1_25_08

Note Title 1/25/2008

Review integration by parts

$$\frac{d}{dt}\int_{-\infty}^{\infty} \Psi^* \Psi \, dx$$

Assume $|\Psi(x,t)|^2$ normalizable

integration over x not t

$$\int_{-\infty}^{\infty} \frac{d}{dt} \Psi^* \Psi \, dx = \int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \, dx$$

If we can replace time derivatives with space derivatives then we can use integ. by parts to simplify. How? use TDSE

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi$$

$$\Rightarrow \quad \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi$$

$$\frac{\partial^* \Psi}{\partial x^2} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^*$$

$$\int_{-\infty}^{\infty} \frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \, dx$$

$$\int_{-\infty}^{\infty} \left(-\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \underline{\frac{i}{\hbar} V \Psi^*} \right) \Psi + \Psi^* \left(\frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \underline{\frac{iV}{\hbar} \Psi} \right) dx$$

$$-\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \frac{\partial^2 \Psi^*}{\partial x^2} \Psi + \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \, dx$$

$$-\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \frac{\partial}{\partial x} \left[\frac{\partial \Psi^*}{\partial x} \Psi + \Psi^* \frac{\partial \Psi}{\partial x} \right] dx$$

$$= -\frac{i\hbar}{2m} \left[\frac{\partial \Psi^*}{\partial x} \Psi + \Psi^* \frac{\partial \Psi}{\partial x} \right]_{-\infty}^{\infty} = 0$$

$$\left.\begin{array}{l} \frac{d}{dt}\langle x \rangle \\ \frac{d}{dt}\langle p \rangle \end{array}\right\}$$ involve same arguments only more complicated.

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$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\,\Psi$$

s. of var. $\Psi(x,t) = \psi(x)\,\varphi(t)$

$$i\hbar \frac{\dot\varphi}{\varphi} = -\frac{\hbar^2}{2m}\frac{\psi''}{\psi} + V(x) \underline{+V_0}$$

in terms of separation of variables this can go on either side

$$i\hbar \frac{\dot\varphi}{\varphi} - V_0 = -\frac{\hbar^2}{2m}\frac{\psi''}{\psi} + V(x) = E$$

$$i\hbar\dot\varphi - (E+V_0)\varphi = 0 \qquad -\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$$

$$\dot\varphi + \frac{i(E+V_0)}{\hbar}\varphi = 0$$

$$\varphi(t) = \varphi_0 e^{-i(E+V_0)/\hbar\, t} = \varphi_0\, e^{-iEt/\hbar}\, e^{-iV_0/\hbar}$$

$$|\Psi|^2 = |\varphi|^2\,|\psi|^2$$

$$|\varphi|^2 = |\varphi_0|^2$$

On the other hand, suppose we put the V_0 on the spatial part

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = \underbrace{(E+V_0)}_{E'}\psi$$

$$H\psi = E'\psi$$ same ε-value problem but w/ shifted ε-values

Stationary states

recall. sep. of var. applied to TDSE gives 2 equations, time and space

time $$\frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi$$ E sep. const

$$\Rightarrow \boxed{\phi = \phi_0 e^{-\frac{iE}{\hbar}t}}$$

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

Spatial part becomes an $\mathcal{E}$-value problem for the operator H.

$$H\psi_n = E_n \psi_n$$

Because H is a Hermitian operator it has a complete set of eigenvectors with real $\mathcal{E}$-values

Each $\mathcal{E}$-vector is a solution of the TISE.

So $\Psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$

is a solution of the TDSE.
These are the stationary states.

Since TDSE is linear

$$\sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$ is

also a solution

To compute the coefficients c_n we need to specify the initial conditions.

$$\psi(x, t=0) = \sum_{n=0}^{\infty} c_n \psi_n(x)$$

since $(\psi_n, \psi_m) = \int \psi_n^* \psi_m \, dx = \delta_{nm}$

$$\int_{-\infty}^{\infty} \psi(x, t=0) \psi_m^* \, dx = \sum_{n=0}^{\infty} c_n \int \psi_m^* \psi_n \, dx$$

$$= \sum c_n \delta_{nm} = c_m$$

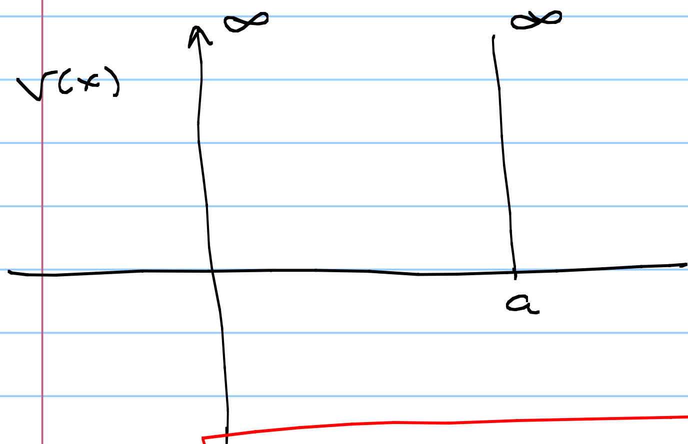
So $\boxed{c_m = \int_{-\infty}^{\infty} \psi(x, t=0) \psi_m^* \, dx}$

This is exactly like a fourier series. with these and

$$\sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$

we have a complete solution to the QM initial value prob.

Recall stationary states of infinite well



$$\psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi x}{a}\right)$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

So $$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi x}{a}\right) e^{-\frac{i n^2\pi^2\hbar}{2ma^2}t}}$$

$$\Psi(x,0) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{a}\right)$$

Mathematica example Griffiths 2.2

Theorem any solution to TDSE can be written as a superposition of S.S.

$$\Psi(x,t) = \sum_{N=1}^{\infty} C_N \sqrt{\frac{2}{a}} \sin\left(\frac{N\pi x}{a}\right) e^{-i\frac{N^2\pi^2\hbar}{2ma^2}t}$$

$$1 = \int_{-\infty}^{\infty} \Psi^* \Psi \, dx = \int_{-\infty}^{\infty} \left[\sum_N C_N^* \sqrt{\ } \sin(\ ) e^{i(\ )t}\right] \left[\sum_{N'} C_{N'} \sqrt{\ } \sin(\ ) e^{-i(\ )t}\right]$$

$$\sum_N \sum_{N'} C_N^* C_{N'} \frac{2}{a} \underbrace{\int \sin\left(\frac{N\pi x}{a}\right) \sin\left(\frac{N'\pi x}{a}\right) dx}_{\frac{a}{2}\delta_{NN'}} \; e^{i(\ )(N'^2 - N^2)}$$

$$= \sum_n |c_n|^2 = 1$$

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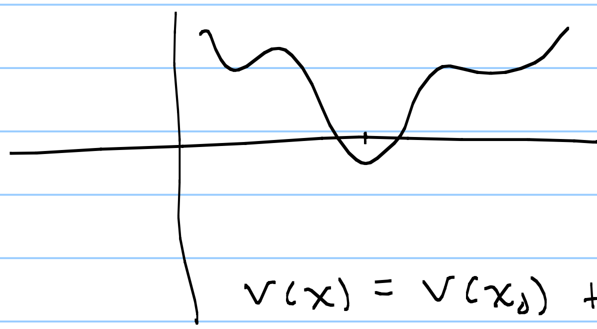

$$V(x) = \underbrace{V(x_0)}_{\text{constant}} + \underbrace{V'(x_0)(x-x_0)}_{=0 \text{ at minimum}} + \frac{1}{2}V''(x_0)(x-x_0)^2 + \dots$$

so $V(x) = \frac{1}{2}V''(x_0)(x-x_0)^2$ Quadratic or Harmonic approx.

$\Rightarrow \quad = \frac{1}{2}k x^2$ shift x so $x_0 = 0$

$$= \frac{1}{2}m\omega^2 x^2$$

TISE $\quad H\psi = E\psi$

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$\Rightarrow \boxed{\frac{-\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \psi = E}$$

2 roads to solution

1) Hard but direct (power series)
2) "easy" but sophisticated (algebraic)

Griffiths Does Both in 2.3 and so will we.

the algebraic approach was invented by Dirac and is fundamental in Quantum Field theory.

it involves operators that "create" and "annhialate" particles

The "modern" way to think about, say, current is in terms of a operator that destroys charge in one place and creates it somewhere else.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\psi = E$$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}}_{\frac{p^2}{2m}}$$

$\frac{p^2}{2m}$ with $p = \frac{\hbar}{i}\frac{d}{dx}$

so $H = \frac{1}{2m}\left[p^2 + (m\omega x)^2\right]$

idea is to factor H. Tricky because operators do not commute.

$$px - xp \neq 0$$

this is an operator equation

To proove it you must apply the operator to a function (any one will do).

$$(px)\psi = -i\hbar\frac{d}{dx}(x\psi)$$

$$= -i\hbar\left[\psi + x\frac{d\psi}{dx}\right]$$

$$(xp)\psi = x\left(-i\hbar\frac{d}{dx}\right)\psi$$

$$= -i\hbar\, x\frac{d\psi}{dx}$$

$$\Rightarrow \quad (px - xp)\psi = -i\hbar\psi$$

Since ψ is arbitrary, we can write this in operator form as.

$$px - xp = i\hbar I$$

└ identity operator