Aula 23 (18/Mar)

Aula de hoje:

* Resolução de exercícios para Prova 1.
  - Exercício 2, Folha 5 (partícula num poço de potencial infinito).
  - Exercício 7, Folha 4. (energia cinética e potencial).

2 Partícula num poço potencial infinito†

Considere uma partícula de massa m num poço de potencial de profundidade infinita definido por

$$V(x) = \begin{cases} 0, & 0 < x < a, \\ +\infty, & x < 0 \text{ e } x > a. \end{cases} \tag{2}$$

Assumamos que no instante $t = 0$ esta partícula está no estado definido por

$$\langle x|\Psi(t=0)\rangle = \Psi(t=0,x) = \begin{cases} \frac{1+i}{\sqrt{2a}} \sin\left(\frac{\pi x}{a}\right) + \frac{1}{\sqrt{a}} \sin\left(\frac{2\pi x}{a}\right), & 0 < x < a, \\ 0, & x < 0 \text{ e } x > a. \end{cases} \tag{3}$$

Relembre que os auto-estados (normalizados) e auto-valores do problema do poço de potencial infinito, $\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$, são dados por

$$\langle x|\varphi_n\rangle = \varphi_n(x) = i\sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a} x\right), \tag{4}$$

e por

$$E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2. \tag{5}$$

(a) Comece por escrever o estado da Eq. (3) como uma combinação linear de auto-estados do poço de potencial infinito $|\varphi_n\rangle$.

$0 < x < a$

$\Psi(x,t) = \frac{1+i}{\sqrt{2a}} \sin\left(\frac{\pi x}{a}\right) + \frac{1}{\sqrt{a}} \sin\left(\frac{2\pi x}{a}\right) \rightarrow \Psi = a_1 \varphi_1 + a_2 \varphi_2$

$\varphi_n(x) = i\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \rightarrow$

$$a_1 \varphi_1 = \frac{1+i}{\sqrt{2a}} \sin\left(\frac{\pi x}{a}\right)$$

$$a_1 \, i \sqrt{\frac{2}{a}} \, \cancel{\sin\left(\frac{\pi x}{a}\right)} = \frac{1+i}{\sqrt{2}\,a} \cancel{\sin\left(\frac{\pi x}{a}\right)}$$

$$\rightarrow \underline{a_1} = \sqrt{\frac{a}{2}} \, \frac{1+i}{i\sqrt{2a}} = \underline{\frac{1+i}{2i}} = i \rightarrow a_1^2 = \frac{1}{2}$$

$$a_2 e_2 = \frac{1}{\sqrt{a}} \sin\left(\frac{2\pi x}{a}\right)$$

$$a_2 \, i \sqrt{\frac{2}{a}} \cancel{\sin\left(\frac{2\pi x}{a}\right)} = \frac{1}{\sqrt{a}} \cancel{\sin\left(\frac{2\pi x}{a}\right)}$$

$$\underline{a_2} = \frac{1}{\sqrt{2}\, i}$$

$$\Psi(t=0,x) = \frac{1+i}{2i} |e_1\rangle + \frac{1}{\sqrt{2}\, i} |e_2\rangle$$

(b) Calcule a norma de $|\Psi(t=0)\rangle$ normalizando este estado se necessário.

$$r_1 = \frac{1-i}{2}$$

$$\Psi(t=0) = \frac{1+i}{2i}|\varphi_1\rangle + \frac{1}{\sqrt{2}\,i}|\varphi_2\rangle$$

$$= \frac{1-i}{2}|\varphi_1\rangle - \frac{i}{\sqrt{2}}|\varphi_2\rangle$$

$$\langle\psi|\psi\rangle = \left[\frac{1+i}{2}\langle\varphi_1| + \frac{i}{\sqrt{2}}\langle\varphi_2|\right]\left[\frac{1-i}{2}|\varphi_1\rangle - \frac{i}{\sqrt{2}}|\varphi_2\rangle\right]$$

$$= \left(\frac{1+i}{2}\right)\left(\frac{1-i}{2}\right) + \frac{i}{\sqrt{2}}\left(\frac{-i}{\sqrt{2}}\right)$$

$$= \frac{1^2-(i)^2}{4} - \frac{(i)^2}{2} = \frac{1}{2} + \frac{1}{2} = 1$$

(c) Calcule $\langle x|\Psi(t)\rangle = \Psi(t,x)$ para $t > 0$.

$$|\psi(t,x)\rangle = e^{-i\frac{Ht}{\hbar}} \, |\psi(t=0)\rangle$$

$$|\psi(t)\rangle = e^{-i\frac{Ht}{\hbar}} \left[a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle \right]$$

$$= a_1 e^{-i\frac{E_1 t}{\hbar}} |\varphi_1\rangle + a_2 e^{-i\frac{E_2 t}{\hbar}} |\varphi_2\rangle$$

$$\langle x|\psi(t)\rangle = \underset{\sim}{a_1} \, e^{-i\frac{E_1 t}{\hbar}} \, i\sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) + \underline{a_2} \, e^{-i\frac{E_2 t}{\hbar}} \, i\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$$

$$\Psi(t,x) = \frac{1-i}{2} \exp\left\{ \frac{-it}{\hbar} \left(\frac{\hbar^2 \pi^2}{2ma^2} \right) \right\} i \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a} \right)$$

$$- \frac{i}{\sqrt{2}} \exp\left\{ \frac{-it}{\hbar} \left(\frac{2\hbar^2 \pi^2}{ma^2} \right) \right\} i \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a} \right)$$

$$\Psi(t,x) = \frac{i+1}{2}\sqrt{\frac{2}{a}}\,\exp\left\{\frac{-it}{\hbar}\left(\frac{\hbar^2\pi^2}{2ma^2}\right)\right\}\sin\left(\frac{\pi x}{a}\right)$$

$$+\frac{1}{\sqrt{a}}\,\exp\left\{\frac{-it}{\hbar}\left(\frac{2\hbar^2\pi^2}{ma^2}\right)\right\}\sin\left(\frac{2\pi x}{a}\right)$$

(d) Para este estado $|\Psi(t)\rangle$ calcule o valor médio da energia total (i.e. o valor esperado do operador hamiltoniano, $\langle \hat{H} \rangle$) para $t > 0$.

$$\hat{H}|\varphi_1\rangle = E_1|\varphi_1\rangle$$

$$\langle \Psi(t)|\hat{H}|\Psi(t)\rangle = \langle \Psi|\hat{H}| \left[a_1 e^{-\frac{iE_1 t}{\hbar}} |\varphi_1\rangle + a_2 e^{-\frac{iE_2 t}{\hbar}} |\varphi_2\rangle \right]$$

$$H\,\hat{a}|\varphi_2\rangle$$

$$= \langle \Psi(t)| \left[a_1 e^{-\frac{iE_1 t}{\hbar}} E_1 |\varphi_1\rangle + a_2 e^{-\frac{iE_2 t}{\hbar}} E_2 |\varphi_2\rangle \right]$$

$$= \left[a_1 e^{\frac{iE_1 t}{\hbar}} \langle \varphi_1| + a_2 e^{\frac{iE_2 t}{\hbar}} \langle \varphi_2| \right] \left[a_1 e^{-\frac{iE_1 t}{\hbar}} E_1 |\varphi_1\rangle + a_2 e^{-\frac{iE_2 t}{\hbar}} E_2 |\varphi_2\rangle \right]$$

$$= a_1^2 E_1 + a_2^2 E_2 = \frac{1}{2} E_1 + \frac{1}{2} E_2 =$$

$$\hat{H}\left(\hat{Q}\,|\psi_n\rangle\right), \quad [\hat{H},\hat{Q}] = \hat{H}\hat{Q} - \hat{Q}\hat{H} = cte$$

$$\hat{H}\hat{Q} = cte + \hat{Q}\hat{H}$$

$$\leadsto \frac{1}{2}E_1 + \frac{1}{2}E_2 = \frac{1}{2}\left(\frac{\hbar^2\pi^2}{2ma^2}\right) + \frac{1}{2}\left(\frac{2\hbar^2\pi^2}{ma^2}\right)$$

$$\langle H\rangle = \frac{1}{4}\left(\frac{\hbar^2\pi^2}{ma^2}\right) + \left(\frac{\hbar^2\pi^2}{ma^2}\right) = \frac{5}{4}\left(\frac{\hbar^2\pi^2}{ma^2}\right)$$

(e) Numa única medição da energia do sistema descrito por $|\Psi(t)\rangle$, qual a probabilidade de medirmos o valor $E = \frac{5\pi^2\hbar^2}{4ma^2}$?

$$E = \frac{5\pi^2\hbar^2}{4ma^2} \rightarrow P = 0$$

$$\Psi(t) = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle \qquad \langle H \rangle = \frac{1}{2}(E_1 + E_2) = \frac{5}{4}\frac{\hbar^2\pi^2}{ma^2}$$

$$H\Psi(t) = \begin{cases} E_1 \\ E_2 \end{cases}$$

(f) Para o n-ésimo estado estacionário do poço de potencial infinito, i.e. $|\varphi_n\rangle$, calcule $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$ e $\langle p^2\rangle$.

(g) Calcule a derivada temporal do valor esperado do operador posição da partícula, i.e. $\frac{d\langle \hat{X}\rangle}{dt}$. Interprete este resultado fisicamente.

$$\langle x | \varphi_n \rangle = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$\langle x \rangle = \int \psi^*(x)\, x\, \psi\, dx = \int x\, |\psi|^2\, dx$$

$$= \frac{2}{a} \int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx \qquad y = \frac{n\pi}{a}x \quad ; \quad dx = \frac{a}{n\pi}\, dy$$

$$= \frac{2}{a} \left(\frac{a}{n\pi}\right)^2 \int_0^{n\pi} y \sin^2(y)\, dy$$

$$\int_0^{n\pi} y\sin^2 y\,dy = \int_0^{n\pi} \frac{y}{2}\left(1-\cos(2y)\right)dy$$

$$= \underbrace{\int_0^{n\pi} \frac{y}{2}\,dy}_{\frac{y^2}{4}\Big|_0^{n\pi} = \frac{(n\pi)^2}{4}} - \underbrace{\int_0^{n\pi} \frac{y}{2}\cos(2y)\,dy}$$

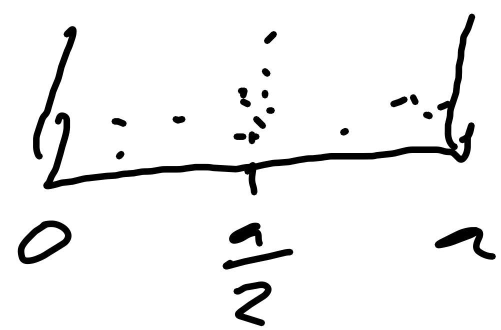
$$\int y\cos(2y)\,dy = y\,\frac{\sin(2y)}{2} - \int \frac{\sin(2y)}{2}\,dy$$

$$= \frac{y\sin(2y)}{2} + \frac{\cos(2y)}{4}$$

$$\langle x\rangle = \frac{2}{a}\left(\frac{a}{n\pi}\right)^2\left[\frac{y^2}{4} - \underbrace{\frac{y\sin y}{4}}_{=0} - \frac{\cos(2y)}{8}\right]\Bigg|_0^{n\pi}$$

$$= \frac{2}{a}\left(\frac{a}{n\pi}\right)^2\left[\frac{(n\pi)^2}{4} - \underbrace{\frac{\cos(2\pi n)}{8}}_{=\frac{1}{8}} + \frac{1}{8}\right]$$

$$\langle x\rangle = \frac{\cancel{2}}{\cancel{a}}\left(\frac{a}{\cancel{n\pi}}\right)^2\frac{\cancel{(n\pi)^2}}{\cancel{4}\,2} = \frac{a}{2}$$



$$\langle x^2 \rangle = \int_0^a x^2 |\psi|^2 dx = \frac{2}{a} \int_0^a x^2 \sin^2\left(\frac{n\pi}{a} x\right) dx$$

$$y = \frac{n\pi x}{a} \qquad dy = \frac{n\pi}{a} dx$$

$$\rightarrow \; = \frac{2}{a}\left(\frac{a}{n\pi}\right)^3 \int_0^{n\pi} y^2 \underbrace{\sin^2 y}_{\frac{1}{2}(1-\cos(2y))} dy = \frac{2}{a}\left(\frac{a}{n\pi}\right)^3 \int_0^{n\pi} \frac{y^2}{2}(1 - \cos(2y)) dy$$

$$= \frac{2}{a}\left(\frac{a}{n\pi}\right)^3 \underbrace{\int_0^{n\pi} \frac{y^2}{2}\,dy}_{\frac{y^3}{6}} - \int_0^{n\pi} \underbrace{\frac{y^2}{2}\cos(2y)\,dy}$$

$$\int y^2 \underbrace{\cos(2y)}\,dy = y^2 \frac{\sin(2y)}{2} - \int \underbrace{y\sin(y)\,dy}$$

$$= \frac{y^2 \sin(2y)}{2} - \frac{\sin(2y)}{4} + \frac{y\cos(2y)}{2}$$

$$= \left(\frac{y^2}{2} - \frac{1}{4}\right)\sin(2y) + \frac{y\cos(2y)}{2}$$

$$\langle x^2 \rangle = \frac{2}{a}\left(\frac{a}{n\pi}\right)^3 \left[\frac{y^3}{6} - \underbrace{\left(\frac{y^2}{2} - \frac{1}{4}\right)\frac{\sin}{2}(2y)}_{=0} + \frac{y \cos y}{4} \right]\Bigg|_0^{n\pi}$$

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

$$\langle x^2 \rangle = \frac{2a^2}{(n\pi)^3} \left[\frac{(n\pi)^2}{\cancel{6}3} - \frac{n\pi \cos(2n\pi)}{4} \right] = \frac{a^2}{3} - \frac{a^2}{2(n\pi)^2}$$

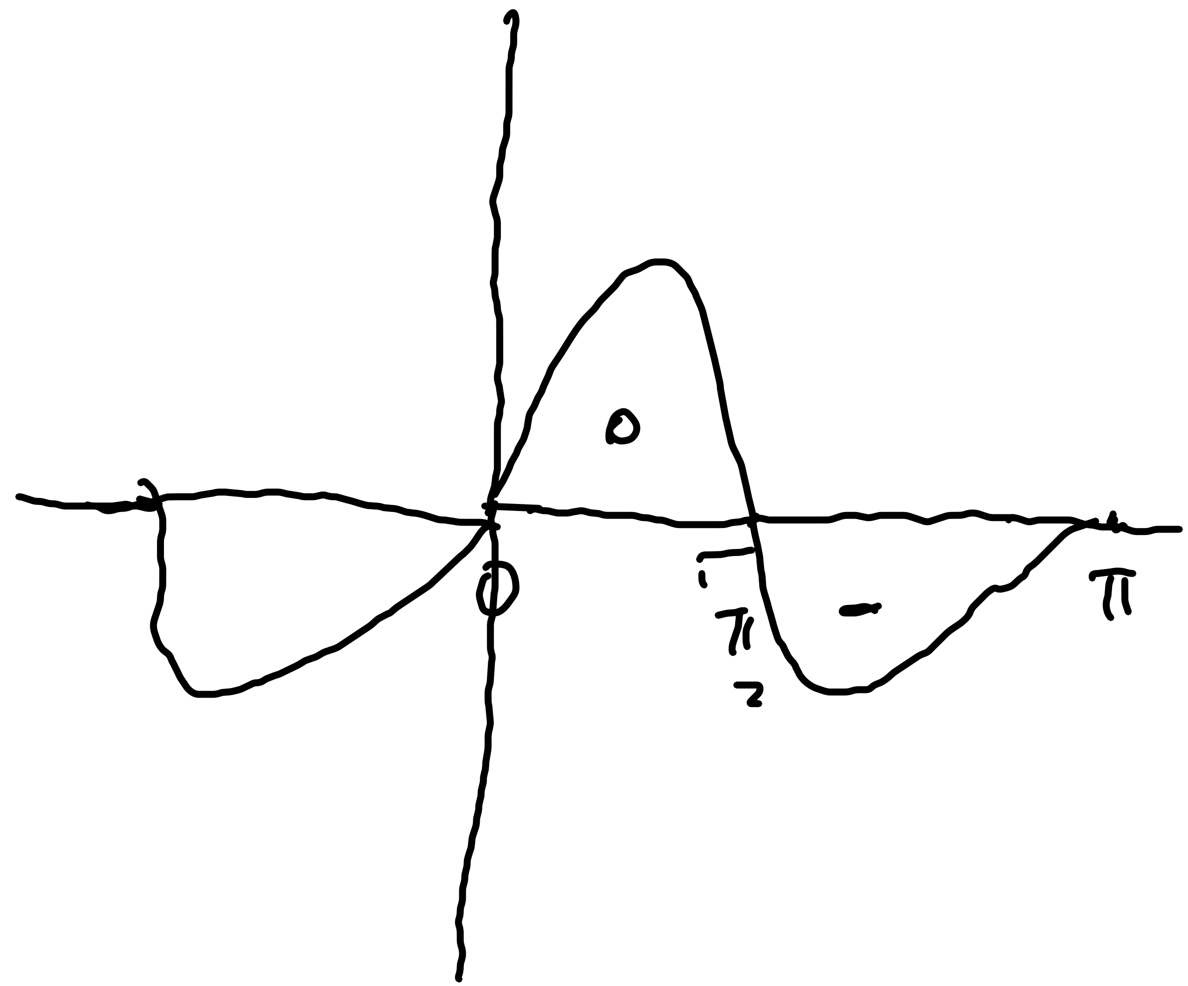
$$\langle p \rangle = \int \psi^* \hat{\underline{p}} \psi \, dx = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \psi \right) dx$$

$$= \frac{2}{a} \int_0^a \sin\left(\frac{n\pi x}{a}\right) C \cos\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{2}{a} C \int_0^a \underbrace{\sin\left(\frac{n\pi x}{a}\right) \cos\left(\frac{n\pi x}{a}\right)}_{=0} dx = 0$$

$\sin(x)\ \cos(x) \rightarrow$

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = 0$$



$$\langle \hat{p}^2 \rangle = \int \psi_n^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi_n \, dx = -\hbar^2 \int \psi_n^* \underbrace{\frac{\partial^2}{\partial x^2} \psi_n}\, dx$$

SG:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n = E_n \psi_n \rightarrow -\hbar^2 \frac{\partial^2}{\partial x^2}\psi_n = \underbrace{2mE\psi_n}$$

$$= 2mE_n \underbrace{\int \psi_n^* \psi_n \, dx}_{=1} = 2mE_n \rightarrow \langle p^2 \rangle = \left(\frac{n\pi\hbar}{a}\right)^2$$

j) $\frac{d\langle \hat{x} \rangle}{dt} = \frac{d}{dt}\left(\frac{a}{2}\right) = 0$

L> CTE DE MOVIMENTO - CONSERVAÇÃO

$\downarrow$

SIMETRIA

$\frac{d\langle \hat{x} \rangle}{dt} = [\hat{H}, \hat{x}] = \frac{\langle p \rangle}{m} = 0$

$\downarrow$

$\frac{p^2}{2m}$

$H = \frac{p^2}{2m} + \underbrace{V(x)}_{\to 0}$

7 Energia cinética e potencial[‡]

Considere o Hamiltoniano $\hat{H}$ de um dado sistema físico, cujos auto-valores e auto-vectores denotamos por E_n e $|\phi_n\rangle$, i.e.

$$\hat{H}\,|\phi_n\rangle \;=\; E_n\,|\phi_n\rangle\;. \tag{4}$$

(a) Mostre que para um operador arbitrário $\hat{A}$ temos a seguinte relação

$$\langle\phi_n|\,[\hat{A},\hat{H}]\,|\phi_n\rangle = 0\,. \tag{5}$$

(b) Considere agora que estamos em 1D, tal que o nosso sistema físico consiste de uma partícula de massa m sujeita a um potencial $V(x)$. Neste caso o Hamiltoniano do nosso sistema será

$$\hat{H} \;=\; \frac{\hat{P}^2}{2m} + V(\hat{X})\,. \tag{6}$$

1. Calcule os seguintes comutadores escrevendo os resultados em termos de $\hat{X}$, $\hat{P}$, $V(\hat{X})$: $[\hat{H},\hat{X}]$, $[\hat{H},\hat{P}]$ e $[\hat{H},\hat{X}\hat{P}]$.
2. Mostre que o elemento de matriz $\langle\phi_n|\hat{P}|\phi_n\rangle$ é zero. No capítulo 5 iremos interpretar este elemento de matriz como o valor esperado do operador momento no estado $|\phi_n\rangle$.
3. Usando os resultados anteriores, estabeleça uma relação entre o valor esperado da energia cinética $E_c \equiv \left\langle\phi_n\,\middle|\,\frac{\hat{P}^2}{2m}\,\middle|\,\phi_n\right\rangle$ e o valor esperado de $\left\langle\phi_n\,\middle|\,\hat{X}\frac{d\hat{V}}{d\hat{X}}\,\middle|\,\phi_n\right\rangle$.
4. Relacione o valor esperado da energia potencial $E_p \equiv \langle\phi_n|V(\hat{X})|\phi_n\rangle$ com o valor esperado da energia cinética, assumindo que $V(\hat{X}) = V_0\hat{X}^{\lambda}$.

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

↳ $V(x)$

$$\psi(x,t) = \varphi(x)\, e^{-i\frac{Et}{\hbar}}$$

→ ESTADOS ESTACIONÁRIOS

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \varphi^*(x)\, e^{\frac{iEt}{\hbar}}\, \varphi(x)\, e^{-\frac{iEt}{\hbar}} = \varphi^*(x)\,\varphi(x) = |\varphi(x)|^2$$

$$\langle Q \rangle = \int \Psi^* Q(x,p)\, \Psi \, dx = \int \varphi^* Q(x,p)\, \varphi \, dx = \langle \varphi | Q | \varphi \rangle$$

↳ $\bar{E}$ CONSTANTE NO TEMPO

↳ $\frac{d}{dt}\langle Q \rangle = 0 \rightarrow \langle [Q, H] \rangle = 0$

b)

$$[\hat{H}, \hat{x}] = \left[\frac{\hat{p}^2}{2m} + V(\hat{x}), \hat{x}\right]$$

$$= \left[\frac{\hat{p}^2}{2m}, \hat{x}\right] = \frac{\hat{p}}{2m}\underbrace{[\hat{p}, x]}_{-i\hbar} + \underbrace{[\hat{p}, x]}_{-i\hbar}\frac{\hat{p}}{2m}$$

$$= \hat{p}\left(\frac{-i\hbar}{2m} - \frac{i\hbar}{2m}\right) = -\frac{\hat{p}}{m} i\hbar$$

$$[\hat{H}, \hat{p}] = \left[\frac{\hat{p}^2}{2m} + V(x), \hat{p}\right] = [V(x), \hat{p}]$$

$$= \left[V(x), \frac{\hbar}{i}\frac{\partial}{\partial x}\right] \rightsquigarrow$$

$$\rightsquigarrow \left[V(x), \frac{\hbar}{i}\frac{\partial}{\partial x}\right]\psi = \frac{\hbar}{i} V \frac{\partial \psi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(V\psi)$$

$$= \cancel{\frac{\hbar}{i} V \frac{\partial \psi}{\partial x}} - \cancel{\frac{\hbar}{i} V \frac{\partial \psi}{\partial x}} - \underbrace{\frac{\hbar}{i} \psi \frac{\partial V}{\partial x}}$$

$$[V(x), \hat{p}]\cancel{\psi} = -\frac{\hbar}{i}\psi\frac{\partial V}{\partial x} = i\hbar\cancel{\psi}\frac{\partial V}{\partial x}$$

$$[V(x), \hat{p}] = i\hbar\frac{\partial V}{\partial x} = [H, \hat{p}]$$

$$[\hat{H}, \hat{X}\hat{P}] = \hat{X}\underbrace{[\hat{H}, \hat{P}]} + \hat{P}\underbrace{[\hat{H}, \hat{X}]}$$

$$= i\hbar\, \hat{X}\frac{\partial V}{\partial x} - i\hbar\, \frac{\hat{P}^2}{m}$$

b 2.

$$\left.\begin{array}{l}\langle \phi_n | \hat{p} | \phi_n \rangle \\ [\hat{x}, \hat{H}] = \hat{p}\,\dfrac{m}{i\hbar}\end{array}\right\} \longrightarrow = \frac{i\hbar}{m} \langle \phi_n | \underbrace{[\hat{x}, \hat{H}] | \phi_n \rangle}_{=0}$$

$$= 0$$

6.3

$$\langle \phi_n | [\hat{H}, \hat{x}\hat{p}] | \phi_n \rangle = \langle \phi_n | \left| i\hbar\, x \frac{\partial V}{\partial x} - i\hbar \frac{p^2}{m} \right| | \phi_n \rangle = 0$$

$$\rightarrow \langle \phi_n | \cancel{i\hbar}\, \hat{x} \frac{\partial V}{\partial x} | \phi_n \rangle - \langle \phi_n | \cancel{i\hbar} \frac{p^2}{m} | \phi_n \rangle = 0$$

$$\underline{\langle \phi_n | \hat{x} \frac{\partial V}{\partial x} | \phi_n \rangle} = 2 \langle \phi_n | \frac{p^2}{2m} | \phi_n \rangle = \underbrace{2 E_c}$$

6.4

$$\langle \phi_n | \hat{x} \frac{\partial V}{\partial x} | \phi_n \rangle = 2 E_c \quad ; \quad \underline{V(x)} = V_0 \hat{x}^{\lambda}$$

$$\langle \phi_n | \hat{x} V_0 \lambda \hat{x}^{\lambda - 1} | \phi_n \rangle = 2 E_c$$

$$\lambda \langle \phi_n | \underbrace{V_0 \hat{x}^{\lambda}}_{V(x)} | \phi_n \rangle = 2 E_c$$

$$\lambda E_p = 2 E_c$$