Problem Sheet 1

Q2(a) If an operator is linear then

$$\hat{A}(f+g) = \hat{A}f + \hat{A}g$$

$$\hat{A}(cf) = c\hat{A}f \qquad \text{where } c = \text{const}$$

So if $f = c_1 f_1 + c_2 f_2$

$$\hat{A}f = \hat{A}(c_1 f_1 + c_2 f_2)$$

$$= \hat{A}c_1 f_1 + \hat{A}c_2 f_2$$

$$= c_1 \hat{A}f_1 + c_2 \hat{A}f_2$$

i) $x(c_1 f + c_2 f_2) = c_1 x f_1 + c_2 x f_2$

$= x f(x)$ so operator x is linear

ii) $\frac{d}{dx}(c_1 f_1 + c_2 f_2) = c_1 \frac{df_1}{dx} + c_2 \frac{df_2}{dx}$

$= df(x)/dx$ so operator $\frac{d}{dx}$ is linear

iii) $c(c_1 f_1 + c_2 f_2) = c_1 c f_1 + c_2 c f_2$

$= c f(x)$ so operator c is linear

iv) $(c_1 f_1 + c_2 f_2) + c = c_1(f_1 + c) + c_2(f_2 + c)$ if $+c$ operator was linear

$\neq f(x) + c$ so operator is not linear

v) $(c_1 f_2 + c_2 f_2)^2 = c_1 f_1^2 + c_2 f_2^2$ if $(\,)^2$ operator was linear

$\neq f(x)^2$ ie operator is not linear

vi) $(c_1 f_1 + c_2 f_2)\frac{d(c_1 f_1 + c_2 f_2)}{dx} = c_1\left(f_1 \frac{df_1}{dx}\right) + c_2\left(f_2 \frac{df_2}{dx}\right)$ if operator was linear

$\neq f(x)\frac{df(x)}{dx}$

vii) $p(x)(c_1 f_1 + c_2 f_2) = c_1 p(x) f_1 + c_2 p(x) f_2$

$= p(x) f(x)$ so operator $p(x)$ is linear

(b) i) x ii) $\frac{d}{dx}$ but $x\frac{df}{dx} \neq \frac{d}{dx}(xf)$ ie operators do not commute

ii) $\frac{d}{dx}$ iii) c (constant) $\frac{d}{dx}cf = c\frac{df}{dx}$ ie operators commute

iii) x vii) $p(x)$ $x\,p(x)\,f(x) = p(x)\,x f(x)$ ie operators commute

ii) $\frac{d}{dx}$ vii) $p(x)$ $\frac{d}{dx}p(x)\,f(x) \neq p(x)\frac{df(x)}{dx}$ ie operators do not commute

Q3 (a) $\hat{A} = d/dx$

If $\hat{A}$ is Hermitian then $\int f_1^*(x)\left(\hat{A} f_2(x)\right)dx = \int\left(\hat{A}f_1(x)\right)^* f_2(x)\,dx$

So $\int f_1^* \frac{df_2}{dx}\,dx \underset{\int \text{by parts}}{=} [f_1^* f_2] - \int \frac{df_1^*}{dx} f_2\,dx$

$= -\int \frac{df_1^*}{dx} f_2\,dx$ assuming that functions are well behaved at boundaries of region

$\neq \int \frac{df_1^*}{dx} f_2\,dx$ $\because$ of sign

(b) $\hat{T} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$ $\because$ $\hat{T} = \frac{\hat{p}_x^2}{2m}$ and $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ $\Rightarrow \hat{T} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$

$\int f_1^* \hat{T} f_2\,dx = \frac{-\hbar^2}{2m}\left\{\cancel{\left[f_1^* df_2/dx\right]}^{\to 0} - \int \frac{df_1^*}{dx}\frac{df_2}{dx}\,dx\right\}$ $\int$ by parts

$= \frac{-\hbar^2}{2m}\left\{-\cancel{\left[\frac{df_1^*}{dx}f_2\right]}^{\to 0} + \int \frac{d^2 f_1^*}{dx^2} f_2\,dx\right\}$ $\int$ " " again

$= \int\left(\hat{T}f_1\right)^* f_2\,dx$ $\Rightarrow$ $\hat{T}$ is a Hermitian operator

[have assumed that functions are well behaved at boundaries of region]

Q5 If the energy eigenfunctions are orthogonal then

$$\int \phi_m^* \phi_n = \delta_{nm}$$

$$n=m: \frac{2}{a}\int_0^a dx \sin^2\left(\frac{n\pi x}{a}\right) = \frac{2}{a}\left[\frac{x}{a} - \frac{a}{4n\pi}\sin\left(\frac{2n\pi}{a}.x\right)\right]_0^a$$

$$= \frac{2}{a}\cdot\frac{a}{2} = 1 \qquad \because \sin 2n\pi = 0,\ \sin 0 = 0$$

$$n\neq m: \frac{2}{a}\int_0^a dx \sin\left(\frac{m\pi x}{a}\right)\sin\left(\frac{n\pi x}{a}\right) = \frac{2}{a}\left[-\frac{\sin\left(\frac{\pi}{a}(m+n)x\right)}{\frac{2\pi}{a}(m+n)} + \frac{\sin\left(\frac{\pi}{a}(m-n)x\right)}{\frac{2\pi}{a}(m-n)}\right]_0^a$$

$$= 0 \qquad \because \sin\pi(m+n) = 0,\ \sin\pi(m-n) = 0,\ \sin 0 = 0$$

Q6 $\psi = \sum_n c_n \phi_n$ so $\psi^*\psi = \sum_{m,n} c_m^* c_n \phi_m^* \phi_n$

$$\therefore \underbrace{\int \psi^*\psi \, d\tau}_{=1} = \sum_{m,n} c_m^* c_n \underbrace{\int \phi_m^* \phi_n \, d\tau}_{=\delta_{mn}}$$

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

Q7(c)

Operator	eigenvalue	eigenfunction	
$\hat{A}$	α_1	$\phi_1 = \frac{2}{\sqrt{13}}\chi_1 + \frac{3}{\sqrt{13}}\chi_2$	(1)
	α_2	$\phi_2 = \frac{3}{\sqrt{13}}\chi_1 \ \frac{-2}{\sqrt{13}}\chi_2$	(2)
$\hat{B}$	β_1	$\chi_1 = \frac{2}{\sqrt{13}}\phi_1 + \frac{3}{\sqrt{13}}\phi_2$	(3)
	β_2	$\chi_2 = \frac{3}{\sqrt{13}}\phi_1 \ \frac{-2}{\sqrt{13}}\phi_2$	(4)

i) Apply $\hat{A}$, measure eigenvalue α_1

$\therefore$ system in state with eigenf^n ϕ_1 as given by eq^n (1)

ii) Apply $\hat{B}$. According to eq^n (1)

prob. of observing eigenvalue $\beta_1 = \left(\frac{3}{\sqrt{13}}\right)^2$

" " " " $\beta_2 = \left(\frac{3}{\sqrt{13}}\right)^2$

The corresponding eigenfunctions χ_1 and χ_2 are given by eq^{n}s (3) & (4), respectively. The measurement associated with $\hat{B}$ destroys any previous information about the system gained by $\hat{A}$

iii) Apply $\hat{A}$ again

If β_1 measured in step ii), eq^n (3) shows that

prob. of observing eigenvalue $\alpha_1 = (2/\sqrt{13})^2$

" " " $\alpha_2 = (3/\sqrt{13})^2$

If β_2 measured in step ii), eq^n (4) shows that

prob. of observing eigenvalue $\alpha_1 = (3/\sqrt{13})^2$

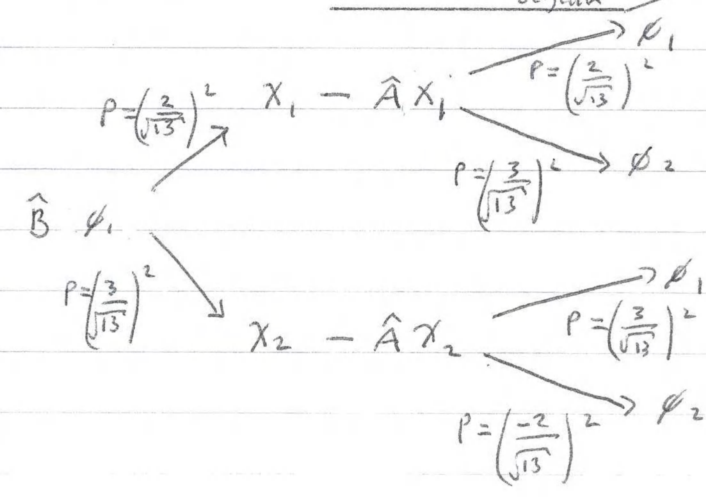
" " " $\alpha_2 = (-2/\sqrt{13})^2$

So prob. of measuring α_1 again is

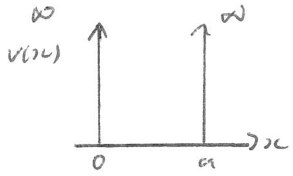
$$\underbrace{\left(\frac{4}{13} \times \frac{4}{13}\right)}_{\text{prob of measuring } \beta_1 \text{ and then } \alpha_1 \text{ again}} + \underbrace{\left(\frac{9}{13} \times \frac{9}{13}\right)}_{\text{prob of measuring } \beta_2 \text{ and then } \alpha_1 \text{ again}} = \frac{97}{169}$$

or

Probability tree



Q8



$\psi(x) = \frac{1}{\sqrt{a}}$

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

$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ energy eigenfunctions

$\therefore \quad c_n = \int \phi_n^* \psi \, dx = \frac{\sqrt{2}}{a} \int_0^a \sin\left(\frac{n\pi x}{a}\right) dx$

$= \frac{2\sqrt{2}}{n\pi}$ for n odd

$= 0$ " n even

Use $\langle \hat{H} \rangle = \sum_n |c_n|^2 E_n = \sum_{n \text{ odd}} \frac{8}{n^2\pi^2} \cdot \frac{\hbar^2 \pi^2 n^2}{2ma^2}$

$= \frac{4\hbar^2}{ma^2} \left(\frac{1^2}{1^2} + \frac{3^2}{3^2} + \cdots \right) = \infty$

or using

$\langle \hat{H} \rangle = \int_0^a dx \, \psi^* \hat{H} \psi$ with $\psi = \frac{1}{\sqrt{a}}$ and $\hat{H} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$

$= 0$

ψ has no x dependence so $\frac{d\psi}{dx} = 0$

So $\psi(x) = \frac{1}{\sqrt{a}}$ cannot be valid. Eg need $\psi(x=0) = \psi(x=a) = 0$ to satisfy the boundary conditions.

i.e. $\psi(x=0) = \psi(x=a) = 0 \neq \frac{1}{\sqrt{a}}$

Q12(c) Stationary states :-

If $V(\underline{r},t)$ in the TDSE $\hat{H}\psi = i\hbar\partial\psi/\partial t$ does not depend on time t, then the energy eigenvalues and eigenfunctions do not depend on time and obey

$$\hat{H}(\underline{r})\phi_n(\underline{r}) = E_n\phi_n(\underline{r}).$$

An arbitrary wavefunction can be written as

$$\psi(\underline{r},t) = \sum_n c_n(t)\phi_n(\underline{r})$$

$$= \sum_n c_n(0)\phi_n(\underline{r})e^{-iE_nt/\hbar}$$

In our case

$$\psi(x,0) = c_1(0)\phi_1(x) + c_2(0)\phi_2(x)$$

where $c_1(0) = c_2(0) = 1/\sqrt{2}$. So

$$\psi(x,t) = c_1(0)\phi_1(x)e^{-iE_1t/\hbar} + c_2(0)\phi_2(x)e^{-iE_2t/\hbar}$$

$$\therefore \quad \hat{H}\psi(x,t) = i\hbar\frac{\partial\psi}{\partial t}$$

$$= E_1c_1(0)\phi_1(x)e^{-iE_1t/\hbar} + E_2c_2(0)\phi_2(x)e^{-iE_2t/\hbar}$$

Hence

$$\langle\hat{H}\rangle = \int_0^a dx\, \psi^*(x,t)\,\hat{H}\,\psi(x,t)$$

$$= \int_0^a dx\left(\frac{\phi_1^*}{\sqrt{2}}e^{+iE_1t/\hbar} + \frac{\phi_2^*}{\sqrt{2}}e^{+iE_2t/\hbar}\right)\left(\frac{E_1}{\sqrt{2}}\phi_1e^{-iE_1t/\hbar} + \frac{E_2\phi_2}{\sqrt{2}}e^{-iE_2t/\hbar}\right)$$

$$= \frac{E_1}{2} + \frac{E_2}{2} \qquad \because \int_0^a \phi_m^*\phi_n\,dx = \delta_{mn}$$

Q12(d) $\langle x(t)\rangle = \int_0^a dx\, \psi^*(x,t)\, x\, \psi(x,t)$

$$= \int_0^a dx \left(\frac{\phi_1^*}{\sqrt{2}} e^{+iE_1t/\hbar} + \frac{\phi_2^*}{\sqrt{2}} e^{iE_2t/\hbar}\right)\left(\frac{x}{\sqrt{2}}\phi_1 e^{-iE_1t/\hbar} + \frac{x}{\sqrt{2}}\phi_2 e^{-iE_2t/\hbar}\right)$$

$$= \int_0^a dx \left(\frac{x}{2}|\phi_1|^2 + \frac{x}{2}|\phi_2|^2 + \frac{x}{2}\phi_1^*\phi_2 e^{i(E_1-E_2)t/\hbar} + \frac{x}{2}\phi_2^*\phi_1 e^{-i(E_1-E_2)t/\hbar}\right)$$

$$= \frac{2}{a}\cdot\frac{1}{2}\left\{\underbrace{\int_0^a x\sin^2\left(\frac{\pi x}{a}\right)dx}_{=a^2/4} + \underbrace{\int_0^a x\sin^2\left(\frac{2\pi x}{a}\right)dx}_{=a^2/4}\right.$$

$$\left. + \int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\underbrace{\left[e^{i(E_1-E_2)t/\hbar} + e^{-i(E_1-E_2)t/\hbar}\right]}_{=2\cos\left(\frac{(E_1-E_2)t}{\hbar}\right)}\right\}$$

$$= \frac{1}{a}\left\{\frac{a^2}{4} + \frac{a^2}{4} + 2\cos\left(\frac{(E_1-E_2)t}{\hbar}\right)\underbrace{\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx}_{=-\frac{8a^2}{9\pi^2}}\right\}$$

$$= \underline{\underline{\frac{a}{2} - \frac{16a}{9\pi^2}\cos\left(\frac{(E_1-E_2)t}{\hbar}\right)}}$$

So the average posn of the particle oscillates about the centre of the well (ie $x=a/2$) with an L^r freq determined by the difference in the energy levels of $\phi_1(x)$ and $\phi_2(x)$

ie $\frac{E_1-E_2}{\hbar} = \frac{\hbar}{\hbar}(\omega_1-\omega_2) = \omega_1-\omega_2$

Q13(a) $$c(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, \psi(x)\, e^{-ikx}$$ for the Gaussian wavepacket

Fourier transform relation

For the ground state energy eigenfunction of an infinite square well in 1D

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

So we want to calculate

$$c(k) = \frac{1}{2\pi}\sqrt{\frac{2}{a}}\int_{0}^{a} dx\, \sin\left(\frac{\pi x}{a}\right) e^{-ikx}$$

The useful integrals give

$$c(k) = \frac{1}{2\pi}\sqrt{\frac{2}{a}}\; \frac{\pi a\left[-1-e^{-ika}\right]}{k^2a^2-\pi^2} = \frac{1}{2\pi}\sqrt{\frac{2}{a}}\; \frac{\pi a\left[1+e^{-ika}\right]}{\pi^2-k^2a^2}$$

(b) $$|c(k)|^2 \propto \frac{(1+e^{-ika})(1+e^{ika})}{(\pi^2-k^2a^2)^2}$$

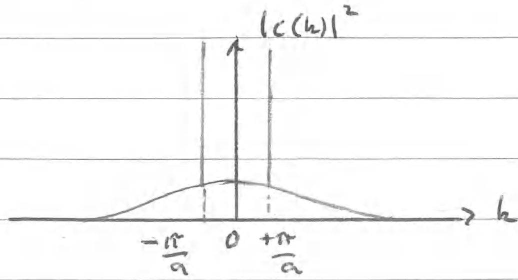
$$= \frac{2(1+\cos ka)}{(\pi^2-k^2a^2)^2} \qquad \text{using } \cos A = \frac{e^{iA}+e^{-iA}}{2}$$

$$\simeq \frac{\cos^2\left(\frac{ka}{2}\right)}{(\pi^2-k^2a^2)^2} \qquad \text{using } \cos^2 A = \frac{1}{2}(1+\cos 2A)$$

$|c(k)|^2$ is symmetrical about $k=0$, so we are equally likely to measure positive or negative momenta. This is consistent with $\langle \hat{p}_x \rangle = 0$ in question 11.

$|c(k)|^2$ is strongly peaked for $k = \pm\pi/a$.

Given that $p = \hbar k$, this is consistent with $\langle \hat{p}_x^2 \rangle = \frac{\pi^2\hbar^2}{a^2}$ in question 11.



Q14 From the lecture notes, we know that the width of a Gaussian wavepacket varies with time as

$$\Delta x(t) = \sqrt{\frac{1}{2a} + \frac{\hbar^2 a t^2}{2m^2}}$$

At time $t=0$, $\Delta x = \sqrt{\frac{1}{2a}} = 1\,\text{Å}$

So, $\frac{1}{2a} = 10^{-20}\,m^2$ or $a = \frac{1}{2\times10^{-20}}\,m^{-2}$

(a) For the wavepacket to double its initial size

$$2.\sqrt{\frac{1}{2a}} = \sqrt{\frac{1}{2a} + \frac{\hbar^2 a t^2}{2m^2}}$$

$$\therefore\ t = \frac{\sqrt{3}\,m}{\hbar a} = \sqrt{3} \times \frac{9.109\times10^{-31} \times 2\times10^{-20}}{1.054\times10^{-34}} = 2.99\times10^{-16}\,s$$

(b) After 1 s

$$\Delta x = \sqrt{\frac{1}{2a} + \frac{\hbar^2 a}{2m^2}}$$

$$\frac{1}{2a} = 10^{-20}\,m^2$$

$$\frac{\hbar^2 a}{2m^2} = \frac{(1.054\times10^{-34})^2}{2\times10^{-20} \times 2\,(9.109\times10^{-31})^2} = 3.347\times10^{11}\ m^2$$

So the first term is negligible

$$\therefore\ \Delta x = \sqrt{3.347\times10^{11}} = 5.785\times10^{5}\ m$$