Numerical solution of Schroedinger equation using matrix Numerov method with Woods - Saxon potential

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Introduction

The Woods-Saxon potential has taken a great deal of interest over the years and has been one of the most useful model to determine the single particle energy levels of nuclei and the nucleus-nucleus interactions [1]. The Woods-Saxon potential is given by

$$V(r) = -\frac{V_0}{1 + e^{(\frac{r-R}{a})}}$$

where V_0 represent the depth of the potential. R and a are the radius of the potential and the width of the surface diffuseness, respectively.

In this work we have considered Woods-Saxon potential for the numerical calculation of eigenvalues by using matrix Numerov method [2].

Theory

Numerovs method is a numerical method developed by Boris Vasilevich Numerov [3, 4]. This method is used to solve ordinary differential equations of second order in which the first-order term does not appear, which is given by

$$\frac{d^2\psi(x)}{dx^2} = f(x)\psi(x) \tag{1}$$

The time independent 1−D Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{2}$$

can be written into the form of (1) as

$$\psi^{(2)}(x) = -\frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = f(x)\psi(x) \tag{3}$$

Where

$$\psi^{(n)}(x) = \frac{d^n\psi(x)}{dx^n}, \quad f(x) = -\frac{2m}{\hbar^2}\left[E - V(x)\right]$$

Numerov's method is a fourth-order linear multi step method. The three term recurrence formula

$$f_i\psi_i = \frac{\psi_{i+1} + psi_{i-1} - 2\psi_i}{d^2} - \frac{1}{12}\left(f_{i+1}\psi_{i+1} + f_{i-1}\psi_{i-1} - 2f_i\psi_i\right) \tag{4}$$

is called the Numerov method for efficient solution of type (1) on a discrete mesh point with variable step-size d of the form $d = x_n - x_{n-1}, n = 0, 1, \cdots, N$.
Where

$$f_{i-1} = f(x-d), \quad f_i = f(x), \quad f_{i+1} = f(x+d)$$
$$\psi_{i-1} = \psi(x-d), \quad \psi_i = \psi(x), \quad \psi_{i-1} = \psi(x-d)$$

Rearranging we have

$$\frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{d^2} = \frac{1}{12}\left(f_{i+1}\psi_{i+1} + f_{i-1}\psi_{i-1} + 10f_i\psi_i\right) \tag{5}$$

Recall that

$$f_{i-1} = -\frac{2m}{\hbar^2}\left(E - V_{i-1}\right), \quad f_i = -\frac{2m}{\hbar^2}\left(E - V_i\right)$$
$$f_{i+1} = -\frac{2m}{\hbar^2}\left(E - V_{i+1}\right)$$

We have

$$-\frac{\hbar^2}{2m}\frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{d^2} + \frac{V_{i-1}\psi_{i-1} + 10V_i\psi_i + V_{i+1}\psi_{i+1}}{12} = E\left[\frac{\psi_{i-1} + 10\psi_i + \psi_{i+1}}{12}\right] \tag{6}$$

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It follows that

$$-\frac{\hbar^2}{2m}A\psi + BV\psi = EB\psi \qquad (7)$$

Where

$$A = \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & -2 & 1 & 0 & 0 & \cdot & \cdot \\ 0 & 1 & -2 & 1 & 0 & \cdot & \cdot \\ 0 & 0 & 1 & -2 & 1 & \cdot & \cdot \\ 0 & 0 & 0 & 1 & -2 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$B = \frac{1}{12}\begin{pmatrix} 10 & 1 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & 10 & 1 & 0 & 0 & \cdot & \cdot \\ 0 & 1 & 10 & 1 & 0 & \cdot & \cdot \\ 0 & 0 & 1 & 10 & 1 & \cdot & \cdot \\ 0 & 0 & 0 & 1 & 10 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$V = \begin{pmatrix} V_1 & 0 & 0 & 0 & 0 & \cdot & \cdot \\ 0 & V_2 & 0 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & V_3 & 0 & 0 & \cdot & \cdot \\ 0 & 0 & 0 & V_4 & 0 & \cdot & \cdot \\ 0 & 0 & 0 & 0 & V_5 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \\ \cdot \end{pmatrix}$$

Multiplying both sides by B^{-1}, we get

$$-\frac{\hbar^2}{2m}B^{-1}A\psi + V\psi = E\psi \qquad (8)$$

which is of the form

$$H\psi = E\psi, \quad H = -\frac{\hbar^2}{2m}B^{-1}A + V \qquad (9)$$

Results and Conclusion

We have solved the Schroedinger equation for the Woods-Saxon potential which is given by

$$V(r) = -\frac{V_0}{1 + e^{(\frac{r-R}{a})}}$$

where V_0 (having dimension of energy) represents the potential well depth. We have used the following parameters : V_0 = 50 MeV, a =0.6 fm and R = 8 fm in our calculation. After substituting the Woods-saxon potential in Eq. 9, we get

$$H = -\frac{\hbar^2}{2m}B^{-1}A - \frac{V_0}{1 + e^{(\frac{r-R}{a})}}$$

We diagonalize the above matrix to obtain the corresponding eigenvalues of the Schroedinger equation for the Woods-Saxon potential. We have developed a mathematica code to calculate the eigenvalues and eigenfunctions of the Schroedinger equation numerically for Woods-Saxon Potential using matrix Numerov method. The table I lists the corresponding eigenvalues obtained by this method.

TABLE I: Numerical results for the quantized energies of the Woods-Saxon potential.

n	Eigenvalue(MeV)
1	-49.9871
2	-49.9484
3	-49.8843
4	-49.7951
5	-49.6812
6	-49.5429

References

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