Quantum wells, wires and dots with finite barrier: analytical expressions of the bound states

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From a careful study of the transcendental equations verified by the bound states energies of a free particle in a quantum well, cylindrical wire or spherical dot with finite potential barrier, we have derived analytical expressions of these energies which reproduce impressively well the numerical solutions of the corresponding transcendental equations for all confinement sizes and potential barriers, without any adjustable parameter. These expressions depend on a unique dimensionless parameter which contains the barrier height and the sphere, wire or well radius.

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The present experimental and theoretical efforts in semiconductor physics are essentially devoted to confined structures: quantum wells, wires or dots. In most calculations, the potential barrier between the confined structure and the outside semiconductor is assumed to be infinitely high for simplicity. When the barrier is finite, the number of bound states, which is infinite for infinite barrier, can be reduced to 1 or even 0 for spherical dots, each energy level being substantially modified by the usual experimental confinements.

The great advantage of the infinite barrier assumption lies in the fact that the energies and wave functions have analytical expressions so that all theoretical calculations using them are rather easy. The introduction of the finite barrier height \( \frac{\hbar}{2mR} \) makes everything much more complicated. Even in the simplest case of one confined direction only, namely the quantum well, the bound states energies are given through a transcendental equation. Its solutions can be obtained either by a numerical calculation or by “reading” their values on a set of curves which makes their use quite inconvenient in quantitative calculations. The cylindrical wire and spherical dot confinement energies being obviously more complicated, the situation is even worse for the energy of these 2D and 3D geometries.

The purpose of this communication is to provide analytical expressions for the energies of any bound state level of these three geometries, valid for all confinements, i.e. all barrier heights and confinement sizes. We will show that these energies have the same analytical form, which depends on a unique dimensionless confinement parameter \( \nu \), in which enter the barrier height and the confinement extension. Let us add that, once the energy levels are known, it is straightforward to get from them the exact wave functions of all these bound states.

1. Results:

We consider a particle of mass \( m \) confined in a sphere or cylinder of radius \( R \) or in a quantum well of width \( 2R \), the energy barrier being \( V \). From \( R \) and \( V \), we can construct the dimensionless parameter \( \nu \) which rules all the physics of these finite barrier problems, namely

\[
V = \frac{h^2
u^2}{2mR^2}
\]

(1)

The infinite barrier limit corresponds to \( \nu \) infinite. From this parameter \( \nu \), we can already note that, as the physical scale for the barrier height is \( \hbar^2/2mR^2 \), a given barrier \( V \) between two semiconductors can appear as high or low depending on the confinement extension: the larger the \( R \), the better the \( V = \infty \) approximation for the same \( V \).

In other words, finite barriers effects are going to be very important for strongly confined systems.

Following Eq.(1), we are led to measure the particle energies in the same unit as \( V \), namely

\[
E = \frac{\hbar^2\alpha^2}{2mR^2} = V - \frac{\hbar^2\beta^2}{2mR^2}
\]

(2)

Note that for \( \beta \approx 0 \), the energy is close to the top of the well while for \( \beta \approx \nu \), \( \alpha \) is close to 0 so that the level is deep inside the well.

From the transcendental equation verified by the various energy levels of these confined geometries given below, we find that the number of bound states is controlled by the position of the parameter \( \nu \) with respect to a set of values \( \nu_{\text{min}} \) at which a bound state gets out of the well, i.e. disappears. A careful study of this transcendental equation shows that the parameter \( \alpha \) of the bound state levels behaves as \( \alpha_{\text{max}}/(1 + \psi^{-1}) \) when \( \nu \rightarrow \infty \), and as \( \nu_{\text{min}} + \gamma(\nu - \nu_{\text{min}}) \) when \( \nu \rightarrow \nu_{\text{min}} \). The three parameters \( (\nu_{\text{min}}, \alpha_{\text{max}}, \gamma) \) of these asymptotic behaviours depend on the geometry of the confinement and the level under consideration.

- For quantum wells, the levels are characterized by one quantum number \( n \), with \( n = 1, 2, 3, \ldots \), the corresponding parameters being \( \nu_{\text{min}} = (n - 1)\pi/2, \alpha_{\text{max}} = n\pi/2 \) and \( \gamma = 1 \).
- For cylindrical wires, the levels are characterized by two quantum numbers \( n \) and \( \pm m \) with \( m = 0, 1, 2, \ldots \). For the \( (n, \pm m) \) levels, the parameter \( \gamma \) is equal to \( 1/\sup(m, 1) \), the parameter \( \alpha_{\text{max}} \) is equal to the \( n^{th} \) zero \( z_{m}^{(n)} \) of the Bessel function \( J_m \) and the threshold \( \nu_{\text{min}} \) for level disappearance is equal to \( z_{m-1}^{(n)} \) for \( m \neq 0, z_{m-1}^{(n-1)} \) for \( m = 0, n \neq 1 \) and 0 for the ground state \( m = 0, n = 1 \).
• For spherical dots, the levels are characterized by three quantum numbers \((n, l, \pm m)\) with \(l = 0, 1, 2, \ldots\); they are degenerate with respect to \(m\). For \(l \neq 0\), the parameters are \(\nu_{\min} = (n - 1/2)\pi\), \(\alpha_{\max} = n\pi\) and \(\gamma = 1\), while for \(l = 0\), they are \(\nu_{\min} = \nu_{\min}^{(n)} = (n - 1)\pi\), \(\alpha_{\max} = \alpha_{\max}^{(n)} = (n + 1)\pi\) and \(\gamma = 1/(l + 1/2)\).

From the numerical resolution of the transcendental equations verified by the energy levels of these three confined geometries, we have checked that the energy parameter \(\alpha\) is amazingly well reproduced, for all levels and all confinement \(\nu\), by the same formula

\[
\chi(\nu) = \frac{\alpha_{\max} \nu}{\nu + 1 + \frac{(\alpha_{\max} - \nu_{\min}^{(n)} - 1)^2}{(\alpha_{\max} - \nu_{\min}^{(n)}) + (\nu - \nu_{\min}^{(n)})(1 + (\gamma - 1)\alpha_{\max}/\nu_{\min}^{(n)})}}
\]

(3)

which is constructed to give the two first terms of the \(\alpha\) behavior for both \(\nu \to \infty\) and \(\nu \to \nu_{\min}\) (see Fig. 3). The solid lines which correspond to the numerical solutions of the energy transcendental equations are hard to distinguish from the dashed lines which correspond to Eq. (3); the discrepancy is indeed extremely small.

In the particular case of the \(n\)th level of a quantum well (which exists for \(\nu > (n - 1)\pi/2\) only), this gives

\[
\alpha^{(n)}(\nu) \simeq \frac{n\pi}{2} \frac{\nu}{\nu + 1 + \frac{(\pi/2 - 1)^2}{(\nu - (n - 1)\pi/2)}}
\]

(4)

while for the \(n\)th level of the \(l = 0\) states of a spherical dot (which exists for \(\nu > (n - 1/2)\pi\) only) this gives

\[
\alpha^{(n)}_{l=0}(\nu) \simeq \frac{n\pi}{\nu + 1 + \frac{(\pi/2 - 1)^2}{(\nu - (n - 1/2)\pi)}}
\]

(5)

2. Derivation:

Let us now outline how we have derived the above results. The Schrödinger equation of a particle of mass \(m\) in the confined geometries considered here reads, in terms of the reduced variable \(\xi = z/R\) for quantum wells, \(\bar{\xi} = (|\mathbf{v}|/R, \varphi)\) for cylindrical wires and \(\check{\xi} = (|\mathbf{r}|/R, \theta, \varphi)\) for spherical dot, as

\[
\left[\Delta_{\xi} + v(\xi)\right] \psi(\xi) = 0
\]

(6)

with \(v(\xi) = \alpha^2 \text{ for } |\bar{\xi}| < 1 \text{ and } v(\xi) = -\beta^2 \text{ for } |\check{\xi}| > 1\).

The bound states of these confined geometries correspond to \((\alpha, \beta)\) real and positive \(3\): \(\alpha\) and \(\beta\) being linked by:

\[
\alpha^2 + \beta^2 = \nu^2
\]

(7)

due to Eq. (3).

a) 1D case: quantum well

In the 1D case, the solution of Eq. (3) is elementary: the wavefunction which cancels at \(\pm \infty\) and has continuous derivatives at \(\pm 1\) can be written as:

\[
\psi(-1 < \xi < 1) = a \left[ e^{2i\alpha} e^{i\alpha \xi} + e^{2i\beta} e^{-i\alpha \xi} \right]
\]

\[
\psi(\xi < -1) = \psi(-1)e^{\beta(\xi-1)}
\]

\[
\psi(\xi > 1) = \psi(1)e^{\beta(\xi-1)}
\]

(8)

with \(\alpha\) and \(\beta\) linked by Eq. (6) and by

\[
\exp 4i\alpha = \exp(4i\arctan \beta/\alpha)
\]

(9)

Eq. (6) is not one of the standard forms of the quantum well transcendental equation found in usual textbooks \(3\). It is however the most convenient one to extract the asymptotic behaviour of \(\alpha\) as we now show.

(i) When \(\nu \to \infty\), the finite values of \(\alpha\) correspond to \(\beta \simeq \nu\) infinite. For such \(\nu\), \(\beta/\alpha\) is large so that \(\arctan \beta/\alpha \simeq \pi/2 - \alpha/\beta\). Eq. (3) then leads to \(4\alpha \simeq 4(\pi/2 - \alpha/\nu)/\beta + 2(n-1)\pi\) i.e. \(\alpha \simeq n\pi/2/(1 + \nu^{-1})\) with \(n = 1, 2, 3, \ldots\).

(ii) The solutions for the bound state disappearance, i.e. for an energy level close to the top of the well, correspond to \(\alpha \simeq \nu\) and \(\beta \simeq 0\). \(\beta/\nu\) is then small so that Eq. (3) gives \(\beta \simeq \nu(\nu - (n - 1)\pi/2)\) i.e. \(\nu \simeq \nu + \mathcal{O}((\nu - (n - 1)\pi/2)^2)\) due to Eq. (3). This gives the values of \(\alpha_{\max}, \nu_{\min}\) and \(\gamma\) listed above.

In order to check the validity of the approximate \(\alpha^{(n)}(\nu)\) given in Eq. (3), it is not necessary to solve Eq. (6) numerically: indeed, while these equations do not give \(\alpha\) in terms of \(\nu\), they do give \(\nu\) in terms of \(\alpha\) as

\[
\nu = \alpha/\cos(\alpha - (n - 1)\pi/2)
\]

(10)

The corresponding curves as well as the various \(\alpha^{(n)}(\nu)\) are shown in Fig. 1. The fit is impressive; the two sets of curves are hard to distinguish, the largest discrepancy is smaller than 4%.

b) 2D case: cylindrical wire

In the 2D case, we have \(\Delta_{\xi} = \frac{1}{\xi^2} \frac{\partial^2}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial}{\partial \xi}\), so that the wave functions write \(\psi(\xi) = f_m(\xi) e^{\pm i m \varphi}\) with \(m = 0, 1, 2, \ldots\). The differential equation obtained for \(f_m\) is just the one of Bessel functions \((J_m, Y_m)\) for \(\xi\) inside the well and \((I_m, K_m)\) for \(\xi\) outside. The solutions which are finite for \(\xi = 0\), tend to 0 for \(\xi \to \infty\) and have a continuous derivative for \(\xi = 1\) read:

\[
f_m(\xi < 1) = A J_m(\alpha \xi)
\]

\[
f_m(\xi > 1) = A \frac{J_m(\alpha)}{K_m(\beta)} K_m(\beta \xi)
\]

(11)

with \(\alpha\) and \(\beta\) linked by Eq. (6) and by

\[
\frac{\alpha_m J_m(\alpha_m)}{J_m(\alpha_m)} = -\frac{\beta_m K_m(\beta_m)}{K_m(\beta_m)}
\]

(12)
In order to get the above expression, we have used $J_{-1} = -J_1$ and $K_{-1} = K_1$ and [10]:

\[
\begin{align*}
(a) & \quad J'_{\nu} = J_{\nu-1} - \nu/z J_{\nu} \\
(b) & \quad K'_{\nu} = -K_{\nu-1} - \nu/z K_{\nu} \\
\end{align*}
\]

(13)

**FIG. 1.** The energy parameter $\alpha$ as defined in Eq.(2) for the $n^{th}$ bound states of a quantum well as obtained from the exact expression of Eq.(13) (solid line) and from the analytical expression Eq.(12) (dashed line). The confinement parameter $\nu$ depends on the barrier height $V$ and half width $R$ through Eq.(1).

(i) When $\nu \to \infty$, the finite values of $\alpha_m$ correspond to $\beta \simeq \nu$ infinite. The $K$ ratio being 1 in this limit, we find $J_{m}(\alpha_m)/\alpha_m J_{m-1}(\alpha_m) \simeq -1/\nu \simeq 0$. The values of $\alpha_m$ are thus close to the zeros of $J_m$. For these $\alpha_m$, we find using Eq.(13a) that the inverse of the LHS of Eq.(12) is close to $(\alpha_m - z_m^{(n)})/z_m^{(n)}$ so that $\alpha_m \simeq z_m^{(n)}/(1 + \nu^{-1})$.

(ii) The solutions close to the top of the well correspond to $\beta_m \simeq 0$ and $\alpha_m \simeq \nu$. For these $\beta_m \simeq 0$ the RHS of Eq.(12) is close to $1/\ln \beta$ for $m = 0$, $\beta^2 \ln \beta$ for $m = 1$ and $-\beta^2/(m-1)$ for $m \geq 2$. Being close to zero in all cases, we conclude that $\alpha_m$ must tend to the zeros of $J_m$. In the particular case of $m = 0$, we find that in addition to the zeros of $J_{-1}$, i.e. the zeros of $J_1$, $\alpha_0$ can also tend to 0 for $\nu \to 0$. Since in this $\beta \sim \nu$ limit, $\alpha \sim \nu$ while the LHS of Eq.(12) is close to $-z_m^{(n)}(\alpha - z_m^{(n)})$ due to Eq.(13a), we get for $m \geq 1$, $\alpha_m \simeq z_m^{(n)}(n) + (\nu - z_m^{(n)})/m$ while for $m = 0$, we find $\alpha_0 \simeq \nu_{\min} + (\nu - \nu_{\min})$ with $\nu_{\min} = 0$ or $z_1^{(n)}$.

We thus recover the values of $(\nu_{\min}, \alpha_{max, \gamma})$ listed above. Fig.2 shows the results of the numerical resolution of Eqs.(12) as well as the value of $\alpha_m^{(n)}$ deduced from the corresponding $(\nu_{\min}, \alpha_{max, \gamma})$ inserted in Eq.(8). The fit is excellent for all confinements, the two curves being hard to distinguish, with an exception for the ground state at intermediate $\nu$: the approximate $\alpha_m^{(n=1)}$ is slightly below the numerical $\alpha$, the largest discrepancy being 14%.

**FIG. 2.** The energy parameters $\alpha$ for the $n^{th}$ level of the $\pm m$ states of the cylindrical wire confinement, as given by the numerical resolution of Eq.(12) (solid line) and by the approximate analytical expressions deduced from Eq.(1) (dashed line). The horizontal dashed lines correspond to $z_m^{(n)} = 2.40$, $z_1^{(n)} = 3.83$, $z_2^{(n)} = 5.13$, $z_3^{(n)} = 5.52$, $z_2^{(2)} = 7.01$ with $z_m^{(n)}$ being the $n^{th}$ zero of the Bessel function $J_m$. The confinement parameter $\nu$ depends on the barrier height and the cylinder radius $R$ through Eq.(1). Note that two curves $\alpha_{m=2}$ and $\alpha_{m=0}$ start each at $\nu \simeq z_1^{(n)}$ (with different slopes).

c) 3D case : spherical dot

In the 3D case, we have $\Delta_E = A J_{l+1/2}^2(\alpha \xi) - \xi^2/\xi^2$, so that the wave functions write $\psi(\xi) = f_l(\xi) Y_l(\theta, \varphi)$, with $l = 0, 1, 2, \ldots$ and $-l \leq m \leq l$. By setting $f_l = y_l/\sqrt{2}$, we find that the differential equation for $y_l$ is just the one of Bessel functions $J_{l+1/2}$ for $y_l$ inside the well, and $(l_{i+1/2}, K_{i+1/2})$ for $y_l$ outside. The solution which are finite for $\xi = 0$, tend to 0 for $\xi \to \infty$ and have a continuous derivative for $\xi = 1$ read:

\[
\begin{align*}
f_l(\xi < 1) &= A J_{l+1/2}(\alpha \xi) \\
f_l(\xi > 1) &= \frac{A J_{l+1/2}(\alpha)}{\sqrt{\xi} K_{l+1/2}(\beta)} K_{l+1/2}(\beta \xi) \\
\end{align*}
\]

with $\alpha$ and $\beta$ linked by Eq.(5) and by

\[
\frac{\alpha_i J_{l-1/2}(\alpha_i)}{J_{l+1/2}(\alpha_i)} = -\beta_i K_{l-1/2}(\beta_i) / K_{l+1/2}(\beta_i)
\]

for $l \geq 1$ (due again to Eq.(13)). For the $l = 0$ states however, it is simpler to use the explicit expression $J_{1/2}(x) = (\frac{x}{2})^{1/2} \sin x$ and $K_{1/2}(x) = (\frac{x}{2})^{1/2} e^{-x}$ in Eq.(14). The continuity of $f'_l$ at $\xi = 1$ then leads to

\[
\frac{\alpha_0}{\tan \alpha_0} = -\beta_0
\]
so that due to Eq.(16), the transcendental equation for the \( l = 0 \) levels of a spherical dot is simply

\[
\nu = \alpha_0 / |\sin \alpha_0| \tag{17}
\]

with \((n-1/2)^2 < \alpha_0 < n\pi\) in order to have \(\beta_0 > 0\).

Let us start with these \( l = 0 \) states.

(i) For \( \nu \to \infty \), Eq.(17) leads to \(|\sin \alpha_0| \to 0\) so that \(\alpha_0 \approx n\pi\). The expansion of the RHS of Eq.(17) close to these maximum values of \(\alpha\) gives \(\alpha_0 \approx n\pi/(1 + \nu^{-1})\).

(ii) For \(\beta_0 \approx 0\), Eq.(13) leads to \(\cos \alpha \approx 0\); so that \(\alpha_0 \approx (n - 1/2)\pi\) only in order to have \(\beta_0 > 0\). The expansion of the LHS of Eq.(14) close to these values gives \(\alpha_0 \approx \nu + O((\nu - (n - 1/2)\pi)^2)\).

We now turn to the \( l \geq 1 \) states.

(i) For \( \nu \to \infty \) and \(\alpha_l \) finite, i.e. \(\beta_l \approx \nu\) infinite, the ratio of \( K \) is equivalent to 1, so that \(J_{l+1/2} \alpha_l / J_{l-1/2} \alpha_l \approx -\nu / \beta_l \approx 0\). \(\alpha_l\) is thus close to a zero of \(J_{l-1/2}\). Using Eq.(13a), the expansion of the inverse of the LHS of Eq.(13) leads to \((\alpha_l - z_{l+1/2}^{(n)}) / z_{l+1/2}^{(n)}\) so that \(\alpha_l \approx z_{l+1/2}^{(n)}(1 + \nu^{-1})\).

(ii) For \(\beta_l \approx 0\), and \(\alpha_l \approx \nu\) finite, the RHS of Eq.(13) goes to zero as \(-\beta_l^2 / (2l - 1)\) so that \(\alpha_l\) is close to a zero of \(J_{l-1/2}\). Close to these values, the LHS of Eq.(13) is equivalent to \(z_{l-1/2}^{(n)}(\alpha_l - z_{l-1/2}^{(n)}) / z_{l-1/2}^{(n)}\) due to Eq.(13a) so that in this limit we have \(\alpha_{l\neq 0} \approx z_{l-1/2}^{(n)}(\nu - z_{l-1/2}^{(n)}) / (l+1/2)\).

This just corresponds to the values of \((\nu_{\text{min}}, \sigma_{\text{max}}, \gamma)\) listed above. Fig.3 shows the results of the numerical resolution of Eq.(13) for the energy parameters \(\alpha\) as given in equation (16). Here again, the fit is incredibility good for all confinement and all energy levels.

d) One specific example:

The above results are of course given in reduced units in order to be universal. Let us apply them to one specific case: \(GaAs/GaAsAl_{1-x}As\). For usual x’s, the electron mass is \(m \approx 0.07\) and the energy barrier for electrons is of the order of \(V \approx 300\,meV\). For quantum well, wire or dot of radius \(R \approx 40\,A\), Eq.(13) gives the confinement parameter \(\nu \approx 3.0\). Figure 4 shows that two bound states exist for quantum well or wire, but only one for quantum dot. Moreover the energies of these levels are significance lower than the energies of the corresponding states for infinite barrier: in the case of a quantum well of half width \(40\,A\), Eq.(13) gives \(\alpha \approx 1.1\) and 2.24 instead of \(\pi/2\) and \(\pi\) which corresponds to 45 and 170 meV instead of 85 and \(340\,meV\).

In conclusion, we have given analytical expressions for the bound states energies of quantum wells, cylindrical wires, and spherical dots, which reproduce impressively well their numerical values, for any level, barrier height and confinement size, without adjustable parameters. From them, we can easily obtain the exact wave functions of these bound states by inserting the corresponding values of \(\alpha, \beta\) into Eq.(13).

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