A New and Simpler Method of Calculating Approximate Energies of Bound-State Potentials using the WKB Approximation

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Abstract

In this article, we discuss a new and simpler method employed to determine the approximate energies of certain bound-state potentials using the WKB approximation. In this method, the potentials are represented by a finite number of equally spaced rectangular step functions. The energy for each step is calculated using the Bohr-Sommerfeld quantization condition $\int pdx = \left(n + \frac{1}{2}\right)\hbar\pi$, where 'p' is the classical momentum and 'n' is a quantum number. The, the total energy would be the sum of the energies determined for all steps in the potential. Specifically, we have determined the approximate energies for the Simple Harmonic Potential, The Double-Ramp Potential and the Quartic Potential. However, this method can be extended, in general, to any bound-state potential.

Keywords: Schrodinger equation, WKB approximation, Bohr-Sommerfeld quantization, Bound-State potential.

1. Introduction

All problems in Non-Relativistic Quantum Mechanics cannot be solved exactly using the Schrodinger equation and therefore one has to resort to approximate methods of solving the same. Some of the well known and commonly used methods are the Perturbation theory, the WKB approximation and the Rayleigh-Ritz Variational Method. We focus on the WKB approximation in this article as it is particularly useful for calculating allowed energies of bound-state potentials. In particular, from the solutions of the WKB wave function, one can arrive at the Bohr-Sommerfeld quantization rule. This is a powerful result as it enables us to determine the approximate allowed energies without having to solve the Schrodinger equation. However, for complex potentials, the integrals become hard to solve. In this article, we present a simpler method in which the integrals encountered in the bound-state potentials are easily solved. We consider three such potentials, namely, the Simple Harmonic potential, the Double-Ramp potential and the Quartic potential. For the sake of convenience, we assume the potentials in this article to be a function of position only. Each of them is represented by a finite number of equally spaced rectangular step functions. The simple harmonic potential and the double-ramp potential have been represented by three, five and seven steps and the quartic potential has been represented by three and five steps. In general, the energy for each step has been determined and the total energy is the sum of the energies determined for each step.

This paper is organized as follows: in Sections 2, 3 and 4 we discuss the allowed energies for the simple harmonic potential, the double-ramp potential and the quartic potential respectively, Section 5 is dedicated to the discussion of results and in Section 6 we express our acknowledgements.

2. Simple Harmonic Potential

We choose to solve the simple harmonic potential first as it is frequently encountered in the literature. Using the standard WKB method, the exact allowed energies for this potential can be obtained. The potential of a simple harmonic oscillator is given by

$$V = \frac{1}{2} m\omega^2 x^2$$

where 'm' is the mass, 'ω' is the angular frequency and 'x' is the position. At the turning points $V = E$ and let $x = A$,

$$V = E = \frac{1}{2} m\omega^2 A^2$$

Solving for

$$A = \left[\frac{2E}{m\omega^2}\right]^{\frac{1}{2}}$$

The potential is now approximated by a finite number of rectangular steps. Consider the potential to be approximated by three steps as shown below.

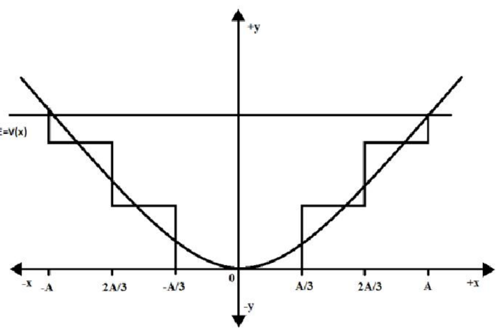

Figure 1: Simple Harmonic Potential approximated by three steps

From equation (2), the potentials at different steps are given by

$$V_1 = \frac{1}{2}m\omega^2\left(\frac{A}{6}\right)^2,$$

$$V_2 = \frac{1}{2}m\omega^2\left(\frac{A}{2}\right)^2,$$

$$V_3 = \frac{1}{2}m\omega^2\left(\frac{5A}{6}\right)^2$$

As $p(x) = [2m\{E - V(x)\}]^{1/2}$ the Bohr-Sommerfeld quantization condition can be written as $\int [2m\{E - V(x)\}]^{1/2}\,dx = \left(n + \frac{1}{2}\right)\hbar\pi$(3)

For the simple harmonic potential as approximated above, we write equation (3) as

$$\int_{-A}^{-5A/6} \sqrt{2m(E - V_3(x))}\,dx + \int_{-5A/6}^{-2A/3} \sqrt{2m(E - V_3(x))}dx + \int_{-2A/3}^{-A/2} \sqrt{2m(E - V_2(x))}dx + \int_{-A/2}^{-A/3} \sqrt{2m(E - V_2(x))}dx + \int_{-A/3}^{-A/6} \sqrt{2m(E - V_1(x))}dx + \int_{-A/6}^{0} \sqrt{2m(E - V_1(x))}dx + \int_{0}^{A/6} \sqrt{2m(E - V_1(x))}dx + \int_{A/6}^{A/3} \sqrt{2m(E - V_1(x))}dx + \int_{A/3}^{A/2} \sqrt{2m(E - V_2(x))}dx + \int_{A/2}^{2A/3} \sqrt{2m(E - V_2(x))}dx + \int_{2A/3}^{5A/6} \sqrt{2m(E - V_3(x))}dx + \int_{5A/6}^{A} \sqrt{2m(E - V_3(x))}dx = \left(n + \frac{1}{2}\right)\hbar\pi$$

Solving the integrals we get,

$$\sqrt{(2m(E-V_3)}\left[\frac{-5A}{6}+A\right]+\sqrt{2m(E-V_3)}\left[\frac{-2A}{3}+\frac{5A}{6}\right]+\sqrt{2m(E-V_2)}\left[\frac{-A}{2}+\frac{2A}{3}\right]$$
$$+\sqrt{2m(E-V_2)}\left[\frac{-A}{3}+\frac{A}{2}\right]+\sqrt{2m(E-V_1)}\left[\frac{-A}{6}+\frac{A}{3}\right]+\sqrt{2m(E-V_1)}\left[\frac{A}{6}\right]$$
$$+\sqrt{2m(E-V_1)}\left[\frac{A}{6}\right]+\sqrt{2m(E-V_1)}\left[\frac{A}{3}-\frac{A}{6}\right]+\sqrt{2m(E-V_2)}\left[\frac{A}{2}-\frac{A}{3}\right]$$
$$+\sqrt{2m(E-V_2)}\left[\frac{2A}{3}-\frac{A}{2}\right]+\sqrt{2m(E-V_3)}\left[\frac{5A}{6}-\frac{2A}{3}\right]+\sqrt{2m(E-V_3)}\left[A-\frac{5A}{6}\right]$$
$$=\left(n+\frac{1}{2}\right)\hbar\pi$$

Simplifying the above we get,

$$\frac{2A}{3}\sqrt{2m(E-V_3)}+\frac{2A}{3}\sqrt{2m(E-V_2)}+\frac{2A}{3}\sqrt{2m(E-V_1)}=\left(n+\frac{1}{2}\right)\hbar\pi$$

$$\frac{2A}{3}(2mE)^{1/2}\left[\left(1-\frac{V_3}{E}\right)^{1/2}+\left(1-\frac{V_2}{E}\right)^{1/2}+\left(1-\frac{V_1}{E}\right)^{1/2}\right]=\left(n+\frac{1}{2}\right)\hbar\pi$$

Using the forms of V_1, V_2 and V_3 in the above equation, we get

$$\frac{2A}{3}(2mE)^{\frac{1}{2}}\left[\left(1-\frac{25}{36}\right)^{\frac{1}{2}}+\left(1-\frac{1}{4}\right)^{\frac{1}{2}}+\left(1-\frac{1}{36}\right)^{\frac{1}{2}}\right]=\left(n+\frac{1}{2}\right)\hbar\pi$$

Substituting for A from equation (2) in the above equation, we get,

$$\frac{4E}{3\omega}(3.206045)=\left(n+\frac{1}{2}\right)\hbar\pi$$

Simplifying the above equation for E, we get

$$E=0.7349\left(n+\tfrac{1}{2}\right)\hbar\omega \qquad (4)$$

Now let us consider the potential to be approximated by five steps. The Bohr-Sommerfeld quantization rule would be now be written as

$$\int_{-A}^{-9A/10} \sqrt{2m(E - V_5(x))}\, dx + \int_{-9A/10}^{-4A/5} \sqrt{2m(E - V_5(x))}\, dx + \int_{-4A/5}^{-7A/10} \sqrt{2m(E - V_4(x))}\, dx$$
$$+ \int_{-7A/10}^{-3A/5} \sqrt{2m(E - V_4(x))}\, dx + \int_{-3A/5}^{-5A/10} \sqrt{2m(E - V_3(x))}\, dx + \int_{-5A/10}^{-2A/5} \sqrt{2m(E - V_3(x))}\, dx$$
$$+ \int_{-2A/5}^{-3A/10} \sqrt{2m(E - V_2(x))}\, dx + \int_{-3A/10}^{-A/5} \sqrt{2m(E - V_2(x))}\, dx + \int_{-A/5}^{-A/10} \sqrt{2m(E - V_1(x))}\, dx$$
$$+ \int_{-A/10}^{0} \sqrt{2m(E - V_1(x))}\, dx + \int_{0}^{A/10} \sqrt{2m(E - V_1(x))}\, dx + \int_{A/10}^{A/5} \sqrt{2m(E - V_1(x))}\, dx$$
$$+ \int_{A/5}^{3A/10} \sqrt{2m(E - V_2(x))}\, dx + \int_{3A/10}^{2A/5} \sqrt{2m(E - V_2(x))}\, dx + \int_{2A/5}^{5A/10} \sqrt{2m(E - V_3(x))}\, dx$$
$$+ \int_{5A/10}^{3A/5} \sqrt{2m(E - V_3(x))}\, dx + \int_{3A/5}^{7A/10} \sqrt{2m(E - V_4(x))}\, dx + \int_{7A/10}^{4A/5} \sqrt{2m(E - V_4(x))}\, dx$$
$$+ \int_{4A/5}^{9A/10} \sqrt{2m(E - V_5(x))}\, dx + \int_{9A/10}^{A} \sqrt{2m(E - V_5(x))}\, dx = \left(n + \frac{1}{2}\right)\pi\hbar$$

where

$$V_1 = \frac{1}{2}m\omega^2\left(\frac{A}{10}\right)^2, V_2 = \frac{1}{2}m\omega^2\left(\frac{3A}{10}\right)^2,$$

$$V_3 = \frac{1}{2}m\omega^2\left(\frac{5A}{10}\right)^2, \qquad V_4 = \frac{1}{2}m\omega^2\left(\frac{7A}{10}\right)^2 \; V_5 = \frac{1}{2}m\omega^2\left(\frac{9A}{10}\right)^2$$

Solving the integrals we get,

$$\sqrt{2mE}\left[\left(1-\frac{V_1}{E}\right)\left(\frac{A}{10}+\frac{A}{5}-\frac{A}{10}+\frac{A}{10}-\frac{A}{10}+\frac{A}{5}\right)+\left(1-\frac{V_2}{E}\right)\left(\frac{3A}{10}-\frac{A}{5}+\frac{2A}{5}-\frac{3A}{10}-\frac{A}{5}+\frac{3A}{10}-\frac{3A}{10}+\frac{2A}{5}\right)\right.$$
$$+\left(1-\frac{V_3}{E}\right)\left(\frac{5A}{10}-\frac{2A}{5}+\frac{3A}{5}-\frac{5A}{10}-\frac{5A}{10}+\frac{3A}{5}-\frac{2A}{5}+\frac{5A}{10}\right)$$
$$+\left(1-\frac{V_4}{E}\right)\left(\frac{7A}{10}-\frac{3A}{5}+\frac{4A}{5}-\frac{7A}{10}-\frac{3A}{5}+\frac{7A}{10}-\frac{7A}{10}+\frac{4A}{5}\right)$$
$$\left.+\left(1-\frac{V_5}{E}\right)\left(\frac{9A}{10}-\frac{4A}{5}+A-\frac{9A}{10}-\frac{9A}{10}+A-\frac{4A}{5}+\frac{9A}{10}\right)\right]=\left(n+\frac{1}{2}\right)\hbar\pi$$

Simplifying the above we get,

$$\sqrt{2mE}\left[\left(1-\frac{V_1}{E}\right)\frac{2A}{5}+\left(1-\frac{V_2}{E}\right)\frac{2A}{5}+\left(1-\frac{V_3}{E}\right)\frac{2A}{5}+\left(1-\frac{V_4}{E}\right)\frac{2A}{5}+\left(1-\frac{V_5}{E}\right)\frac{2A}{5}\right]=\left(n+\frac{1}{2}\right)\hbar\pi$$

Using the forms of V_1, V_2, V_3, V_4 and V_5 in the above equation, we get

$$\frac{2A}{5}\sqrt{2mE}\left[\left(1-\frac{1}{100}\right)+\left(1-\frac{9}{100}\right)+\left(1-\frac{25}{100}\right)+\left(1-\frac{49}{100}\right)+\left(1-\frac{81}{100}\right)\right]=\left(n+\frac{1}{2}\right)\hbar\pi$$

or

$$\frac{4E}{5\omega}\left[\left(\frac{99}{100}\right)^{1/2}+\left(\frac{91}{100}\right)^{1/2}+\left(\frac{75}{100}\right)^{1/2}+\left(\frac{51}{100}\right)^{1/2}\left(\frac{19}{100}\right)^{1/2}\right]=\left(n+\frac{1}{2}\right)\hbar\pi$$

Simplifying the above equation for E, we get

$$E=0.99066\left(n+\tfrac{1}{2}\right)\hbar\omega \qquad (5)$$

Now let us consider the potential to be approximated by seven steps. The Bohr-Sommerfeld quantization rule would be now be written as

$$\int_{-A}^{-13A/14} \sqrt{2m(E-V_7(x))}\,dx + \int_{-13A/14}^{-6A/7} \sqrt{2m(E-V_7(x))}\,dx + \int_{-6A/7}^{-11A/14} \sqrt{2m(E-V_6(x))}\,dx$$
$$+ \int_{-11A/14}^{-5A/7} \sqrt{2m(E-V_6(x))}\,dx + \int_{-5A/7}^{-9A/14} \sqrt{2m(E-V_5(x))}\,dx + \int_{-9A/14}^{-4A/7} \sqrt{2m(E-V_5(x))}\,dx$$
$$+ \int_{-4A/7}^{-A/2} \sqrt{2m(E-V_4(x))}\,dx + \int_{-A/2}^{-3A/7} \sqrt{2m(E-V_4(x))}\,dx + \int_{-3A/7}^{-5A/14} \sqrt{2m(E-V_3(x))}\,dx$$
$$+ \int_{-5A/14}^{-2A/7} \sqrt{2m(E-V_3(x))}\,dx + \int_{-2A/7}^{-3A/14} \sqrt{2m(E-V_2(x))}\,dx + \int_{-3A/14}^{-A/7} \sqrt{2m(E-V_2(x))}\,dx$$
$$+ \int_{-A/7}^{-A/14} \sqrt{2m(E-V_1(x))}\,dx + \int_{-A/14}^{0} \sqrt{2m(E-V_1(x))}\,dx + \int_{0}^{A/14} \sqrt{2m(E-V_1(x))}\,dx$$
$$+ \int_{A/14}^{A/7} \sqrt{2m(E-V_1(x))}\,dx + \int_{A/7}^{3A/14} \sqrt{2m(E-V_2(x))}\,dx + \int_{3A/14}^{2A/7} \sqrt{2m(E-V_2(x))}\,dx$$
$$+ \int_{2A/7}^{5A/14} \sqrt{2m(E-V_3(x))}\,dx + \int_{5A/14}^{3A/7} \sqrt{2m(E-V_3(x))}\,dx + \int_{3A/7}^{A/2} \sqrt{2m(E-V_4(x))}\,dx$$
$$+ \int_{A/2}^{4A/7} \sqrt{2m(E-V_4(x))}\,dx + \int_{4A/7}^{9A/14} \sqrt{2m(E-V_5(x))}\,dx + \int_{9A/14}^{5A/7} \sqrt{2m(E-V_5(x))}\,dx$$
$$+ \int_{5A/7}^{11A/14} \sqrt{2m(E-V_6(x))}\,dx + \int_{11A/14}^{6A/7} \sqrt{2m(E-V_6(x))}\,dx + \int_{6A/7}^{13A/14} \sqrt{2m(E-V_7(x))}$$
$$+ \int_{13A/14}^{A} \sqrt{2m(E-V_7(x))} = \left(n+\frac{1}{2}\right)\hbar\pi$$

where $V_1 = \frac{1}{2}m\omega^2\left(\frac{A}{14}\right)^2, V_2 = \frac{1}{2}m\omega^2\left(\frac{3A}{14}\right)^2, V_3 = \frac{1}{2}m\omega^2\left(\frac{5A}{14}\right)^2, V_4 = \frac{1}{2}m\omega^2\left(\frac{A}{2}\right)^2$

$$V_5 = \frac{1}{2}m\omega^2\left(\frac{9A}{14}\right)^2, V_6 = \frac{1}{2}m\omega^2\left(\frac{11A}{14}\right)^2, V_7 = \frac{1}{2}m\omega^2\left(\frac{13A}{14}\right)^2$$

Simplifying in a similar way as done in the three steps and five steps, we obtain

$$E = 0.9941\left(n + \frac{1}{2}\right)\hbar\omega$$

3.The Double-Ramp Potential

The Double-Ramp potential or also called the Gravitational Potential is given by

$$V = mg|x|$$

At turning points; $E = V$

$$E = mg|x|$$

$$x = \frac{E}{mg} \qquad (7)$$

Consider the potential to be approximated by three steps as shown below.

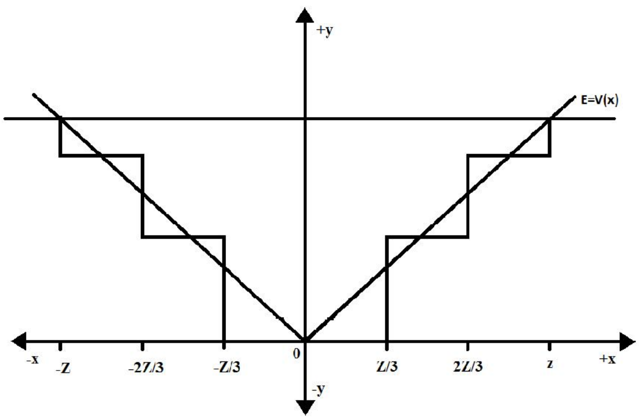

Figure 2: The Double-Ramp Potential approximated by three steps.

From equation (7), the potentials at different steps are given by

$$V_1 = mg\left|\frac{x}{6}\right|;\ V_2 = mg\left|\frac{x}{2}\right|; V_3 = mg\left|\frac{5x}{6}\right|$$

The Bohr-Sommerfeld quantization condition is written as,

$$\int_{-Z}^{-5Z/6} \sqrt{2m(E-V_3(x))}\,dx + \int_{-5Z/6}^{-2Z/3} \sqrt{2m(E-V_3(x))}\,dx + \int_{-2Z/3}^{-Z/2} \sqrt{2m(E-V_2(x))}\,dx$$
$$+ \int_{-Z/2}^{-Z/3} \sqrt{2m(E-V_2(x))}\,dx + \int_{-Z/3}^{-Z/6} \sqrt{2m(E-V_1(x))}\,dx + \int_{-Z/6}^{0} \sqrt{2m(E-V_1(x))}\,dx$$
$$+ \int_{0}^{Z/6} \sqrt{2m(E-V_1(x))}\,dx + \int_{Z/6}^{Z/3} \sqrt{2m(E-V_1(x))}\,dx + \int_{Z/3}^{Z/2} \sqrt{2m(E-V_2(x))}\,dx$$
$$+ \int_{Z/2}^{2Z/3} \sqrt{2m(E-V_2(x))}\,dx + \int_{2z/3}^{5Z/6} \sqrt{2m(E-V_3(x))}\,dx + \int_{5z/6}^{z} \sqrt{2m(E-V_3(x))}\,dx$$
$$= \left(n+\frac{1}{2}\right)\hbar\pi$$

Simplifying in the same way as in Section 2, we get:

$$E = 0.649\left(n+\tfrac{1}{2}\right)^{2/3}(\pi^2\hbar^2 mg^2)^{1/3} \qquad (8)$$

Similarly, when the potential is approximated by 5 steps, we get:

$$E = 0.652\left(n+\tfrac{1}{2}\right)^{2/3}(\pi^2\hbar^2 mg^2)^{1/3} (9)$$

And when approximated by 7 steps, we get:

$$E = 0.653\left(n+\tfrac{1}{2}\right)^{2/3}(\pi^2\hbar^2 mg^2)^{1/3} (10)$$

4.The Quartic Potential.

The potential of a quartic oscillator is given by:
$V = \lambda x^4$

At turning points: $E = V$ and let $x = A$

$$E = \lambda A^4$$
$$A = \left(\frac{E}{\lambda}\right)^{1/4} \qquad (11)$$

Consider the potential to be approximated by three steps as shown below.

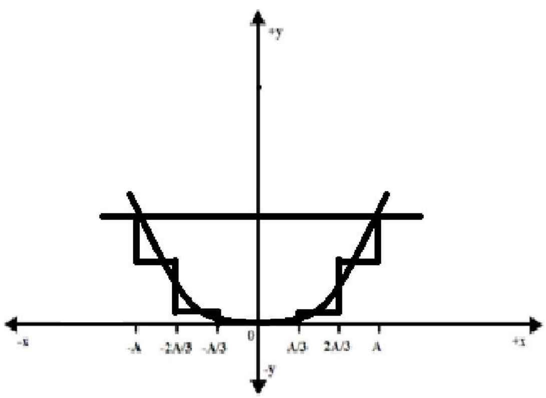

Figure 3: The Quartic Potential approximated by three steps.

From equation (11), the potentials at different steps are given by

$$V_1 = \lambda\left(\frac{A}{6}\right)^4 ;\ V_2 = \lambda\left(\frac{A}{2}\right)^4 ;\ V_3 = \lambda\left(\frac{5A}{6}\right)^4$$

The Bohr-Sommerfeld quantization condition is written as,

$$\int_{-A}^{-5A/6} \sqrt{2m(E - V_3(x))}\,dx + \int_{-5A/6}^{-2A/3} \sqrt{2m(E - V_3(x))}\,dx + \int_{-2A/3}^{-A/2} \sqrt{2m(E - V_2(x))}\,dx$$
$$+ \int_{-A/2}^{-A/3} \sqrt{2m(E - V_2(x))}\,dx + \int_{-A/3}^{-A/6} \sqrt{2m(E - V_1(x))}\,dx + \int_{-A/6}^{0} \sqrt{2m(E - V_1(x))}\,dx$$
$$+ \int_{0}^{A/6} \sqrt{2m(E - V_1(x))}\,dx + \int_{A/6}^{A/3} \sqrt{2m(E - V_1(x))}\,dx + \int_{A/3}^{A/2} \sqrt{2m(E - V_2(x))}\,dx$$
$$+ \int_{A/2}^{2A/3} \sqrt{2m(E - V_2(x))}\,dx + \int_{2A/3}^{5A/6} \sqrt{2m(E - V_3(x))}\,dx + \int_{5A/6}^{A} \sqrt{2m(E - V_3(x))}\,dx$$
$$= \left(n + \frac{1}{2}\right)\hbar\pi$$

Simplifying in the same way as in Sections 2 and 3, we get:

$$E = 0.289\left(n + \tfrac{1}{2}\right)^{4/3}\left(\frac{\hbar^4\pi^4\lambda}{m^2}\right)^{1/3} \qquad (12)$$

Similarly, when the potential is approximated by 5 steps, we get:

$$E = 0.29\left(n + \tfrac{1}{2}\right)^{4/3}\left(\frac{\hbar^4\pi^4\lambda}{m^2}\right)^{1/3} \qquad (13)$$

4.Results and Discussion.

At the very first glance, we see that the accuracy of the calculations increases as we increase the number of rectangular steps in each of the potentials. The best possible values of the approximate energies so obtained are summarized in the table below.

Simple harmonic potential	$E = 0.99066\left(n + \frac{1}{2}\right)\hbar\pi$

Quartic potential	$E = 0.29\left(n+\frac{1}{2}\right)^{\frac{4}{3}}\left(\frac{\hbar^4\pi^4\lambda}{m^2}\right)^{\frac{1}{3}}$
Gravitational potential	$E = 0.653\left(n+\frac{1}{2}\right)^{\frac{2}{3}}(\pi^2\hbar^2 m g^2)^{\frac{1}{3}}$

The potentials that we have discussed in this article are fairly simple. The method can also be extended to complex potentials of physical interest such as the Morse potential in Molecular Spectroscopy or the Wood-Saxon potential in Nuclear Physics and so on. The spacing between the rectangular steps and the number of steps can be appropriately varied, depending on the nature of the potential, to achieve the desired convergence of energy eigenvalues.

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