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Asymptotic Iteration Method in Single and Multilayered Quantum Dots

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Abstract:

The asymptotic iteration method (AIM) has been applied to calculate the ground state and binding energy of an impurity located at the center of a single and multilayered spherical quantum dot.Regarding the single quantum dot (QD) the results obtained for the ground state energy and for the first approximation of the binding energy agree entirely with the results of the ordinary perturbation technique obtained in earlier treatments.

Besides, the second approximation of the binding energy differs by about 16.5 % in both treatments which is quite reasonable.

The results obtained in the case of multilayered spherical quantum dot (MSQD) showed a reasonable quantitative agreement with the results obtained in an earlier treatment by applying an entire numerical technique. They are also distinguished by exhibiting a peak similar to the results obtained before by applying the variational method in analogous problems.

Keywords: Asymptotic iteration method, Single and multilayered quantum dots, Parabolic confining potential, Central impurity, Ground energy state.

1. Introduction

The exact solutions of the Schrödinger equation can be derived for very few problems of specific forms of confining potential. In most of the cases approximate analytical and numerical techniques have to be applied to obtain the solution. The well known approximate techniques are the first and second order perturbation theory, the strong perturbation technique and the variational method. Also, the asymptotic iteration method has been applied more recently.

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The perturbation technique has been employed by Bose [1], Xie [2] and Yuan and Liu [3] to determine an electron binding energy in a spherical quantum dot with a parabolic confining potential. On the other hand, the variational method has been applied with different forms of the trial wave function. Zhu and Chen [4] used a trial wave function in the form of linear expansion where the coefficients have been taken as the variational parameters. Alternative forms for the trial wave functions were employed in Wang and Yang [5], Merchancano et al [6] and Mikhail and Ismail [7]. Mikhail and El Sayed [8, 9] have derived analytical expressions for the energy expectation value and for the binding energy of central and off - central impurities.

The strong perturbation technique was introduced originally by Jiang [10] and was applied for the calculation of the binding energy of a central impurity in a quantum dot by Kassim [11]. Mikhail and Ismail [12] investigated the variational and strong perturbation techniques and showed that the variational method leads to better results and is accordingly more powerful.

The asymptotic iteration method (AIM) deals with a more complicated confining potential that consists of three terms. The first term represents the coulomb potential due to a central impurity, the second term stands for a linear potential while the third term represents the parabolic confining potential which is the familiar term used in most of the previous studies. The method was originally introduced by Ciftci et al [13], [14], [15] and was applied by Barkat [16]. More recent applications have been performed by Ismail, Saad and his coworkers [17, 18, 19, 20, 21].

Also, it may be worthwhile pointing out that the asymptotic iteration method can be applied in many other branches of applied mathematics and theoretical physics such as quantum optics (Makram-Allah et al [22]) and stability of dynamical systems (Hamza et al [23]).

The aim of the present work is to investigate further the asymptotic iteration method (AIM) to calculate the ground state and binding energy of an impurity located at the center of a single and multilayered spherical quantum dots. In section 2 a comparison has been made between the results of the perturbation and asymptotic iteration methods. The results of the ground state energy and the first perturbation obtained from the two methods agree entirely while the results of the second approximation differ by about 16.5 % which is a very reasonable result. Moreover, the

result obtained by using the asymptotic iteration method is the lower one. This indicates that it is much nearer to the exact negative result since it represents a better lower bound.

In section 3 the asymptotic expansion method has been applied to obtain the solution of the Schrödinger equation in the dot regions of a multilayered spherical structure where the confining potential has been taken in complicated parabolic forms.

Section 4 has been devoted to perform a comparison between the results obtained in the present work and the result of the entirely numerical technique used in Akgül et al [24]. The comparison indicated that the present results are very reasonable. They are distinguished by exhibiting a peak similar to the results obtained before by applying a variational method in analogous problems (Mikhail and Ismail [7, 25] and Mikhail and El Sayed [8, 9]).

2. Asymptotic Iteration Method

In this section we deal with the asymptotic iteration method (AIM) which was originally introduced by Ciftci et al ([13], [14], [15]) and was applied in Barakat [16] to find a solution for the Schrödinger equation with potential

$$V(r) = -\frac{Z}{r} + g\,r + \lambda\,r^2 \ , \tag{1}$$

where g, Z, λ are arbitrary and r is the electron position vector. The Schrödinger equation in spherical polar coordinates is given

$$\frac{sin^2\theta}{R}\,\frac{d}{dr}\,r^2\,\frac{d\,R}{d\,r} + \frac{sin\,\theta}{\Theta}\,\frac{d}{d\theta}\,sin\,\theta\,\frac{d\Theta}{d\theta} + \frac{1}{\phi}\,\frac{d^2\phi}{d\,\varphi^2} - \frac{2\,m^*\,r^2 sin^2\theta}{\hbar^2}\,(V(r) - E) = 0. \tag{2}$$

If we further take,

$$R = \frac{x}{r}, \tag{3}$$

and substitute in Eq. (2) it can be shown after using the Rydberg and Bohr radius units that

$$-\frac{d^2x}{dr^2} + \frac{1}{r^2}\,\ell(\ell+1)x + V\,x = E\,x. \tag{4}$$

The transformations

$$r = u^2\ ,\ x = \phi(u)e^{-P(u)/2}\ ,\quad \grave{P}\ (u) = \frac{-1}{u}, \tag{5}$$

leads, in turn to

$$\frac{d^2\phi}{du^2} - \left[\frac{\grave{\ell}\,(\grave{\ell}+1)}{u^2} + 4\,gu^4 + 4\,\lambda u^6 - 4\,Z - 4\,E\,u^2\right]\phi = 0\,, \tag{6}$$

where

$$\grave{\ell}\,(\grave{\ell}+1) = 4\,\ell(\ell+1) + \frac{3}{4}\,. \tag{7}$$

Finally, $\phi(u)$ can be changed to *f(u)* by using the transformation

$$\phi(u) = u^{\grave{\ell}+1}\,e^{-\alpha u^4/4}\,f(u)\,,\alpha^2 = 4\,\lambda\ . \tag{8}$$

It can consequently be shown after some manipulations that

$$\grave{\hat{f}} = \lambda_0\,\grave{f} + S_0 f\,, \tag{9}$$

where,

$$\lambda_0 = 2\left(\alpha\,u^3 - \frac{\grave{\ell}+1}{u}\right), \tag{10 a}$$

$$S_0 = \left(-\,\varepsilon_{n\ell}\,u^2 + 4\,\tilde{\gamma}(g\,u^4 - Z)\right), \tag{10 b}$$

$$\varepsilon_{n\ell} = 4\,E - \left(2\,\grave{\ell} + 5\right)\alpha\,. \tag{10 c}$$

In Eq. (10 b) $\tilde{\gamma}$ is artificially introduced perturbation expansion parameter to be equal to 1 at the end of the calculation.

Now, within the framework of AIM (Refs. [13], [14], [15]) we apply a mathematical induction procedure to prove by successively differentiating Eq. (9) that

$$\mathrm{f}^{(\mathrm{n}+2)} = \lambda_n(u)\,\grave{f} + S_n(u)f\ \ , n = 0,1,2,\ldots \tag{11}$$

where

$$\lambda_n = \grave{\lambda}_{n-1} + S_{n-1} + \lambda_0\lambda_{n-1}\ \ , \tag{12 a}$$

and

$$S_n = \lambda_{n-1}S_0 + \grave{S}_{n-1}\,. \tag{12 b}$$

It then, follows from Eqs. (11), (12 a, b) that

$$\frac{d}{du}\ln f^{(n+1)} = \frac{f^{(n+2)}}{f^{(n+1)}} = \frac{\lambda_n(\grave{f}+\frac{S_n}{\lambda_n}f)}{\lambda_{n-1}\left(\grave{f}+\frac{S_{n-1}}{\lambda_{n-1}}f\right)} . \quad (13)$$

We now introduce the "asymptotic" aspect of the method that implies for some $n\rangle 0$

$$\frac{S_n}{\lambda_n} = \frac{S_{n-1}}{\lambda_{n-1}} = \rho(u,\tilde{\gamma}) . \quad (14)$$

Substitution from Eq. (14) in Eq. (13) gives

$$\frac{d}{du}\ln(f^{(n+1)}) = \frac{\lambda_n(\grave{f}+\rho f)}{\lambda_{n-1}(\grave{f}+\rho f)} = \frac{\lambda_n}{\lambda_{n-1}}, \quad (15)$$

which yields

$$f^{(n+1)}(u) = C_1 \exp[\int^u(\frac{\grave{\lambda}_{n-1}(t)}{\lambda_{n-1}(t)} + \frac{S_{n-1}(t)}{\lambda_{n-1}(t)} + \lambda_0(t))dt]$$

$$= C_1\lambda_{n-1}(u)exp(\int^u(\rho+\lambda_0)dt) . \quad (16)$$

We then replace n by (n+1) in Eq. (16) and use Eqs. (11), (14) to find

$$\grave{f} + \rho f = C_1 \exp(\int^u(\rho+\lambda_0)dt) , \quad (17)$$

The basic achievement of the previous calculations is the replacement of the second order differential equation (9) by the first order linear differential equation (17). The latter can then be solved by multiplying both sides of the equation by an integrating factor $e^{\int^u \rho\, dt}$. It can be shown that

$$\frac{d}{dt}(f(u)\, e^{\int^u \rho(t,\tilde{\gamma})dt}) = Q(u)\, e^{\int^u \rho(t,\tilde{\gamma})dt} , \quad (18)$$

where

$$Q(u) = C_1 \exp(\int^u(\rho+\lambda_0)dt) . \quad (19)$$

Thus by integrating Eq. (18) with respect to *u* we find

$$f(u) = \exp\left(-\int^u \rho\, dt\right)\left[C_2 + C_1\int^u \exp(\int^t\left(\lambda_0(\tau)+2\rho(\tau)\right)d\tau)\, dt\right]. \quad (20)$$

Moreover, in the AIM (asymptotic iteration method) we define

$$\delta_k(u,\tilde{\gamma}) \equiv S_{\mathrm{k}}\lambda_{\mathrm{k+1}} - S_{\mathrm{k+1}}\lambda_{\mathrm{k}} \equiv 0\ . \tag{21}$$

If we expand $\delta_k(u,\tilde{\gamma})$ around $\tilde{\gamma}=0$ we get the following series

$$\delta_k(u,\tilde{\gamma}) = \delta_k(u,0) + \frac{\tilde{\gamma}}{1!}\frac{\partial\delta_k(u,\tilde{\gamma})}{\partial\tilde{\gamma}}\Big|_{\tilde{\gamma}=0} + \frac{\tilde{\gamma}^2}{2!}\frac{\partial^2\delta_k}{\partial\tilde{\gamma}^2}\Big|_{\tilde{\gamma}=0} + \frac{\tilde{\gamma}^3}{3!}\frac{\partial^3\delta_k}{\partial\tilde{\gamma}^3}\Big|_{\tilde{\gamma}=0} + \cdots . \tag{22}$$

According to the procedure of AIM, $\delta_k(u,\tilde{\gamma})$must be zero; if this to be true for every $\tilde{\gamma}$ value, then every term of the series must be zero. That is to say

$$\delta_k^{(j)}(u,\tilde{\gamma}) = \frac{\tilde{\gamma}^j}{j!}\frac{\partial^j\delta(u,\tilde{\gamma})}{\partial\tilde{\gamma}^j}\Big|_{\tilde{\gamma}=0} = 0\ , \quad j = 0,1,2,\ldots\ . \tag{23}$$

Up to this point, it is also convenient to expand $\varepsilon_{n\ell}$,

$$\varepsilon_{n\ell} = \varepsilon_{n\ell}^{(0)} + \tilde{\gamma}\varepsilon_{n\ell}^{(1)} + \tilde{\gamma}^2\varepsilon_{n\ell}^{(2)} + \tilde{\gamma}^3\varepsilon_{n\ell}^{(3)} + \tilde{\gamma}^4\varepsilon_{n\ell}^{(4)} + \cdots . \tag{24}$$

A quantitative estimate for $\varepsilon_{n\ell}$ expansion terms can be obtained by comparing the terms with the same order of $\tilde{\gamma}$ in Eqs. (22) and (24). Therefore, it is clear that the roots of $\delta_k^{(0)}(u,\gamma)=0$ give us the leading contribution energy terms $\varepsilon_{n\ell}^{(0)}$. Likewise, the roots of $\delta_k^{(1)}(u,\gamma)=0$ gives us the first correction terms to $\varepsilon_{n\ell}^{(1)}$and so on. Accordingly, the general solution for the eigenenergies $E_{n\ell}$in conjunction with Eq.(10 c) is

$$E_{n\ell} = \frac{1}{4}\Big(\big(2\grave{\ell}+5\big)\alpha + \varepsilon_{n\ell}^{(0)} + \tilde{\gamma}\varepsilon_{n\ell}^{(1)} + \tilde{\gamma}^2\varepsilon_{n\ell}^{(2)} + \tilde{\gamma}^3\varepsilon_{n\ell}^{(3)} + \tilde{\gamma}^4\varepsilon_{n\ell}^{(4)} + \cdots\Big). \tag{25}$$

To obtain the leading energy term $\varepsilon_{n\ell}^{(0)}$, one should simply switch off $\tilde{\gamma}$ in Eq. (9), which will lead to an exactly solvable eigenvalue problem within the framework of AIM

$$\grave{f}(u) = 2\left(\alpha u^3 - \frac{(\grave{\ell}+1)}{u}\right)\grave{f}(u) - \varepsilon_{n\ell}\,u^2\,f_{n\ell}(u) \quad . \tag{26}$$

In general the choice of u is critical to speed the convergence of the method. Thus following Barakat [16] we choose $u_c = (\frac{\grave{\ell}+1}{\alpha})^{1/4}$. This implies that the function $\frac{\phi(u)}{f(u)} = u^{\grave{\ell}+1}\,e^{-\alpha u^4/4}$ in Eq. (8) is extremum. Moreover $\lambda_0 = 0\ at\ u = u_c$

A mathematica programme has been prepared to calculate $\delta_k^{(0,1,2)}(u,\tilde{\gamma})$ up to a sufficiently high accuracy. The three equations

$$\delta_k^{(0,1,2)}(u_c,0)=0\,, \tag{27}$$

have then been solved for

$$\lambda=\frac{1}{2}\frac{m^*{\omega_0}^2{a^*}^2}{R^*}=\gamma^2,\ \ Z=2,\ g=0\ . \tag{28}$$

It has been found that

$$\varepsilon^{(0)}=0\,,\quad \varepsilon^{(1)}=-7.449\,,\quad \varepsilon^{(2)}=-1.247\,. \tag{29}$$

The above results lead to

$$E^{(0)}=\frac{1}{4}\big(2\grave{\ell}+5\big)\alpha,\quad E^{(1)}=\frac{\varepsilon^{(1)}}{4}=-1.8622\,,\quad E^{(2)}=\frac{\varepsilon^{(2)}}{4}=-0.3117 \tag{30}$$

Moreover, it follows from Eqs. (7), (8) that

$$\ell=0,\quad \grave{\ell}=\frac{1}{2}\,,\quad \alpha=2\sqrt{\lambda}=2\gamma, \tag{31}$$

the first of Eq. (32) together with Eq. (33) give

$$E^{(0)}=3\gamma=2.0427\,. \tag{32}$$

The results obtained in (30), (32) for $E^{(0)}$, $E^{(1)}$agree entirely with those found by applying the ordinary time independent perturbation theory. This theory also implies that the second approximation $E^{(2)}=-0.2601$. Thus, the value of $E^{(2)}$given in Eq. (30) differs from this value by about 16.5 %.

3. A Detailed Investigation of a Multilayered Spherical Quantum Dot with a Parabolic Confinement

In this section we reconsider the problem of multilayered spherical quantum dot with a parabolic confining potential in the core and well layers which was originally introduced in Akgűl et al [24]. The investigation is performed in the absence and presence of impurity. An analytical approach is applied to obtain the solution unlike Akgűl et al [24] where the solution was retrieved

entirely by utilizing a numerical treatment that depends on the shooting and finite difference methods.

The confining potential in the different regions of the multilayered structure is given by

$$V_n(r) = \begin{cases} \frac{V_0}{{R_1}^2} r^2 & ,0 < r < R_1 \quad , \\ V_0 & ,R_1 < r < R_2 \quad , \\ \frac{V_0}{(R_2 - a)^2}(r-a)^2 & ,R_2 < r < R_3 \quad , \\ V_0 & , \quad r > R_3 \quad , \end{cases} \tag{33}$$

where $a = (R_2 + R_3)/2$. Also, the coulomb potential due to a central impurity is defined by

$$V_c = \frac{-e^2}{4\pi\varepsilon r} = \frac{-2}{r} . \tag{34}$$

The second result is defined in the Rydberg and Bohr radius units.

In the case of spherical symmetry the eigenfunctions of the Schrödinger equation can be expressed as $\psi(r,\theta,\phi) = C\, Y_{\ell m}(\theta,\phi) R(r)$, where $R(r)$ is the solution of the radial Schrödinger equation that is given in Rydberg and Bohr radius units by

$$\left[\frac{\mathrm{d}^2}{\mathrm{dr}^2} + \frac{2}{\mathrm{r}}\frac{\mathrm{d}}{\mathrm{dr}} - \frac{\ell(\ell+1)}{\mathrm{r}^2}\right] \mathrm{R} = -(\mathrm{E} - \mathrm{V})\mathrm{R} , \tag{35}$$

the potential $V(r)$ in Eq. (35) is defined as V_n *and* $V_n + V_c$ in the absence and presence of impurity respectively. We then take

$$\mathrm{R(r)} = \frac{\mathrm{X(r)}}{\mathrm{r}} , \tag{36}$$

to find

$$\left[\frac{\mathrm{d}^2}{\mathrm{dr}^2} - \frac{\ell(\ell+1)}{\mathrm{r}^2}\right] \mathrm{X} = -(\mathrm{E} - \mathrm{V})\mathrm{X} . \tag{37}$$

For the ground state $\ell = 0$ and accordingly Eq. (37) takes the form

$$\frac{\mathrm{d}^2\mathrm{X}}{\mathrm{dr}^2} = -(\mathrm{E} - \mathrm{V})\mathrm{X} . \tag{38}$$

We now proceed to consider the solution of Eq. (38) in the different regions of the multilayered. We start by the case in which the impurity is absent. In the first region ($0 < r < R_1$) the potential is parabolic and consequently the solution is given by

$$\psi_1^{(0)}(\mathrm{r}) = \mathrm{A}\, \mathrm{e}^{-\gamma_1 \mathrm{r}^2/2}\, {}_1\mathrm{F}_1(-\mathrm{n}, \tfrac{3}{2}, \gamma_1\, \mathrm{r}^2)\,, \tag{39}$$

where

$$\gamma_1 = \frac{\sqrt{\mathrm{V}_0}}{\mathrm{R}_1},\ \hbar\omega_1 = 2\gamma_1,\ \mathrm{n} = \frac{\mathrm{E}}{4\gamma} - \frac{3}{4}, \tag{40 a}$$

and the superscript (0) refers to the case in the absence of impurity. In Eq. (39) we preferred to use the hypergeometric function ${}_1F_1$ instead of Laguerre polynomial. They are related by the relation (Bell [26])

$${}_1\mathrm{F}_1(-\mathrm{n}, \alpha + 1, \xi) = \mathrm{L}_\mathrm{n}^{\alpha}(\xi)\, \frac{\mathrm{n!}\ \alpha!}{(\mathrm{n}+\alpha)!}\,. \tag{40 b}$$

Also in regions 2 and 4 *($R_1 < r < R_2$, $r > R_3$)* , $V(r) = V_0$.

Accordingly

$$\psi_2^{(0)} = \mathrm{B}\, \frac{\mathrm{e}^{\beta \mathrm{r}}}{\mathrm{r}} + \mathrm{C}\, \frac{\mathrm{e}^{-\beta \mathrm{r}}}{\mathrm{r}}\,, \tag{41}$$

$$\psi_4^{(0)} = \mathrm{D}\, \frac{\mathrm{e}^{-\beta \mathrm{r}}}{\mathrm{r}}\,, \tag{42}$$

where

$$\beta = \sqrt{\mathrm{V}_0 - \mathrm{E}}\,. \tag{43}$$

Finally, in region 3 the confining potential can be expressed as

$$\mathrm{V}_\mathrm{n} = \frac{\mathrm{V}_0}{(\mathrm{R}_2 - \mathrm{a})^2}\, (\mathrm{r}^2 - 2\mathrm{ar} + \mathrm{a}^2)\,. \tag{44}$$

We thus apply the asymptotic iteration method (AIM) which has been discussed in section 2. The values of the parameters Z, g, λ can be taken as

$$\mathrm{Z} = 0, \qquad \lambda = \frac{\mathrm{V}_0}{(\mathrm{R}_2 - \mathrm{a})^2}\,, \qquad \mathrm{g} = \frac{-2\mathrm{aV}_0}{(\mathrm{R}_2 - \mathrm{a})^2}\,. \tag{45}$$

The last term in Eq. (44) can be included in the energy term. We, in turn, define

$$E` = E - \frac{a^2 V_0}{(R_2 - a)^2} . \quad (46)$$

Moreover

$$\alpha = 2\sqrt{\lambda}\,, \grave{\ell}\left(\grave{\ell}+1\right) = 4\ell(\ell+1) + \frac{3}{4} = \frac{3}{4}\,, \qquad \grave{\ell} = \frac{1}{2}\,. \quad (47)$$

Also, it can be shown from Eqs. (2), (8), (20) that

$$\psi_3^{(0)}(r) = e^{-\sqrt{\lambda} r^2/2} f(u), \quad u^2 = r\,, \quad (48)$$

where

$$f(u) = e^{-\int_{u_2}^{u} \rho(\grave{u})d\grave{u}} \left[f(u_2) + F(u_2) \int_{u_2}^{u} \exp\{\int_{u_2}^{\grave{u}} (\lambda_0(\grave{\grave{u}}) + 2\rho(\grave{\grave{u}}))d\grave{\grave{u}}\}\, d\grave{u}\right], \quad (49)$$

$f(u_2)$, $F(u_2)$ are constants which have to be determined and $u_2 = \sqrt{R_2}$. Moreover it can be shown from Eqs. (48), (17) that

$$\frac{d\psi_3^{(0)}(r)}{dr} = -r\sqrt{\lambda}\psi_3^{(0)}(r) + e^{-\sqrt{\lambda} r^2/2} \frac{df}{du}\frac{1}{2u}\,, \quad (50)$$

where

$$\frac{df}{du} = \grave{f}(u) = F(u) - \rho(u)f(u) = F(u_2)\, e^{\int_{u_2}^{u} (\lambda_0(\grave{u}) + \rho(\grave{u}))d\grave{u}} - \rho(u)f(u). \quad (51)$$

Eqs. (50), (51) imply that

$$\frac{d\psi_3^{(0)}(r)}{dr} = -\left(r\sqrt{\lambda} + \frac{\rho(u)}{2u}\right) \psi_3^{(0)}(r) + \frac{F(u_2)}{2u}\, e^{-\sqrt{\lambda} r^2/2}\, e^{\int_{\sqrt{R_2}}^{u} (\lambda_0(\grave{u}) + \rho(\grave{u}))d\grave{u}}. \quad (52)$$

The boundary conditions necessitate that

$$\psi_i^{(0)}(R_i) = \psi_{i+1}^{(0)}(R_i), \quad i = 1,2,3$$

$$\left(\frac{d\psi_i^{(0)}}{dr}\right)_{r=R_i} = \left(\frac{d\psi_{i+1}^{(0)}}{dr}\right)_{r=R_i}\,, \qquad i = 1,2,3\,, \quad (53)$$

which are sufficient to determine the constants $B, C, D, f(u_2), F(u_2)$ in terms of A which can be taken equal to unity or determined from the normalization condition.

Now in the presence of a central impurity, we have to apply the (AIM) with $Z = 2$ in regions 1 and 3 . For region 1 we take

$$Z = 2\,, \quad \lambda = \frac{V_0}{R_1{}^2}\,, \quad g = 0\,. \tag{54}$$

Accordingly

$$\psi_1(r) = e^{-\sqrt{\lambda}r^2/2}\, f_1(u)\,, \tag{55}$$

where

$$f_1(u) = e^{-\int_{u_1}^{u}\rho(\grave{u})du}\left[f_1(u_1) + F_1(u_1)\int_{u_1}^{u}\exp\left(\int_{u_1}^{\grave{u}}\{\lambda_0(\grave{u}) + 2\rho(\grave{u})\}d\grave{u}\right)du\right]. \tag{56}$$

Also, $\psi_1(0) = 0$ and hence

$$F_1(u_1) = \frac{f_1(u_1)}{\int_0^{u_1}\exp[-\int_{\grave{u}}^{u_1}\{\lambda_0(\grave{u})+2\rho(\grave{u})\}d\grave{u}]du}\,. \tag{57}$$

It then, follows that

$$\left(\frac{d\psi_1}{dr}\right)_{R_1} = \psi_1(R_1)\{-R_1\sqrt{\lambda} + \frac{1}{2u_1}[-\rho(u_1) + \frac{1}{\int_0^{u_1}\exp(-\int_{\grave{u}}^{u_1}(\lambda_0(\grave{u})+2\rho(\grave{u}))d\grave{u})du}]\}. \tag{58}$$

Regarding region 3, we apply the (AIM) with $Z = 2$ and the other parameters as defined by Eq. (45). Also È and $\psi_3(r)$ will be defined in a similar manner as Eqs. (46) and (48) respectively.

In regions 2 and 4, the results of Mikhail and El Sayed [27] for a central impurity with constant confining potential will be applied. Accordingly,

$$\psi_2(r) = e^{-\tilde{\rho}/2}[\grave{B}\,{}_1F_1(1-\tilde{\lambda},2,\tilde{\rho}) + \grave{C}\,U(1-\tilde{\lambda},2,\tilde{\rho})]\,, \tag{59}$$

and

$$\psi_4(r) = \grave{D}e^{-\tilde{\rho}/2}U(1-\tilde{\lambda},2,\tilde{\rho})\quad, \tag{60}$$

where

$$\tilde{\rho} = \tilde{\gamma}r\,, \quad \tilde{\gamma} = 2\sqrt{V_0 - E}\,, \quad \tilde{\lambda} = \frac{2}{\tilde{\gamma}} = \frac{1}{\sqrt{V_0 - E}}\,. \tag{61}$$

The boundary conditions in this case are equivalent to Eqs. (53) but with the superscript (0) being dropped. The resulting equations will give the values of $\grave{B}, \grave{C}, \grave{D}, f(u_2), F(u_2)$ in terms of $f_1(u_1)$ which can be taken equal to one or has to be calculated from the normalization condition. Here, the constants $f(u_2), F(u_2)$ should take new values owing to the new value of the parameter Z ($Z = 2$).

4. Numerical Calculations

The multilayered quantum dot considered here is composed of two *Ga As* dots, the one within the other. They are defined by the parabolic electronic potentials. Also, they are separated by $Ga_{1-x}\ Al_x\ As$ layers that build finite potential barriers (V_0) in between the dots and outside the whole system. Here, the subscript x represents the Aluminum (*Al*) concentration and accordingly it takes a value between 0 and 1. The confining potentials are given by Eq. (33). The inner dot is of radius R_1 while the outside dot has the inner radius R_2 and outer radius R_3 . The thickness of the outside dot and the barrier between the dots are

$$\mathrm{T_w = R_3 - R_2} \text{ and } \mathrm{T_s = R_2 - R_1}. \tag{62}$$

The input parameters are taken from Casey [28] and Adachi [29]. They are given by

$$\mathrm{m^* = 0.067\ m_0},\ \ \in = 13.18\ \epsilon_0,\ \ \mathrm{R^* = 5.8\ mev}\ \text{and}\ \mathrm{a^* = 100\ A^0}\ , \tag{63}$$

where m_0 is the bare mass of the electron and ϵ_0 is the dielectric constant of free space. Following Akgül et al [24] we further take

$$\mathrm{V_0 = 225\ mev}\ ,\ \ \mathrm{T_s = 0.2\ a^*}\ . \tag{64}$$

For the ground state (0s) we take $l = 0$. The results obtained in the absence and presence of impurity are shown in Figs. (1), (2) for $T_w = 0.6\ a^*$ and $0.4\ a^*$ respectively. The comparison with the corresponding results of Akgül et al [24] showed a reasonable agreement.

We have preferred here to restrict ourselves to the ground state (*I=0*). We found that this is enough to compare the results with those obtained in Akgül et al [24] by using an entirely numerical technique. The other excited states will be considered in a separate article where the

results obtained by applying the (AIM) will be compared with those obtained by applying the variational method and other numerical techniques.

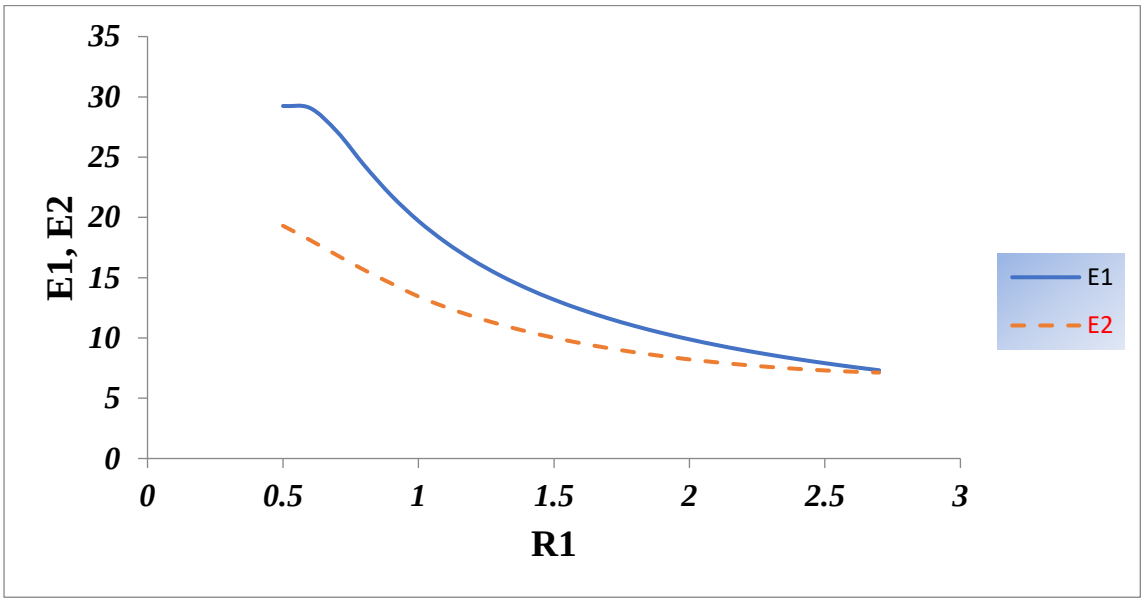

Fig. 1: Graph of the energy ground states (E_1,E_2) (L=0) against R_1 for $T_w = 0.4\ a^*$. Here E_1, E_2 are the energies in absence and presence of impurity.

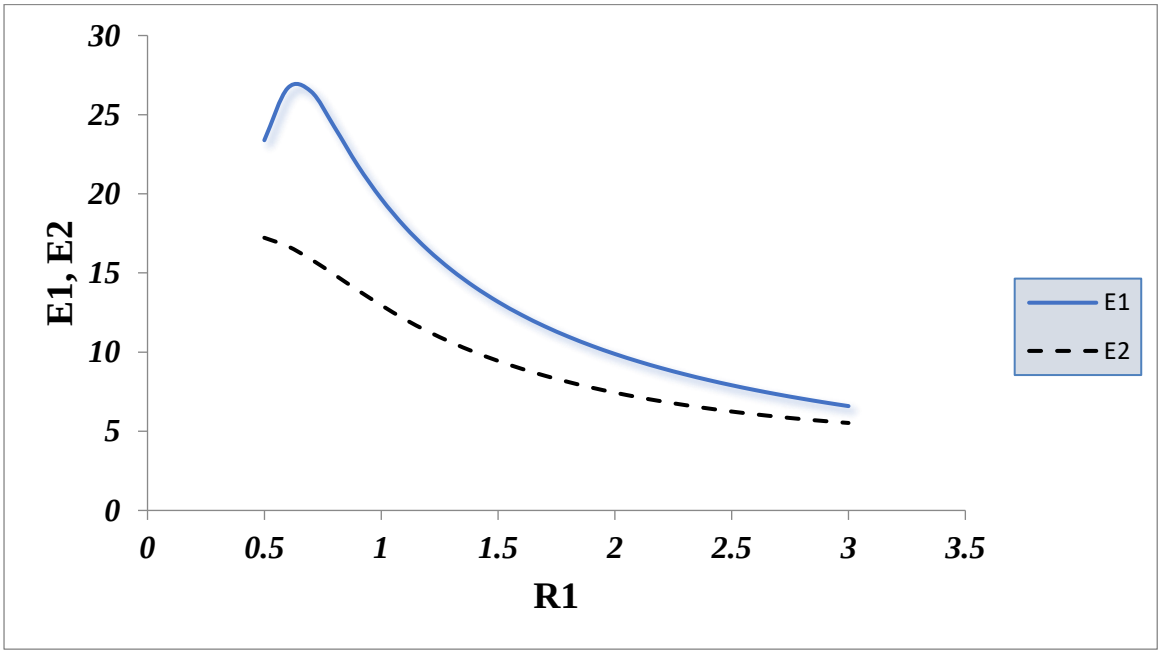

Fig. 2: Plot of the energy ground states (E_1,E_2) (L=0) versus R_1 for $T_w = 0.6\ a^*$.

5. Conclusion

The importance of the asymptotic iteration method in determining the binding energy of a central impurity in both single and multilayered quantum dots has been emphasized. To the best of our knowledge this method has not been employed anywhere before to determine the impurity binding energy. In a single quantum dot subject to a parabolic confining potential this method has led to a result which agrees entirely with the result of the time independent perturbation technique up to the first approximation. Also, in a multilayered spherical quantum dot (MSQD) subject to a very complicated parabolic potential in the different regions the results obtained from the (AIM) showed reasonable agreement with the results obtained by using entirely numerical techniques.

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الملخص العربى

طريقة التكرار التقاربية في النقاط الكمية المنفردة والمتعددة الطبقات

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الملخص العربى

استخدمت طريقة التقارب التكرارية التي لم تستخدم من قبل لحساب طاقة الترابط للشائبة. ولقد اعطت هذه الطريقة تطابق مع نتائج نظرية الاضطراب بالنسبة للشائبة المركزية حتى التقريب الاول بينما يختلف التقريب الثاني للطريقتين بحوالي 16.5 % وهذه نتيجة منطقية .

كما تم تطبيق طريقة التقارب التكرارية لحساب طاقة الارتباط لشائبة مركزية في نقطة مادية متعددة الطبقات في وجود جهد محدد على صورة معقدة للقطع المكافئ وتختلف من طبقة الى اخرى .

قد اعطت الطريقة نتائج تتفق الى حد كبير مع النتائج التي تم الحصول عليها لآخرين باستخدام الطرق العددية . ولذلك فقد اظهرت الدراسة الحالية اهمية طريقة التقارب التكرارية في حل معادلة شرودنجر النصف قطرية في وجود جهد محدد معقد .

كما تم حساب طاقة الارتباط لشائبة مركزية او لا مركزية موضوعة في نقطة كمية كروية باستخدام نظرية الاضطراب . كما تم دراسة طريقة التقارب التكرارية . ولقد تم تطبيق الطريقتين لحساب مستوى الطاقة في وجود شائبة مركزية.

كما تم دراسة الشائبة المركزية في نقطة كمية كروية متعددة الطبقات في وجود جهد محدد على صورة معقدة للقطع المكافئ بحيث تختلف من منطقة الى اخرى . ولقد تم بنجاح.