PH 651 Solutions of HW #5

Problem #1 Sakurai 1.23

$$V = \begin{cases} 0, & 0 < x < a \\ \infty, & \text{otherwise} \end{cases} \Rightarrow \psi_n = \sqrt{\frac{2}{a}} \sin\frac{\pi n x}{a}$$

$$\langle \hat{X} \rangle_n = \int_0^a x\, |\psi_n(x)|^2 dx = \frac{2}{a}\int_0^a x \underbrace{\sin^2\frac{\pi n x}{a}}_{= \frac{1 - \cos\frac{2\pi n x}{a}}{2}} dx = \frac{a}{2}$$

$$\langle \hat{X}^2 \rangle_n = \int_0^a x^2 |\psi_n(x)|^2 dx = \frac{2}{a}\int_0^a \frac{x^2}{2}\left(1 - \cos\frac{2\pi n x}{a}\right) dx =$$

$$= \frac{a^2}{3} - \frac{1}{2}\left(\frac{a}{\pi n}\right)^2$$

$$\langle \hat{P} \rangle_n = \int_0^a \psi_n^*(x)\left(-i\hbar \frac{d}{dx}\right)\psi_n(x)\, dx = -i\hbar \cdot \frac{2}{a} \cdot \int_0^a \sin\frac{\pi n x}{a} \cdot$$

$$\cdot \frac{\pi n}{a} \cos\frac{\pi n x}{a}\, dx = 0$$

$$\uparrow \int_0^a \sin\frac{2\pi n x}{a} dx$$

$$\langle \hat{P}^2 \rangle_n = \frac{2}{a}(-\hbar^2)\int_0^a \sin\frac{\pi n x}{a} \cdot \left(\frac{\pi n}{a}\right)^2 \cdot \left(-\sin\frac{\pi n x}{a}\right) dx =$$

$$= \frac{2}{a}\hbar^2 \left(\frac{\pi n}{a}\right)^2 \underbrace{\int_0^a \sin^2\frac{\pi n x}{a} dx}_{= \frac{a}{2}} = \hbar^2 \left(\frac{\pi n}{a}\right)^2$$

$$\langle (\Delta \hat{X})^2 \rangle_n = \frac{a^2}{3} - \frac{1}{2}\left(\frac{a}{\pi n}\right)^2 - \frac{a^2}{4} = a^2\left[\frac{1}{12} - \frac{1}{2(\pi n)^2}\right]$$

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$$\langle (\Delta\hat{p})^2\rangle_n = \hbar^2\left(\frac{\pi n}{a}\right)^2$$

$$\langle(\Delta x)^2\rangle_n \langle(\Delta\hat{p})^2\rangle_n = \frac{\cancel{a^2}}{2}\left[\frac{1}{6}-\frac{1}{(\pi n)^2}\right]\cdot\frac{\hbar^2}{\cancel{a^2}}(\pi n)^2 =$$

$$= \frac{\hbar^2}{2}\left[\frac{(\pi n)^2}{6}-1\right] = \frac{\hbar^2}{4}\left[\frac{(\pi n)^2}{3}-2\right]$$

$$\langle[\hat{x},\hat{p}]\rangle_n = i\hbar \Rightarrow \frac{1}{4}\left|\langle[\hat{x},\hat{p}]\rangle_n\right|^2 = \frac{\hbar^2}{4}$$

Since $\frac{(\pi n)^2}{3}-2>1$ for any $n \Rightarrow$

$\frac{\hbar^2}{4}\left[\frac{(\pi n)^2}{3}-2\right] > \frac{\hbar^2}{4}$ for any n

Note that as
- $n\to\infty \Rightarrow \Delta x \to \frac{a}{2\sqrt{3}}$, but $\Delta p \to \infty$
- $n\uparrow \Rightarrow \Delta x, \Delta p \uparrow \Rightarrow$

minimal uncertainty at $n=1$ (ground state)

Solutions of HW #5 (ctd)

Problem #2 (Sakurai 1.29)

(a) $A|a'\rangle = a'|a'\rangle$

$$\langle b''|f(A)|b'\rangle \underset{\uparrow}{=} \sum_{a',a''} \langle b''|a'\rangle \underbrace{\langle a'|f(A)|a''\rangle}_{\substack{\| \\ f(a')\delta_{a',a''}}}$$

assuming $\langle a'|b'\rangle$ is known

$$\cdot \langle a''|b'\rangle = \sum_{a'} f(a') \langle b''|a'\rangle \langle a'|b'\rangle$$

(b) $\langle \vec{p}''| \underbrace{F(r)}_{\leftarrow \text{operator}} |\vec{p}'\rangle = ?$ $\quad r = \sqrt{x^2+y^2+z^2}$ ← operator

$$\langle \vec{p}''|F(r)|\vec{p}'\rangle = \int d^3\vec{r}'\, d^3\vec{r}'' \langle \vec{p}''|\vec{r}'\rangle \langle \vec{r}'|F(r)|\vec{r}''\rangle \cdot \langle \vec{r}''|\vec{p}'\rangle \underset{\uparrow}{=} \int d^3\vec{r}'\, d^3\vec{r}'' \frac{1}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}\vec{p}''\cdot\vec{r}'} \langle \vec{r}'|F(r)|\vec{r}''\rangle \cdot e^{\frac{i}{\hbar}\vec{p}'\cdot\vec{r}''} =$$

Lecture #13
$$\langle \vec{r}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

⇒

What is $\langle \vec{r}'' | \underbrace{F(r)}_{\text{operator}} | \vec{r}' \rangle$? (4)

$\Downarrow$

Recall: $A|\psi\rangle = a|\psi\rangle \Rightarrow F(A)|\psi\rangle = F(a)|\psi\rangle$

If $r^2 = X^2 + Y^2 + Z^2 \Rightarrow$

$$(X^2+Y^2+Z^2)\underbrace{|\vec{r}'\rangle}_{\substack{\parallel \\ |x', y', z'\rangle}} = \underbrace{(x'^2+y'^2+z'^2)}_{\substack{\parallel \\ r'^2 \\ \uparrow \\ \text{eigenvalue}}}|\vec{r}'\rangle$$

$\Downarrow$

$$F(\underset{\substack{\uparrow \\ \sqrt{\ }}}{f}(r^2))\,|\vec{r}'\rangle = F(\underset{\substack{\uparrow \\ \sqrt{\ }}}{f}(\underset{\substack{\uparrow \\ \text{eigenvalue}}}{r'^2}))\,|\vec{r}'\rangle$$

Then, $\langle \vec{r}'' | F(r) | \vec{r}' \rangle = F(r') \underbrace{\langle \vec{r}'' | \vec{r}' \rangle}_{\substack{\parallel \\ \delta^{(3)}(\vec{r}''-\vec{r}')}}$

$$\Rightarrow = \frac{1}{(2\pi\hbar)^3}\int d^3\vec{r}'\, d^3\vec{r}''\; F(r')\, e^{\frac{i}{\hbar}(\vec{p}'\cdot\vec{r}'' - \vec{p}''\cdot\vec{r}')}\,\delta^{(3)}(\vec{r}''-\vec{r}')$$

$$= \frac{1}{(2\pi\hbar)^3}\int d^3\vec{r}'\; F(r')\, e^{\frac{i}{\hbar}(\vec{p}'-\vec{p}'')\cdot\vec{r}'} \underset{\substack{\nearrow \\ \text{spherical coordinates}}}{=} \frac{1}{(2\pi\hbar)^3} \cdot$$

$$\cdot \int r'^2 dr' \sin\theta' d\theta' d\varphi'\; F(\underset{\substack{\uparrow \\ =|\vec{r}'|}}{r'})\, e^{\frac{i}{\hbar}\Delta\vec{p}\cdot\vec{r}'}, \quad \Delta\vec{p} = \vec{p}' - \vec{p}''$$

$$\Delta\vec{p}\cdot\vec{r}' = |\Delta\vec{p}|\cdot r'\cos\theta'$$

$$= \frac{1}{(2\pi\hbar)^3} \cdot \underbrace{2\pi}_{\int_0^{2\pi} d\varphi} \cdot \int_0^\infty r'^2 F(r') dr' \underbrace{\int_0^\pi e^{\frac{i}{\hbar}|\Delta\vec{p}| r' \cos\theta'} \sin\theta' d\theta}_{\parallel}$$

$$\frac{e^{\frac{i}{\hbar}|\Delta\vec{p}|r'} - e^{-\frac{i}{\hbar}|\Delta\vec{p}|r'}}{\frac{i}{\hbar}|\Delta\vec{p}|r'} = \frac{\hbar}{|\Delta\vec{p}|r'} \cdot 2\sin\frac{|\Delta\vec{p}|r'}{\hbar}$$

$$= \frac{1}{(2\pi)^2\hbar^3} \int_0^\infty \frac{2\hbar}{|\Delta\vec{p}|r'} r'^2 F(r') \cdot \sin\frac{|\Delta\vec{p}|r'}{\hbar} dr' =$$

$$= \frac{1}{2\pi^2\hbar^2 |\vec{p}' - \vec{p}''|} \int_0^\infty r' \sin\frac{|\vec{p}' - \vec{p}''|r'}{\hbar} F(r') dr' =$$

$$= \langle \vec{p}'' | F(r) | \vec{p}' \rangle$$

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Problem #3

$$\langle X^2\rangle = \int_{-\infty}^{+\infty} dx' \langle\alpha|x'\rangle\, x'^2 \langle x'|\alpha\rangle =$$

$$= \int_{-\infty}^{+\infty} dx'\, x'^2\, |\psi_\alpha(x')|^2 = \frac{1}{\sqrt{\pi}\, d} \int_{-\infty}^{+\infty} e^{-x'^2/d^2}\, x'^2 dx' =$$

$$= \frac{1}{\cancel{\sqrt{\pi}}\, d} \cdot \cancel{\sqrt{\pi}} \cdot \frac{1}{2} \left(\frac{1}{d^2}\right)^{-3/2} = \frac{d^2}{2}$$

$$\int_{-\infty}^{+\infty} x^2 e^{-\alpha x^2} dx = -\frac{\partial}{\partial\alpha} \underbrace{\int_{-\infty}^{+\infty} e^{-\alpha x^2} dx}_{= \sqrt{\frac{\pi}{\alpha}}} = \sqrt{\pi} \cdot \frac{1}{2} \alpha^{-3/2}$$

Alternatively,

$$\langle X^2\rangle = \int_{-\infty}^{+\infty} dp' dp'' \langle\alpha|p'\rangle\langle p'|X^2|p''\rangle\langle p''|\alpha\rangle.$$

$$= \int_{-\infty}^{+\infty} dp' dp''\, \varphi_\alpha^*(p')\, \underbrace{\langle p'|X^2|p''\rangle}_{\Downarrow\ ?}\, \varphi_\alpha(p'')$$

$$\langle X^2\rangle = -\hbar^2\int_{-\infty}^{+\infty} dp'\, \varphi_\alpha^{*}(p')\frac{\partial^2}{\partial p'^2}\varphi_\alpha(p') =$$

$$= -\hbar^2\cdot\frac{d}{\hbar}\,\frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty} dp'\, e^{-\frac{(p'-\hbar k)^2}{\hbar^2}d^2}\left[-\frac{d^2}{\hbar^2}+\frac{(p'-\hbar k)^2}{\hbar^4}d^4\right] \circleddash$$

$\uparrow$

$$\frac{d^2\varphi_\alpha(p')}{dp'^2} = \sqrt{\frac{d}{\hbar}}\,\frac{1}{\pi^{1/4}}\, e^{-\frac{(p'-\hbar k)^2 d^2}{2\hbar^2}}\left[-\frac{d^2}{\hbar^2}+\frac{(p'-\hbar k)^2}{\hbar^4}d^4\right]$$

$$\circleddash -\frac{\hbar d}{\sqrt{\pi}}\left[-\frac{d^{\cancel{2}}}{\hbar^{\cancel{2}}}\cdot\frac{\sqrt{\pi}\,\cancel{\hbar}}{\cancel{d}}+\frac{d^4}{\hbar^4}\frac{-\partial}{\partial\alpha}\underbrace{\int_{-\infty}^{+\infty} d(p'-\hbar k)\, e^{-\alpha(p'-\hbar k)^2}}_{=\sqrt{\frac{\pi}{\alpha}}}\right] =$$

$$\sqrt{\frac{\pi}{\alpha}},\quad \alpha = \frac{d^2}{\hbar^2}$$

$$= -\frac{\hbar d}{\sqrt{\pi}}\left[-\frac{d}{\hbar}\sqrt{\pi}+\frac{d^4}{2\hbar^4}\left(\frac{d^2}{\hbar^2}\right)^{-3/2}\sqrt{\pi}\right] =$$

$$= -\frac{\hbar d}{\sqrt{\pi}}\left[-\frac{d}{\hbar}\sqrt{\pi}+\frac{d^4}{2\hbar^4}\cdot\frac{\cancel{\hbar^3}}{\cancel{d^3}}\sqrt{\pi}\right] = -\frac{\cancel{\hbar} d}{\cancel{\sqrt{\pi}}}\cdot\frac{-d\cancel{\sqrt{\pi}}}{2\cancel{\hbar}} = \frac{d^2}{2}$$

Now $\langle P^2\rangle$:

$$\langle P^2\rangle = \int_{-\infty}^{+\infty} dp'\,dp''\,\langle\alpha|p'\rangle\langle p'|P^2|p''\rangle\langle p''|\alpha\rangle =$$

$$= \int_{-\infty}^{+\infty} dp'\,|\varphi_\alpha(p')|^2 p'^2 = \frac{d}{\hbar\sqrt{\pi}}\int_{-\infty}^{+\infty} dp'\, e^{-\frac{(p'-\hbar k)^2}{\hbar^2}d^2}p'^2 \underset{p'-\hbar k = p}{=}$$

$$= \frac{d}{\hbar\sqrt{\pi}} \int_{-\infty}^{+\infty} dp\, e^{-\frac{p^2 d^2}{\hbar^2}} (p+\hbar k)^2 = \frac{d}{\hbar\sqrt{\pi}} \Big[\int_{-\infty}^{+\infty} dp\, e^{-\frac{p^2 d^2}{\hbar^2}} p^2 +$$

$$+ 2\hbar k \int_{-\infty}^{+\infty} dp\, e^{-\frac{p^2 d^2}{\hbar^2}} p + (\hbar k)^2 \int_{-\infty}^{+\infty} e^{-\frac{p^2 d^2}{\hbar^2}} dp \Big] =$$

$$= \frac{d}{\hbar\sqrt{\pi}} \Big[-\frac{\partial}{\partial \alpha} \sqrt{\frac{\pi}{\alpha}} + 0 + (\hbar k)^2 \cdot \sqrt{\frac{\pi}{\alpha}} \Big] = \frac{d}{\hbar\sqrt{\pi}} \Big[\sqrt{\pi} \cdot \frac{1}{2} \cdot \left(\frac{d^2}{\hbar^2}\right)^{-3/2}$$

$$\alpha = \frac{d^2}{\hbar^2}$$

$$+ (\hbar k)^2 \sqrt{\pi} \cdot \frac{\hbar}{d} \Big] = \frac{1}{2} \frac{\hbar^2}{d^2} + \hbar^2 k^2$$

Alternatively,

$$\langle P^2 \rangle = \int_{-\infty}^{+\infty} dx' dx'' \langle \alpha | x' \rangle \langle x' | P^2 | x'' \rangle \langle x'' | \alpha \rangle =$$

$$= \int_{-\infty}^{+\infty} dx'\, \psi_\alpha^*(x') (-\hbar^2) \frac{\partial^2}{\partial x'^2} \psi_\alpha(x') = -\frac{\hbar^2}{\sqrt{\pi} d} \int_{-\infty}^{+\infty} e^{-\frac{x'^2}{d^2}} \cdot$$

Lecture #13

$$\frac{d^2 \psi_\alpha(x)}{dx^2} = \frac{1}{\pi^{1/4}\sqrt{d}} e^{ikx - \frac{x^2}{2d^2}} \left[-\frac{1}{d^2} + \left(ik - \frac{x}{d^2}\right)^2 \right]$$

$$\cdot \left[-\frac{1}{d^2} + \left(ik - \frac{x'}{d^2}\right)^2 \right] dx' = -\frac{\hbar^2}{\sqrt{\pi} d} \Big[\left(-\frac{1}{d^2} - k^2\right) \sqrt{\pi} d - 0$$

$$+ \frac{1}{d^4} \underbrace{\int_{-\infty}^{+\infty} e^{-x'^2/d^2} x'^2 dx}_{\frac{d^3}{2}\sqrt{\pi}} \Big] = \frac{\hbar^2}{d^2} + \hbar^2 k^2 + \frac{1}{d^4} \cdot \frac{-\hbar^2}{d} \cdot \frac{d^3}{2} = \frac{\hbar^2}{2d^2} + \hbar^2 k^2$$

Problem #4

$$\Psi(x,0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right)$$

(a) Recall that $\int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx =$

$$= \frac{a}{2} \delta_{mn}$$

Denote $\varphi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \leftarrow$ normalized function

Then $\Psi(x,0) = \frac{A}{\sqrt{a}} \cdot \sqrt{\frac{a}{2}}\, \varphi_1(x) + \sqrt{\frac{3}{5a}} \cdot \sqrt{\frac{a}{2}}\, \varphi_3(x) +$

$+ \frac{1}{\sqrt{5a}} \cdot \sqrt{\frac{a}{2}}\, \varphi_5(x) = \frac{A}{\sqrt{2}} \varphi_1(x) + \sqrt{\frac{3}{10}}\, \varphi_3(x) + \frac{1}{\sqrt{10}} \varphi_5(x)$

Since $\langle \varphi_n | \varphi_m \rangle = \delta_{nm} \Rightarrow$

$$\langle \Psi | \Psi \rangle = 1 = \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} = \frac{A^2}{2} + \frac{2}{5} \Rightarrow$$

$$A^2 = \frac{6}{5} \Rightarrow A = \sqrt{\frac{6}{5}}$$

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(b) For a particle in the infinite potential well,
$V = 0$ at $[0, a]$ and $V = \infty$ elsewhere

$$\Downarrow \quad H\varphi_n = E_n \varphi_n$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_n = E_n\varphi_n \Rightarrow \quad \varphi_n'' = \underbrace{-\frac{2mE_n}{\hbar^2}}_{=-k^2}\varphi_n,$$

$$\varphi_n'' + k^2\varphi_n = 0 \Rightarrow$$

$$\varphi_n = \overbrace{C_1}^{=\sqrt{\frac{2}{a}}} \sin kx + C_2 \cos kx$$

$$\varphi_n(0) = \varphi_n(a) = 0 \Rightarrow C_2 = 0 \; ;$$

$$\Downarrow \qquad ka = \pi n \Rightarrow \quad (n \text{ integer})$$

$$\sin ka = 0 \Longrightarrow \quad k = \frac{\pi n}{a} = \sqrt{\frac{2mE_n}{\hbar^2}}$$

$$\Downarrow$$

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

eigenvalues of energy

$$\mathcal{P}(E_n) = |\langle\varphi_n|\Psi(0)\rangle|^2 \Rightarrow$$

↑
probability
to measure E_n

$$\sum_n \mathcal{P}(E_n) = \frac{3}{5} + \frac{3}{10} + \frac{1}{10} = 1 \checkmark$$

$$\mathcal{P}(E_1) = \frac{A^2}{2} = \frac{6}{10} = \underbrace{\frac{3}{5}} \Rightarrow$$

$$\mathcal{P}(E_3) = \underline{\frac{3}{10}} \; ; \quad \mathcal{P}(E_5) = \underline{\frac{1}{10}}$$

(c) $$\langle E \rangle = \sum_n \mathcal{P}(E_n)\, E_n = \frac{3}{5} E_1 + \frac{3}{10} E_3 + \frac{1}{10} E_5 = \frac{\pi^2 \hbar^2}{2ma^2} \underbrace{\left[\frac{3}{5} \cdot 1 + \frac{3}{10} \cdot 9 + \frac{1}{10} \cdot 25 \right]}_{\frac{3}{5} + \frac{27}{10} + \frac{25}{10} = \frac{58}{10} = \frac{29}{5}} =$$

$$= \frac{\pi^2 \hbar^2}{ma^2} \cdot \frac{29}{10}$$

(d) $$\Psi(x,t) = \sqrt{\frac{3}{5}}\, e^{-\frac{i}{\hbar} E_1 t}\, \varphi_1(x) + \sqrt{\frac{3}{10}}\, e^{-\frac{i}{\hbar} E_3 t} \cdot \varphi_3(x) + \frac{1}{\sqrt{10}}\, e^{-\frac{i}{\hbar} E_5 t}\, \varphi_5(x)$$

(e) $$\mathcal{P} = |\langle \varphi(t) | \Psi(t) \rangle|^2 = \left| \int_0^a \varphi^*(x,t)\, \Psi(x,t)\, dx \right|^2$$

$$\varphi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{5\pi x}{a}\right) \cdot e^{-iE_5 t/\hbar}$$

$$= \left| \sqrt{\frac{2}{a}} \cdot \frac{1}{\sqrt{10}} \int_0^a \sin\left(\frac{5\pi x}{a}\right) \cancel{e^{\frac{i}{\hbar} E_5 t}}\ \cancel{e^{-\frac{i}{\hbar} E_5 t}} \cdot \sqrt{\frac{2}{a}} \sin\frac{5\pi x}{a}\, dx \right|^2$$

other terms vanish due to orthogonality

$$= \frac{1}{10}$$

(f) $$\mathcal{P} = |\langle \chi(t) | \Psi(t) \rangle|^2 = 0$$

$$0 = \langle \varphi_2 | \varphi_1 \rangle = \langle \varphi_2 | \varphi_3 \rangle = \langle \varphi_2 | \varphi_5 \rangle$$