An efficient approximation for accelerating convergence of the numerical power series. 

Results for the $1D$–Schrödinger’s equation

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The numerical matrix Numerov algorithm is used to solve the stationary Schrödinger equation for central Coulomb potentials. An efficient approximation for accelerating the convergence is proposed. The Numerov method is error–prone if the magnitude of grid–size is not chosen properly. A number of rules so far, have been devised. The effectiveness of these rules decrease for more complicated equations. Efficiency of the technique used for accelerating the convergence is tested by allowing the grid–sizes to have variationally optimum values. The method presented in this study eliminates the increased margin of error while calculating the excited states. The results obtained for energy eigenvalues are compared with the literature. It is observed that, once the values of grid–sizes for hydrogen energy eigenvalues are obtained, they can simply be determined for the hydrogen iso–electronic series as, $h_e(Z) = h_e(1)/Z$.

**Keywords:** Numerov method, Screened Coulomb potential, Schrödinger equation

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I. INTRODUCTION

The wave–function that holds all the required information of a system is obtained from analytical or numerical solution of the quantum mechanical wave–equation such as Schrödinger or Dirac equation. Characteristics of the potential determines an exact analytical solution for the wave–equation whether available or not. If the potential function $V(r,r_0)$ is separable depending on its variables $r,r_0$ into two factors [1] may be reduced to solvable form. Such simplicity however, appears only for a few idealized systems. Complexity increases and the potential function may not be separable for more realistic representations. In this case, an analytical solution based on the approximation methods is required. Among these approximations, the perturbation, variation and Wentzel–Kramers–Brillouin (WKB) methods have generally been used in the literature [2, 3]. Although these analytical approaches are preferred for use in atomic and molecular calculations, they are limited in terms of applications [2]. A solution free from symmetry properties of a potential inevitably leads to numerical approaches [4].

Numerical integration formula for integrating the time–independent Schrödinger equation [5]

$$ -\frac{\hbar}{2m} \psi''(x) + V(x) \psi(x) \approx E \psi(x) \quad x \in [a,b] \quad (1)$$

which was suggested in the early days of quantum mechanics by Numerov [6, 7]. The Numerov’s method takes advantage of specific structure of the Eq. [1]. It involves no first derivative and it is linear in $\psi$. The Eq. [1] may be transformed to dimensionless form as,

$$ \psi''(x) - f(x) \psi(x) = 0, \quad (2)$$

where, $f(x) = -2m(E - V(x))/\hbar^2$.

The solution $\psi(x)$ at the nodes of $N$ uniform grid points, namely, $x_0, x_1, x_2, ..., x_N$ with $h_x = x_{i+1} - x_i$, where $h_x$ grid–size for $\epsilon$th energy state. The Numerov’s algorithm includes higher order terms than the well–known finite–difference with an error term that is of order $O(h^2)$. It is derived by considering conjointly the forward, backward Taylor expansion of $\psi(x)$ up to order $O(h^6)$ [8]. The following relation is finally obtained $[\psi_i \equiv \psi(x_i), f_i \equiv f_i(x_i)]$,

$$ \psi_{i+1} - 2\psi_i + \psi_{i-1} = -\frac{h^2}{12}(f_{i+1}\psi_{i+1} + 10f_i\psi_i + f_{i-1}\psi_{i-1}) + O(h^6). \quad (3)$$

The Eq. (3) is a numerical one–dimensional pattern [9]. The wavefunction $\psi(x)$ is calculated iteratively [10]. An initial guess for $E$ is required. The interval $[a,b]$ is finite and implicit the Dirichlet boundary conditions at $\psi_0 = \psi(a) = 0$, $\psi_N = \psi(b) = 0$ [8]. Richardson extrapolation [5] or Cooley’s correction formula [11, 12] which are based on perturbation theory, may be used to improve the approximation for the energy with each iteration. Several other variants in order to increase both stability and accuracy while calculating the resonance problems and high–lying bound states were proposed. Generalization of the algorithm to an error of arbitrary order [13, 25] and its extension for solution of differential equations with more than one–dimension [8, 20, 35] form the...
main framework of the studies. A Numerov–type exponentially fitted method was suggested [18–20, 32, 34–43], accordingly. Here, the coefficients in the Eq. (3) are replaced by some arbitrary parameters. It is assumed that the solution is a linear combination of the exponential functions. The parameters are then obtained from the resulting system of differential equations. Another method derived from the Eq. (4) is so called re-normalized Numerov method. It was obtained by making two transformations [44–45]. The first transformation is used to decrease the number of steps required for calculation and the second one is used to replace the three–point recurrence relation with two–point relations by defining a ratio. If the iteration is stopped at any point, the last two elements of the ratio are immediately available. They are used to calculate the wave–function ($\psi$) around that point within a normalized factor [44]. Non–uniform grid–size $h_i, h_{i+1} = x_{i+1} - x_i$ was also considered to be use [43, 54]. It is derived due to the need to solve the transport model for semiconductor devices where, the standard Numerov procedure with uniform grid–size is not applicable [53, 54]. The range of application of the Numerov’s algorithm is indubitably not limited to the aforementioned examples [17, 45, 50, 53, 54]. It is used to determine presence of the energetics for short intramolecular $O–H\ldots O$ in enzyme and photo centers by nuclear motion of the involved hydrogen atom [5], to solve the Schrödinger equation with complex potential in the Schrödinger equation. Due to singularity of the Coulomb potential, hydrogen-like eigen–functions have non–continuous derivatives at $r = 0$ [61]. Correctly representation of the radial wave–function require use of tremendous grid points such that, one has to consider how to compute Eq. (4) effectively. The solution of the Schrödinger equation for the central Coulomb potential is therefore examined as a sample. The error term is embedded in a certain weight to the matrix that represents the effective potential. Such weight leads to approximately determine the grid–size. Variational stability is tested via the optimization procedure. The results are presented for hydrogen-like atoms.

II. MODIFIED MATRIX NUMEROV REPRESENTATION FOR THE HAMILTONIAN

Taking into account the Eqs. (12) the exact second derivative for $\psi(x)$ is given as,

$$\psi''(x) = -\frac{2m}{\hbar^2} [E - V(x)] \psi(x).$$

(5)

The Eq. (5) from the perspective of numerical integration, may be represented by the following statement;

$$\text{Exact} = \text{Numerical} + \mathcal{O}(\hbar^6).$$

By inserting the Eq. (5) in the above statement and assuming that the error term is of order $\mathcal{O}(\hbar^6)$ we have the following property,

$$\hat{\beta}(\hbar^6) \psi(x) = \mathcal{O}(\hbar^6) \psi(x),$$

(6)

$$\text{Numerical} = -\frac{2m}{\hbar^2} [E - V(x) \pm \beta(\hbar^6)] \psi(x).$$

(7)

If the potential term defined as,

$$V'(x) = V(x) \pm \beta(\hbar^6),$$

(8)

the Eq. (7) becomes analogous to Eq. (2). It is unlikely to find a definition for $\beta(\hbar^6)$. Instead the potential $V(x)$ may be replaced by the one involving a screening parameter $\mu$ (more precisely a function). Thus,

$$V'(x) = V_\mu(x).$$

(9)

In general we can say that the function $\mu$ is a function of number of grid–points. It must be a function such that it satisfies the conditions given for the screened potential as below;

$$\lim_{\mu \to 0} V_\mu(x) = V(x),$$

(10)

$$\lim_{N \to \infty} V_\mu(x) = V(x).$$

(11)

We have derived two variants of $\mu$ in order to solve the radial stationary Schrödinger equation of an electron moving through the Coulomb potential.
III. A METHOD TO DETERMINE THE FUNCTION $\mu (N)$

Depending on the number of grid—points $N$ and angular momentum quantum number $l$, the two versions of the $\mu$ function in this study are defined as,

$$\mu_1 (N, l, \nu_1) = \exp \left[ \frac{1}{N\nu_1(l+1)} \right] - 1,$$

$$\mu_2 (N, l, \nu_2) = \text{Erf} \left[ \frac{1}{N\nu_2(l+1)} \right],$$

where, $\{\nu_1, \nu_2\} \in \mathbb{R}^+$, $1 \leq \{\nu_1, \nu_2\} < \infty$. Minimum and maximum values to be found for energy eigenvalues correspond to the $\nu = 1$ and $\nu = \infty$ $(\mu \to 0$, represents the pure Coulomb potential), respectively. According to the value of $\nu$ the interval for numerically obtained energy eigenvalues are determined as,

$$E_1 \leq E_\nu \leq E_\infty = E_{\text{Coulomb}}.$$

The Eqs. (12, 13) for any value of angular momentum quantum number $l$ satisfy the following property,

$$\lim_{N \to \infty} \mu (N, l, \nu) = 0.$$

The Eq. (14) is solved iteratively since it is now depends to the values of $\nu$. The number of iterations are sensitive to the choice of initial values of $\nu$. Large number of grid—points approximate both values of the $\mu$ and the grid—size $h$ to zero. A simple approach as $\mu_1 (N, l, \nu_1) = h_1^2$, $\mu_2 (N, l, \nu_2) = h_2^2$, or visa versa (see the Table I) that promise better initial values for $\nu$ (or if $\nu$ is known for $h$) is used, accordingly. Alternatively, one can chose a large value of $\nu$ as an initial input. Two upper limit of summations (number of grid—points) are selected. The calculations are performed for these two upper limit of summations using the $\nu_1$. If the energy eigenvalues are increasing, then the $\nu_2$ is used. The iteration is terminated. Else, $\nu_1$ is used in the Eq. (13) to derive a new $\nu_1$. This new value of $\nu_1$ is used in the Eq. (12). The calculations are performed until the energy eigenvalues start to increasing. An algorithm for the above procedure may be summarized as,

Step 1. Choose two upper limit of summation $(N_1, N_2)$.

Step 2. Choose a grid—size for each upper limit of summation or use the ones given in the Table I.

Step 3. Obtain initial values of $\nu_1$ and $\nu_2$ for each $N$ by solving the equations $\mu_1 (N, l, \nu_1) = h_1^2$, $\mu_2 (N, l, \nu_2) = h_2^2$, $i = 0$ (iteration number).

Step 4. Calculate the energy eigenvalues $E_{N_i} (h_1, \nu_1)$,
TABLE III. Results of computation for electronic energy spectrum of hydrogen atom with screened Coulomb potential in atomic units (a. u.) where, \( \nu \neq 0 \) and \( \mu (N, 0, \nu) \neq 0 \).

| \( N \) | \( E_{1a} (N, h_1, \nu) \) | \( E_{2a} (N, h_2, \nu) \) | \( E_{3a} (N, h_3, \nu) \) | \( E_{4a} (N, h_4, 0) \) | \( E_{5a} (N, h_5, \nu) \) | \( E_{10a} (N, h_{10}, \nu) \) |
|------|----------------|----------------|----------------|----------------|----------------|----------------|
| 500  | 0.49999 8138 | 0.12499 3530 | 0.05555 0098 | 0.03124 4397 | 0.01999 4397 | 0.00499 4636 |
| 1000 | 0.49999 9566 | 0.12499 8145 | 0.05555 3903 | 0.03124 8101 | 0.01999 7811 | 0.00499 5772 |
| 1500 | 0.49999 9841 | 0.12499 9161 | 0.05555 4814 | 0.03124 9116 | 0.01999 8934 | 0.00499 9505 |
| 2000 | 0.49999 9939 | 0.12499 9539 | 0.05555 5155 | 0.03124 9512 | 0.01999 9394 | 0.00499 9609 |
| 2500 | 0.49999 9969 | 0.12499 9708 | 0.05555 5306 | 0.03124 9694 | 0.01999 9612 | 0.00499 9709 |
| 5000 | 0.50000 0010 | 0.12499 9933 | 0.05555 5506 | 0.03124 9936 | 0.01999 9913 | 0.00499 9920 |
| 7500 | 0.49999 9960 | 0.12499 9968 | 0.05555 5534 | 0.03124 9972 | 0.01999 9962 | 0.00499 9965 |
| 10000| 0.50000 0037 | 0.12499 9986 | 0.05555 5548 | 0.03124 9989 | 0.01999 9984 | 0.00499 9986 |
| 15000| 0.50000 0036 | 0.12499 9995 | 0.05555 5548 | 0.03124 9998 | 0.01999 9995 | 0.00499 9997 |

\( i = 3 \) \quad i = 1 \quad i = 2 \quad i = 4 \quad i = 6 \quad i = 15

\( * i \) is the number of iterations

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\( E_{N_2} (h_2, \nu_1) \).

**Step 5.** If \( E_{N_1} (h_1, \nu_1) < E_{N_2} (h_2, \nu_1) \) and \( i = 0 \)
Print \( E_{N_2} (h_2, \nu_2) \). Break.

**Step 6.** Else if \( E_{N_1} (h_1, \nu_1) > E_{N_2} (h_2, \nu_1) \)
Insert the \( \nu_1 \) in the Eq. (13). Obtain new values for \( \mu_2 \).
Solve the equation \( (N, \nu_1, \nu_1) = \mu_2 \). This derives a new
value for \( \nu_1, i = i + 1 \). Go to step 4.

**Step 7.** Write,

\[
\nu_1^{2i} E_{N_2}^{i-1} + \nu_2^{2i} E_{N_2}^i
\]

Note that \( E_N^i \equiv E_N (h, \mu) = E_{ni} [h, \mu (N, l, \nu)] \) of \( i^{th} \)
iteration. \( n = 1, 2, 3, ..., l = n - 1 \), represent the corre-
sponding energy state. \( \nu_1^{2i}, \nu_2^{2i} \) represent \( i^{th} \) values of \( \nu_1 \) and \( \nu_2 \) for grid–points \( N_1, N_2 \) with \( p = 1 \) or \( p = 2 \),
respectively. \( h_1 \) and \( h_2 \) are the grid–sizes for the corre-
sponding energy eigenvalues in \( N_1, N_2 \). The convergence
properties and the algorithm of the procedure with an explicit
application are given in the Figures 1, 2.

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**IV. EXAMPLE: HYDROGEN–LIKE ATOMS**

The radial Schrödinger equation for an electron in a
spherically symmetric potential has the following form

\[
\hat{H}_r \Psi (r) = E_r \Psi (r),
\]

where,

\[
\hat{H}_r = -\frac{1}{2} \left( \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} \right) + \frac{1}{r},
\]

is the one–electron Hamilton operator [in atomic units
(a. u.); \( h = 1, m = 1 \) and \( e^2/4\pi \varepsilon_0 = 1 \)]. Note that, the
Eq. (16) depends upon \( l \) yet, the exact solution of the
Eq. (15) with \( \hat{H}_r \) for hydrogen atom is \( n^2–fold \) degen-
erate. It is referred to as **accidental degeneracy**. The dis-
cussion on the origin of such degeneracy for hydrogen
atom is treated rigorously in [62]. The results obtained
from numerical solution of the Schrödinger equation
using the standard Numerov’s method for \( \hat{H}_r \) operator do
not posses \( n^2–fold \) degeneracy (see the following section
for more detail). The Numerov’s method with a modified
effective potential on the other hand, reveals the **acciden-
tal degeneracy**.

In order to apply the Numerov method with a modified
effective potential, the Eq. (15) is transformed into a
linear finite–difference equation. The effective potential
is defined as,

\[
V' \equiv V_{eff} (r) = \frac{1}{2} \left[ \frac{(l+1)}{r^2} + \frac{1}{r^{1-\mu}} \right].
\]

The standard Numerov algorithm given in the Eq. 3
is used in following. The resulting equation can be rear-
 ranged into the following form \( (\Psi \equiv \Psi (r)) \) [51 58].

\[
-\frac{1}{2} \left( \Psi_{i-1} - 2\Psi_i + \Psi_{i+1} \right)
\]

\[
+ \frac{1}{h^2} \left( V'_{i-1} \Psi_{i-1} + 10V' \Psi_i + V'_{i+1} \Psi_{i+1} \right)
\]

\[
= E (\Psi_{i-1} + 10\Psi_i + \Psi_{i+1}).
\]

**N** equations of the linear system given above in the matrix
form are written as,

\[
-\frac{1}{2} A \Psi + B V' \Psi = EB \Psi,
\]

where, \( \Psi \) as the column vector \( \left( ...\Psi_{i-1}, \Psi_i, \Psi_{i+1}... \right) \),
\( A = (I_1 + 2I_0 + I_1)/h^2, \) \( B = (I_1 - 2I_0 + I_1)/2, \)
\( V' = \text{diag} (V'_{i-1}, V', V'_{i+1},...) \), \( I_p \) is a matrix of \( 1 \)s along the
\( pth \) diagonal and zero elsewhere. The boundary condi-
tions \( \Psi (0) = \Psi (R) = 0 \) for some large \( R \) are imple-
mented by taking \( N \times N \) sub–matrices of \( A \) and \( B \). The
optimized values of \( h \) is obtained by minimizing the en-
ergy eigenvalues. Then, the solution for \( \Psi \) is found at the
interval \( [0, R], R = N \times h \).
V. RESULTS AND DISCUSSIONS

The modified Numerov algorithm proposed in the present paper is based on the potential function has a screening parameter, $\mu$. Such a potential is first suggested to calculate the matrix elements of molecular properties such as quadrupole coupling tensor, electron–photon hyperfine interaction, chemical shift and spin–orbit coupling [63]. Later on, an exponential function was embedded into this potential function [64]. It was referred to as non–central interaction potential [65]. This type of potential was used to improve Hartree–Fock self–consistent field calculations [67]. It is on the other hand, obvious that the real values of $\mu$ may cause variational instability.

Based on the perspective of numerical integration, the aforementioned method in this study regards $\mu$ as a function enables the exact value for the second order derivative of $\psi(x)$ to be acquired at a finite number of grid–points. The function $\mu$ is chosen depending on the conditions given in the Eq. (10) and the Eq. (14). The values of $\mu$ functions for certain number of grid–point are determined through the Eqs. (12) [66]. The Eqs. (12) depend on the angular momentum quantum number $l$ and their values significantly decrease by increasing the $l$.

The energy eigenvalues are usually calculated by requiring the eigen–functions to satisfy certain boundary conditions [68]. The method presented in this study avoids dependence of energy eigenvalues to the eigen–functions. It suggests first to calculate the eigenvalues. The corresponding eigen–functions are then calculated easily. In this case all the energy eigenvalues should be tried up to a certain precision. This approximation was used previously in [65]. An infinite potential barrier at some radius $C$ added to a potential. The correct eigenvalue is then obtained in the limit $C \rightarrow \infty$. It is referred to as hardwall method. The number of significant digits provided by this method is limited to a few. In this work, an explicit function that satisfy the conditions given in the Eqs. (10) is alternatively added to the potential. The presented algorithm provides arbitrary number of significant digit because the range of values of $\mu$ indicates where the exact energy eigenvalue is (see Figure 2). This yields the variational instability to be eliminated as well. The parameter $\mu$ in the non–central interaction potential free from restriction and the energy eigenvalues are unbounded from below unless the Eqs. (10) are taken into account.

![Figure 1](image_url)

**FIG. 1.** Results for the 4s electronic energy state depending on the upper limit of summation ($N$) in atomic units (a. u.). The dotted, dashed, dot–dashed and black lines represents $E(h, \nu_1)$ with values of $\nu_1$ obtained from $2^{th}$ ($i = 2$), $3^{th}$ ($i = 3$), $4^{th}$ ($i = 4$), $5^{th}$ ($i = 5$) iterations, respectively.

The time–independent one–dimensional Schrödinger equation given in the previous section is solved as a sample. The method of solution has been incorporated into a computer program written in the Mathematica programming language. Variationally optimum values for the grid–size $h$ are used in calculations. The optimization procedure is implemented in order to test stability of the suggested method.

Results for the 4s electronic energy state of hydrogen atom depending on the upper limit of summation ($N$) are given in the Figure 1. This figure demonstrates how the correct energy eigenvalues to be found by using the procedure presented in the Section III. It can be seen from this Figure that, the first four iterations convergence from above while the fifth convergences from below. This convergence property exposes at which iteration the algorithm should decide to stop. The algorithm of the procedure with an application for ground state energy calculation is given in the Figure 2.
states are presented. The matrix form approach is used to solve the Eq. (4) for Coulomb and screened Coulomb potentials, respectively. They are compared with the results given in [5] obtained via Richardson’s extrapolation and with the results obtained via band matrix technique that recently have been published in [69]. The most accurate results that the standard Numerov method with error term is of order $O(h^4)$ can provide, were presented in [69]. The eigenvalue problem for large matrices must be overcome for such work. The modified subroutines from the LINPACK library: dgbsl.f, dgbfa.f were accordingly, performed in [69]. Fairly large number
of grid—points (i.e., \( \approx 25000 \)) were used. It was reported that the Numerov’s method for \( s \) state with error term only is of order \( \mathcal{O}(h^2) \) due to singularity of Coulomb potential. Note that, for the \( p \) states is \( \mathcal{O}(h^3) \) and for the \( d \) states is \( \mathcal{O}(h^4) \).

The results given in the Tables [11][11] are presented for \( s \) states, accordingly. Although less number of grid—points are used, more accurate than the ones presented in both Table [11] and [69] are given the Table [11]. In this table, instead of using large number of grid—points as in [69], the range of values of \( \nu \) are reduced. The following conclusions are achieved consequently:

- The method suggested in this study accelerating the convergence of numerical power series related with the Numerov method.
- Difficulty of obtaining the eigenvalues for large matrices is eliminated.
- The standart Numerov method is limited to error term is of order \( \mathcal{O}(h^5) \). Table [11] show that, the technique developed here, improves the accuracy for any energy state. It permits to find the energy eigenvalues with more then \( \mathcal{O}(h^4) \) even for potential with a singularity.
- Extension of the Numerov method to error term is of arbitrary order is problematic because \( B^{-1}A \) in the Eq. (19) is not sparse and not symmetric [33]. Such necessity may also be eliminated. Instead, the range of values of \( \nu \) may be further constrained.

Solution of Hartree–Fock equations for atoms and molecules provides essential input information in investigating the internal structures and reaction dynamics of complex systems in fields like condensed matter physics, quantum chemistry, and plasma physics. [71][73]. The Hartree–Fock equations are solved by self–consistent field method. It is an iterative solution obtained by rewriting each Hartree–Fock equation in the form of the Schrödinger equation with the non–local potential. In addition to field of studies referred in the Section [1], the convergence acceleration method for numerical power series suggested in this work is also useful to improve the numerical solutions for Hartree–Fock equations.

The computational aspect of the formulae given in the present work for numerical calculation of the two– and three–dimensional Schrödinger equations will be the subject of the next work.

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