Chapter 2

Time-Independent Schrödinger Equation

Problem 2.1

(a)

$$\Psi(x,t) = \psi(x)e^{-i(E_0+i\Gamma)t/\hbar} = \psi(x)e^{\Gamma t/\hbar}e^{-iE_0t/\hbar} \Longrightarrow |\Psi|^2 = |\psi|^2 e^{2\Gamma t/\hbar}.$$

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = e^{2\Gamma t/\hbar} \int_{-\infty}^{\infty} |\psi|^2 dx.$$

The second term is independent of t, so if the product is to be 1 for all time, the first term ($e^{2\Gamma t/\hbar}$) must also be constant, and hence $\Gamma = 0$. QED

(b) If ψ satisfies Eq. 2.5, $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{dx^2} + V\psi = E\psi$, then (taking the complex conjugate and noting that V and E are real): $-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{dx^2} + V\psi^* = E\psi^*$, so ψ^* *also* satisfies Eq. 2.5. Now, if ψ_1 and ψ_2 satisfy Eq. 2.5, so too does any linear combination of them ($\psi_3 \equiv c_1\psi_1 + c_2\psi_2$):

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2\psi_3}{dx^2} + V\psi_3 &= -\frac{\hbar^2}{2m}\left(c_1\frac{\partial^2\psi_1}{dx^2} + c_2\frac{\partial^2\psi_2}{\partial x^2}\right) + V(c_1\psi_1 + c_2\psi_2) \\
&= c_1\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V\psi_1\right] + c_2\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2\right] \\
&= c_1(E\psi_1) + c_2(E\psi_2) = E(c_1\psi_1 + c_2\psi_2) = E\psi_3.
\end{aligned}$$

Thus, $(\psi + \psi^*)$ and $i(\psi - \psi^*)$ – both of which are *real* – satisfy Eq. 2.5. *Conclusion:* From any complex solution, we can always construct two *real* solutions (of course, if ψ is already real, the second one will be zero). In particular, since $\psi = \frac{1}{2}[(\psi + \psi^*) - i(i(\psi - \psi^*))]$, ψ can be expressed as a linear combination of two real solutions. QED

(c) If $\psi(x)$ satisfies Eq. 2.5, then, changing variables $x \to -x$ and noting that $\partial^2/\partial(-x)^2 = \partial^2/\partial x^2$,

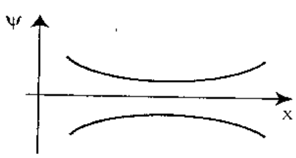
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{dx^2} + V(-x)\psi(-x) = E\psi(-x);$$

so if $V(-x) = V(x)$ then $\psi(-x)$ *also* satisfies Eq. 2.5. It follows that $\psi_+(x) \equiv \psi(x) + \psi(-x)$ (which is *even*: $\psi_+(-x) = \psi_+(x)$) and $\psi_-(x) \equiv \psi(x) - \psi(-x)$ (which is *odd*: $\psi_-(-x) = -\psi_-(x)$) both satisfy Eq.

2.5. But $\psi(x) = \frac{1}{2}(\psi_+(x) + \psi_-(x))$, so any solution can be expressed as a linear combination of even and odd solutions. QED

Problem 2.2

Given $\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V(x) - E]\psi$, if $E < V_{\min}$, then ψ'' and ψ always have the same sign: If ψ is positive(negative), then ψ'' is also positive(negative). This means that ψ always curves away from the axis (see Figure). However, it has got to go to zero as $x \to -\infty$ (else it would not be normalizable). At some point it's got to *depart* from zero (if it *doesn't*, it's going to be identically zero *everywhere*), in (say) the positive direction. At this point its slope is positive, and *increasing*, so ψ gets bigger and bigger as x increases. It can't ever "turn over" and head back toward the axis, because that would requuire a negative second derivative—it always has to bend away from the axis. By the same token, if it starts out heading negative, it just runs more and more negative. In neither case is there any way for it to come back to zero, as it must (at $x \to \infty$) in order to be normalizable. QED



Problem 2.3

Equation 2.20 says $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$; Eq. 2.23 says $\psi(0) = \psi(a) = 0$. If $E = 0$, $d^2\psi/dx^2 = 0$, so $\psi(x) = A + Bx$; $\psi(0) = A = 0 \Rightarrow \psi = Bx$; $\psi(a) = Ba = 0 \Rightarrow B = 0$, so $\psi = 0$. If $E < 0$, $d^2\psi/dx^2 = \kappa^2\psi$, with $\kappa \equiv \sqrt{-2mE}/\hbar$ real, so $\psi(x) = Ae^{\kappa x} + Be^{-\kappa x}$. This time $\psi(0) = A + B = 0 \Rightarrow B = -A$, so $\psi = A(e^{\kappa x} - e^{-\kappa x})$, while $\psi(a) = A\left(e^{\kappa a} - e^{i\kappa a}\right) = 0 \Rightarrow$ either $A = 0$, so $\psi = 0$, or else $e^{\kappa a} = e^{-\kappa a}$, so $e^{2\kappa a} = 1$, so $2\kappa a = \ln(1) = 0$, so $\kappa = 0$, and again $\psi = 0$. In all cases, then, the boundary conditions force $\psi = 0$, which is unacceptable (non-normalizable).

Problem 2.4

$$\langle x\rangle = \int x|\psi|^2 dx = \frac{2}{a}\int_0^a x\sin^2\left(\frac{n\pi}{a}x\right)dx. \qquad \text{Let } y \equiv \frac{n\pi}{a}x, \text{ so } dx = \frac{a}{n\pi}dy; \quad y: 0 \to n\pi.$$

$$= \frac{2}{a}\left(\frac{a}{n\pi}\right)^2\int_0^{n\pi} y\sin^2 y\,dy = \frac{2a}{n^2\pi^2}\left[\frac{y^2}{4} - \frac{y\sin 2y}{4} - \frac{\cos 2y}{8}\right]\Bigg|_0^{n\pi}$$

$$= \frac{2a}{n^2\pi^2}\left[\frac{n^2\pi^2}{4} - \frac{\cos 2n\pi}{8} + \frac{1}{8}\right] = \boxed{\frac{a}{2}.} \quad \text{(Independent of } n.)$$

$$\langle x^2\rangle = \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{n\pi}{a}x\right)dx = \frac{2}{a}\left(\frac{a}{n\pi}\right)^3\int_0^{n\pi} y^2\sin^2 y\,dy$$
$$= \frac{2a^2}{(n\pi)^3}\left[\frac{y^3}{6} - \left(\frac{y^2}{4}-\frac{1}{8}\right)\sin 2y - \frac{y\cos 2y}{4}\right]_0^{n\pi}$$
$$= \frac{2a^2}{(n\pi)^3}\left[\frac{(n\pi)^3}{6} - \frac{n\pi\cos(2n\pi)}{4}\right] = \boxed{a^2\left[\frac{1}{3}-\frac{1}{2(n\pi)^2}\right].}$$

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = \boxed{0.}\quad (\textit{Note}: \text{Eq. 1.33 is much faster than Eq. 1.35.})$$

$$\langle p^2\rangle = \int \psi_n^*\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2\psi_n\,dx = -\hbar^2\int\psi_n^*\left(\frac{d^2\psi_n}{dx^2}\right)dx$$
$$= (-\hbar^2)\left(-\frac{2mE_n}{\hbar^2}\right)\int\psi_n^*\psi_n\,dx = 2mE_n = \boxed{\left(\frac{n\pi\hbar}{a}\right)^2.}$$

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2\left(\frac{1}{3}-\frac{1}{2(n\pi)^2}-\frac{1}{4}\right) = \frac{a^2}{4}\left(\frac{1}{3}-\frac{2}{(n\pi)^2}\right);\quad \boxed{\sigma_x = \frac{a}{2}\sqrt{\frac{1}{3}-\frac{2}{(n\pi)^2}}.}$$

$$\sigma_p^2 = \langle p^2\rangle - \langle p\rangle^2 = \left(\frac{n\pi\hbar}{a}\right)^2;\quad \boxed{\sigma_p = \frac{n\pi\hbar}{a}.}\quad \therefore \sigma_x\sigma_p = \boxed{\frac{\hbar}{2}\sqrt{\frac{(n\pi)^2}{3}-2}.}$$

The product $\sigma_x\sigma_p$ is $\boxed{\text{smallest for } n=1;}$ in that case, $\sigma_x\sigma_p = \frac{\hbar}{2}\sqrt{\frac{\pi^2}{3}-2} = (1.136)\hbar/2 > \hbar/2.$ ✓

Problem 2.5

(a)

$$|\Psi|^2 = \Psi^2\Psi = |A|^2(\psi_1^*+\psi_2^*)(\psi_1+\psi_2) = |A|^2[\psi_1^*\psi_1+\psi_1^*\psi_2+\psi_2^*\psi_1+\psi_2^*\psi_2].$$
$$1 = \int|\Psi|^2dx = |A|^2\int[|\psi_1|^2+\psi_1^*\psi_2+\psi_2^*\psi_1+|\psi_2|^2]dx = 2|A|^2 \Rightarrow \boxed{A = 1/\sqrt{2}.}$$

(b)

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1 e^{-iE_1t/\hbar} + \psi_2 e^{-iE_2t/\hbar}\right]\quad \left(\text{but } \frac{E_n}{\hbar} = n^2\omega\right)$$
$$= \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\left[\sin\left(\frac{\pi}{a}x\right)e^{-i\omega t} + \sin\left(\frac{2\pi}{a}x\right)e^{-i4\omega t}\right] = \boxed{\frac{1}{\sqrt{a}}e^{-i\omega t}\left[\sin\left(\frac{\pi}{a}x\right)+\sin\left(\frac{2\pi}{a}x\right)e^{-3i\omega t}\right].}$$

$$|\Psi(x,t)|^2 = \frac{1}{a}\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\left(e^{-3i\omega t}+e^{3i\omega t}\right) + \sin^2\left(\frac{2\pi}{a}x\right)\right]$$
$$= \boxed{\frac{1}{a}\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin^2\left(\frac{2\pi}{a}x\right) + 2\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\cos(3\omega t)\right].}$$

(c)

$$\langle x\rangle = \int x|\Psi(x,t)|^2 dx$$
$$= \frac{1}{a}\int_0^a x\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin^2\left(\frac{2\pi}{a}x\right) + 2\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\cos(3\omega t)\right]dx$$

$$\int_0^a x\sin^2\left(\frac{\pi}{a}x\right)dx = \left[\frac{x^2}{4} - \frac{x\sin\left(\frac{2\pi}{a}x\right)}{4\pi/a} - \frac{\cos\left(\frac{2\pi}{a}x\right)}{8(\pi/a)^2}\right]\Bigg|_0^a = \frac{a^2}{4} = \int_0^a x\sin^2\left(\frac{2\pi}{a}x\right)dx.$$

$$\int_0^a x\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)dx = \frac{1}{2}\int_0^a x\left[\cos\left(\frac{\pi}{a}x\right) - \cos\left(\frac{3\pi}{a}x\right)\right]dx$$

$$= \frac{1}{2}\left[\frac{a^2}{\pi^2}\cos\left(\frac{\pi}{a}x\right) + \frac{ax}{\pi}\sin\left(\frac{\pi}{a}x\right) - \frac{a^2}{9\pi^2}\cos\left(\frac{3\pi}{a}x\right) - \frac{ax}{3\pi}\sin\left(\frac{3\pi}{a}x\right)\right]_0^a$$

$$= \frac{1}{2}\left[\frac{a^2}{\pi^2}(\cos(\pi) - \cos(0)) - \frac{a^2}{9\pi^2}(\cos(3\pi) - \cos(0))\right] = -\frac{a^2}{\pi^2}\left(1 - \frac{1}{9}\right) = -\frac{8a^2}{9\pi^2}.$$

$$\therefore \langle x\rangle = \frac{1}{a}\left[\frac{a^2}{4} + \frac{a^2}{4} - \frac{16a^2}{9\pi^2}\cos(3\omega t)\right] = \boxed{\frac{a}{2}\left[1 - \frac{32}{9\pi^2}\cos(3\omega t)\right].}$$

Amplitude: $\boxed{\frac{32}{9\pi^2}\left(\frac{a}{2}\right) = 0.3603(a/2);}$ *angular frequency:* $\boxed{3\omega = \frac{3\pi^2\hbar}{2ma^2}.}$

(d)

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = m\left(\frac{a}{2}\right)\left(-\frac{32}{9\pi^2}\right)(-3\omega)\sin(3\omega t) = \boxed{\frac{8\hbar}{3a}\sin(3\omega t).}$$

(e) You could get either $\boxed{E_1 = \pi^2\hbar^2/2ma^2}$ or $\boxed{E_2 = 2\pi^2\hbar^2/ma^2,}$ with equal probability $\boxed{P_1 = P_2 = 1/2.}$

So $\langle H\rangle = \boxed{\frac{1}{2}(E_1 + E_2) = \frac{5\pi^2\hbar^2}{4ma^2};}$ it's the *average* of E_1 and E_2.

Problem 2.6

From Problem 2.5, we see that

$$\Psi(x,t) = \boxed{\frac{1}{\sqrt{a}}e^{-i\omega t}\left[\sin\left(\frac{\pi}{a}x\right) + \sin\left(\frac{2\pi}{a}x\right)e^{-3i\omega t}e^{i\phi}\right];}$$

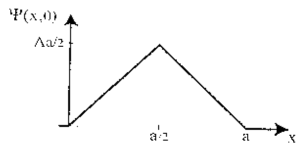
$$|\Psi(x,t)|^2 = \boxed{\frac{1}{a}\left[\sin^2\left(\frac{\pi}{a}x\right) + \sin^2\left(\frac{2\pi}{a}x\right) + 2\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}x\right)\cos(3\omega t - \phi)\right];}$$

and hence $\boxed{\langle x\rangle = \frac{a}{2}\left[1 - \frac{32}{9\pi^2}\cos(3\omega t - \phi)\right].}$ This amounts physically to starting the clock at a different time (i.e., shifting the $t = 0$ point).

If $\phi = \frac{\pi}{2}$, so $\Psi(x,0) = A[\psi_1(x) + i\psi_2(x)]$, then $\cos(3\omega t - \phi) = \sin(3\omega t)$; $\langle x\rangle$ starts at $\frac{a}{2}$.

If $\phi = \pi$, so $\Psi(x,0) = A[\psi_1(x) - \psi_2(x)]$, then $\cos(3\omega t - \phi) = -\cos(3\omega t)$; $\langle x\rangle$ starts at $\frac{a}{2}\left(1 + \frac{32}{9\pi^2}\right)$.

Problem 2.7



(a)

$$1 = A^2\int_0^{a/2} x^2 dx + A^2\int_{a/2}^{a}(a-x)^2 dx = A^2\left[\frac{x^3}{3}\Big|_0^{a/2} - \frac{(a-x)^3}{3}\Big|_{a/2}^{a}\right]$$
$$= \frac{A^2}{3}\left(\frac{a^3}{8} + \frac{a^3}{8}\right) = \frac{A^2a^3}{12} \Rightarrow \boxed{A = \frac{2\sqrt{3}}{\sqrt{a^3}}.}$$

(b)

$$c_n = \sqrt{\frac{2}{a}}\frac{2\sqrt{3}}{a\sqrt{a}}\left[\int_0^{a/2} x\sin\left(\frac{n\pi}{a}x\right)dx + \int_{a/2}^{a}(a-x)\sin\left(\frac{n\pi}{a}x\right)dx\right]$$
$$= \frac{2\sqrt{6}}{a^2}\left\{\left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{a}x\right) - \frac{xa}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right]\Big|_0^{a/2}\right.$$
$$\left. + a\left[-\frac{a}{n\pi}\cos\left(\frac{n\pi}{a}x\right)\right]\Big|_{a/2}^{a} - \left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{a}x\right) - \left(\frac{ax}{n\pi}\right)\cos\left(\frac{n\pi}{a}x\right)\right]\Big|_{a/2}^{a}\right\}$$
$$= \frac{2\sqrt{6}}{a^2}\left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{2}\right) - \frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right) - \frac{a^2}{n\pi}\cos n\pi + \frac{a^2}{n\pi}\cos\left(\frac{n\pi}{2}\right)\right.$$
$$\left. + \left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi}{2}\right) + \frac{a^2}{n\pi}\cos n\pi - \frac{a^2}{2n\pi}\cos\left(\frac{n\pi}{2}\right)\right]$$
$$= \frac{2\sqrt{6}}{a^2}2\frac{a^2}{(n\pi)^2}\sin\left(\frac{n\pi}{2}\right) = \frac{4\sqrt{6}}{(n\pi)^2}\sin\left(\frac{n\pi}{2}\right) = \begin{cases} 0, & n \text{ even},\\ (-1)^{(n-1)/2}\frac{4\sqrt{6}}{(n\pi)^2}, & n \text{ odd}.\end{cases}$$

So $\boxed{\Psi(x,t) = \frac{4\sqrt{6}}{\pi^2}\sqrt{\frac{2}{a}}\sum_{n=1,3,5,\dots}(-1)^{(n-1)/2}\frac{1}{n^2}\sin\left(\frac{n\pi}{a}x\right)e^{-iE_nt/\hbar},}$ where $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$.

(c)

$$P_1 = |c_1|^2 = \frac{16 \cdot 6}{\pi^4} = \boxed{0.9855.}$$

(d)

$$\langle H \rangle = \sum |c_n|^2 E_n = \frac{96}{\pi^4} \frac{\pi^2 \hbar^2}{2ma^2} \underbrace{\left(\frac{1}{1} + \frac{1}{3^2} + \frac{1}{5^2} + \frac{1}{7^2} + \cdots \right)}_{\pi^2/8} = \frac{48\hbar^2}{\pi^2 m a^2} \frac{\pi^2}{8} = \boxed{\frac{6\hbar^2}{ma^2}.}$$

Problem 2.8

(a)

$$\boxed{\Psi(x,0) = \begin{cases} A, & 0 < x < a/2; \\ 0, & \text{otherwise.} \end{cases}} \quad 1 = A^2 \int_0^{a/2} dx = A^2 (a/2) \Rightarrow \boxed{A = \sqrt{\frac{2}{a}}.}$$

(b) From Eq. 2.37,

$$c_1 = A\sqrt{\frac{2}{a}} \int_0^{a/2} \sin\left(\frac{\pi}{a}x\right) dx = \frac{2}{a}\left[-\frac{a}{\pi}\cos\left(\frac{\pi}{a}x\right)\right]\Big|_0^{a/2} = -\frac{2}{\pi}\left[\cos\left(\frac{\pi}{2}\right) - \cos 0\right] = \frac{2}{\pi}.$$

$$P_1 = |c_1|^2 = \boxed{(2/\pi)^2 = 0.4053.}$$

Problem 2.9

$$\hat{H}\Psi(x,0) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[Ax(a-x)\right] = -A\frac{\hbar^2}{2m}\frac{\partial}{\partial x}(a-2x) = A\frac{\hbar^2}{m}.$$

$$\begin{aligned} \int \Psi(x,0)^* \hat{H}\Psi(x,0)\, dx &= A^2 \frac{\hbar^2}{m} \int_0^a x(a-x)\, dx = A^2 \frac{\hbar^2}{m} \left(a\frac{x^2}{2} - \frac{x^3}{3} \right)\Big|_0^a \\ &= A^2 \frac{\hbar^2}{m} \left(\frac{a^3}{2} - \frac{a^3}{3} \right) = \frac{30}{a^5} \frac{\hbar^2}{m} \frac{a^3}{6} = \boxed{\frac{5\hbar^2}{ma^2}} \end{aligned}$$

(same as Example 2.3).