

Fig. 1. Twice the binding energy of the centered impurity as a function of $gL$. Points are variational calculations satisfying $L \leq 1/\sqrt{g}$.

Fig. 2. Twice the binding energy as a function of $L$ when $L \geq 2.6/\sqrt{g}$.

Fig. 3. The dependence of $\sqrt{g}L_\text{c}$ on $g$. 
