Testing the Bohr-Sommerfield Approximation for Various Oscillators

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ABSTRACT

Analogous to the classical situation of a spring connected to a ball and forced into a continuous periodic motion, a harmonic oscillator is a system in which an object is moved in an oscillatory fashion towards a center by a restoring force whose magnitude varies with position. This problem is generally modeled by solving an equation describing a particle's state developed by the Schrödinger. The results of this method have been repeatedly proven, both theoretically and experimentally, to be correct; however, the calculations are complex and time consuming. The much simpler Bohr-Sommerfield approximation has been shown to provide the same results for a certain system. We proceeded to use the approximation on oscillators of different non-zero potentials to test whether the results are consistent with the Schrödinger Equation.

I. Introduction

Quantum Mechanics is a realm of physics very different than the definite, continuous world we are used to. Through the works of many minds, the modern theory of quantum mechanics surfaced, based in the fundamental mathematical structures developed independently by Werner Heisenberg and Erwin Schrödinger. Despite the accuracy of the results given by this method, the complex nature of quantum mechanics still remains its biggest drawback. One way to challenge this is by modifying simpler methods to achieve the same results. Bohr proposed that the electrons in atoms could only exist in certain well-defined, stable orbits, which satisfied the Bohr-Sommerfield quantization condition,

$$\oint p \cdot dx = nh, \quad n \in \mathrm{N}$$

Where p is the momentum and x is the position coordinate of an electron in three-dimensional space; the integral is performed over some closed orbit in space {p, x}. Considering the electron as a wave with wavelength λ = h/p, this Bohr-Sommerfield quantization condition ensures that the wave is described by a function that is single-valued.

The energy of an oscillator is given by the equation

$$\frac{p^2}{2m}=E-V(x)$$

The simplest example of an oscillator would be the case in which the potential V(x) is zero. This would be a box in which a particle collides with a wall, meets an infinite potential and returns in the opposite direction with the same magnitude of momentum until it meets another similar wall. This situation is known as the infinite square well with magnitude of momentum p given by

$$p=\pm\sqrt{2mE}$$

The Bohr-Summerfield approximation is based on a realization that the units of plank's constant can be interpreted in a different manner. The units of plank’s constant h are

$$[h]=joules\cdot seconds$$

Where the units of a joule are

$$joule=(\frac{ml}{sec^2})l$$

It is apparent that the units of plank’s constant are equivalent to momentum multiplied by distance

$$h=(\frac{ml}{sec^2})l\cdot sec=(\frac{ml}{sec})l$$

This suggests that the integral of the momentum between the walls would be equivalent to plank's constant times a constant

$$nh=\int_0^L\sqrt{2mE}\,dx+\int_L^0(-\sqrt{2mE})dx=2L\sqrt{2mE}$$

It is an assumption related to the quantized nature of the miniscule world that the values of n will be whole numbers. Rearranging the equation to solve for the energy gives the result:

$$E_n=\frac{n^2h^2}{8mL^2}$$

To verify the result received by the Bohr-Summerfield method, the problem must be solved rigorously. The energy of the particle can be derived most accurately by using the Schrödinger equation.

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

Since the particle does not have potential energy while traversing the region between the two walls, V(x)=0.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$$

Rearranging the equation gives us

$$\frac{d^2\psi}{dx^2}=-\frac{-2mE}{\hbar^2}\psi$$

Since it is a second order differential equation, the wave function, ψ, will be of the form

$$\psi(x)=A\sin\sqrt{\frac{2mE}{\hbar^2}}\,x+B\cos\sqrt{\frac{2mE}{\hbar^2}}\,x$$

Using the fact that at the boundaries ψ is zero, the coefficient B must be zero, leaving

$$\psi(x)=A\sin\sqrt{\frac{2mE}{\hbar^2}}\,x$$

Since at the boundary, a distance L from the origin, has a zero value of ψ:

$$0=A\sin\sqrt{\frac{2mE}{\hbar^2}}\,L$$

For ψ to be equal to zero, either A must be zero, or sin must be taken of a multiple of π. Since the first would be a trivial, uninformative solution, the former is taken. Thus the following equation holds true

$$n\pi=\sqrt{\frac{2mE}{\hbar^2}}\,L$$

□ is defined in the following way

$$\hbar=\frac{h}{2\pi}$$

So, solving for energy yields

$$E_n = \frac{n^2 h^2}{8mL^2}$$

This is the definite quantum mechanical result.

The two methods arrive at exactly the same results for the simplest harmonic oscillator in the case of the potential energy function equating to zero when not at the barriers. Since the Bohr-Sommerfield method is mathematically simpler, it is natural to ask if this method, when modified, works for other particle systems with non-zero potential.

Firstly, the momentum is derived from the total energy and the potential.

$$p = \pm\sqrt{2m(E-V(x))}$$

The integral is then be generalized to

$$nh = 2\int_{x_1}^{x_2} \sqrt{2m(E-V(x))}\ dx$$

Where x_1 and x_2 are the end points, which can be found by solving for the positions where the momentum is zero. We assume that the momentum must be purely real.

To check whether or not the method holds for different functions of potential, the values for E in which n is an integer, calculated by using the Bohr-Summerfield method, are compared to the values given by the Schrödinger equation. In the calculations, $\hbar$ is equal to 1 to simplify the problem. Thus, h=2π. Solving the equation for n, we get

$$\frac{1}{\pi}\int_{x_1}^{x_2} \sqrt{2m(E-V(x))}\ dx = n$$

II. Calculations and Results

To calculate the results given by the Bohr-Sommerfield method, a program in Java using Eclipse was created with the following steps, with an accuracy of 5 decimal places.

1. Use Newton's method to approximate roots when V(x)=E
2. Loop through different E values
3. Integrate using mid-point approximation with roots as bounds
4. Check to see if value returned is an integer with an accuracy function

Using this program we calculated Energy level values for various different particle systems with non-zero potential.

Example 1

For the potential V(x),

$$V(x)=\frac{x^2}{2}$$

When plugged into the equation, and making the assumption that m=1, we end up with the integral,

$$\frac{1}{\pi}\int_{x_1}^{x_2}\sqrt{2E-x^2}\,dx=n$$

After running the program, the results we get for this particle system are

	n
E_1	0.00000
E_2	1.00000
E_3	2.00000
E_4	3.00000

We can see the general trend of E=n which is also consistent with Schrödinger's wave equation result.

Example 2

For the potential V(x),

$$V(x)=3x^4-8x^2$$

When plugged into the equation, and making the assumption that m=1, we end up with the integral,

$$\frac{1}{\pi}\int_{x_1}^{x_2}\sqrt{2E-6x^4+16x^2}\,dx=n$$

After running the program, the results we get for this particle system are

	n
E_1	-2.66194
E_2	-0.42968
E_3	1.44553
E_4	4.09841

However, when compared to the results given by the Schrödinger's wave equation (shown below) we see that these values are very different and leads us to believe that the Bohr-Sommerfield method does not work for this particle system.

	n
E_1	-2.16970
E_2	-1.40647
E_3	3.10247
E_4	7.08793

III. Conclusion

The Bohr-Sommerfield method fails to re-create the solutions given by Schrödinger's wave equation when tested for different non-zero potentials with the exception of several simple functions such as V(x)=x^2/2.