

Confined states in fullerenes and quantum dots calculated by Analytic Continuation Method

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Abstract. The Schrödinger equation with a Gaussian potential to model a confined system as a quantum dot or a fullerene is solved using the Analytic Continuation Method. The use of the Rodrigues formula allows us to obtain in an easy way the coefficients of the power series expansion of the Gaussian potential in terms of the Hermite polynomials. Recurrence formulas have been obtained for the series of the states of an electron confined by that potential. This method is simpler and computationally more efficient than others employed to model quantum dots using Gaussian potentials.

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1 Introduction

The Gaussian confining potential is a particular case of the power-exponential potentials [1]:

$$V(r) = -w_0 \exp \left[- \left(\frac{r - r_c}{\sigma} \right)^p \right], \quad (1)$$

where w_0 is the depth of the potential ($w_0 > 0$), r is the radial coordinate, r_c is the radial distance from the origin to the minimum of the potential, σ is the range of the potential and $p \geq 1$. Changing the value of the parameter p we can change the shape of the potential from the Gaussian one for $p = 2$ to the rectangular well for $p \rightarrow \infty$.

In 1977, Buck et al. [2] used the Gaussian potential as the nucleus-nucleus interaction potential to calculate the α - α scattering phase shifts. They solved the Schrödinger equation by direct integration and obtained a satisfactory agreement with experiment.

Since then, several methods have been applied to calculate the eigenvalues of the Schrödinger equation (2D or 3D) with a radial Gaussian potential: Stephenson [3] used the Liouville-Green uniform asymptotic method, Bessis et al. [4] applied a perturbational and a variational treatment, Crandal [5] used a Prüfer transformation to the Schrödinger equation that provides fast algorithms to calculate eigenvalues in one-dimensional problems, and Lai [6] determined the eigenvalues using the hypervirial-Padé scheme.

In 2000, Adamowski et al. [7] considered the Gaussian potential to study two electrons confined in quantum dots (QD) in a variational approach while Ciurla et al. [1] applied a finite-difference numerical method with the

higher-order approximation of the Laplacian described in Chelikowsky et al. [8], showing that the attractive Gaussian potential was more suitable to describe QD than previously used potentials as square-well or parabolic ones. Thus, in the last years, many works used the Gaussian potential to investigate the electronic structure of QD and their properties [9–12]. Also, a Gaussian potential has been used to model other confined systems as a C_{60} fullerene [13].

There is an increasing interest not only in eigenvalues but in eigenfunctions too for the bound states of the Gaussian potential. Nascimento et al. [13] applied a variational approach expanding the wave function using a finite basis obtained by the p-version of finite-element method, an approach known as self-consistent finite-element method (SC-FEM). Boda and Chatterjee [14] chose as trial wave functions the product of a gaussian function with a Jastrow factor using three variational parameters. Al-Hayek and Sandouqa [15] calculated the spectra of an electron and a donor in QD confined by a Gaussian potential and applied the shifted $1/N$ expansion method (N is the number of spatial dimensions) but only reported the eigenvalues in their paper. Recently, Mutuk [16] used the asymptotic iteration method that consists in expanding the Gaussian potential in a power series and truncating it for the r^{-10} term. He also worked with a variational method using as trial functions the radial part of the three-dimensional harmonic oscillator wave function with one variational parameter. Sari et al. [11] reported the first six confined levels for a GaAs QD using a Gaussian potential to model the QD and a perturbation expansion method to obtain energies and wave functions. Bai et al. [9] described the electron confined in a QD by an asymmetric Gaussian potential and computed the ground and first excited state energies and wave functions using the Pekar-type varia-

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tional method. All these works have calculated approximate bound state wave functions using perturbational or variational methods.

In 1985, Holubec and Stauffer [17] proposed to approximate the solution of a differential equation with an initial value at point x_0 by a truncated Frobenius series instead of a truncated Taylor series. This Frobenius series is used to evaluate the derivatives at x_0 and a Taylor series at $x_1 = x_0 + h$ is constructed. In this way they obtain an analytic continuation of the solution of the differential equation. The solution is also an approximate one but the method works for arbitrary order and is superior in speed and accuracy to conventional methods. It works very well if the potential can be expanded in a Taylor series so analytic coefficients can be obtained [18,19].

Therefore, in this work, we apply the analytic continuation method (ACM) proposed by Holubec and Stauffer to calculate the eigenvalues and eigenfunctions of the Schrödinger equation with a radial Gaussian potential in order to model a QD or a fullerene. The coefficients of the series for the Gaussian potential are computed using the Rodrigues formula for the Hermite polynomials [20]. This paper is organized as follows. In Section 2, a description of the analytic continuation method for a symmetric Gaussian potential is done. In Section 3, the numerical energy states, wave functions and other interesting magnitudes are presented. Finally, the conclusions are provided in Section 4.

2 Methodology

Given a spherically symmetric potential $V_c(r)$ to describe a confining environment, the Hamiltonian for the one-electron problem containing this potential can be expressed as

$$H = -\frac{1}{2}\nabla^2 - \frac{Z}{r} + V_c(r) \quad (2)$$

where the Laplacian term corresponds to the kinetic energy of the confined electron and the second right-term represents the Coulomb interaction with the atomic nucleus ($Z = 1$ models a Hydrogen atom inside a fullerene whereas $Z = 0$ can model a quantum dot). Atomic units have been used through out this work.

The confining potential $V_c(r)$ is considered to be an attractive short-range spherical Gaussian-type potential not centred in the origin, given by equation 1 with $p = 2$ [13]. In this case, r_c corresponds to the position of the confining shell or the quantum dot given by the minimum of the potential, w_0 indicates the confinement strength, and σ represents a measure of the size of the confining shell.

Owing to the spherical symmetry of the confining potential, the Schrödinger equation for a stationary state $\Psi_{nlm}^c(\mathbf{r})$,

$$H^c\Psi_{nlm}^c(\mathbf{r}) = E_{nl}^c\Psi_{nlm}^c(\mathbf{r}) \quad (3)$$

can be reduced to the radial form as

$$\frac{d^2 u_{nl}^c(r)}{dr^2} + \left[2E_{nl}^c + \frac{2Z}{r} - \frac{l(l+1)}{r^2} - 2V_c(r) \right] u_{nl}^c(r) = 0 \quad (4)$$

where E_{nl}^c is the energy of the state, $u_{nl}^c(r)$ is the reduced radial function ($\Psi_{nlm}^c(\mathbf{r}) = \frac{u_{nl}^c(r)}{r} Y_{lm}(\Omega)$), and nlm are the quantum numbers of the state.

As stated before, the analytic continuation method has been employed to obtain the radial functions of the confined states [17–19, 21, 22]. To apply this method, it is necessary to discretize the interval of integration along r-axis in a series of tabular points r_0, r_1, \dots, r_N . These points do not need to be equally spaced. The ACM approximates the solution of the differential equation in the neighbourhood of each tabular point by a truncated series, so the radial function is expressed as a piecewise polynomial function.

The Gaussian potential can be expanded in the neighbourhood of a point r_i by a Taylor series in the form:

$$V_c(r) = \sum_{k=0}^{\infty} V_k (r - r_i)^k \quad (5)$$

where V_k is proportional to the kth-order derivative of the Gaussian function. This derivative is calculated using the Rodrigues formula for the Hermite polynomials [20] and we get

$$V_k = \frac{1}{k!\sigma^k} (-1)^{k+1} w_0 \left[e^{-x^2} H_k(x) \right] \Big|_{x=\frac{r_i-r_c}{\sigma}} \quad (6)$$

where H_k is the kth-order Hermite polynomial.

It is well known that the solution around the origin ($r_i = r_0 = 0$) can be written as a Frobenius series of the form [23]

$$u(r) = \sum_{j=0}^{\infty} b_j r^{l+j+1} \quad (7)$$

where l is the quantum number associated to the angular momentum. For $l = 0$ we obtain the *s-states*, for $l = 1$ the *p-states* and so on.

Substituting Eqs. (7) and (5) into Eq. (4) we get for the coefficients b_j :

$$b_0 \neq 0 \quad (8)$$

$$b_1 = -\frac{b_0}{l+1} \quad (9)$$

$$b_j = \frac{-2}{j(j+2l+1)} (Zb_{j-1} + Eb_{j-2} - \sum_{k=0}^{j-2} V_k b_{j-2-k}), \quad j \geq 2 \quad (10)$$

This solution can be extended analytically to other tabular points $r_t \neq 0$, $t = 1, 2, \dots$. Thus, as it has been done previously, the solution around r_t can be written as a series of the form

$$u(r) = \sum_{j=0}^{\infty} c_j (r - r_t)^j \quad (11)$$

Substituting Eqs. (11) and (5) into Eq. (4) we obtain

$$c_0 = u(r_t) \quad (12)$$

$$c_1 = u'(r_t) \quad (13)$$

$$c_2 = -c_0 \left[\frac{2 - l(l+1) + \underline{2r_t Z} + 2(E - V_0)r_t^2}{2r_t} \right] \quad (14)$$

$$c_3 = \frac{1}{6r_t} \left\{ -4r_t c_2 - [\underline{2r_t Z} + 2r_t^2 E - l(l+1)] c_1 - [\underline{2Z} + 4r_t(E - V_0)] c_0 + 2r_t^2 \sum_{k=0}^1 V_k c_{1-k} \right\} \quad (15)$$

$$c_j = \frac{1}{r_t j(j-1)} \left\{ -2r_t c_{j-1}(j-1)(j-2) - c_{j-2} [(j-2)(j-3) - l(l+1) + \underline{2r_t Z} + 2r_t^2 E] - (\underline{2Z} + 4r_t E) c_{j-3} + 2r_t^2 \sum_{k=0}^{j-2} V_k c_{j-2-k} + 4r_t \sum_{k=0}^{j-3} V_k c_{j-3-k} + 2 \sum_{k=0}^{j-4} V_k c_{j-4-k} \right\}, \quad j \geq 4 \quad (16)$$

with c_0 and c_1 for r_t calculated from the series at r_{t-1} .

If we considered the Schrödinger equation only for the Gaussian potential without the Coulomb interaction with the atomic nucleus, the sets of coefficients would be simpler. In the case of the coefficients b_j , b_0 would be zero and each b_j would not depend on b_{j-1} , and for the c_j , we have underlined in Eqs. (14)-(16) the terms that correspond to the Coulomb potential and are absent for the Gaussian potential only. This would be the case, for example, of the absence of donor atom in a quantum dot.

Equations (10) and (14)-(16) include the eigenvalue E , so we have applied a shooting method to carry out inward and outward integrations imposing the continuity of the log derivative at an intermediate point to get the eigenvalue [21].

Equally spaced tabular points with step size $\sim 10^{-4}$ have been employed in most cases. Calculations were carried out in double precision on an AMD OpteronTM 6376.

Once energies and wave functions are known, it is possible to obtain other interesting magnitudes such as the binding energy for quantum dots, which is defined by the difference of energy for a state in the absence of donor atom ($Z = 0$) and in its presence ($Z = 1$), or the hyperfine splitting constant, which contributes to the coupling between the nuclear spin and the electron and is defined as [24]

$$A = \frac{2}{3} g \beta g_n \beta_n |R_{1s}(0)|^2 \quad (17)$$

where g is the electron gyromagnetic ratio, g_n is the dimensionless nuclear g-factor, β is the electron magnetic moment, β_n is the nuclear magneton, and $R_{1s}(0)$ is the radial wave function evaluated at the origin.

3 Results and discussion

Firstly, Hydrogen energies are computed for the Coulomb and attractive non-centred Gaussian potentials for $r_c = 6.69$ so as to model a C_{60} fullerene [25] and compare to previous results obtained using the SC-FEM [13]. In order to assert the highest possible accuracy, we have previously studied the convergence of the energy values as a function of N , the degree of the polynomial in the series expansion, as it is shown in Table 1. We present to 8 decimal places the results of applying the method for $N = 3, 5, 10$ and 20 and it is observed that energy values are not modified for $N \geq 5$. CPU times for the calculus of the $1s$ state as a function of N are also included. As the order of magnitude for computational times are seconds, a polynomial expansion of degree $N = 20$ has been used through out this work to ensure a great accuracy. This method precision is supported by previous studies where it was tested for well-known problems [17-19].

$1s$ to $4s$ energy levels are computed and compared with those from the SC-FEM as it is seen in Table 2 (other orbitals with $l \neq 0$ can be calculated using the same recurrence formulas, Eqs. (8)-(10) and (12)-(16)). Our results are equal or lower than those of SC-FEM as expected. SC-FEM is a variational method so it gives an upper bound to the energies. Only 4 decimal places are included in order to compare with values reported but as indicated before, we have obtained 8 decimal places.

In addition, wave functions have been computed as it is shown in Fig. 1, where the reduced radial function of the $3s$ state is plotted for $r_c = 6.69$, $\sigma = 1.08$ and different values of the well depth, w_0 , which is representative for the rest of cases. As the well depth increases, the charge density is attracted by the confining potential so it is more localised between the origin and the well ($w_0 = 1$ and $w_0 = 2$). From certain value of well depth ($w_0 = 5$) the electron is practically confined in that region because a lower orbital is localised around the well and the $3s$ takes its place near the origin. For deeper wells ($w_0 = 7$), almost all the wave function is inside the well including all its nodes, so the density is bounded to the well due to its strong attraction. This result is in good agreement with other results [13].

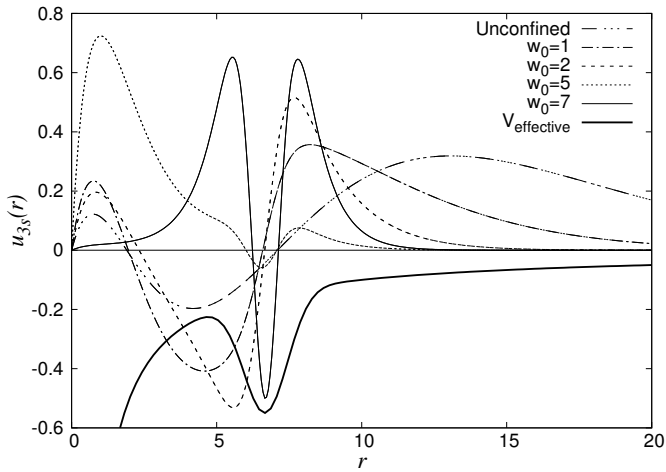
Moreover, energy values only for the attractive Gaussian potential centred in the origin ($r_c = 0$) have also been calculated. This potential can model different physical phenomena such as the absence of an impurity in a spherical quantum dot. Table 3 shows our results for the $1s$ to $4f$ energy states for $w_0 = 200$ and $\sigma = 1$ compared with previous calculations obtained from the use of the hypervirial-Padé scheme [6], the Numerov's integration method [26], the diagonalization of the Hamiltonian matrix [26], the shifted $1/N$ expansion method [15], and the asymptotic iteration method [16]. Our results are in very good agreement with those from different approximation methods but present some advantages against them. Thus, the shifted $1/N$ expansion method only allows to calculate the spectra without giving any information about the wave functions. The case of the Hypervirial-Padé Method is similar but it permits to obtain information about mean

Table 1. Convergence for the 1s to 4s energy levels of H for the attractive Gaussian potential for $r_c = 6.69$, $w_0 = 0.5$ and $\sigma = 3.01$. CPU time for the calculus of the 1s state is also included.

Energy levels					CPU time (s)
N	1s	2s	3s	4s	1s
3	-0.55841238	-0.48920712	-0.24808437	-0.07087828	0.07
5	-0.55841252	-0.48920779	-0.24808456	-0.07087825	0.09
10	-0.55841252	-0.48920779	-0.24808456	-0.07087825	0.18
20	-0.55841252	-0.48920779	-0.24808456	-0.07087825	0.48

Table 2. Energy of the 1s to 4s states of H for the attractive Gaussian potential for $r_c = 6.69$ and different values of w_0 and σ .

Energy levels									
		1s		2s		3s		4s	
w_0	σ	SC-FEM [13]	Our work	SC-FEM [13]	Our work	SC-FEM [13]	Our work	SC-FEM [13]	Our work
0.500	0.49	-0.5002	-0.5002	-0.2224	-0.2227	-0.0565	-0.0565	-0.0316	-0.0316
	1.08	-0.5013	-0.5013	-0.3418	-0.3419	-0.0639	-0.0639	-0.0362	-0.0363
	3.01	-0.5584	-0.5584	-0.4892	-0.4892	-0.2480	-0.2481	-0.0708	-0.0709
0.324	0.49	-0.5001	-0.5001	-0.1804	-0.1806	-0.0562	-0.0562	-0.0314	-0.0314
	1.08	-0.5006	-0.5006	-0.2504	-0.2504	-0.0599	-0.0599	-0.0336	-0.0336
	3.01	-0.5280	-0.5280	-0.3603	-0.3603	-0.1594	-0.1595	-0.0491	-0.0492
0.162	0.49	-0.5000	-0.5001	-0.1495	-0.1495	-0.0559	-0.0559	-0.0313	-0.0313
	1.08	-0.5002	-0.5002	-0.1799	-0.1799	-0.0575	-0.0575	-0.0322	-0.0322
	3.01	-0.5128	-0.5128	-0.2382	-0.2382	-0.0918	-0.0918	-0.0406	-0.0406
free		-0.5000	-0.5000	-0.1250	-0.1250	-0.0556	-0.0556	-0.0312	-0.0313

**Fig. 1.** Reduced radial function, $u(r)$, of the confined 3s state for $r_c = 6.69$, $\sigma = 1.08$ and $w_0 = 1, 2, 5$ and 7 . The unconfined radial orbital and the effective potential in arbitrary units are also shown.

values of powers of r . In contrast, ACM gives not only the energy spectra but also the wave functions. Although Gómez and Romero [26] calculate the wave functions too, they do it in a basis set composed by Cartesian Gaussian functions and they need 140 functions to describe states with $l \leq 4$ and 360 ones for states with $l \leq 7$. Our results are obtained with a power series of only 20 terms for any value of l and as discussed before, results converge till 8 decimal places with only 5 terms. Similar to ACM, asymptotic iteration method expands the Gaussian potential near the origin but the description is limited to

10th-power of r . Our method is more general as it allows to have the Gaussian potential not centered in the origin.

Other physical properties as binding energies for quantum dots or the hyper-fine splitting constant can also be computed. On one hand, Fig. 2 displays the binding energy, E_B , of the 1s to 4s and of the 3s to 3d states as a function of the dot size, σ , for potential depth $w_0 = 25$. The binding energy rises as the dot size decreases until it reaches a maximum value. The highest binding energy corresponds to the ground state. Similar results have been obtained in other works[15].

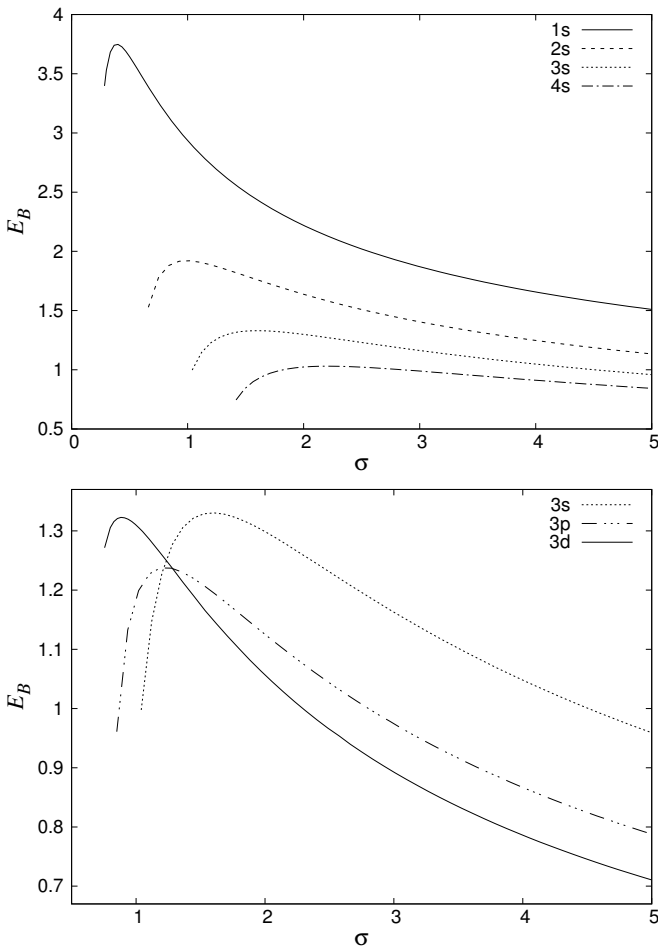
On the other hand, Fig. 3 shows the hyper-fine splitting constant, A , as a function of the well depth, w_0 , for $r_c = 6.745$ and $\sigma = 0.945$ in order to compare with a previous work by Martínez-Flores and Cabrera-Trujillo [27]. As it can be seen, there is a decrease around a critical value of $w_0 = 0.8$ and then, there is no further contribution to the splitting constant, which means that the 1s state is mainly bounded to the well. This behaviour is similar to the one described in the aforementioned work.

4 Conclusions

Analytic Continuation Method is well suited for the resolution of the Schrödinger equation with a Gaussian potential. The use of the Rodrigues formula allows us to obtain in an easy way the coefficients of the power series expansion of the Gaussian potential in terms of the Hermite polynomials. Thus, recurrence formulas have been calculated for the series of the states of an electron confined by a Gaussian potential. As it has been explained, this method is simpler and computationally more efficient than others

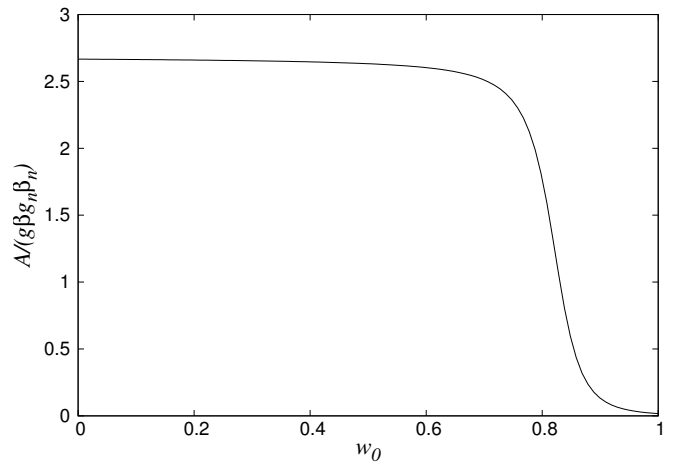
Table 3. Energy of the 1s to 4f states for the attractive Gaussian potential for $r_c = 0$, $w_0 = 200$ and $\sigma = 1$.

Energy levels	Hypervirial Padé [6]	Numerov [26]	Diagon. [26]	Shifted $1/N$ exp.[15]	Asymptotic Iteration[16]	Our work
1s	-170.9476	-170.946	-170.948	-170.948	-170.948	-170.9476
2s	-134.8223	-134.820	-134.822	-134.822	-134.822	-134.8222
2p	-152.2314	-152.232	-152.232	-152.232	-152.232	-152.2314
3s	-101.9918	-101.990	-101.992	-101.999	-101.979	-101.9918
3p	-117.7250	-117.725	-117.223	-117.723	-117.735	-117.7250
3d	-134.0554	-134.056	-134.055	-134.056	-134.056	-134.0554
4s	-72.6890	-72.687	-72.686	-72.716	-72.567	-72.6889
4p	-86.6222	-86.622	-86.578	-86.629	-86.611	-86.6222
4d	-101.2157	-101.216	-101.214	-101.216	-101.208	-101.2156
4f	-116.4377	-116.448	-116.425	-116.439	-116.437	-116.4377


Fig. 2. Upper panel: Binding energy, E_B , of the 1s to 4s states as a function of the dot size, σ , for $w_0 = 25$. Lower panel: The same for 3s to 3d states.

described to model quantum dots using Gaussian potentials.

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Fig. 3. Hyper-fine splitting constant, A , for $r_c = 6.745$ and $\sigma = 0.945$ as a function of the potential depth, w_0 .

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Authors contributions

All the authors were involved in the preparation of the manuscript. All the authors have read and approved the final manuscript.

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