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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$-2sa_0x^s + (\lambda - 1)a_n x^s = 0$$

Assuming the series coefficients and variables are nonzero we have:

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

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

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

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

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

So, we make the conjecture:

$$\lambda = 2n + 1$$

And thus

$$\frac{d^2\mathrm{H}_n}{dx^2} - 2x\frac{d\mathrm{H}_n}{dx} + 2n\mathrm{H}_n = 0$$

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 position and momentum commutator vanishes:

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

Annihilation and creation:

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

[2]

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.