1a) The eigenfunctions are orthonormal:

$$\underline{\underline{\int_{-\infty}^{\infty}\phi_n^*\phi_m\,dx}} = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\cdot\sin\left(\frac{m\pi x}{L}\right)dx \underset{\substack{u=\frac{\pi x}{L}\\ \frac{du}{dx}=\frac{\pi}{L}\\ dx=\frac{L}{\pi}\cdot du}}{=} \frac{2}{L}\cdot\frac{L}{\pi}\int_0^{\pi}\sin(nu)\cdot\sin(mu)\,du \overset{\substack{\text{Bronstein p. 82,}\\ \text{equation 2.117}}}{=} \frac{1}{\pi}\int_0^{\pi}\left[\cos((n-m)u)-\cos((n+m)u)\right]du$$

$$= \frac{1}{\pi}\cdot\left\{\frac{1}{n-m}\cdot\sin[(n-m)u]_0^{\pi} - \frac{1}{n+m}\sin[(n+m)u]_0^{\pi}\right\} \quad \underline{\underline{=0 \text{ for } m\neq n}}$$

For $m=n$: $$\underline{\underline{\int_{-\infty}^{\infty}|\phi_n|^2dx}} = \frac{2}{L}\int_0^L\sin^2\left(\frac{n\pi x}{L}\right)dx \underset{\substack{\text{Bronstein p. 1067}\\ \text{equation 275}}}{=} \frac{2}{L}\left[\frac{x}{2}-\frac{L}{4n\pi}\cdot\sin\left(\frac{2n\pi x}{L}\right)\right]_0^L = \underline{\underline{1}}$$ (normalized eigenfunctions!)

These results can be written as $\underline{\underline{\int_{-\infty}^{\infty}\phi_n^*\phi_m\,dx = \delta_{mn}}}$

b) For a given $X(x)$ we can obtain the decomposition into eigenfunctions by

$$\underline{\underline{\int_{-\infty}^{\infty}\phi_n^*(x)X(x)\,dx}} = \int_{-\infty}^{\infty}\phi_n^*(x)\left[\sum_m c_m\phi_m(x)\right]dx = \sum_m c_m\underbrace{\int_{-\infty}^{\infty}\phi_n^*\phi_m\,dx}_{=\delta_{nm}} = \underline{\underline{c_n}}$$

c) Goal: decompose initial state $\psi(x,t=0)$ into eigenfunctions of the full-width square well potential ϕ_n, i.e. $\psi(x,t)=\sum_n a_n\cdot\phi_n$

From b): $$a_n = \int_{-\infty}^{\infty}\phi_n^*\psi(x,t=0)\,dx = \underset{\text{from }\phi_n}{\sqrt{\frac{2}{L}}}\cdot\underset{\text{from }\psi}{\frac{2}{\sqrt{L}}}\int_{L/2}^{L}\sin\left(\frac{n\pi x}{L}\right)\cdot\sin\left(\frac{2\pi x}{L}-\pi\right)dx$$ (boundaries limited by ψ)

$$\overset{\sin(-x)=-\sin(x)}{=} -\frac{2\sqrt{2}}{L}\int_{L/2}^{L}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)dx \underset{\substack{u=\frac{\pi x}{L}\\ du=\frac{\pi}{L}dx}}{=} -\frac{2\sqrt{2}}{\pi}\int_{\pi/2}^{\pi}\sin(nu)\cdot\sin(2u)\,du$$

$$\overset{\substack{\text{Bronstein p. 82}\\ \text{eq. 2.117}}}{=} -\frac{\sqrt{2}}{\pi}\int_{\pi/2}^{\pi}\left[\cos((n-2)u)-\cos((n+2)u)\right]du$$

$$= -\frac{\sqrt{2}}{\pi}\left\{\frac{1}{n-2}\cdot\sin[(n-2)u]_{\pi/2}^{\pi} - \frac{1}{n+2}\sin[(n+2)u]_{\pi/2}^{\pi}\right\}$$

Distinguish different cases: (i) $n\neq 2$, n even $\Rightarrow$ all terms have the form $\underbrace{\sin(\text{even}\cdot\pi)}_{=0}$

$$\Rightarrow \underline{\underline{a_n = 0 \text{ for } n \text{ even}, n\neq 0}}$$

(ii) $n=2$: $\underline{\underline{a_2}} = -\frac{2\sqrt{2}}{\pi}\int_{\pi/2}^{\pi}\sin^2(2u)\,du \underset{\uparrow}{=} -\frac{2\sqrt{2}}{\pi}\left[\frac{u}{2}-\frac{1}{8}\cdot\sin(4u)\right]_{\pi/2}^{\pi} = -\frac{2\sqrt{2}}{\pi}\left[\frac{\pi}{2}-\frac{\pi}{4}-0-0\right] = \underline{\underline{-\frac{1}{\sqrt{2}}}}$

Bronstein p. 1067, eq. 275

(iii) $\underline{n \text{ odd}}$:

$$\underline{\underline{a_n}} = -\frac{\sqrt{2}}{\pi}\left\{\frac{1}{n-2}\sin(n\pi-2\pi) - \frac{1}{n-2}\sin\left(\frac{n\pi}{2}-\pi\right) - \frac{1}{n+2}\sin(n\pi+2\pi) + \frac{1}{n+2}\sin(n\pi/2+\pi)\right\}$$

$$= -\frac{\sqrt{2}}{\pi}\left\{\frac{1}{n-2}\underbrace{\sin(n\pi)}_{\substack{=0\\(n\text{ odd!})}} + \frac{1}{n-2}\sin\left(\frac{n\pi}{2}\right) - \frac{1}{n+2}\underbrace{\sin(n\pi)}_{\substack{=0\\(n\text{ odd!})}} - \frac{1}{n+2}\sin\left(\frac{n\pi}{2}\right)\right\}$$

$$= -\frac{\sqrt{2}}{\pi}\left\{\frac{1}{n-2}\sin\left(\frac{n\pi}{2}\right) - \frac{1}{n+2}\sin\left(\frac{n\pi}{2}\right)\right\} = -\frac{\sqrt{2}}{\pi}\sin\left(\frac{n\pi}{2}\right)\cdot\left[\frac{1}{n-2}-\frac{1}{n+2}\right] = -\frac{\sqrt{2}}{\pi}\sin\left(\frac{n\pi}{2}\right)\cdot\frac{4}{n^2-4}$$

$$\underset{\uparrow}{=} \frac{-4\sqrt{2}}{\pi(n^2-4)}\sin(m\pi+\pi/2) = \frac{-4\sqrt{2}}{\pi(n^2-4)}\underbrace{\cos(m\pi)}_{=(-1)^m} = \underline{\underline{\frac{-4\sqrt{2}}{\pi(n^2-4)}\cdot(-1)^{\frac{n-1}{2}}}}$$

$n=2m+1$, $m=0,1,\dots$

1d) $$\Psi(x,t) = \sum_n a_n\cdot \underset{\substack{\uparrow\\\text{time dependence of eigenfunctions}}}{e^{-i\frac{E_n}{\hbar}t}}\cdot\phi_n(x) = \underbrace{-\frac{1}{\sqrt{2}}}_{a_2}e^{-i\overbrace{\frac{4\pi^2\hbar}{2mL^2}}^{E_2/\hbar}\cdot t}\underbrace{\sqrt{\tfrac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)}_{\phi_2(x)} - \frac{4}{\pi\sqrt{L}}\sum_{n\text{ odd}}\frac{(-1)^{\frac{n-1}{2}}}{n^2-4}\cdot\underbrace{\sin\left(\frac{n\pi x}{L}\right)}_{\text{from }\phi_n}\cdot\underbrace{e^{-i\frac{n^2\pi^2\hbar}{2mL^2}t}}_{\text{time dependence of }\phi_n}$$

e) $$\underline{\underline{P(E=E_1) = |a_1|^2}} = \left|\frac{-4\sqrt{2}}{\pi(1-4)}\cdot(-1)^0\right|^2 = \frac{16\cdot 2}{\pi^2\cdot 9} = \frac{32}{9\pi^2} \approx \underline{\underline{0.36}}$$

f) $$\underline{\underline{\langle E\rangle}} = \sum_n P(E=E_n)\cdot E_n = \sum_n |a_n|^2\cdot E_n = \frac{1}{2}E_2 + \sum_{n\text{ odd}}\frac{16\cdot 2}{\pi^2(n^2-4)^2}\cdot E_n$$

$$= \frac{\pi^2\hbar^2}{mL^2} + \frac{32}{\pi^2}\cdot\frac{\pi^2\hbar^2}{2mL^2}\underbrace{\sum_{n\text{ odd}}\frac{n^2}{(n^2-4)^2}}_{\pi^2/16} = \underline{\underline{\frac{2\pi^2\hbar^2}{mL^2}}}\ (= E_2)$$

2) Schrödinger equation: $i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \Rightarrow \frac{\partial\Psi}{\partial t} = -\frac{i}{\hbar}\cdot H\Psi$; $\frac{\partial\Psi^*}{\partial t} = \frac{i}{\hbar}H\Psi^*$

$$\langle\hat{p}\rangle = \int_{-\infty}^{\infty}\Psi^*\underbrace{\left(-i\hbar\frac{\partial}{\partial x}\right)}_{\hat{p}\text{ in real space}}\Psi\,dx$$

summation and spatial derivative commute with time derivative

$$\frac{\partial}{\partial t}\langle\hat{p}\rangle = \frac{\partial}{\partial t}\int_{-\infty}^{\infty}\Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi\,dx = \int_{-\infty}^{\infty}\underbrace{\frac{\partial\Psi^*}{\partial t}}_{\frac{i}{\hbar}(H\Psi^*)}\left(-i\hbar\frac{\partial\Psi}{\partial x}\right)dx + \int_{-\infty}^{\infty}\Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\underbrace{\frac{\partial\Psi}{\partial t}}_{-\frac{i}{\hbar}(H\Psi)}dx$$

$$= \int_{-\infty}^{\infty}(H\Psi^*)\cdot\frac{\partial\Psi}{\partial x}dx - \int_{-\infty}^{\infty}\Psi^*\frac{\partial}{\partial x}(H\Psi)\,dx = \dots$$ (next page)

$$\ldots \overset{\text{explicitly: Schrödinger eq.}}{=} \int_{-\infty}^{\infty}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}+V(x)\psi^*\right]\cdot\frac{\partial\psi}{\partial x}\,dx \;-\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi\right]dx$$

$$= \int_{-\infty}^{\infty} -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}\cdot\frac{\partial\psi}{\partial x}\,dx + \cancel{\int_{-\infty}^{\infty} V\psi^*\frac{\partial\psi}{\partial x}\cdot dx} \underbrace{- \int_{-\infty}^{\infty}\overbrace{\psi^*}^{f}\left(-\frac{\hbar^2}{2m}\overbrace{\frac{\partial^3\psi}{\partial x^3}}^{g'}\right)dx}_{\text{partial integration:}} - \int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\cdot\psi\,dx \cancel{-\int_{-\infty}^{\infty}\psi^*\cdot V\cdot\frac{\partial\psi}{\partial x}\,dx}$$

partial integration:

$fg - \int f'g\,dx$

$$= \underbrace{\left[-\frac{\hbar^2}{2m}\psi^*\frac{\partial^2\psi}{\partial x^2}\right]_{-\infty}^{\infty}}_{=0 \text{ since } \psi^*\to 0 \text{ for } x\to\pm\infty \text{ (normalization)}} + \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{\partial\psi^*}{\partial x}\cdot\frac{\partial^2\psi}{\partial x^2}\,dx$$

$$= -\int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\psi\,dx - \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\Bigg[\underbrace{\overset{g'}{\frac{\partial^2\psi^*}{\partial x^2}}\cdot\overset{f}{\frac{\partial\psi}{\partial x}}}_{\text{another partial integration}} + \cancel{\frac{\partial^2\psi}{\partial x^2}\cdot\frac{\partial\psi^*}{\partial x}}\Bigg]dx$$

another partial integration

$$fg - \int f'g\,dx = \underbrace{\frac{\partial\psi}{\partial x}\cdot\frac{\partial\psi^*}{\partial x}\Big|_{-\infty}^{\infty}}_{=0 \text{ (normalization)}} \cancel{-\int_{-\infty}^{\infty}\frac{\partial^2\psi}{\partial x^2}\frac{\partial\psi^*}{\partial x}\,dx}$$

$$\underline{\underline{= -\int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\psi\,dx \equiv -\left\langle\frac{\partial V}{\partial x}\right\rangle}} \overset{!}{\underset{\text{where we started}}{=}} \underline{\underline{\frac{\partial}{\partial t}\langle p\rangle}}$$