Phys 5701 1 Oct 2020

From Last Class

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2 u_E(\vec{x}) + V(\vec{x})\,u_E(\vec{x}) = E\,u_E(\vec{x})$$

with wave function $\psi(\vec{x},t) = e^{-iEt/\hbar}\,u_E(\vec{x})$

we will be solving this differential equation for the next few classes $\Rightarrow$ No "primes"

TODAY: Two Examples
- Free particle in 3D
- SHO in 1D

Free Particle i.e. $V(\vec{x}) = 0$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2 u_E(\vec{x}) = E\,u_E(\vec{x})$$

$$E = \frac{\hbar^2}{2m}\vec{k}^2 \qquad \vec{k}^2 = k_x^2 + k_y^2 + k_z^2$$

$$\Leftrightarrow \vec{\nabla}^2 u_E(\vec{x}) = -\vec{k}^2 u_E(\vec{x})$$

Solution: $u_E(\vec{x}) = C\,e^{i\vec{k}\cdot\vec{x}}$ $\quad (\vec{\nabla}^2 = \vec{\nabla}\cdot\vec{\nabla})$

$$\Leftrightarrow \psi(\vec{x},t) = C\,e^{i(\vec{k}\cdot\vec{x} - \omega t)} \qquad E = \hbar\omega$$

Degeneracy

"How many states w/ energy b/w $E, E+dE$"
dN

i.e. What is $\frac{dN}{dE}$? "Density of states"

"Big Box" Normalization w/ Periodic BC

Cube of size L

$u_E(x+L, y, z) = u_E(x, y, z)$
etc...

$\vec{k} = \frac{2\pi}{L}\vec{n} \quad \vec{n} = \underline{n_x}\hat{i} + \underline{n_y}\hat{j} + \underline{n_z}\hat{k}$
= Integers

For large $|\vec{n}|$ count states as follows:

$$dN = 4\pi|\vec{n}|^2 d|\vec{n}|$$

$$E = \frac{\hbar^2}{2m}|\vec{k}|^2 \Rightarrow dE = \frac{\hbar^2}{m}|\vec{k}|d|\vec{k}|$$

But $|\vec{n}| = L/2\pi \, |\vec{k}|$

$$\frac{dN}{dE} = \frac{4\pi|\vec{n}|^2 d|\vec{n}|}{\hbar^2|\vec{k}|d|\vec{k}|/m} = \frac{4\pi m}{\hbar^2}\left(\frac{L}{2\pi}\right)^2|\vec{k}|\left(\frac{L}{2\pi}\right)$$

$$\frac{dN}{dE} = \frac{4\pi m}{\hbar^2}\left(\frac{L}{2\pi}\right)^3\left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

$$= \frac{m^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}\,E^{1/2}\,L^3$$

HW #4: 2D

Simple Harmonic Oscillator in 1D

$$-\frac{\hbar^2}{2m}\frac{d^2u_E(x)}{dx^2} + \frac{1}{2}m\omega^2x^2u_E(x) = E\,u_E(x)$$

$$\text{with } \int_{-\infty}^{\infty}dx\,|u_E(x)|^2 = 1$$

Scales: $x_0 \equiv (\hbar/m\omega)^{1/2} \Rightarrow y \equiv x/x_0$

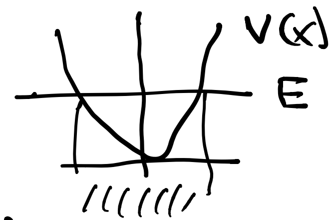
$$\varepsilon \equiv E/(\tfrac{1}{2}\hbar\omega) = 2E/\hbar\omega$$

Put $u(y) = u_E(x)$ and $x = y x_0$

$$\Rightarrow \boxed{\frac{d^2u}{dy^2} + (\varepsilon - y^2)\,u(y) = 0}$$

Consider $y \to \pm\infty$

want $u(y) \to 0$



$$\frac{d^2w}{dy^2} = y^2 w \qquad w(y) = e^{\pm y^2/2}$$ "+ is no good"

$$\Rightarrow \quad \boxed{u(y) = h(y)\, e^{-y^2/2}}$$

$$\Rightarrow \quad \boxed{\frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (\varepsilon - 1)\, h(y) = 0}$$

Generating Function

$$g(x,t) \equiv \exp\left(-t^2 + 2xt\right)$$

Define "Hermite Polynomials" $H_n(x)$

$$g(x,t) = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}$$

• $g(x,t) = 1 + \cdots \Rightarrow H_0(x) = 1$

• $g(0,t) =$ Expansion of e^{-t^2}
has only even powers of t
$\Rightarrow H_n(0) = 0$ if n is odd

• $g(0,t) = e^{-t^2} = \sum_{n \text{ even}} (-1)^{n/2} \dfrac{t^n}{(n/2)!}$

$$= \sum_{n \text{ even}} \frac{(-1)^{n/2}\, n!}{(n/2)!} \frac{t^n}{n!} \Rightarrow H_n(0) = \frac{(-1)^{n/2}\, n!}{(n/2)!}$$

For n even

Build $H_n(x)$ by considering $\partial g/\partial x$

$$\frac{\partial g}{\partial x} = 2t\, g(x,t) = \sum_{n=0}^{\infty} 2H_n(x) \frac{t^{n+1}}{n!}$$

$$= \sum_{n=0}^{\infty} \boxed{H_n'(x)} \frac{t^n}{n!}$$

But $\sum_n 2H_n(x) \dfrac{t^{n+1}}{n!} = \sum_{n=0}^{\infty} 2(n+1) H_n(x) \dfrac{t^{n+1}}{(n+1)!}$

$$= \sum_{n=0}^{\infty} \boxed{2n H_{n-1}} \frac{t^n}{n!}$$

$$H_n'(x) = 2n H_{n-1}(x) \qquad H_0(x) = 1$$

Also $H_n(0) = 0$ or $(-1)^{n/2}\, n!/(n/2)!$

e.g. $H_1'(x) = 2 \Rightarrow H_1(x) = 2x + C$

$$H_1(0) = 0 \Rightarrow H_1(x) = 2x$$

$$H_2'(x) = 8x \Rightarrow H_2(x) = 4x^2 + C$$

$$H_2(0) = (-1)\,2/1 = -2$$

$$\Rightarrow H_2(x) = 4x^2 - 2$$

$$g(x,t) = e^{-t^2+2xt} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

$$\frac{\partial g}{\partial t} = \sum_{n=0}^{\infty} n H_n \frac{t^{n-1}}{n!} = \sum_{n=1}^{\infty} n H_n \frac{t^{n-1}}{n!}$$

$$= \sum_{n=1}^{\infty} H_n \frac{t^{n-1}}{(n-1)!} = \boxed{\sum_{n=0}^{\infty} H_{n+1}(x)\frac{t^n}{n!}}$$

$$= \boxed{-2t\, g(x,t) + 2x\, g(x,t)}$$

$$= \boxed{\sum_{n=0}^{\infty} 2x H_n \frac{t^n}{n!}}$$

$$2t\,g(x,t) = \sum_{n=0}^{\infty} 2H_n(x)\frac{t^{n+1}}{n!}$$

$$= \sum_{n=0}^{\infty} 2(n+1)H_n(x)\frac{t^{n+1}}{(n+1)!}$$

$m = n+1$

$$= \sum_{m=1}^{\infty} 2m\,H_{m-1}(x)\frac{t^m}{m!}$$

$$= \boxed{\sum_{n=0}^{\infty} 2n\,H_{n-1}(x)\frac{t^n}{n!}}$$

$$H_{n+1}(x) = -2n\,H_{n-1}(x) + 2x\,H_n(x)$$

$$2n\,H_{n-1}(x) = 2x\,H_n(x) - H_{n+1}(x)$$

or $$2(n-1)\,H_{n-2}(x) = 2x\,H_{n-1}(x) - H_n(x)$$

But $$H_n'(x) = 2n\,H_{n-1}(x)$$

$$H_n''(x) = 2n\,H_{n-1}'(x)$$

$$= 2n\cdot 2(n-1)\,H_{n-2}(x)$$

$$= 2n\left[2x\,H_{n-1}(x) - H_n(x)\right]$$

$$= 2x\,H_n'(x) - 2n\,H_n(x)$$

$$H_n''(x) - 2x H_n'(x) + 2n H_n(x) = 0$$

$$h''(y) - 2y h'(y) + (\varepsilon - 1) h(y) = 0$$

Same Equation! i.e. $h(y) = H_n(y)$

$$u(y) = \underline{\underline{C}}\, e^{-y^2/2} H_n(y)$$

$$\varepsilon - 1 = \frac{2E}{\hbar\omega} - 1 = 2n \Rightarrow \underline{\underline{E = (n + 1/2)\hbar\omega}}$$

<u>Note</u>: Find C with generating function.

Easy!

ε

$(\hbar\omega)$