Resonance states in a cylindrical quantum dot with an external magnetic field

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Abstract
Bound and resonance states of quantum dots play a significant role in photo-absorption processes. In this work, we analyse a cylindrical quantum dot, its spectrum and, in particular, the behaviour of the lowest resonance state when a magnetic field is applied along the symmetry axis of the cylinder. To obtain the energy and width of the resonance we use the complex rotation method. As expected, the structure of the spectrum is strongly influenced by the Landau levels associated to the magnetic field. We show how this structure affects the behaviour of the resonance state and that the binding of the resonance has a clear interpretation in terms of the Landau levels and the probability of localization of the resonance state. The localization probability and the fidelity of the lowest energy state allow identification of two different physical regimes, a large field–small quantum dot radius regime and a small field–large quantum dot radius, where the binding of the resonance is dominated by the field strength or the potential well, respectively.

Keywords: quantum dots, resonance, binding, fidelity

1. Introduction
The availability of quantum devices with a characteristic length of only a few nanometres allows the implementation of a number of experimental setups that put the very foundations of quantum mechanics under test. The fact that the radius of a Landau level (LL) is only a few nanometres for magnetic field strengths of around 10 Tesla allows the verification of the Aharonov–Bohm effect in quantum rings [1], which leads to the presence of persistent currents [2]. These persistent currents have been measured even for one-electron states [3]. The quantum rings are formed by only one semiconductor material, and the fabrication of multiple concentric quantum rings (up to five) can be achieved with high quality and reliability [4].

The early realization that quantum dots presented an ideal scenario to study transitions between electrically confined states and Landau-type magnetic levels [5], originated numerous theoretical and experimental works attempting to explain the effect of the confinement potential over the observed spectrum. For example, Peeters and collaborators studied the spectral properties of a two-dimensional parabolic confinement potential [6], the effect of the confinement in the direction of the field (or $z$ direction) [7, 8], and the spectral properties of an electron confined in an artificial molecule [9]. Anyway, even in the case of a finite confinement potential in the $z$ direction [8], these studies were restricted to the discrete spectrum of each problem.

On the other hand, the quantum dot has been appointed as one of the most promising implementations of a single qubit [10, 11]. There has been a huge amount of work to circumvent the numerous associated problems: decoherence [12], the coupling between two qubits (to implement a two-qubit quantum gate) in double quantum dots has been studied extensively, in particular how it can be tuned using electric fields [13], magnetic fields [14], or the effect of the confinement of the double quantum dot in a quantum wire [15], etc.

When dealing with applied magnetic fields, most theoretical studies on quantum dots focus on strongly localized states, achieved many times using always-bounding potentials, as the three-dimensional harmonic potential or impenetrable...
walls. The presence of a constant magnetic field, anyway, is equivalent to a two-dimensional harmonic potential in the plane orthogonal to the field direction. Conversely, there are far fewer examples of studies considering finite potentials, in particular those whose shapes or features allow the presence of resonance states. There is a number of reasons to study finite potentials, from charge transport situations to the effect of resonance states in luminescent quantum dots. Bylicki and Jaskólski [16] analysed the binding of shape resonances through the application of an external magnetic field. They considered a one-electron spherical quantum dot–quantum well structure. In this work we consider a closely related problem with the purpose of a better understanding of the transition from a resonance state to a bounded one.

As has been said above, a constant magnetic field induces a two-dimensional harmonic potential that precludes the appearance of resonances in the plane orthogonal to the field, i.e., the loss of particles can take place only in the direction of the field, closing a number of decaying channels that would be available in absence of the field. In this sense, it renders what particular shape the binding potential has almost irrelevant, as long as it allows the appearance of resonances in the direction of the field. So, to avoid unnecessary complications, we consider a quantum dot model with cylindrical symmetry whose axis has the same direction as the magnetic field, besides we use the effective mass approximation. As is well known, in this approximation the many-body interactions of the electron trapped in the quantum dot are reduced to a (simple) binding potential, and all the parameters of the Hamiltonian, mass, dielectric constants and so on are taken as equal to the bulk parameters.

Despite its apparent simplicity, the calculation of the resonance states of one electron trapped in a binding potential with an external magnetic field is far from trivial, in particular for small enough strengths of the field since the LLs are bunched when the strength of the field goes to zero. To obtain the energy and width of the resonance states we employ the complex scaling method [17] that, together with a square-root approximation for the wave function, has been very fruitful to analyse bound and resonance states in many-body models, is near the ionization threshold or to a transition from a resonance state to a bounded one.

Even with the introduction of the external field, the angular momentum \( L_z \) is a conserved quantity, and its eigenvalues give quantum numbers. So, we focus on states with zero angular momentum. In this case, the Hamiltonian reads

\[
H_0 = -\frac{1}{2\mu} \left( \nabla \cdot \nabla + \nabla^2 \right) + V(\rho, z),
\]

where \( V(\rho, z) \) is given by equation (1), \( \mu \) is the effective mass of the electron in the semiconductor material. The equation is written in atomic units. If a magnetic field \( B = Bz \) is applied, there is a new term that must be incorporated to the RHS of equation (2), which results in the following Hamiltonian [16]:

\[
H = H_0 + \frac{B^2}{8\mu} \rho^2.
\]

The discrete spectrum and the resonance states of the model given by equation (3) can be obtained approximately using square-integrable variational functions \( \Psi_j^\rho \) [18, 19, 24, 25]. So, if \( \Psi_j \) are the exact eigenfunctions of the Hamiltonian, we look for variational approximations

\[
\Psi_j \simeq \sum_{i=1}^{N} c_{i}^{j}(\Phi_i, \psi_i), \quad j = 1, \ldots, N,
\]

where the \( \Phi_i \) must be chosen adequately, \( N \) is the basis set size, and the \( \psi_i \) are the linear variational parameters of the Rayleigh–Ritz method.

Since we are interested in null angular momentum eigenfunctions, and taking into account the symmetries of the Hamiltonian (3), we choose as basis functions

\[
\Phi_i(\rho, z) = \psi_\eta(\rho)\psi_\nu(z),
\]

where

\[
\psi_\eta(\rho) = \frac{1}{\sqrt{n+1}} \eta e^{-\eta^2/2} L_n^{(1)}(\eta\rho),
\]

and

\[
\psi_\nu(z) = \frac{1}{\sqrt{2}} e^{-v|z|^2/2} L_0^{(0)}(|v|z)|.\]

The paper is organized as follows, the quantum dot model and the variational approximation that provides approximate eigenvalues and eigenfunctions are presented in section 2. The analysis of the resonance using complex exterior scaling and the influence of the LLs are presented in section 3, while the binding process is studied, using different methods, in sections 3–5. Finally, we summarize and discuss our results in section 6. Some rather lengthy and technical results, mostly matrix elements are deferred to the appendices.

**2. Model**

The binding potential of the quantum dot is given by a piecewise function

\[
V(\rho, z) = \begin{cases} V_1, & \rho < a_\rho, \frac{\eta}{2} < |z| < \frac{\eta+b}{2}, \\ -V_2, & \rho < a_\rho, |z| < \frac{\eta}{2}, \\ 0, & \text{otherwise} \end{cases},
\]

i.e., the potential is a cylindrical well aligned with the \( z \)-axis, with two potential steps at the top and bottom of the cylinder, where the radius of the cylinder is \( a_\rho \), its height \( \eta \), the depth of the potential well, \(-V_2\), and the height of the potential steps, \( V_1 \). This ensures that, for properly chosen constants \( a_\rho, b, a_\rho, V_1 \) and \( V_2 \), the one-electron problem has resonance states without an external field.

Despite its apparent simplicity, the calculation of the resonance states of one electron trapped in a (simple) binding potential with an external field.

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\]

and

\[
\psi_\nu(z) = \frac{1}{\sqrt{2}} e^{-v|z|^2/2} L_0^{(0)}(|v|z)|.\]
Figure 1. The four panels show details of the variational spectrum and the LLs. (a) The variational spectrum obtained with a basis set size \(N = 2500\). Each black curve corresponds to a single eigenvalue and the red curves correspond to the exact LLs. (b) This panel shows the zone around the second LL (red solid line). It can be seen how the levels that cross above the second LL have several avoided crossings before they reach the third one. (c) This panel shows the levels that cross above the second LL have several avoided crossings before they reach the third one. (d) This panel shows the spectrum of a two-electron quantum dot [7, 19]. When a magnetic field is applied, each LL works as the bottom of a continuum. Another salient feature of the spectrum appears for large enough magnetic fields; one isolated eigenvalue with lower energy than the lowest LL. From a physical point of view, the origin of this state can be understood as follows: for intermediate values of the magnetic fields the wave function of the electron looks like an harmonic oscillator wave function in the \((\rho, \phi)\) plane and as a free particle in the \(z\) direction. The spatial extent of the wave function on the plane is roughly equivalent to the radius of a LL, that is larger than the radius (in the plane) of the quantum dot. When the strength of the magnetic field is increased the radius of the lowest LL becomes smaller and smaller reaching, at some point, a size similar to the radius of the quantum dot, at this point the state becomes localized. As we will show, the mechanism of localization can be quantified and strongly influences the behaviour of the resonance states whose energy lies near the localization point, in particular this mechanism is responsible for the binding of the resonance for a large enough magnetic field [16], we will return to this point in section 4.

The similarities between the behaviour of the spectrum analysed in figure 1 near the point where \(E_1 < E_{L1} (0,0)\), and the spectrum of a two-electron quantum dot near the ionization threshold are striking. So, it comes as no surprise that the resonance states of both models also show some similarities, as we will show later on.

3. Detecting the resonance states using complex exterior scaling

The calculation of the energy and width of resonance states offers a number of challenges that repeatedly leads to the formulation of new methods. Among the most widely used methods that can be mentioned are the complex scaling (or complex dilation) method [17], the complex absorbing potential method [27] and the density of states method [28]. Each one of these has its advantages and drawbacks. Because we are dealing with a piecewise potential we resort to the exterior complex scaling (see, for example, [17]). This method is particularly appealing in our case since for \(B \neq 0\), the complex scaling should be applied only to the \(z\) variable because this is the only direction available to the electron to get away from the bounding potential. The exterior of the method refers to the exterior of the region where the potential is not zero so, for \(B \neq 0\) the exterior complex scaling asks that

\[
z \leftrightarrow \begin{cases} 
 z' & \text{if } |z| \leq \frac{a + b}{2} \\
 e^{i\theta}z' & \text{if } |z| \geq \frac{a + b}{2}
\end{cases},
\]

where \(z\) is the coordinate to be complex scaled, and \(\theta\) is the rotation angle. The complex scaling turns the resonance states into a complex plane.
The exterior complex scaling method works nicely for intermediate values of the magnetic field. Anyway, if \( B \leq 5T \), or \( B \geq 16T \), the convergence of the method is, at least, questionable, see figure 3. For small fields the method struggles to provide a reliable value for the resonance eigenvalue because, as can be appreciated from figure 2, for \( B \approx 5T \) the resonance ‘enters’ in the continuum above the second LL. In this region the approximate eigenvalues that enter from the region above the first LL ‘collide’ with the eigenvalues that lie between the first and second LL. The successive collisions, and the corresponding avoided crossings, can be well appreciated in figure 1(b).

The binding of the resonance, i.e., the fact that the width of the resonance becomes zero for large enough field strengths cannot be understood by only studying the spectrum. In the next section, we will introduce a quantity that will allow us to study the associated eigenstates. As we will show, the analysis of the eigenstate corresponding to the isolated eigenvalue that appears below the first LL, see figure 1(a), gives a physical picture of the binding process.

In what follows, and up to the end of this section, we want to focus on the results of the complex rotation method between LLs. The scenario between LLs can be better appreciated in figure 3. The figure shows the complex spectrum obtained when the complex rotation is performed accordingly with equation (10) for different values of \( \theta \). In this figure it is clear why the method is termed complex rotation, the continuum part of the spectrum now lies in the complex plane over straight lines, the angle between the lines and the real axis equal to \( 2\theta \). When \( B \neq 0 \), the data for different \( \theta \) values form ‘hand-fans’ of data, i.e., sets of straight lines with a common origin in the real axis. Each one of these sets can be associated to a single LL, the leftmost hand-fan corresponds to the first LL, the middle one to the second LL, and the rightmost to the third LL. Again, this structure can be attributed to the role that each LL plays as the bottom of a continuum of levels. Effectively, the distance between the origins of each set of lines, over the real axis, is exactly equal to the distance between the LL at the magnetic field strength considered. As the magnetic field strength decreases, the data of the different fans overlap making it very difficult to distinguish the eigenvalues corresponding to the resonance.

Figure 3(b) shows the trajectory in the complex plane of the eigenvalue associated to the resonance state. As can be appreciated, the eigenvalues are scattered much less in energy than in width. This feature is typical of the complex rotation method.

Above the second LL, the complex rotation method should be complemented with some \textit{ad hoc} assumptions to identify the points that belong to the \( \theta \)-trajectory. The main assumption is rather physical; the complex rotated eigenvalues can be approximated by \( E_{LL} + \tan (2\theta) E_\nu \), i.e., they form a straight line in the complex plane that forms an angle of \( 2\theta \) with the \( x \)-axis, \( E_\nu \) is a variational eigenvalue. This approximation works nicely except near a resonance. The second assumption is similar: a given complex eigenvalue \( E_\nu (\theta) \) should not change too much if \( \theta \) is changed, say

\[
|E_\nu (\theta + \delta \theta) - E_\nu (\theta)| \lesssim \delta \theta |E_\nu (\theta)|, \tag{13}
\]

where \( \delta \theta \) is small enough. Applying these assumptions and discarding complex eigenvalues that jump from a hand-fan to another (see figure 3(a)) it is feasible to obtain stabilized values for \( E_{\text{res}} \) above the second LL.

---

**Figure 2.** The real and imaginary parts of the resonance eigenvalue \( E(\theta) \) versus the magnetic field strength. (a) The solid square (blue) dots correspond to the energy of the resonance and the solid lines correspond to the two lowest LL energies. The value for \( B = 0 \) was obtained performing the complex rotation in the coordinates \( \rho \) and \( z \). (b) The width of the resonance versus the magnetic field. As the magnetic field increases its value the width of the resonance goes to zero, signalling its binding.
4. Detecting the resonance states using localization probability

As we will show in this section, the binding of the resonance for large enough magnetic field is a consequence of the strong localization experienced by the wave function corresponding to the lowest eigenvalue. As a matter of fact, the localization allows the resonance through the spectrum to be followed. To quantify the localization of an approximate eigenfunction $\Psi_j$, we calculate the probability that the electron is localized in the potential well,

$$P_j = \int_{-\pi/2}^{\pi/2} \int_0^{\alpha_j} |\Psi_j(\rho, z)|^2 \, d\rho \, dz,$$

(14)

where $P_j$ is the probability attributable to the localization of $\Psi_j$.

Figure 4(a) shows the probability $P_1$ as a function of the magnetic field strength for the lowest variational eigenvalue, while figure 4(b) shows the probability $P_j$ for $j = 2, 3, \ldots, 8$. The curves are shown in different panels because of their respective scale.

It is worth mentioning that despite the variational eigenvalues not showing any sudden changes near $B \sim 17T$, except for the lowest one when it crosses the first LL, the probability of localization into the well shows a well-defined maximum for a large number of eigenvalues.

For small values of the magnetic field, the probability of localization $P_1 \lesssim 10^{-3}$ and is a very smooth function of $B$. This behaviour changes abruptly near $B \sim 17T$, and for larger values of $B$ the localization probability grows up to values larger than 0.1, see figure 4(a). It is clear that this behaviour is not compatible with an extended wave function. Since we are approximating the exact solutions of the eigenvalue problem with square-integrable functions, the value of the localization probability cannot drop to zero, in the continuum region and far away from a resonance state, the variational eigenfunctions resemble a plane wave that is extended in a cylindrical spatial region with radius $R \sim 1/\eta$ and length $L \sim 1/\nu$, where $\eta$ and $\nu$ are the nonlinear variational parameters. For this reason, in the continuum region and far away from a resonance, we estimate the localization probability as $P_1 \sim a_d \alpha_d \eta \nu \sim 10^{-3}$.

The localization of $\Psi_j$ can be further analysed using the expectation value

$$\langle |z| \rangle_1 = \int_{-\pi/2}^{\pi/2} \int_0^{\alpha_j} |\Psi_j(\rho, z)|^2 |z| \, d\rho \, dz,$$

(15)
We interpret that the peak in a given localization probability appears when the corresponding eigenvalue is a reasonable approximation for the resonance energy at that particular value of $B$. In other words, $E_{res}(B_j^{\text{peak}}) \approx E_j(B_j^{\text{peak}})$, where $B_j^{\text{peak}}$ is the value of the magnetic field where $P_j$ attains its maximum. The $E_j(B_j^{\text{peak}})$ allow the resonance states to be tracked down from the localization point up to the second LL, above the second LL the spectrum shows a multiple-continua region, generating multiple avoided crossings due to two-continua interaction that this method cannot distinguish from the avoided crossings due to resonances. The $E_j'(B_j^{\text{peak}})$ are shown in figure 7, where they are compared to the resonance energies obtained using the other methods discussed in this work.

5. Detecting the resonance states using the fidelity

For a given quantum state $\psi$, that depends on a parameter $\lambda$, a measure of how much it changes when the parameter is varied is given by the fidelity, $F$, which is defined as

$$F_{\Delta \lambda}(\lambda) = \left| \langle \psi(\lambda - \Delta \lambda) | \psi(\lambda + \Delta \lambda) \rangle \right|^2,$$

(16)

where $\Delta \lambda$ is a small variation of the parameter.

The fidelity has been extensively used to characterize the analytical properties of quantum states near a quantum phase transition in quantum spin chains models [29], quantum phases of matter [30], or bound and resonance states in atomic or quantum dot models [18]. In two-electron quantum dots, it has been shown that the fidelity of the approximate variational eigenstates detect the resonance states and allow its energy to be calculated approximately [18]. To achieve this, the fidelity of many eigenstates should be calculated as a function of the external parameter that drives the system from bound to unbounded states. In this work, this parameter is the magnetic field strength.

From its definition, equation (16), it is clear that most of the time $F_{\Delta \lambda} \approx 1$, except for very special cases. On the other hand, the fidelity should drop to zero if the system experiences a rather sudden change [29]. For this reason, it is often convenient to study the function

$$G_n(\lambda) = 1 - \left| \langle \Psi_n^\ast(\lambda - \Delta \lambda) | \Psi_n(\lambda + \Delta \lambda) \rangle \right|^2.$$

(17)

Figure 5 shows the behaviour of the $G_n$ function for $n = 1, 2, \ldots, 6$, as a function of the magnetic field strength. Each curve has a more or less well-defined peak for a given value of the magnetic field, $B_n$. The values $E_n(B_n)$, i.e., the value of the variational eigenvalues at their respective peaks of the function $G_n$, give a very good approximation for the resonance energy at the points $B_n$. Obtaining an estimation for the resonance energy in this way does not allow it to be obtained for arbitrary magnetic field strength values since the values $B_n$ are not chosen at will, they are obtained from the fidelity data and depend on the basis set size, the nonlinear variational parameters, the basis functions used, and so on; this has been pointed out previously in [18]. Nevertheless, the method provides another tool to analyse resonance states. The fidelity method works best when the width of the resonance is

![Figure 5. The function $G_n$ versus the magnetic field. The figure shows the function for the first six variational eigenvalues, $G_1$, $G_2$, $G_3$, $G_4$, $G_5$, $G_6$, solid (---), dotted (-----), short-dashed (---), long-dashed (---), dot-dashed (---) and double dot-dashed (---) lines, respectively. The peak where each curve attains its maximum value is clearly appreciable. $B_n$ is given by the abscissa of the peak (see the text).](image-url)
The critical fields $B_p(a_\rho)$ and $B_F(a_\rho)$ versus the quantum dot radius. The localization probability critical field (red squared dots) and the fidelity critical field (solid black dots) is shown for several quantum dot radii. The (blue) dashed curve corresponds to the radius of the lowest LL as a function of the magnetic field. It is clear that for small quantum dot radius, the localization takes place when the cylindrical wave function enters the critical field. For the larger QD’s radius, the localization is dominated by the quantum well potential and not by the magnetic field.

not too wide, so it is to be expected that it will be more precise near the localization point.

Before presenting the results of the localization and fidelity methods with respect to the resonant states, we want to stress the relationship between both quantities. Let us call $B_p(a_\rho)$ the critical value of the magnetic field such that the localization probability of the first variational eigenvalue becomes noticeable for a given quantum dot radius $a_\rho$, and $B_F(a_\rho)$ the magnetic field value such that the function $G_1$ attains its maximum value as a function of $B$. Figure 6 shows the values of both quantities, $B_p(a_\rho)$ and $B_F(a_\rho)$, for several values of the quantum dot radius $a_\rho$. The agreement between both critical quantities is striking.

At this point, we can summarize our results in figure 7. The figure shows the energy of the resonant state as a function of $B$, as it is obtained from the complex rotation, fidelity and localization methods.

From figure 7, it is rather clear that both the localization method and the fidelity are able to follow the resonance from the localization point until the second LL. Anyway, a word of caution is necessary here. The complex rotation method implies a stabilization procedure that, when properly used, gives an idea about the accuracy of the results obtained. This is not true for the fidelity method. The best recipe to obtain stabilized results from the fidelity method implies picking the largest possible basis set size, $N$, with $N_z = N_\rho$. Otherwise, the convergence of the fidelity data, i.e., the values obtained for the resonance’s energy from the fidelity, is not uniform. Figure 8 shows the behaviour of the resonance energy obtained following the fidelity method with different basis set sizes. It is worth mentioning that the resonance energies obtained with $N = 900$ and $N = 3600$ differ by less than 5%.

Again, as is the case with the localization probability method to find estimations for the resonance energy, the fidelity method works properly as long as the resonance state is well isolated, i.e., the only avoided crossings present in a given region of the spectrum should be the one associated to the resonance. As has been said previously, above the second LL there is a very large number of avoided-crossings for each eigenvalue due to a multiple-continua scenario. Each $G_n$ has a peak associated to every single avoided-crossing, making it extremely hard to decide which peak corresponds to the resonance state.

6. Discussion and conclusions

The external magnetic field precludes the escape of the electron on the $(\rho, \phi)$ plane, for this reason the quantum dot bounding potential consists of a potential well and a potential step, to ensure the presence of resonance states. In this sense, the problem has several characteristic lengths, the quantum dot radius, the LLs’ radii, the length of the quantum dot along the $z$ axis, and so on. The two lengths that come into play varying the...
magnetic field strength, for the set of parameters considered in this work, are the quantum dot radius and the lowest LL radius. The potential well depth and the other parameters of the QD were chosen to ensure that for \( B = 0 \) there were no bound states.

The localization probability is able to track down the resonance states from the localization point up to the second LL. Above the second LL, the eigenvalues have too many avoided crossings, because of the multiple continua interacting in this region of the spectrum, rendering the method useless. The many avoided crossings also prevent the use of the fidelity to detect the resonance above the second LL. Moreover, despite the fact that the width of the resonance state analysed is not small when compared with the resonance energy, the fidelity method provides a good estimation of the last. Anyway, some precaution must be exercised to obtain accurate and stable results.

Finally, both critical fields, \( B_{c1}(a_r) \) and \( B_{c2}(a_r) \), show two clearly distinguishable regimes, for a small quantum dot radius their values are given by the lowest LL radius, so both are proportional to \( 1/a_r^2 \). For a large enough quantum dot radius both critical fields show a different behaviour and, apparently, both are proportional to \( (\alpha - \beta a_r)^2 \), where \( \alpha \) and \( \beta \) are constants. The extent of the small field regime can be tuned changing the parameters of the bounding potential, equation (1), extending or reducing it. The critical behaviour of the eigenvalues in the transition region between the large-field–small quantum dot radius and the small field–large quantum dot radius will be analysed elsewhere.

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Appendix. Some matrix elements

It is convenient to separate the kinetic energy matrix elements into two contributions, one corresponding to the radial coordinate,

\[
\langle \psi_n | T_{r} | \psi_s \rangle = \left( \psi_n - \frac{1}{2\mu} \nabla^2_r \psi_s \right) 
= \frac{\eta}{\mu \sqrt{(n+1)(s+1)}} \left( \frac{1}{4} T_1 + \frac{1}{2} (T_2 + T_3) + T_0 \right)
\]

(A.1)

and the other corresponding to the \( z \) coordinate,

\[
\langle \phi_t | T_{z} | \phi_s \rangle = \left( \phi_t - \frac{1}{2\mu} \nabla^2_z \phi_s \right) 
= \frac{2\mu}{\eta \sqrt{(n+1)(s+1)}} 
\times \left( \frac{1}{4} T_{1z} + \frac{1}{2} (T_{2z} + T_{3z}) + T_{0z} \right),
\]

(A.2)

where

\[
T_1 = (n+1) \delta_{n,s}, \\
T_2 = \sum_{p=0}^{n} \sum_{q=0}^{s-1} \frac{(-1)^{p+q}(n+1)!(s+1)!(p+q+1)!}{(n-1-p)!(2+p)!p!(s-q)!(1+q)!q!}, \\
T_3 = \sum_{p=0}^{n-1} \sum_{q=0}^{s} \frac{(-1)^{p+q}(n+1)!(s+1)!(p+q+1)!}{(n-p)!(1+p)!p!(s-1-q)!(2+q)!q!}, \\
T_4 = \sum_{p=0}^{n-1} \sum_{q=0}^{s} \frac{(-1)^{p+q}(n+1)!(s+1)!(p+q+1)!}{(n-1-p)!(2+p)!p!(s-1-q)!(2+q)!q!}, \\
T_5 = \delta_{n,s},
\]

(A.3)

and

\[
T_{1z} = \delta_{n,s}, \\
T_{2z} = \sum_{d=0}^{r} \sum_{f=0}^{r-1} \frac{(-1)^{d+f}!(d+f)!}{(d-f)!f!(f)!}, \\
T_{3z} = \sum_{d=0}^{r} \sum_{f=0}^{r-1} \frac{(-1)^{d+f}!(d+f)!}{(d-f)!f!(f)!}, \\
T_{4z} = \sum_{d=0}^{r} \sum_{f=0}^{r-1} \frac{(-1)^{d+f}!(d+f)!}{(d-f)!f!(f)!}, \\
T_{5z} = \delta_{n,s},
\]

(A.4)

while

\[
\langle \psi_n | V(\rho, z) | \psi_s \rangle = -(V_2 I_{v2} + V_1 I_{v1} \delta_{n,s}),
\]

(A.8)

the barrier term is, obviously, proportional to \( V_1 \), while the term proportional to \( V_2 \) corresponds to the matrix element of the potential well. The matrix elements \( I_{v2} \) and \( I_{v1} \) are given by

\[
I_{v2} = \frac{1}{\sqrt{(n+1)(s+1)}} \sum_{p=0}^{n} \sum_{q=0}^{s} \frac{(-1)^{p+q}(n+1)!(s+1)!I_{v21}}{(n-p)!(1+p)!p!(s-q)!(1+q)!q!} \times \sum_{d=0}^{r} \sum_{f=0}^{r-1} \frac{(-1)^{d+f}!(d+f)!}{(d-f)!f!(f)!},
\]

(A.9)

and

\[
I_{v1} = \frac{1}{\sqrt{(n+1)(s+1)}} \sum_{d=0}^{r} \sum_{f=0}^{r-1} \frac{(-1)^{d+f}!(d+f)!}{(d-f)!f!(f)!} \times \sum_{d=0}^{r} \sum_{f=0}^{r-1} \frac{(-1)^{d+f}!(d+f)!}{(d-f)!f!(f)!},
\]

(A.10)

and

\[
I_{v21} = (p+q+1)! - e^{-\eta a} \sum_{k=0}^{p+q+1} \frac{(p+q+1)!(an)^{p+q+1-k}}{(p+q+1-k)},
\]

(A.11)

\[
I_{v22} = (d+f)! - e^{-\nu a/2} \sum_{g=0}^{d+f} \frac{(d+f)!}{(d+f-g)!} \frac{(-\nu a)^{d+f-g}}{2},
\]

(A.12)
\[ I_{11} = \sum_{k=0}^{d_f} \frac{(d_f + f)!}{(d_f + f - k)!} \times \left( e^{-\frac{a\nu}{2}} \left( \frac{a\nu}{2} \right)^{d_f + f - k} - e^{-\frac{(a+b)\nu}{2}} \left( \frac{(a+b)\nu}{2} \right)^{d_f + f - k} \right). \]  
\((A.13)\)

The matrix element of the magnetic field term reads
\[
\langle \psi_n | H_c | \psi_s \rangle = \frac{B^2}{8\mu^2 \eta^2 \sqrt{(n+1)(s+1)}} \times \sum_{p=0}^{n} \sum_{q=0}^{s} \frac{(-1)^{p+q} (n+1)! (s+1)! (p+q+3)!}{(n-p)! (1+p)! (s-q)! (1+q)! q!}.
\]  
\((A.14)\)

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