SQ 28

$\boxed{\text{Aim: Study the properties of Hermitian Operators}}$

(a) Is $i\frac{d^2}{dx^2}$ a Hermitian operator?

Definition: If $\int f^* \hat{A} g \, d\tau = \int (\hat{A} f)^* g \, d\tau$, (*)
then $\hat{A}$ is a Hermitian Operator.

Let $\hat{B} = i\frac{d^2}{dx^2}$, the question is whether $\hat{B}$ satisfy (*).

Checking:

$$\int_{-\infty}^{\infty} f^*(x) \hat{B} g(x) \, dx$$

$$= i\int_{-\infty}^{\infty} f^*(x) \frac{d^2 g}{dx^2} dx$$

$$= i f^*(x) \frac{dg}{dx}\Big|_{-\infty}^{\infty} - i\int_{-\infty}^{\infty} \frac{df^*}{dx}\frac{dg}{dx} dx \text{ (Integration by parts).}$$

$$= (0) - i\int_{-\infty}^{\infty} \frac{df^*}{dx}\frac{dg}{dx} dx$$

$$= -i g(x)\frac{df^*}{dx}\Big|_{-\infty}^{\infty} + i\int_{-\infty}^{\infty} \frac{d^2 f^*}{dx^2} g(x) \, dx$$

$$= 0 - \int_{-\infty}^{\infty} \left(i\frac{d^2}{dx^2} f(x)\right)^* g(x) \, dx$$

$$= -\int_{-\infty}^{\infty} (\hat{B} f)^* g \, dx.$$

Therefore, $\hat{B}$ doesn't satisfy (*) and is not a Hermitian operator.

(b). Property 1. Sum of two Hermitian operators $(\hat{A}+\hat{B})$ is also a Hermitian operator.

Proof:

In our case, $\hat{A}$ and $\hat{B}$ are hermitian:

$$\begin{cases} \int f^* \hat{A} g \, d\tau = \int (\hat{A} f)^* g \, d\tau. \\ \int f^* \hat{B} g \, d\tau = \int (\hat{B} f)^* g \, d\tau \end{cases}$$

We want to show

$$\int f^* (\hat{A}+\hat{B}) g \, d\tau = \int [(A+B) f]^* g \, d\tau.$$

$$\begin{aligned} LHS &= \int f^* (\hat{A}+\hat{B}) g \, d\tau \\ &= \int f^* \hat{A} g \, d\tau + \int f^* \hat{B} g \, d\tau \\ &= \int (\hat{A} f)^* g \, d\tau + \int (\hat{B} f)^* g \, d\tau. \\ &= \int [(\hat{A}+\hat{B}) f]^* g \, d\tau. \\ &= RHS. \end{aligned}$$

$\therefore$ Sum of two Hermitian operators is also a hermitian operator.

(c) Property 2. if $\hat{A}$ is a heritian operator, the expection of $\hat{A}^2$ for any state Ψ cannot be negative, i.e. $\langle \hat{A}^2 \rangle \geq 0$.

$$\langle \hat{A}^2 \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \hat{A}^2 \Psi(x) dx$$

$$= \int_{-\infty}^{\infty} [\Psi(x)]^* \hat{A} [\hat{A}\Psi(x)] dx \quad (\hat{A}^2 = \hat{A}\hat{A})$$

$$= \int_{-\infty}^{\infty} [f(x)]^* \hat{A} g(x) dx \quad \left(\begin{array}{l} \text{Let } f(x) = \Psi(x) \\ \quad g(x) = \hat{A}\Psi(x) \end{array} \right)$$

$$= \int_{-\infty}^{\infty} [\hat{A} f(x)]^* g(x) dx \quad (\hat{A} \text{ is hermitian})$$

$$= \int_{-\infty}^{\infty} (\hat{A}\Psi(x))^* (\hat{A}\Psi(x)) dx$$

$$= \int_{-\infty}^{\infty} |\hat{A}\Psi(x)|^2 dx.$$

$$\geq 0.$$

In fancy notation,

$$\langle \hat{A}^2 \rangle = \langle \Psi | \hat{A}^2 \Psi \rangle$$

$$= \langle \Psi | \hat{A} (\hat{A}\Psi) \rangle \quad (\hat{A}^2 = \hat{A}\hat{A})$$

$$= \langle f | \hat{A} g \rangle \quad \left(\begin{array}{l} \text{Let } f(x) = \Psi(x) \\ \quad g(x) = \hat{A}\Psi(x) \end{array} \right)$$

$$= \langle \hat{A} f | g \rangle \quad (\hat{A} \text{ is hermitian})$$

$$= \langle \hat{A}\Psi | \hat{A}\Psi \rangle \geq 0.$$

SQ 29.

Aim: Knowing the definition of the function of operators and the property of $e^{-\frac{i\hat{H}t}{\hbar}}$

Definition of a function of operator:

$$f(\hat{A}) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \hat{A}^n .$$

(a) $f(x) = e^{-\frac{it}{\hbar}x}$, where x is a scalor.

$f^{(n)}(x) = \left(-\frac{it}{\hbar}\right)^n e^{-\frac{it}{\hbar}x}$

$f^{(n)}(0) = \left(-\frac{it}{\hbar}\right)^n$

Using the definition

$$\hat{\tau} = f(\hat{H}) = e^{-\frac{i\hat{H}t}{\hbar}} = \sum_{n=0}^{\infty} \frac{\left(\frac{-it}{\hbar}\right)^n}{n!} \hat{H}^n$$

(b) If we have a general state

$$\Phi = \sum_{m=0}^{\infty} C_m \psi_m ,$$

$\{\psi_m\}$ is the complete set of energy eigenstate.

What is $\hat{\tau}\Phi$?

$\hat{\tau}\Phi$

$$= \sum_{n=0}^{\infty} \frac{\left(\frac{-it}{\hbar}\right)^n}{n!} \left(\hat{H}^n \sum_{m=0}^{\infty} C_m \psi_m\right)$$

$$= \sum_{n=0}^{\infty} \frac{\left(\frac{-it}{\hbar}\right)^n}{n!} \sum_{m=0}^{\infty} C_m \left(\hat{H}^n \psi_m\right)$$

Since $\hat{H}\psi_m = E_m\psi_m$,

$$\begin{aligned}\hat{H}^n\psi_m &= (\hat{H}^{n-1})\,\hat{H}\psi_m \\ &= (\hat{H}^{n-1})(E_m\psi_m) \\ &= E_m(\hat{H}^{n-1}\psi_m). \\ &= E_m(E_m\hat{H}^{n-2}\psi_m) \\ &\;\;\vdots \\ &= E_m^n\psi_m.\end{aligned}$$

$$\begin{aligned}\therefore \hat{\tau}\Phi &= \sum_{n=0}^{\infty}\frac{\left(\frac{-it}{\hbar}\right)^n}{n!}\sum_{m=0}^{\infty}C_m(E_m^n\psi_m) \\ &= \sum_{m=0}^{\infty}C_m\left(\sum_{n=0}^{\infty}\frac{\left(\frac{-it}{\hbar}E_m\right)^n}{n!}\right)\psi_m \\ &= \sum_{m=0}^{\infty}C_m\, e^{-\frac{iE_mt}{\hbar}}\psi_m.\end{aligned}$$

It must remind you of the initial value problem in QM.

In QM, You are given $-\frac{\hbar^2}{2m}\vec{\nabla}^2\Phi + V\Phi = E\Phi$, with $\Phi(\vec{x},t=0) = f(\vec{x})$. (*)

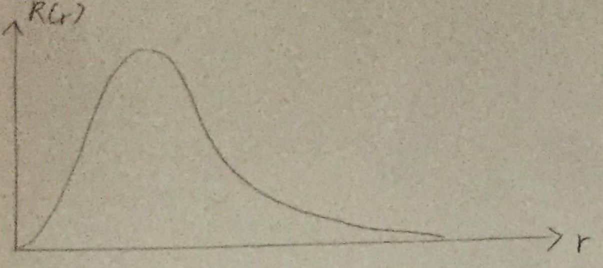
You always expand $f(\vec{x})$ using the eigenfunctions $\{\psi_m\}$ of the system and corresponding energies are $\{E_m\}$.

i.e. $\Phi(\vec{x},t=0) = f(\vec{x}) = \sum_{m=0}^{\infty} C_m\psi_m$

After some time, you can find $\Phi(x,t)$ to be $\sum_{m=0}^{\infty} C_m e^{-\frac{iE_mt}{\hbar}}\psi_m$ by solving (*) using eigenfunctions expansion. This is exactly the same as $\hat{\tau}\Phi(\vec{x},t=0) = \sum_{m=0}^{\infty} C_m e^{-\frac{iE_mt}{\hbar}}\psi_m$.

SQ27)

For 3d state, $R_{32}(r) = A r^2 e^{-\alpha r}$, where $A = \frac{4}{81\sqrt{30}\, a_0^{\frac{3}{2}}} \frac{1}{a_0^2}$ and $\alpha = \frac{1}{3a_0}$.



$$P_{32}(r) = r^2 [R_{32}(r)]^2$$

$$= A^2 r^6 e^{-2\alpha r}$$

$$\frac{dP_{32}(r)}{dr} = A^2 [6r^5 e^{-2\alpha r} - 2\alpha r^6 e^{-2\alpha r}] = 0$$

$$6 - 2\alpha r = 0$$

$$r = \frac{3}{\alpha}$$

$$= 9a_0$$

Most probable distance is $r = 9a_0$ as stated at lecture notes.