Solution of the Time Independent Schrödinger Equation for the Quantum Mechanical Harmonic Oscillator © Thursday, May 16, 2024, by James Pate Williams, Jr.

The Hamiltonian is defined by the equation:

$$H = T + V$$

Where T is the kinetic energy and V is the potential energy. The classical Hamiltonian for the harmonic oscillator is given by:

$$H = \frac{p^2}{2m} + \frac{kx^2}{2}$$

where p is the linear momentum and k is Hooke's constant. Introducing the quantum mechanical momentum operator yields the Hamiltonian for the quantum mechanical harmonic oscillator:

$$H = -\frac{h^2}{8\pi^2 m} \frac{d^2}{dz^2} + \frac{m\omega^2 z^2}{2}$$

The time independent Schrödinger equation is:

$$-\frac{h^2}{8\pi^2 m}\frac{d^2\Psi}{dz^2} + \frac{m\omega^2 z^2}{2}\Psi = E\Psi$$

Now perform the transformation:

$$x = \alpha z, \alpha = \sqrt{\frac{4\pi^2 m\omega}{h^2}}, \lambda = \frac{4\pi E}{h\omega}, z = \frac{x}{\alpha}, \psi(x) = \Psi\left(\frac{z}{\alpha}\right)$$

$$\frac{d\psi}{dx} = \frac{dz}{dx} \frac{d\Psi}{dz} = \frac{1}{\alpha} \frac{d\Psi}{dz}$$

$$\frac{d^2\psi}{dx^2} = \frac{d^2z}{dx^2} \frac{d\Psi}{dz} + \frac{1}{\alpha^2} \frac{d^2\Psi}{dz^2} = \frac{1}{\alpha^2} \frac{d^2\Psi}{dz^2}$$

$$\frac{d^2\psi}{dx^2} + (\lambda - x^2)\psi = 0$$

$$\varphi(x) = e^{x^2/2}\psi(x)$$

$$\psi(x) = e^{-x^2/2}\varphi(x)$$

$$\frac{d\psi}{dx} = e^{-x^2/2} \frac{d\varphi}{dx} - xe^{-x^2/2}\varphi$$

$$e^{-x^{2}/2}\frac{d^{2}\varphi}{dx^{2}} - 2xe^{-x^{2}/2}\frac{d\varphi}{dx} - e^{-x^{2}/2}\varphi + x^{2}e^{-x^{2}/2}\varphi - x^{2}e^{-x^{2}/2}\varphi + \lambda e^{-x^{2}/2}\varphi = 0$$

$$\frac{d^{2}\varphi}{dx^{2}} - 2x\frac{d\varphi}{dx} + (\lambda - 1)\varphi = 0$$

Now we solve the previous equation using Frobenius' method using a special infinite power series:

$$\varphi(x) = x^{s} \sum_{n=0}^{\infty} a_{n} x^{n}$$

$$\frac{d\varphi}{dx} = \sum_{n=0}^{\infty} (n+s) a_{n} x^{n+s-1}$$

$$\frac{d^{2} \varphi}{dx^{2}} = \sum_{n=0}^{\infty} (n+s) (n+s-1) a_{n} x^{n+s-2}$$

$$\sum_{n=0}^{\infty} (n+s) (n+s-1) a_{n} x^{n+s-2} - 2 \sum_{n=0}^{\infty} (n+s) a_{n} x^{n+s} + (\lambda - 1) \sum_{n=0}^{\infty} a_{n} x^{n+s} = 0$$

$$-2s a_{0} x^{s} + (\lambda - 1) a_{n} x^{s} = 0$$

Assuming the series coefficients and variables are nonzero we have:

$$\lambda = -2s + 1 = 1, for \ s = 0, n = 0$$

$$\lambda = 2(s+1) + 1 = 3for \ s = 0, n = 1$$

$$\lambda = -(s+2)(s+1) + 2(s+2) + 1 = 0 + 4 + 1 = 5for \ s = 0, n = 2$$

$$\lambda = -(s+4)(s+3) + 2(s+3) + 1 = 7for \ s = 0, n = 3$$

$$\lambda = -(s+4)(s+3) + 2(s+4) + 1 = 9for \ s = 0, n = 4$$

So, we make the conjecture:

$$\lambda = 2n + 1$$

And thus

$$\frac{d^2H_n}{dx^2} - 2x\frac{dH_n}{dx} + 2nH_n = 0$$

H is the physicist Hermite polynomial. Remember the equation:

$$\lambda = \frac{4\pi E}{h\omega}$$

The total energy is:

$$E = \frac{\lambda h \omega}{4\pi} = \frac{(2n+1)h\omega}{4\pi} = \left(n + \frac{1}{2}\right) \frac{h\omega}{2\pi}$$

[1]

Next, we introduce the ladder operations also known as annihilation and creation operators. These two operators are self-adjoint, Q is the position operator and P is the momentum operator:

$$a = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{2\pi m\omega}{h}} Q + \frac{i}{\sqrt{2\pi m\omega h}} P \right)$$

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{2\pi m\omega}{h}} Q - \frac{i}{\sqrt{2\pi m\omega h}} P \right)$$

We introduce a new operator:

$$N = \hat{a}a$$

$$N = \frac{2\pi m\omega}{2h} Q^2 + \frac{2\pi}{\omega mh} - \frac{2\pi i}{2h} (PQ - QP)$$

$$N = \frac{2\pi I}{\omega h} H - \frac{I}{2}$$

$$a\hat{a} = \frac{2\pi I}{\omega h} H + \frac{I}{2}$$

The following commutator vanishes:

$$[a, \hat{a}] = a\hat{a} - \hat{a}a = 0$$

Annihilation and creation:

$$a\phi_n = \sqrt{n}\phi_{n-1}$$

$$\hat{a}\phi_n = \sqrt{n+1}\phi_{n+1}$$

References

- [1] Baring, "Hermite Polynomials," Rice University, [Online]. Available: https://www.ruf.rice.edu/~baring/phys516/phys516_2021_lec_041321.pdf. [Accessed 16 May 2024].
- [2] A. Boehm, "Algebra of the Harmonic Oscillator," in *Quantum Mechanics*, New York, Springer-Verlag, 1979, pp. 15-20.