PH2255 Course:
Quantum Harmonic Oscillators

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Abstract

Every introduction into the paradigm of Quantum Mechanics culminates in the understanding of its mathematical cornerstone: the Schrödinger Equation. This equation governs the wave function of any system in quantum mechanics, which encapsulates all observable quantities of the system, most notably position and momentum. However, the Schrödinger equations themselves are not easily observable, or understood with day-to-day phenomena. To understand the effects of the Schrdinger equations, and the closely related Heisenberg Uncertainty Principles, we can apply the concepts of the classical harmonic oscillator (governed by Hooke's law) to the quantum realm. This allows us to understand the vibrational motion of atoms, and is one of very few quantum systems for which we can derive exact analytical solutions.

1 TISE and Hooke's Law

To begin our understanding of the quantum harmonic oscillator (QHM), we begin - as most analysis of quantum mechanics does - with the Schrödinger Equations, specifically the Time-Independent (TISE) form, in one dimension:

$$\frac{-\hbar^2}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

This notation uses the *nabla* function, as defined by $\nabla f(\vec{r}) = \frac{\partial f}{\partial \vec{r}}$. Next, we introduce our model of the atom as a harmonic oscillator. Hooke's law gives us a model for the force needed to extend or compress a spring by a distance x as $F = kx$. From this, by using simple differentiation, we can calculate the work done to compress the spring as $W = \frac{1}{2}kx^2$.

To apply this spring model to an atom, we first interpret the work done on the spring as the change in potential energy, ΔPE, and then assign it to the potential variable, $V(x)$, in one dimension. Next, we analyse the spring constant not as a classical characteristic of a spring's stiffness, but in terms of angular frequency, using $\omega = \sqrt{k/m}$:

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2 \tag{2}$$

Finally, by substituting Equation 2 into the potential variable in Equation 1, we obtain our Schrödinger equation for the system, where ω_c is used to denote the *classical* angular frequency of the system:

$$\frac{-\hbar^2}{2m}\nabla^2\psi(x) + \frac{1}{2}m\omega_c^2x^2\psi(x) = E\psi(x) \tag{3}$$

2 Reducing Dimensionality

To make analytical solutions easier, we substitute out our displacement variable x and energy variable E with dimensionless equivalents. To obtain a dimensionless variable y, we use a substitution with $a = \sqrt{\hbar/m\omega_c}$:

$$y = \frac{x}{a} = \sqrt{\frac{m\omega_c}{\hbar}} \cdot x \tag{4}$$

To obtain a dimensionless energy ε, we again use the reduced Planck constant:

$$\varepsilon = \frac{E}{\hbar\omega_c/2} \tag{5}$$

By substituting Equations 4 and 5 into Equation 3, we obtain a homogeneous formulation of the Schrödinger equation:

$$\nabla^2\psi(y) + (\varepsilon - y^2)\psi(y) = 0 \tag{6}$$

3 Boundary Conditions and Differential Equation Solution

Now that we have a homogeneous differential equation, intuition tells us that we need an understanding of the boundary conditions of the model. If we assume energy E to be finite, our substituted ε must be finite too, so in the boundary condition of y approaching infinities, our equation reduces to zero, as energy becomes negligible with the y^2 term:

$$\text{As } y \to \pm\infty \text{ then } \psi(y) \to 0 \tag{7}$$

Considering this asymptotic regime, we can begin to solve the differential equation with a trial solution $\psi(y) = y^n \cdot \exp(-y^2/2)$, for some positive n. We choose this trial solution, as we can see in Equation 6 that we need the function $\psi(y)$ to have some terms of $\psi(y)y^2$ (seen in the second term of the equation) when differentiated twice (seen in the first term of the equation). As exponentials survive differentiation, we use this trial solution. To solve the differential equation, we then differentiate the trial solution twice:

$$\psi(y)' = [ny^{n-1} + y^n(-y)] \cdot e^{-y^2/2} \tag{8}$$

$$\psi(y)'' = [n(n-1)y^{n-2} + ny^{n-1}(-y) - (n+1)y^n - y^{n+1}(-y)] \cdot e^{-y^2/2} \tag{9}$$

As we are considering the asymptotic regime, we can see that the higher order powers of y dominate over the smaller powers. From this, we can establish an inequality:

$$y^{n+2} \gg\sim y^{n-2}, \sim y^n \tag{10}$$

Having established this, we can simplify Equation 9:

$$\psi'' \approx y^{n+2}e^{-y^2/2} \tag{11}$$