Research Article

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The problem of a hydrogen atom in a cavity: Oscillator representation solution versus analytic solution

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Abstract: A solution to the problem of a hydrogenic atom in a homogeneous dielectric medium with a concentric spherical cavity using the oscillator representation method (ORM) is presented. The results obtained by the ORM are compared with a known exact analytic solution. The energy levels of the hydrogenic atom in a spherical cavity exhibit a shallow-deep instability as a function of the cavity radius. The sharpness of the transition depends on the value of the dielectric constant of the medium. The results of the ORM agree well with the results obtained by the analytic solution when the shallow-deep transition is not too sharp (i.e., when the dielectric constant is not too large) for all values of the cavity radius. The ORM results in the zeroth order approximation diverge significantly in the region of the shallow-deep transition (i.e., for the values of the radius where the shallow-deep transition occurs) when the dielectric constant is high and as a result the transition is sharp. Even for the sharp transition, the ORM results again agree very well with the analytic results at least for the ground state when a commonly used approximation in the ORM is removed. The ORM methodology for the cavity model presented in this article can potentially be used for two-electron systems in a quantum dot.

Keywords: hydrogenic impurity cavity model, oscillator representation method, quantum dot, shallow-deep energy level transition

1 Introduction

We consider a hydrogen-like atom of nuclear charge e in a medium of dielectric constant ϵ with a concentric

spherical cavity of radius r_0 around the nucleus and free space dielectric constant ϵ_0 . The following potential represents such a system:

$$V(r) = \left[-\frac{e^2}{\epsilon_0 r} + \left(1 - \frac{\epsilon_0}{\epsilon} \right) \frac{e^2}{\epsilon_0 r_0} \right] \theta(r_0 - r) - \frac{e^2}{\epsilon r} \theta(r - r_0), \quad (1)$$

where $\theta(x)$ is the Heaviside function which is 0 for $x < 0$ and 1 for $x \geq 0$.

Chaudhuri and Coon [1] treated a more general version of this problem in which the effective mass of the electron is also different in the medium outside the cavity and provided an exact analytic solution. Von Roos [2] pointed out that the Hamiltonian with position-dependent mass is not Hermitian and hence should be abandoned. Still it has been widely and successfully used in semiconductor physics particularly in quantum well problems. Considerable interest and work on the position-dependent effective mass have continued (see ref. [3] and references therein). It is not clear how to treat the position-dependent effective mass in the oscillator representation method (ORM) and it is not so important for our purposes either. So we have not included the position-dependent effective mass in the problem treated in this article. It should also be noted that the second term in $V(r)$ was added [1] to ensure the continuity of the potential at r_0 although it is not an absolute requirement that the potential must be continuous. While this term makes the potential continuous, the electric field is still discontinuous.

It is clear from a simple inspection of the potential that in the limits of $r_0 \rightarrow \infty$ and $r_0 \rightarrow 0$, the energy levels are identical to those of a hydrogen atom in free space and in the medium of dielectric constant ϵ , respectively. Thus, the energy undergoes a transition from a shallow to a deep level in some range of r_0 as it increases from 0 to ∞ . The magnitude of the transition is proportional to ϵ^2 . As discussed in ref. [1], the reason for this transition is as

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follows. If the free space wavefunction, or more accurately the probability function, fits almost entirely inside the cavity, then the effect of the medium outside the cavity is small. If, on the other hand, the cavity size is such that significant portions of the free space wavefunction fall both inside and outside the cavity, then there is a competition to squeeze in and to stretch out the wavefunction by the two regions resulting in an intermediate energy value. The sharpness of the transition increases as the value of ϵ increases. This transition is akin to a second-order phase transition.

In Section 2, we reproduce the solution to the Schrödinger equation (SE) with the potential in equation (1) provided in ref. [1]. In Sections 3 and 4, we outline the general principles of the ORM developed by Dineykhani and Efimov [4] and present the results of the application of the ORM to the current problem, respectively. In Section 5, we compare and discuss the results obtained by the two methods for different parameters.

2 Cavity model: analytic solution

The SE with the potential given in equation (1) is spherically symmetric. Consequently, the wavefunction can be separated in spherical coordinates and written as¹

$$\Psi_{vlm} = N_{vlm} R_{vl}(r) Y_{lm}(\theta, \phi), \quad (2)$$

where N_{vlm} is the normalization constant, R_{vl} is the radial part of the wavefunction, and Y_{lm} s are the spherical harmonics. The radial part of the SE in dimensionless form is written as:

$$\left[\rho^* \frac{d^2}{d\rho^{*2}} + (2l + 2 - \rho^*) \frac{d}{d\rho^*} + (\nu^* - l - 1)\rho^* \right] \times u_{vl}(\rho^*) = 0 \quad \text{for } r < r_0, \quad (3a)$$

$$\left[\rho \frac{d^2}{d\rho^2} + (2l + 2 - \rho) \frac{d}{d\rho} + (\nu - l - 1)\rho \right] \times v_{vl}(\rho) = 0 \quad \text{for } r > r_0, \quad (3b)$$

¹ It should be noted that the hydrogen atom being a two-body problem, strictly speaking, the SE even with spherically symmetric potential is not separable into the center-of-mass and relative coordinates. The separation is possible only when the medium is completely homogenous and the medium in the cavity model is not. However, given the electron to the nucleus mass ratio is very small, considering the relative coordinate r as the electron radial coordinate would not introduce any appreciable error for all practical purposes.

where $\rho^* = 2r/(v^* a_B)$, $\rho = 2r\epsilon_0/(v\epsilon a_B)$, and $a_B = \frac{\epsilon_0 \hbar^2}{me^2}$ is the Bohr radius. The radial wavefunction $R(r)$ has been written in terms of u and v in the two regions

$$R(r) = \begin{cases} R_{<}(r) = Au_{vl}(\rho^*)^l \exp(-\rho^*/2) & \text{for } r < r_0 \\ R_{>}(r) = Bv_{vl}\rho^l \exp(-\rho/2) & \text{for } r > r_0. \end{cases} \quad (4)$$

The constants A and B are obtained by matching the wavefunctions at $r = r_0$ and from the normalization condition. The energy eigenvalue E is related to the effective principal quantum number ν by

$$E = -\frac{me^4}{\epsilon^2 \hbar^2} \frac{1}{2\nu^2}, \quad (5)$$

and ν^* is related to ν by

$$\frac{1}{2\nu^{*2}} = \left(\frac{\epsilon_0}{\epsilon}\right)^2 \frac{1}{2\nu^2} + \left(1 - \frac{\epsilon_0}{\epsilon}\right) \frac{a_B}{r_0}. \quad (6)$$

Equations 3(a) and 3(b) are confluent hypergeometric equations, each of which has two independent solutions. To obtain a physical solution, the solutions of equations 3(a) and 3(b) are selected so that they are regular at $r = 0$ and $r = \infty$, respectively. Chaudhuri et al. [1] provided the following energy eigenvalue condition² by matching the logarithmic derivative of the radial wavefunctions corresponding to the two selected solutions appropriate for the two regions:

$$\left[1 - \frac{-\nu + l + 1}{l + 1} \frac{\Phi(l + 2 - \nu^*, 2l + 3; \rho_0^*)}{\Phi(l + 1 - \nu^*, 2l + 2; \rho_0^*)} \right] + \frac{\nu^* \epsilon_0}{\nu \epsilon} \left[1 - \frac{2}{\rho_0} \frac{\Psi(-\nu - l - 1, -2l - 1; \rho_0)}{\Psi(-\nu - l, -2l; \rho_0)} \right] = 0. \quad (7)$$

The functions Φ and Ψ are confluent hypergeometric functions related to the confluent hypergeometric series ${}_1F_1$ and ${}_2F_0$, respectively. While the series representation of the function Φ (see equation (15) in ref. [1]) is convergent for all finite values of ρ^* , the series representation of Ψ has zero radius of convergence. However, an integral representation of Ψ (see equation (16) in ref. [1]) that satisfies the convergence requirements is used to calculate the function. The eigenvalues ν for a given value of the angular momentum quantum number l can be calculated by locating the zeroes of the expression in equation (7).

² It should be noted that there are two typographical errors in equation (20) in ref. [1]. The ν^* in the first bracket should be replaced by $-\nu^*$ and the $-$ sign between the two brackets should be changed to $+$.

3 ORM

Dineykhon and Efimov [4] developed the ORM arising from ideas and methods of the quantum field theory. Using the ORM they calculated the binding energies of a number of systems with various types of potentials including the Coulomb and power-law potentials, exponentially screened Coulomb potential, logarithmic potential [4,5], and a two-electron quantum dot in a magnetic field [6]. The ORM results for the Coulomb and power law, the exponentially screened Coulomb, and logarithmic potentials agree very well with the results obtained by variational numerical methods. Amin and El-Asser have applied the ORM to calculate the energy spectrum of hydrogen-like atoms in a van der Waals potential [7].

The first key step in the ORM is a transformation of the variables in the SE such that the wavefunction takes a Gaussian asymptotic form. Schrödinger in a paper [8] on solving eigenvalue problems by factorization pointed out the existence of such a transformation in which the Kepler problem is transformed into an oscillator problem in four dimensions. The modified SE in the new expanded space having the Gaussian asymptotic solution exhibit oscillator behavior at large distances.

In the next steps, the canonical variables (coordinate and momentum) in the transformed space are represented in terms of creation and annihilation operators $a^\dagger$ and a , and the Hamiltonian is written in terms of *normal ordered products* over $a^\dagger$ and a . The *normal order* operation (also known as Wick's transform) is an operation in which all the creation operators $a^\dagger$ are moved to the left and all the annihilation operators a are moved to the right. The *normal order* operation is frequently used in quantum field theory. Wick's transform $:q^n:$ yields the n th order Hermite polynomial in q which, of course, is the harmonic oscillator wavefunction apart from the exponential term. Wick's transform is in fact used in quantum field theory to eliminate infinity arising from the zero-point energy. See ref. [9] for an exposition on Wick's calculus. The pure oscillator part with some yet unknown frequency, ω , is extracted from the Hamiltonian written in the form $H = H_0 + H_I + \varepsilon_0$, where $H_0 = \omega a^\dagger a$. In addition, a requirement is imposed that the interaction part, H_I , does not contain terms quadratic in the canonical variables so that they are completely absorbed in the oscillator part. This requirement leads to the following condition:

$$\frac{\partial \varepsilon_0}{\partial \omega} = 0, \quad (8)$$

which determines ω , the oscillator frequency. This condition is known as the oscillator requirement condition (ORC).

Another interesting aspect of the ORM is that the dimension of the hyperspace can be a variational parameter and as a result can be non-integer. Even though an integer dimension is used to derive the energy equations, the dimension appears in the end results just as a parameter and thus can be varied to obtain the energy minimum.

Dineykhon and Efimov [4] used the following transformations that provide the Gaussian asymptotic wavefunction behavior:³

$$r = q^{2\rho}, \quad (9)$$

$$r\psi(r) = q^a\phi(q). \quad (10)$$

The radial part of the SE in the new variable q in the expanded space is then obtained as follows:

$$\left[-\frac{1}{2} \left(\frac{\partial^2}{\partial q^2} + \frac{d-1}{q} \frac{\partial}{\partial q} \right) + W_l(q; E) \right] \phi(q) = \varepsilon(E) \phi(q), \quad (11)$$

where

$$W_l(q; E) = -\frac{K(l, \rho, d)}{2q^2} + 4\rho^2(q^2)^{(2\rho-1)}(V(q^2) - E), \quad (12)$$

$$d = 2a - 2\rho + 2, \quad \text{and} \quad (13)$$

$$K(l, \rho, d) = \frac{1}{4}[(d-2)^2 - 4\rho^2(2l+1)^2]. \quad (14)$$

It should be noted here that d is the dimension of the hyperspace, the energy E is now incorporated in the new potential W_l , and $q^2 = q_i q_i$ summed over the repeated index i from 1 to the dimension d . As mentioned earlier, d is assumed to be an integer for the calculations of $\varepsilon_0, \varepsilon, W_l$, until at the end when ρ and d can be treated as non-integer variational parameters. We also note that the SE is written in dimensionless form by using the length unit as $\hbar^2/me^2$ and the energy unit as $me^4/\hbar^2$.

The energy spectrum E_{nl} of the original system is obtained from the radial excitation spectrum $\varepsilon^{[n_r]}$ of the Hamiltonian of equation (11)

$$H(E_{nl})\phi^{[n_r]}(q) = \varepsilon^{[n_r]}\phi^{[n_r]}(q), \quad (n_r = 0, 1, 2, \dots), \quad (15)$$

and it is determined by

$$\varepsilon^{[n_r]}(E_{nl}) = \varepsilon^{[n_r]}(l, \rho, d; E) = 0, \quad (16)$$

where n_r is the radial quantum number.

³ We should note that in the context of the ORM ρ is a parameter, while ρ was used as the scaled radius variable r in the analytic model section.

If the potential $V(r)$ does not have a repulsive character as $r_0 \rightarrow 0$, $K(l, \rho, d)$ is typically chosen to be zero and that leads to the equation for the dimension,

$$d = 4\rho l + 2\rho + 2. \quad (17)$$

The oscillator representation is then obtained by writing the Hamiltonian H in the form

$$H = \frac{1}{2}(p^2 + \omega^2 q^2) + \left(W_l(q) - \frac{1}{2}\omega^2 q^2 \right), \quad (18)$$

and by introducing the usual creation and annihilation operators, $a^\dagger$ and a , respectively, in terms of the canonical variables q_j and p_j ($j = 1, 2, \dots, d$), as:

$$q_j = \frac{1}{\sqrt{2\omega}}(a_j + a_j^\dagger), \quad p_j = \frac{1}{i}\sqrt{\frac{\omega}{2}}(a_j - a_j^\dagger). \quad (19)$$

The creation and annihilation operators satisfy the standard commutation relation

$$[a_j, a_k^\dagger] = \delta_{jk}, \quad j, k = 1, 2, \dots, d. \quad (20)$$

After normal ordering the products over $a^\dagger$ and a , in which all the creation operators are moved to the left and the annihilation operators are moved to the right as if they commute and some manipulation the ORM Hamiltonian is obtained as

$$H = H_0 + H_l + \varepsilon_0, \quad (21)$$

where

$$H_0 = \omega a_j^\dagger a_j, \quad (22)$$

$$H_l = \int_{-\infty}^{\infty} \left(\frac{dk}{2\pi} \right)^d \tilde{W}(k) \exp\left(\frac{-k^2}{4\omega} \right) : e_2^{(kq)} :, \quad \text{and} \quad (23)$$

$$\varepsilon_0 = \frac{d\omega}{4} + \int_{-\infty}^{\infty} \left(\frac{dk}{2\pi} \right)^d \tilde{W}(k) \exp\left(-\frac{k^2}{4\omega} \right). \quad (24)$$

As mentioned earlier, the symbol $:*$ represents the *normal ordering* of the products over $a^\dagger$ and a . In $kq = k_j q_j$ as well as in k^2 and q^2 summation over repeated indices are assumed and the notation $e_2^x = e^x - 1 - x - \frac{1}{2}x^2$ is introduced. The function $\tilde{W}$ is the Fourier transform of $W(q)$ in d -dimension and given as

$$\tilde{W}(k) = \int_{-\infty}^{\infty} (d\xi)^d W_l(\xi) \exp(ik\xi), \quad k\xi = k_j \xi_j. \quad (25)$$

The energy spectrum is then obtained by calculating the contribution of the interaction part H_l of the Hamiltonian in the perturbation approach. In the zeroth

order approximation, the energy spectrum is determined by

$$2n_r \omega + \langle n_r | H_l | n_r \rangle + \varepsilon_0 = 0. \quad (26)$$

See ref. [4] for the details of the calculation of the radial eigenstates $|n_r\rangle$ and the matrix elements $\langle n_r | H_l | n_r \rangle$. In this article, we will consider only the zeroth order approximation in H_l .

4 Cavity model: ORM solution

In this section, we will apply the ORM to the cavity model defined by the potential in equation (1). We note that the calculation of the energy spectrum using the wavefunction matching method is a natural one when the potential is discontinuous. However, to apply the ORM to the cavity model it may be useful for the calculations of various terms to write the potential in a continuous form as follows:

$$V(r) = -\frac{1}{r} - \frac{(B-1)}{r_0} \theta(r_0 - r) - \frac{(B-1)}{r} \theta(r - r_0), \quad (27)$$

$$\theta(x) = P(\tau) e^{-ix\tau} = \lim_{\sigma \rightarrow 0^+} \int_{-\infty}^{+\infty} \frac{e^{-ix\tau}}{\tau + i\sigma} d\tau, \quad (28)$$

where $B = (\epsilon_0/\epsilon)$. The second and the third terms can be treated as exponential and screened Coulomb potentials, respectively, with complex exponentials by using equation (28) for the Heaviside function. The final results are obtained by applying the operation $P(\tau)$ over the functions of $(i\tau)$.

Now we make the typical approximation in which there is no repulsive character in the potential by setting $K(l, \rho, d) = 0$ and then d is given by equation (17). With this approximation, we obtain after some manipulations the pertinent ORM equations for the cavity model potential given in equation (27):

$$\begin{aligned} \varepsilon_0 = & a_0 \omega - \frac{4E\rho^2}{\omega^{2\rho-1}} \frac{\Gamma\left(\frac{d}{2} + 2\rho - 1\right)}{\Gamma\left(\frac{d}{2}\right)} - \frac{a_1}{\omega^{\rho-1}} \\ & - \frac{a_2}{\omega^{2\rho-1}} \gamma_l \left(\frac{d}{2} + 2\rho - 1, \omega r_0^{\frac{1}{\rho}} \right) \\ & - \frac{a_3}{\omega^{\rho-1}} \gamma_u \left(\frac{d}{2} + \rho - 1, \omega r_0^{1/\rho} \right), \end{aligned} \quad (29)$$

$$\begin{aligned} \langle n_r | H_l | n_r \rangle = & -a_1 \frac{BT(\rho-1)}{\omega^{\rho-1}} - \frac{4E\rho^2}{\omega^{2\rho-1}} \Gamma(d/2 + 2\rho - 1) \\ & \times T(2\rho - 1) - a_4 T_{12}(\rho), \end{aligned} \quad (30)$$

where

$$a_0 = \frac{d}{4}, \quad a_1 = \frac{4\rho^2\Gamma(d/2 + \rho - 1)}{\Gamma(d/2)}, \quad a_2 = \frac{4(B-1)\rho^2\Gamma(d/2 + 2\rho - 1)}{r_0\Gamma(d/2)}, \quad a_3 = \frac{4(B-1)\rho^2\Gamma(d/2 + \rho - 1)}{\Gamma(d/2)}, \quad \text{and} \quad (31a)$$

$$a_4 = \frac{4(B-1)\rho^2}{\Gamma(d/2)}$$

$$T(x) = \frac{\Gamma(d/2)\Gamma(n_r + 1)}{\Gamma(d/2 + n_r)} \left[\frac{x(x-1)\Gamma(d/2 + n_r + 1)\theta(n_r - 1)}{\Gamma(d/2 + 2)\Gamma^3(n_r)} + \sum_{t=2}^{n_r} \sum_{p=t}^{2t} 2^{2t-p} \cdot (x)_p \cdot (p)_t \cdot (t)_{2t-p} \right. \\ \left. \times \frac{\Gamma(d/2 + p + n_r - t)}{\Gamma(p+1)\Gamma(t+1)\Gamma(d/2 + p)\Gamma^3(n_r - t + 1)\Gamma(p-t+1)\Gamma(2t-p+1)} \right]; \quad (31b)$$

$$(x)_p = x(x-1)(x-2)\dots(x-p+1); \quad (31c)$$

$$T_{12}(\rho) = -\frac{\rho(\omega r_0^{1/\rho})^{d/2+\rho-1}}{\omega^{\rho-1}} \times \sum_{k=0}^{\infty} (-1)^k \frac{(\omega r_0^{1/\rho})^k T(-d/2-k)}{(d/2+2\rho-1+k)(d/2+\rho-1+k)\Gamma(k+1)}; \quad (31d)$$

and γ_l and γ_u are incomplete gamma functions defined as

$$\gamma_l(a, x) = \frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t} dt, \quad \gamma_u(a, x) = \frac{1}{\Gamma(a)} \int_x^{\infty} t^{a-1} e^{-t} dt. \quad (31e)$$

In order to obtain the energy spectrum we use the ORC in equation (8) with ε_0 and $\langle n_r | H_I | n_r \rangle$ given in equations (29) and (30). We solve the ORC equation for E and plug in the expression for E in equations (26) and (30) to obtain the equation for ω as follows:

$$\left[\left(1 + \frac{T(2\rho-1)}{2\rho} \right) a_0 + \frac{n_r(2\rho-1)}{\rho} \right] \omega \\ - \left[\frac{a_1}{2} \left(1 + \frac{B(2\rho-1)}{\rho} T(\rho-1) - \frac{(\rho-1)}{\rho} T(2\rho-1) \right) \right. \\ \left. + \frac{a_3}{2} \gamma_u(d/2 + \rho - 1, \omega r_0^{1/\rho}) \left(1 - \frac{(\rho-1)}{\rho} T(2\rho-1) \right) \right] \omega^{1-\rho} \\ + \frac{a_2(2\rho-1)}{2\rho} \gamma_l(d/2 + 2\rho - 1, \omega r_0^{1/\rho}) T(2\rho-1) \omega^{1-2\rho} \\ - \frac{a_4(2\rho-1)}{2\rho} T_{12}(\rho) = 0. \quad (32)$$

With a solution for ω obtained from equation (32) the energy spectrum E is then obtained from equations (8) and (30) as

$$E(n_r, l; \rho) = -\frac{\Gamma(d/2)\omega^{2\rho}}{4\rho^2(2\rho-1)\Gamma(d/2+2\rho-1)} \\ \times [a_0 + a_1(\rho-1)\omega^{-\rho} + a_2(2\rho-1)\gamma_l(d/2+2\rho-1, \omega r_0^{1/\rho})\omega^{-2\rho} \\ + a_3(\rho-1)\gamma_u(d/2+\rho-1, \omega r_0^{1/\rho})\omega^{-\rho}]. \quad (33)$$

The energy spectrum given by equation (33) is still a function of the parameter ρ . The energy spectrum $E(n_r, l)$ is obtained by minimizing $E(n_r, l; \rho)$ with respect to ρ as

$$E(n_r, l) = E(n_r, l; \rho_{\min}) = \min_{\rho} E(n_r, l; \rho), \quad (34)$$

in which ω for a given value of ρ is determined by finding the solution to equation (32).

An inspection of equations (31b) and (31d) indicates that $T(0) = T(1) = T_{12} = 0$ for $n_r = 0$ states (i.e., 1s, 2p, 3d...). Therefore, there is no contribution from the interaction part of the Hamiltonian, H_I , for these states.

In the limiting case of $B = 1$, the solution of equation (32) yields $\omega = 2/n$, where $n = n_r + l + 1$ is the principal quantum number, and the energy spectrum appropriately reduces to that of a free space hydrogen atom, $E(n_r, l) = -\left(\frac{1}{2n^2}\right)$. In the limiting case of $r_0 \rightarrow 0$, $\omega = 2B/n$, and the energy spectrum correctly reduces to that of a hydrogen atom in a medium of dielectric constant ϵ , i.e., $E(n_r, l) = -\left(\frac{B^2}{2n^2}\right)$. In the limiting case of $r_0 \rightarrow \infty$, it can be shown that $T(0) = T(1) = T_{12} = 0$ as the parameter ρ tends to 1 and the energy spectrum reduces to that of the free space hydrogen atom.

In some situations, fixing the parameter ρ to a value 1 may be sufficient. Noting that $T(0) = T(1) = 0$ when $\rho = 1$, equations (32) and (33) reduce to the simpler forms:

$$\omega - \frac{2}{n} - \frac{2}{n} [\gamma_l(2l+2, r_0\omega) + B\gamma_u(2l+2, r_0\omega)] \\ - \frac{2}{n} \frac{(B-1)}{\Gamma(2l+2)} T_{12}(1) = 0, \quad (35)$$

$$E_{nl} = -\frac{\omega^2}{8} \left[1 + \frac{8(B-1)}{r_0\omega^2} \gamma_l(2l+3, r_0\omega) \right], \quad \text{and} \quad (36)$$

$$T_{12}(1) = -(\omega r_0)^{2l+2} \sum_{k=0}^{\infty} (-1)^k \times \frac{(\omega r_0)^k T(-2l-2-k)}{(2l+3+k)(2l+2+k)\Gamma(k+1)}. \quad (37)$$

As mentioned earlier, $T_{12} = 0$ for $n_r = 0$ states (i.e., 1s, 2p, 3d...).

5 Results and discussion

First, we consider the ground state, i.e., the 1s state for which $n = 1$, $n_r = 0$, and $l = 0$. In Figure 1(a–d), we have plotted ν as a function of r_0 for a set of parameters B (0.088, 0.25, 0.5, and 0.75) obtained by the two methods presented earlier for the 1s state. For the ORM, we have computed the values of E_{1s} for the $\rho = 1$ case by using equations (35–37). As noted earlier, $T(\rho) = T(2\rho - 1) = T_{12}(\rho) = 0$ even when $\rho \neq 1$ for the 1s state. The values of ν are then obtained by using equation (5). We have computed the values of ν for the analytic solution directly by solving equation (7) for ν . The value of $B = 0.088$ corresponds to silicon for which the dielectric constant $\epsilon = 11.4\epsilon_0$.

As seen from the analytic results the shallow to deep transition of the energy level occurs near $r_0 = 1$, where the wavefunction is maximum. Evidently, the ORM results agree very well with the analytic results for all values of r_0 when the dielectric constant of the medium outside the cavity does not differ significantly from that of the free space cavity. However, the ORM results diverge significantly in the neighborhood of r_0 where the energy level undergoes shallow to deep transition when the dielectric constant of the medium outside the cavity differs significantly from that of the free space cavity. For the realistic case of silicon ($B = 0.088$) the disagreement is stark.

Now in order to eliminate the $\rho = 1$ restriction we computed the 1s energy level $E_{1s}(\rho_{\min})$ by finding the minima of the energy with respect to ρ following equations (32), (33), and (34). The dashed line in Figure 2 represents $E_{1s}(\rho_{\min})$ as a function of r_0 . The value of $\rho_{\min}$ was found to vary between 1 and 2.14. As expected, the values of $\rho_{\min}$ differ from 1 only in the transition region. With the minimization of the energy with respect to the parameter ρ , or equivalently, the dimension d , the ORM results agree very well with the exact analytic results including in the transition region even for the case of sharp transition ($B = 0.088$).

For all states for which $n_r = 0$ that includes the ground state (1s), the contribution from the interaction

Figure 1: Principal quantum number ν for the 1s state as a function of r_0 with $\rho = 1$ for four values of (a) $B = 0.088$, (b) 0.25, (c) 0.5, and (d) 0.75. The upper and lower dashed lines represent the values of ν for $r_0 = 0$ and $r_0 = \infty$, which are 1.0 and $B = (\epsilon_0/\epsilon)$, respectively.

part $\langle n_r | H_I | n_r \rangle$ is zero since $T(x) = T_{12} = 0$. The first state for which the contribution from the interaction part is

Figure 2: Principal quantum number ν for the 1s state for $B = 0.088$ with varying parameter ρ . The dash-dotted line represents the results with $\rho = 1$ presented earlier. The dashed curve represents the results with $\rho = \rho_{\min}$ that minimizes the energy. The upper and lower dashed lines represent the values of ν for $r_0 = 0$ and $r_0 = \infty$, which are 1.0 and $B = (\epsilon_0/\epsilon)$, respectively.

non-zero is the 2s state. We present the results in Figure 3(a and b) for the values of $B = 0.088$ and 0.5.

The solid lines in Figure 3(a and b) represent the analytic results. The 2s radial probability function has two lobes with maxima at $r = 0.76$ and at $r = 5.24$. Consequently, there are two sharp transitions close to these two values of r_0 with a plateau in between.

The ORM results with $\rho = 1$ diverge widely in the transition region for the 2s state. So we have shown the ORM results only with $\rho = \rho_{\min}$ that minimizes the energy. The value of $\rho_{\min}$ was found to vary between 1 and 2.45 (i.e., $d = 4$ to 6.9) for $B = 0.088$ and from 1 to 1.28 (i.e., $d = 4$ to 4.56) for $B = 0.5$. Even with the minimization with respect to ρ , the ORM result for the sharp transition case ($B = 0.088$) differs significantly from the analytic result in the transition region. The origin of the discrepancy for this case can be attributed to the extremely shallow zero-crossing of the ω function given in equation (32), where the value of the ω function remains very close to zero for a wide range of ω values. A small change in the ω function would move the zero-crossing from the left to the right of the wide shallow region of ω . A small error in the ω function thus would change the calculated energy significantly. This indicates that higher order perturbation terms in the interaction part may be necessary to obtain better ORM results for sharp transition cases for states with $n_r \geq 1$.

From this analysis, it appears that at least for the ground state in which there is no contribution from the interaction part of the Hamiltonian, H_I , the ORM provides excellent results when the energy is minimized with respect to the parameter, ρ . On the other hand, for states

Figure 3: Principal quantum number ν for the 2s state for two values of $B = 0.088$ and 0.5. The solid lines in (a) and (b) represent the analytic results and the dashed curves represent the ORM results with $\rho = \rho_{\min}$ that minimizes the energy. The upper and lower dashed lines represent the values of ν for $r_0 = 0$ and $r_0 = \infty$, which are 2.0 and $B = 2(\epsilon_0/\epsilon)$, respectively.

where the interaction part is non-zero, such as the 2s state, the ORM results are not so accurate in the transition region when the transition is sharp. It appears that for these cases higher order perturbation terms in the interaction contribution are necessary for more accurate results.

Dineykhani and Nazmitdinov [6] provided analytical results for a two-electron quantum dot in a magnetic field

with a harmonic oscillator potential for the quantum dot using the ORM. The problem of a quantum dot in a magnetic field was treated using numerical method [10,11] and analytical method with some approximations [12]. A singlet to triplet state transition was predicted for the ground state in a quantum dot as a function of the applied magnetic field. These transitions were experimentally observed by Ashoori et al. [13]. The harmonic oscillator potential has been used [10,11,13] to represent the confining potential in a quantum dot. However, a quantum dot having a finite size, a finite potential should provide a better model. Ashoori et al. conjectured that the discrepancy of their experimental values of the magnetic fields at which the singlet to triplet transition occurs with the theoretical values to the strictly harmonic confining potentials used in the theoretical calculations. Recently, Chaudhuri [14] obtained analytic expressions for the energy levels of a 2-electron system in a 2-dimensional quantum dot modeled with a finite Gaussian potential and subjected to a magnetic field using an ORM approach like the one presented in this article. In the appropriate limits, the results are shown to match very well with previous analytical and numerical results. Using the expressions, the magnetic field at which the spin-singlet to spin-triplet ground state crossing occurs is calculated. The calculated value is closer to the experimental value compared with the infinite harmonic potential results in previous theoretical models.

References

- [1] Chaudhuri S, Coon DD. Analytic solution of the cavity model for interstitial impurities in semiconductors. *Phys Rev B*. 1984;30:3338–43.
- [2] von Roos O. Position-dependent effective masses in semiconductor theory. *Phys Rev B*. 1983;27:7547–52.
- [3] Abdalla MS, Eleuch H. *AIP Adv*. 2016;6(055011):1.
- [4] Dineykhon M, Efimov GV. *Rep Math Phys*. 1995;36:287.
- [5] Dineykhon M, Efimov GV. The oscillator representation and the stability of three-body Coulomb systems. *Few-Body Syst*. 1994;16:59–90.
- [6] Dineykhon M, Nazmitdinov RG. Two-electron quantum dot in a magnetic field: analytical results. *Phys. Rev B*. 1997;55(20):13707–14.
- [7] Amin ME, El-Asser MA. An analytical treatment of the energy spectrum of hydrogen-like atoms perturbed by a generalized van der Waals potential. *Braz J Phys*. 2009;39(2):301–5.
- [8] Schrödinger E. *Proc R Irish Acad*. 1941;46:183.
- [9] Wurm A, Berg M. Wick calculus. *Am J Phys*. 2008;76(1):65–72.
- [10] Maksym PA, Chakrabarty T. Quantum dots in a magnetic field: role of electron-electron interactions. *Phys Rev Lett*. 1990;65:108–11.
- [11] Wagner M, Merkt U, Chaplik AV. Spin-singlet–spin-triplet oscillations in quantum dots. *Phys Rev B*. 1992;45:1951–4.
- [12] Taut M. Two electrons in a homogeneous magnetic field: particular analytical solutions. *J Phys A*. 1994;27:1045–55.
- [13] Ashoori RC, Stormer HL, Weiner JSPLN, Baldwin KW, West KW. N-electron ground state energies of a quantum dot in magnetic field. *Phys Rev Lett*. 1993;71:613–6.
- [14] Chaudhuri S. Two-electron quantum dot in a magnetic field: Analytic solution for finite potential model. *Phys E Low Dimens Syst Nanostruct*. 2021;128:114571.