5.1 The commutation operator is defined by its action on a state vector $|\psi\rangle$ as:

$$[\hat{x},\hat{p}]|\psi\rangle = \hat{x}\hat{p}|\psi\rangle - \hat{p}\hat{x}|\psi\rangle$$

In wave function language (the position representation), we express position as a multiplicative factor, $\hat{x} \doteq x$ and momentum as a derivative operator $\hat{p} \doteq -i\hbar\, d/dx$, and the state vector is represented by $|\psi\rangle \doteq \psi(x)$. Then the commutator becomes

$$[\hat{x},\hat{p}]|\psi\rangle \doteq x\left(-i\hbar\frac{d}{dx}\right)\psi(x) - \left(-i\hbar\frac{d}{dx}\right)x\psi(x)$$

The second term requires the chain rule, yielding

$$\begin{aligned}[\hat{x},\hat{p}]|\psi\rangle &\doteq -i\hbar x\frac{d\psi(x)}{dx} + i\hbar x\frac{d\psi(x)}{dx} + i\hbar\psi(x)\\ &\doteq i\hbar\psi(x)\end{aligned}$$

This is very clearly non-zero, and tells us that the position and momentum operators do not commute.

5.2 a) Initial state vector is $|\psi(t=0)\rangle = A\big(|E_1\rangle - |E_2\rangle + i|E_3\rangle\big)$ where $|E_n\rangle$ are energy eigenstates. To normalize, we require

$$\begin{aligned}1 = \langle\psi|\psi\rangle &= A^*\big(\langle E_1| - \langle E_2| - i\langle E_3|\big)A\big(|E_1\rangle - |E_2\rangle + i|E_3\rangle\big)\\ &= A^*A\big(\langle E_1|E_1\rangle + \langle E_2|E_2\rangle + \langle E_3|E_3\rangle\big)\\ &= 3|A|^2\end{aligned}$$

Therefore: $A = 1/\sqrt{3}$ and $|\psi(t=0)\rangle = \big(1/\sqrt{3}\big)\big(|E_1\rangle - |E_2\rangle + i|E_3\rangle\big)$

(b) The only possible outcome of an energy measurement is an energy eigenvalue

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2};\quad n = 1,2,3...$$

The probability of measuring an energy eigenvalue is

$$\mathcal{P}_{E_n} = \left|\langle E_n|\psi(0)\rangle\right|^2$$

Clearly all probabilities for measuring eigenstates other than 1,2, and 3 are zero. What remains then is:

$$\begin{aligned}\mathcal{P}_{E_1} &= \left|\langle E_1|\psi(0)\rangle\right|^2 = \left|\langle E_1|\big(1/\sqrt{3}\big)\big(|E_1\rangle - |E_2\rangle + i|E_3\rangle\big)\right|^2\\ &= \left|\big(1/\sqrt{3}\big)\big(\langle E_1|E_1\rangle - \langle E_1|E_2\rangle + i\langle E_1|E_3\rangle\big)\right|^2 = \left|\big(1/\sqrt{3}\big)(1-0+i0)\right|^2 = \tfrac{1}{3}\end{aligned}$$

and likewise

$$\mathcal{P}_{E_2} = \left|\langle E_2|\psi(0)\rangle\right|^2 = \left|\langle E_2|\left(1/\sqrt{3}\right)\left(|E_1\rangle - |E_2\rangle + i|E_3\rangle\right)\right|^2 = \tfrac{1}{3}$$

$$\mathcal{P}_{E_3} = \left|\langle E_3|\psi(0)\rangle\right|^2 = \left|\langle E_3|\left(1/\sqrt{3}\right)\left(|E_1\rangle - |E_2\rangle + i|E_3\rangle\right)\right|^2 = \tfrac{1}{3}$$

(c) The average value of the energy is

$$\langle E\rangle = \sum_{n=1}^{\infty}\mathcal{P}_{E_n}E_n = \sum_{n=1}^{\infty}\left|\langle E_n|\psi(0)\rangle\right|^2 n^2\frac{\pi^2\hbar^2}{2mL^2} = \sum_{n=1}^{\infty}\frac{1}{3}n^2\frac{\pi^2\hbar^2}{2mL^2} = \frac{\pi^2\hbar^2}{6mL^2}\left(1^2+2^2+3^2\right)$$
$$= \frac{7\pi^2\hbar^2}{3mL^2} = \frac{14}{3}E_1$$

(d) Using the Schrödinger recipe, the time-evolved state is

$$|\psi(t)\rangle = \left(1/\sqrt{3}\right)\left(e^{-iE_1t/\hbar}|E_1\rangle - e^{-iE_2t/\hbar}|E_2\rangle + ie^{-iE_3t/\hbar}|E_3\rangle\right)$$
$$= \left(1/\sqrt{3}\right)\left(e^{-i\pi^2\hbar t/2mL^2}|E_1\rangle - e^{-i4\pi^2\hbar t/2mL^2}|E_2\rangle + ie^{-i9\pi^2\hbar t/2mL^2}|E_3\rangle\right)$$

(e) At time $t = \hbar/E_1$, the possible outcomes of a measurement of the energy are the energy eigenvalues. The probabilities are

$$\mathcal{P}_{E_1} = \left|\langle E_1|\psi(t)\rangle\right|^2 = \left|\langle E_1|\left(1/\sqrt{3}\right)\left(e^{-i}|E_1\rangle - e^{-4i}|E_2\rangle + ie^{-9i}|E_3\rangle\right)\right|^2 = \tfrac{1}{3}$$

$$\mathcal{P}_{E_2} = \left|\langle E_2|\psi(t)\rangle\right|^2 = \left|\langle E_2|\left(1/\sqrt{3}\right)\left(e^{-i}|E_1\rangle - e^{-4i}|E_2\rangle + ie^{-9i}|E_3\rangle\right)\right|^2 = \tfrac{1}{3}$$

$$\mathcal{P}_{E_3} = \left|\langle E_3|\psi(t)\rangle\right|^2 = \left|\langle E_3|\left(1/\sqrt{3}\right)\left(e^{-i}|E_1\rangle - e^{-4i}|E_2\rangle + ie^{-9i}|E_3\rangle\right)\right|^2 = \tfrac{1}{3}$$

which are independent of time, as expected.

5.3 Assume the solution

$$\varphi_E(x) = Ae^{ikx} + Be^{-ikx}$$

The boundary conditions yield

$$\varphi_E(0):\quad A + B = 0 \quad\Rightarrow\quad B = -A$$
$$\varphi_E(L):\quad Ae^{ikL} + Be^{-ikL} = 0 \quad\Rightarrow\quad A\left(e^{ikL} - e^{-ikL}\right) = 2iA\sin kL = 0$$

Hence wave vectors that satisfy the equation are

$$kL = n\pi$$

$$k_n = n\frac{\pi}{L};\quad n = 1,2,3,\ldots$$

just as before. The allowed energies are thus

$$E_n = \frac{\hbar^2k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2};\quad n = 1,2,3\ldots$$

The allowed eigenstates are

$$\varphi_n(x) = Ae^{in\pi x/L} - Ae^{-in\pi x/L} = 2Ai\sin\frac{n\pi x}{L}$$

which after normalization are

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}, \qquad n = 1,2,3,...$$

5.4 Assume the real solutions

$$\varphi_E(x) = A\sin kx + B\cos kx$$

The boundary conditions yield

$$\begin{aligned} &\varphi_E(-a): \quad -A\sin ka + B\cos ka = 0 \quad \Rightarrow \quad B\cos ka = A\sin ka \\ &\varphi_E(a): \quad A\sin ka + B\cos ka = 0 \quad \Rightarrow \quad 2A\sin ka = 0 \;\; or \;\; 2B\cos ka = 0 \end{aligned}$$

This yields two quantization equations:

$$\begin{aligned} &\sin ka = 0 \quad \Rightarrow \quad ka = n\pi \\ &\cos ka = 0 \quad \Rightarrow \quad ka = \left(n' + \tfrac{1}{2}\right)\pi \end{aligned}$$

and quantized energies:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \begin{cases} \dfrac{n^2\pi^2\hbar^2}{2ma^2}; \quad n = 1,2,3... \\ \dfrac{\left(n' + \frac{1}{2}\right)^2 \pi^2\hbar^2}{2ma^2}; \quad n' = 0,1,2... \end{cases}$$

Hence the energies are

$$\begin{aligned} E_n &= \frac{1}{8}\frac{\pi^2\hbar^2}{ma^2}, \; \frac{1}{2}\frac{\pi^2\hbar^2}{ma^2}, \; \frac{9}{8}\frac{\pi^2\hbar^2}{ma^2}, \; \frac{4}{2}\frac{\pi^2\hbar^2}{ma^2}, \; \frac{25}{8}\frac{\pi^2\hbar^2}{ma^2}, \; \cdots \\ &= 1^2\frac{\pi^2\hbar^2}{2m(2a)^2}, \; 2^2\frac{\pi^2\hbar^2}{2m(2a)^2}, \; 3^2\frac{\pi^2\hbar^2}{2m(2a)^2}, \; 4^2\frac{\pi^2\hbar^2}{2m(2a)^2}, \; 5^2\frac{\pi^2\hbar^2}{2m(2a)^2}, \; \cdots \end{aligned}$$

which are the same as the 0->L well, BUT with the full width now $2a$. The quantization condition $\sin ka = 0$ requires that $B = 0$, so the solutions are sine functions, whereas $\cos ka = 0$ requires that $A = 0$, so the solutions are cosine functions. The normalization requirement for the sine functions is

$$1 = \langle\psi|\psi\rangle = \int_{-a}^{a}|\varphi_n(x)|^2\,dx = \int_{-a}^{a}\left|A\sin\left(\tfrac{n\pi x}{a}\right)\right|^2 dx = |A|^2\int_{-a}^{a}\sin^2\left(\tfrac{n\pi x}{a}\right)dx = |A|^2\,a$$

The cosine functions yield the same normalization, so the normalized eigenstates are

$$\varphi_n(x) = \begin{cases} \sqrt{\dfrac{1}{a}}\sin\dfrac{n\pi x}{a} & n = 1,2,3,... \\ \sqrt{\dfrac{1}{a}}\cos\dfrac{\left(n'+\frac{1}{2}\right)\pi x}{a} & n' = 0,1,2,... \end{cases}$$

These look the same inside the well as the 0->L case, but we need both functions in this case.

5.5 The expectation value of the position for a particle in any energy eigenstate state of an infinite square potential energy well is

$$\begin{aligned}\langle x\rangle &= \langle E_n|x|E_n\rangle = \int_{-\infty}^{\infty}\varphi_n^*(x)x\varphi_n(x)dx = \int_{-\infty}^{\infty}x|\varphi_n(x)|^2 dx \\ &= \tfrac{2}{L}\int_0^L x\sin^2\left(\tfrac{n\pi x}{L}\right)dx = \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^2\int_0^{n\pi}y\sin^2(y)dy = \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^2\left[\tfrac{y^2}{4}-\tfrac{y\sin 2y}{4}-\tfrac{\cos 2y}{8}\right]_0^{n\pi} \\ &= \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^2\left[\tfrac{n^2\pi^2}{4}-\tfrac{n\pi\sin(2n\pi)}{4}-\tfrac{\cos(2n\pi)}{8}+\tfrac{1}{8}\right] = \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^2\left[\tfrac{n^2\pi^2}{4}\right] = \tfrac{L}{2}\end{aligned}$$

as expected. To find the uncertainty, we first need the expectation value of the square of the position:

$$\begin{aligned}\langle x^2\rangle &= \langle E_n|x^2|E_n\rangle = \int_{-\infty}^{\infty}x^2|\varphi_n(x)|^2 dx = \tfrac{2}{L}\int_0^L x\sin^2\left(\tfrac{n\pi x}{L}\right)dx \\ &= \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^3\int_0^{n\pi}y^2\sin^2(y)dy = \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^3\left[\tfrac{y^3}{6}-\tfrac{(2y^2-1)\sin 2y}{8}-\tfrac{y\cos 2y}{4}\right]_0^{n\pi} \\ &= \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)^3\left[\tfrac{n^3\pi^3}{6}-\tfrac{n\pi\cos(2n\pi)}{4}\right] = L^2\left[\tfrac{1}{3}-\tfrac{1}{2n^2\pi^2}\right]\end{aligned}$$

The uncertainty of the position is

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{L^2\left(\tfrac{1}{3}-\tfrac{1}{2n^2\pi^2}\right)-\left(\tfrac{L}{2}\right)^2} = L\sqrt{\tfrac{1}{12}-\tfrac{1}{2n^2\pi^2}}$$

The expectation value of the momentum is

$$\begin{aligned}\langle p\rangle &= \langle E_n|p|E_n\rangle = \int_{-\infty}^{\infty}\varphi_n^*(x)\left(-i\hbar\tfrac{d}{dx}\right)\varphi_n(x)dx = \tfrac{2}{L}\int_0^L\sin\left(\tfrac{n\pi x}{L}\right)\left(-i\hbar\tfrac{d}{dx}\right)\sin\left(\tfrac{n\pi x}{L}\right)dx \\ &= -i\hbar\tfrac{2}{L}\int_0^L\sin\left(\tfrac{n\pi x}{L}\right)\left(\tfrac{n\pi}{L}\right)\cos\left(\tfrac{n\pi x}{L}\right)dx = -i\hbar\tfrac{1}{L}\left[\sin^2\left(\tfrac{n\pi x}{L}\right)\right]_0^L = 0\end{aligned}$$

The expectation value of the square of the momentum is:

$$\begin{aligned}\langle p^2\rangle &= \langle E_n|p^2|E_n\rangle = \int_{-\infty}^{\infty}\varphi_n^*(x)\left(-i\hbar\tfrac{d}{dx}\right)^2\varphi_n(x)dx = -\tfrac{2}{L}\hbar^2\int_0^L\sin\left(\tfrac{n\pi x}{L}\right)\left(\tfrac{d^2}{dx^2}\right)\sin\left(\tfrac{n\pi x}{L}\right)dx \\ &= \tfrac{2}{L}\hbar^2\left(\tfrac{n\pi}{L}\right)^2\int_0^L\sin^2\left(\tfrac{n\pi x}{L}\right)dx = \tfrac{2}{L}\hbar^2\left(\tfrac{n\pi}{L}\right)^2\tfrac{L}{2} = \left(\tfrac{n\pi\hbar}{L}\right)^2\end{aligned}$$

The uncertainty of the momentum is

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\left(\tfrac{n\pi\hbar}{L}\right)^2 - 0} = \left(\tfrac{n\pi\hbar}{L}\right)$$

5.6 To calculate the probability of finding the particle in the interval, use Eq. (5.28). For an energy eigenstate, the result is

$$\mathcal{P}_{3L/4<x<L} = \int_{3L/4}^{L} \left|\psi(x)\right|^2 dx = \int_{3L/4}^{L} \left|\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{n\pi x}{L}\right)\right|^2 dx = \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)\int_{3n\pi/4}^{n\pi} \sin^2 y\, dy$$
$$= \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)\left[\tfrac{y}{2} - \tfrac{\sin 2y}{4}\right]_{3n\pi/4}^{n\pi} = \tfrac{2}{L}\left(\tfrac{L}{n\pi}\right)\left[\tfrac{n\pi}{2} - \tfrac{\sin 2n\pi}{4} - \tfrac{3n\pi}{8} + \tfrac{\sin(3n\pi/2)}{4}\right] = \tfrac{1}{4}\left(1 + \tfrac{2}{n\pi}\sin\left(3n\pi/2\right)\right)$$

For the first three states, the results are

$$\mathcal{P}_{3L/4<x<L} = \tfrac{1}{4}\left(1 - \tfrac{2}{\pi}\right),\ \tfrac{1}{4},\ \tfrac{1}{4}\left(1 + \tfrac{2}{3\pi}\right) \cong 0.09,\ 0.25,\ 0.30$$

5.7 The initial state vector is $\left|\psi(t=0)\right\rangle = \left(\left|E_1\right\rangle - 2i\left|E_2\right\rangle\right)/\sqrt{5}$. Using the Schrödinger recipe, the time evolved state is

$$\left|\psi(t)\right\rangle = \tfrac{1}{\sqrt{5}}\left(e^{-iE_1t/\hbar}\left|E_1\right\rangle - 2ie^{-iE_2t/\hbar}\left|E_2\right\rangle\right) = \tfrac{1}{\sqrt{5}}e^{-iE_1t/\hbar}\left(\left|E_1\right\rangle - 2ie^{-i\omega_{21}t}\left|E_2\right\rangle\right)$$

with the Bohr frequency

$$\omega_{21} = \frac{3\pi^2\hbar}{2mL^2}$$

The expectation value of the position is

$$\langle x\rangle(t) = \left\langle\psi(t)\right|x\left|\psi(t)\right\rangle = \tfrac{1}{\sqrt{5}}e^{+iE_1t/\hbar}\left(\left\langle E_1\right| + 2ie^{+i\omega_{21}t}\left\langle E_2\right|\right)x\tfrac{1}{\sqrt{5}}e^{-iE_1t/\hbar}\left(\left|E_1\right\rangle - 2ie^{-i\omega_{21}t}\left|E_2\right\rangle\right)$$
$$= \tfrac{1}{5}\left(\left\langle E_1\right|x\left|E_1\right\rangle + 2ie^{+i\omega_{21}t}\left\langle E_2\right|x\left|E_1\right\rangle - 2ie^{-i\omega_{21}t}\left\langle E_1\right|x\left|E_2\right\rangle + 4\left\langle E_2\right|x\left|E_2\right\rangle\right)$$
$$= \tfrac{1}{5}\left(x_{11} + 2ie^{+i\omega_{21}t}x_{21} - 2ie^{-i\omega_{21}t}x_{12} + 4x_{22}\right)$$

where the matrix elements are defined as

$$\langle x\rangle_{nk} = \left\langle E_n\right|x\left|E_k\right\rangle = \int_0^L \varphi_n^*(x)\ x\ \varphi_k(x)dx$$

The diagonal matrix elements are

$$\langle x\rangle_{nn} = \int_0^L \varphi_n^*(x)\ x\ \varphi_n(x)dx\ = \int_0^L x\left|\varphi_n(x)\right|^2 dx\ = \frac{L}{2}$$

as found in Problem 5.5. The off-diagonal matrix elements are

$$\langle x\rangle_{nk} = \langle E_n|x|E_k\rangle = \int_0^L \varphi_n^*(x)\ x\ \varphi_k(x)dx\ = \frac{2}{L}\int_0^L \sin\frac{n\pi x}{L}x\sin\frac{k\pi x}{L}dx$$
$$= \frac{2}{L}\left(\frac{L}{\pi}\right)^2\int_0^\pi y\sin(ny)\sin(ky)dy\ = \frac{2}{L}\left(\frac{L}{\pi}\right)^2\int_0^\pi y\tfrac{1}{2}\left[\cos(n-k)y-\cos(n+k)y\right]dy$$
$$= \frac{1}{L}\left(\frac{L}{\pi}\right)^2\left[\frac{\cos(n-k)y}{(n-k)^2}+\frac{y\sin(n-k)y}{(n-k)}-\frac{\cos(n+k)y}{(n+k)^2}-\frac{y\sin(n+k)y}{(n+k)}\right]_0^\pi$$
$$= \frac{1}{L}\left(\frac{L}{\pi}\right)^2\left[\frac{\cos(n-k)\pi}{(n-k)^2}-\frac{\cos(n+k)\pi}{(n+k)^2}-\frac{1}{(n-k)^2}+\frac{1}{(n+k)^2}\right]$$
$$= \frac{L}{\pi^2}\left[\frac{1}{(n+k)^2}-\frac{1}{(n-k)^2}\right]\left[1-(-1)^{n+k}\right] = \frac{-4Lnk}{\pi^2\left(n^2-k^2\right)^2}\left[1-(-1)^{n+k}\right]$$

Hence,

$$x_{11} = x_{22} = \frac{L}{2};\quad x_{12} = x_{21} = -\frac{16L}{9\pi^2}$$

So the expectation value of the position is

$$\langle x\rangle(t) = \tfrac{1}{5}\left(\tfrac{L}{2}-2ie^{+i\omega_{21}t}\tfrac{16L}{9\pi^2}+2ie^{-i\omega_{21}t}\tfrac{16L}{9\pi^2}+4\tfrac{L}{2}\right) = L\left(\tfrac{1}{2}+\tfrac{64}{45\pi^2}\sin\omega_{21}t\right)$$

5.8 The initial wave function is $\psi(x,t=0) = Ax(L-x)$. To find the time evolution using the Schrödinger recipe, we must first normalize the state, and then write it in terms of the energy eigenstates. The normalization requirement is

$$1 = \langle\psi|\psi\rangle = \int_0^L|\psi(x)|^2dx = \int_0^L|Ax(L-x)|^2dx = |A|^2\int_0^L\left(x^2L^2-2Lx^3+x^4\right)dx$$
$$= |A|^2\left(\tfrac{1}{3}x^3L^2-\tfrac{1}{2}Lx^4+\tfrac{1}{5}x^5\right)_0^L = |A|^2\left(\tfrac{1}{3}L^5-\tfrac{1}{2}L^5+\tfrac{1}{5}L^5\right) = \tfrac{1}{30}L^5|A|^2$$

Hence the normalized wave function is $\psi(x,t=0) = \sqrt{30}x(L-x)\big/\left(L^2\sqrt{L}\right)$. Now we write the wave function in the energy basis using the projections on the energy eigenstates:

$$\psi(x,0) = \sum_{n=1}^{\infty}c_n\varphi_n(x)$$
$$c_n = \langle E_n|\psi(0)\rangle = \int_0^L\varphi_n^*(x)\psi(x,0)dx = \int_0^L\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)Ax(L-x)dx$$
$$= \frac{4\sqrt{15}}{n^3\pi^3}\left[1-(-1)^n\right]\ = \frac{8\sqrt{15}}{j^3\pi^3};\ \ j\ \ odd$$

The wave function has even parity with respect to the well center, which is why only odd numbered (even parity) states contribute. The time-evolved state is

$$\psi(x,t)=\sum_{n=1}^{\infty}c_n e^{-iE_nt/\hbar}\varphi_n(x)=\frac{8\sqrt{15}}{\pi^3}\sqrt{\frac{2}{L}}\sum_{j\ odd}^{\infty}\frac{1}{j^3}e^{-iE_jt/\hbar}\sin\left(\frac{j\pi x}{L}\right)$$

Now find the expectation value of the position:

$$\langle x\rangle(t)=\langle\psi(t)|x|\psi(t)\rangle=\left(\sum_{m=1}^{\infty}c_m^* e^{+iE_mt/\hbar}\langle E_m|\right)x\left(\sum_{n=1}^{\infty}c_n e^{-iE_nt/\hbar}|E_n\rangle\right)$$

$$=\sum_{m,n=1}^{\infty}c_m^*c_n e^{+i(E_m-E_n)t/\hbar}\langle E_m|x|E_n\rangle$$

The off-diagonal matrix elements of the position are zero for states with the same parity (see Problem 5.7), which we have here. So only the diagonal elements of the sum survive. The diagonal elements are all equal to $L/2$ (see Problem 5.5), so we get

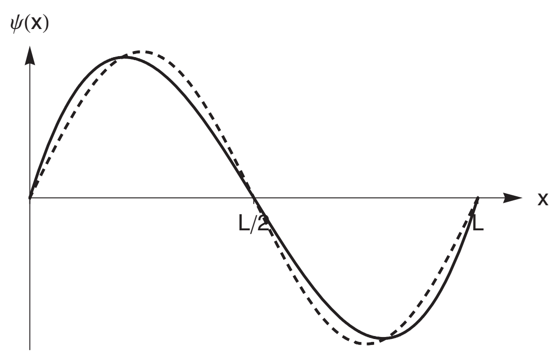
$$\langle x\rangle(t)=\sum_{n=1}^{\infty}c_n^*c_n\langle E_n|x|E_n\rangle=\frac{L}{2}\sum_{n=1}^{\infty}|c_n|^2=\frac{L}{2}$$

So the expectation value of the position is time independent.

5.9 The initial wave function is

$$\psi(x,0)=A\left[\left(\frac{x}{L}\right)^3-\frac{3}{2}\left(\frac{x}{L}\right)^2+\frac{1}{2}\left(\frac{x}{L}\right)\right]$$

which looks similar to the $n=2$ state (dashed):



(a) To find the time evolution using the Schrödinger recipe, we must first normalize the state, and then write it in terms of the energy eigenstates. The normalization requirement is

$$1=\langle\psi|\psi\rangle=\int_0^L|\psi(x,0)|^2\,dx$$

$$=|A|^2\int_0^L\left[\left(\frac{x}{L}\right)^3-\frac{3}{2}\left(\frac{x}{L}\right)^2+\frac{1}{2}\left(\frac{x}{L}\right)\right]^2dx=|A|^2\frac{L}{840}$$

Hence the normalized wave function is

$$\psi(x,0) = \sqrt{\frac{840}{L}}\left[\left(\frac{x}{L}\right)^3 - \frac{3}{2}\left(\frac{x}{L}\right)^2 + \frac{1}{2}\left(\frac{x}{L}\right)\right].$$

Now perform the overlap integral to find the expansion coefficients:

$$\begin{aligned} c_n &= \langle E_n|\psi\rangle = \int_{-\infty}^{\infty}\varphi_n^*(x)\psi(x,0)\,dx \\ &= \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\sqrt{\frac{840}{L}}\left[\left(\frac{x}{L}\right)^3 - \frac{3}{2}\left(\frac{x}{L}\right)^2 + \frac{1}{2}\left(\frac{x}{L}\right)\right]dx \\ &= \frac{12\sqrt{105}}{n^3\pi^3}\left[1+(-1)^n\right] = \frac{24\sqrt{105}}{j^3\pi^3};\ \ j\ \ even \end{aligned}$$

The first few coefficients are

$$c_1 = 0;\ \ c_2 = 0.991;\ \ c_3 = 0;\ \ c_4 = 0.124$$

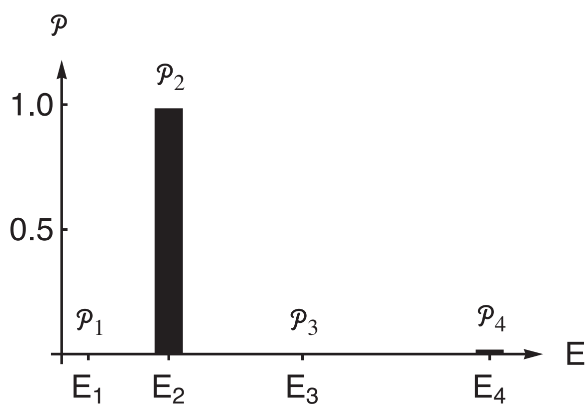
so the state mostly comprises the first excited state, as expected. The time-evolved state is

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n e^{-iE_n t/\hbar}\varphi_n(x) = \frac{8\sqrt{15}}{\pi^3}\sqrt{\frac{2}{L}}\sum_{j\ \ odd}^{\infty}\frac{1}{j^3}e^{-iE_j t/\hbar}\sin\left(\frac{j\pi x}{L}\right)$$

(b) The probabilities of measuring the energy eigenvalues are the squares of the expansion coefficients:

$$\mathcal{P}_n = \left|\langle E_n|\psi(t)\rangle\right|^2 = |c_n|^2 = \frac{60480}{n^6\pi^6};\ \ n\ \ even$$

The energy probabilities are shown in the histogram below, reflecting the predominance of the 2nd state.



(c) The expectation value of the energy is

$$\begin{aligned} \langle H\rangle &= \sum_n \mathcal{P}_n E_n = \sum_n |c_n|^2 E_n = \sum_{n\ \ even}^{\infty}\frac{60480}{n^6\pi^6}\left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right) \\ &= \frac{60480}{\pi^4}\frac{\hbar^2}{2mL^2}\sum_{n\ \ even}^{\infty}\frac{1}{n^4} = \frac{60480}{\pi^6}\frac{\pi^2\hbar^2}{2mL^2}\frac{\pi^4}{1440} = \frac{42}{\pi^2}E_1 \cong 4.26E_1 \end{aligned}$$

which is slightly larger than the energy ($E_2 = 4E_1$) of the first excited state, as expected from the histogram above.

5.10 The probability density is uniform over the right half, so the wave function must also be uniform (with a possible overall phase that we neglect):

$$\psi(x,0) = \begin{cases} 0 & ;0 < x \le L/2 \\ A & ;L/2 < x < L \end{cases}$$

Now find the normalization constant *A*:

$$1 = \langle\psi|\psi\rangle = \int_0^L |\psi(x)|^2\, dx = \int_{L/2}^L |A|^2\, dx = |A|^2 \frac{L}{2} \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}$$

Giving the wave function:

$$\psi(x,0) = \begin{cases} 0 & ;0 < x \le lL/2 \\ \sqrt{\frac{2}{L}} & ;L/2 < x < L \end{cases}$$

Now find the probability of an energy measurement

$$\mathcal{P}_{E_n} = \left|\langle E_n|\psi(0)\rangle\right|^2$$

$$\langle E_n|\psi(0)\rangle = \int_0^L \psi_n^*(x)\psi(x,0)\,dx = \int_{L/2}^L \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\sqrt{\frac{2}{L}}\,dx$$

$$= -\frac{2}{L}\frac{L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)\Bigg|_{L/2}^{L} = \frac{2}{n\pi}\left[\cos\left(\frac{n\pi}{2}\right) - (-1)^n\right] \;;\; n = 1,2,3,...$$

$$= \frac{2}{n\pi}[1,-2,1,0,1,-2,1,0,1,-2,1,0,1,-2,1,0,......]$$

The probabilities of the first three states are

$$\langle E_1|\psi(0)\rangle = \frac{2}{\pi}; \quad \langle E_2|\psi(0)\rangle = \frac{-2}{\pi}; \quad \langle E_3|\psi(0)\rangle = \frac{2}{3\pi}$$

$$\mathcal{P}_{E_1} = \left|\langle E_1|\psi(0)\rangle\right|^2 = \left(\frac{2}{\pi}\right)^2 = \frac{4}{\pi^2} = 0.405$$

$$\mathcal{P}_{E_2} = \left|\langle E_2|\psi(0)\rangle\right|^2 = \left(\frac{-2}{\pi}\right)^2 = \frac{4}{\pi^2} = 0.405$$

$$\mathcal{P}_{E_3} = \left|\langle E_3|\psi(0)\rangle\right|^2 = \left(\frac{2}{3\pi}\right)^2 = \frac{4}{9\pi^2} = 0.045$$

The expectation value of the energy is given by the following sum, which does not converge:

$$\begin{aligned}\langle E\rangle &= \sum_{n=1}^{\infty}\mathcal{P}_{E_n}E_n = \sum_{n=1}^{\infty}\left|\langle E_n|\psi(0)\rangle\right|^2 n^2\frac{\pi^2\hbar^2}{2ma^2}\\ &= \sum_{n=1}^{\infty}\left|\frac{2}{n\pi}\left[\cos\left(\frac{n\pi}{2}\right)-(-1)^n\right]\right|^2 n^2\frac{\pi^2\hbar^2}{2ma^2} = \frac{2\hbar^2}{ma^2}\sum_{n=1}^{\infty}\left|\left[\cos\left(\frac{n\pi}{2}\right)-(-1)^n\right]\right|^2\\ &= \frac{2\hbar^2}{ma^2}\left[1+4+1+0+1+4+1+0+1+4+1+0+.....\right] = \infty\end{aligned}$$

This sum is infinite because of the step function in the wave function. Fourier analysis tells us that this requires high frequency components, and our calculation tells us these components scale as $1/n$.

A more realistic wave function might have position dependent phase, which would make the integrals much more complicated. Linear and quadratic phases give results not too different than the uniform phase result.

5.11 The particle is initially in the ground state of a box of size L. Hence the initial state is

$$\psi_{initial}(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

between 0 and L and zero elsewhere. If the box is expanded "suddenly," this means the wave function remains unaltered. Now we want the probabilities that the particle in the expanded box is in the ground state and first excited state of the expanded box. The probability that the initial state $|\psi_{initial}\rangle \doteq \psi_{initial}(x)$ is measured to be in the final state $|\psi_{final}\rangle \doteq \psi_{final}(x)$ is the square of the projection of the two states:

$$\begin{aligned}\mathcal{P}_{i\to f} &= \left|\langle\psi_{final}|\psi_{initial}\rangle\right|^2\\ &= \left|\int_{-\infty}^{\infty}\psi^*_{final}(x)\psi_{initial}(x)dx\right|^2\end{aligned}$$

The energy eigenfunctions of the <u>expanded</u> box are

$$\varphi_n(x) = \sqrt{\frac{2}{3L}}\sin\left(\frac{n\pi x}{3L}\right)$$

between 0 and $3L$.

(i) We are interested in the term with $n = 1$; this is the ground state of the new box. Break the integral over the new box into two pieces, with one piece being zero:

$$\mathcal{P}_{i\to n=1} = \left|\int_{-\infty}^{\infty}\varphi_1^*(x)\psi_{initial}(x)\,dx\right|^2$$
$$= \left|\int_0^L \sqrt{\frac{2}{3L}}\sin\left(\frac{\pi x}{3L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)dx + \int_L^{3L}\sqrt{\frac{2}{3L}}\sin\left(\frac{\pi x}{3L}\right)\cdot 0\,dx\right|^2$$
$$= \left|\frac{2}{\sqrt{3}L}\int_0^L \sin\left(\frac{\pi x}{3L}\right)\sin\left(\frac{\pi x}{L}\right)dx\right|^2 = \left|\frac{2\sqrt{3}}{\pi}\left[\cos\left(\frac{\pi x}{3L}\right)\sin\left(\frac{\pi x}{3L}\right)^3\right]_0^L\right|^2$$
$$= \left|\frac{9}{8\pi}\right|^2 = \frac{81}{64\pi^2} \cong 0.13$$

There is a 13% chance that the particle is measured in the ground state of the expanded box.

(ii) Now the $n = 2$ state:

$$\mathcal{P}_{i\to n=2} = \left|\int_{-\infty}^{\infty}\varphi_2^*(x)\psi_{initial}(x)\,dx\right|^2$$
$$= \left|\int_0^L \sqrt{\frac{2}{3L}}\sin\left(\frac{2\pi x}{3L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)dx + \int_L^{3L}\sqrt{\frac{2}{3L}}\sin\left(\frac{2\pi x}{3L}\right)\cdot 0\,dx\right|^2$$
$$= \left|\frac{2}{\sqrt{3}L}\int_0^L \sin\left(\frac{2\pi x}{3L}\right)\sin\left(\frac{\pi x}{L}\right)dx\right|^2 = \left|\left[\frac{4\sqrt{3}}{5\pi}\left(3+2\cos\left(\frac{2\pi x}{3L}\right)\right)\sin\left(\frac{\pi x}{3L}\right)^3\right]_0^L\right|^2$$
$$= \left|\frac{9}{5\pi}\right|^2 = 0.33$$

There is a 33% chance of finding the particle in the second state. This seems reasonable because the second state of the bigger box is a better match to the first state of the smaller box.

5.12 The orthogonality relation is (for $n \neq m$):

$$\langle E_n|E_m\rangle = \int_{-\infty}^{\infty}\varphi_n^*(x)\varphi_m(x)\,dx = \int_0^L\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{n\pi x}{L}\right)\sqrt{\tfrac{2}{L}}\sin\left(\tfrac{m\pi x}{L}\right)dx = \tfrac{2}{L}\left(\tfrac{L}{\pi}\right)\int_0^\pi \sin ny\sin my\,dy$$
$$= \frac{2}{\pi}\left[\frac{\sin(n-m)y}{2(n-m)} - \frac{\sin(n+m)y}{2(n+m)}\right]_0^\pi = \frac{2}{\pi}\left[\frac{\sin(n-m)\pi}{2(n-m)} - \frac{\sin(n+m)\pi}{2(n+m)}\right] = 0$$

showing that the states are orthogonal.

5.13 Start with the normalization condition $1 = \langle\psi|\psi\rangle$, and then insert the unity operator in the form of the closure relation:

$$1 = \langle\psi|\psi\rangle = \langle\psi|\mathbf{1}|\psi\rangle = \langle\psi|\left[\sum_n |E_n\rangle\langle E_n|\right]|\psi\rangle$$

The sum can be pulled outside the bracket to give

$$1 = \langle \psi | \psi \rangle = \sum_n \langle \psi | E_n \rangle \langle E_n | \psi \rangle = \sum_n \left| \langle E_n | \psi \rangle \right|^2$$

5.14 Assume a solution of the form

$$\varphi_E(x) = \begin{cases} Ae^{qx} + Be^{-qx} & x < -a \\ C\sin kx + D\cos kx & -a < x < a \\ Fe^{qx} + Ge^{-qx} & x > a \end{cases}$$

This boundary condition at infinity requires that $B = F = 0$. The boundary conditions at the right side of the well ($x = a$) give

$$\varphi_{even}(a) : C\sin(ka) + D\cos(ka) = Ge^{-qa}$$

$$\left.\frac{d\varphi_{even}(x)}{dx}\right|_{x=a} : kC\cos(ka) - kD\sin(ka) = -qGe^{-qa}$$

The boundary conditions at the left side of the well ($x = -a$) give

$$\varphi_{even}(-a) : -C\sin(ka) + D\cos(ka) = Ae^{-qa}$$

$$\left.\frac{d\varphi_{even}(x)}{dx}\right|_{x=-a} : kC\cos(ka) + kD\sin(ka) = qAe^{-qa}$$

Add and subtract the wave function and derivative equations respectively to get

$$\begin{aligned} 2D\cos(ka) &= (A+G)e^{-qa} \\ 2C\sin(ka) &= (-A+G)e^{-qa} \\ 2C\cos(ka) &= \tfrac{q}{k}(A-G)e^{-qa} \\ 2D\sin(ka) &= \tfrac{q}{k}(A+G)e^{-qa} \end{aligned}$$

Eliminate the A and G terms from the C and D equations to get

$$\begin{aligned} 2C\left[\sin(ka) + \tfrac{k}{q}\cos(ka)\right] &= 0 \\ 2D\left[\cos(ka) - \tfrac{k}{q}\sin(ka)\right] &= 0 \end{aligned}$$

So either C=0 or D=0 (if both =0 then there is no wave function). This leaves us with either sin or cos solutions. For the even cos solutions (C=0), the quantization condition is

$$\left[\cos(ka) - \tfrac{k}{q}\sin(ka)\right] = 0 \quad \Rightarrow \quad k\tan(ka) = q$$

as we found before. For the odd sin solutions (D=0), the quantization condition is

$$\left[\sin(ka) + \tfrac{k}{q}\cos(ka)\right] = 0 \quad \Rightarrow \quad -k\cot(ka) = q$$

as we found before.

5.15 The odd solutions are

$$\varphi_{odd}(x) = \begin{cases} Ae^{qx} & x < -a \\ C\sin(kx) & -a \le x \le a \\ -Ae^{-qx} & x > a \end{cases}$$

The boundary conditions at the right side of the well ($x = a$) give

$$\varphi_{even}(a) : C\sin(ka) = -Ae^{-qa}$$
$$\left.\frac{d\varphi_{even}(x)}{dx}\right|_{x=a} : kC\cos(ka) = qAe^{-qa}$$

The boundary conditions at the left side of the well ($x = -a$) give

$$\varphi_{even}(a) : -C\sin(ka) = Ae^{-qa}$$
$$\left.\frac{d\varphi_{even}(x)}{dx}\right|_{x=a} : kC\cos(ka) = qAe^{-qa}$$

Dividing the equations for either set eliminates the normalization constants to yield

$$-k\cot(ka) = q$$

as quoted in the text.

5.16 Normalize the finite well eigenstates by using the boundary conditions to relate the wave function coefficients inside and outside the well and then integrating over all space. For the even states, Eq. (5.82) gives

$$A = De^{qa}\cos(ka)$$

The normalization integral is

$$\begin{aligned}
1 = \langle E_n | E_n \rangle &= \int_{-\infty}^{\infty} |\varphi_n(x)|^2 \, dx \\
&= \int_{-\infty}^{-a} \left|Ae^{qx}\right|^2 dx + \int_{-a}^{a} |D\cos(kx)|^2 dx + \int_{a}^{\infty} \left|Ae^{-qx}\right|^2 dx \\
&= \left|De^{qa}\cos(ka)\right|^2 \int_{-\infty}^{-a} e^{2qx} dx + |D|^2 \int_{-a}^{a} \cos^2(kx) dx + \left|De^{qa}\cos(ka)\right|^2 \int_{a}^{\infty} e^{-2qx} dx \\
&= |D|^2 \left\{ e^{2qa}\cos^2(ka)\frac{e^{-2qa}}{2q} + a + \frac{\sin(2ka)}{2k} + e^{2qa}\cos^2(ka)\frac{e^{-2qa}}{2q} \right\} \\
&= |D|^2 \left\{ \cos^2(ka)\frac{1}{q} + a + \frac{\sin(2ka)}{2k} \right\}
\end{aligned}$$

Using the quantization condition for even states $k\tan(ka) = q$, we get

$$1=|D|^2\left\{\cos^2(ka)\frac{1}{k\tan(ka)}+a+\frac{\sin(2ka)}{2k}\right\}=|D|^2\left\{a+\frac{1}{k}\left(\frac{\cos^3(ka)}{\sin(ka)}+\frac{2\sin(ka)\cos(ka)}{2}\right)\right\}$$
$$=|D|^2\left\{a+\frac{\cos(ka)}{k}\left(\frac{\cos^2(ka)}{\sin(ka)}+\frac{\sin^2(ka)}{\sin(ka)}\right)\right\}=|D|^2\left\{a+\frac{1}{k\tan(ka)}\right\}=|D|^2\left\{a+\frac{1}{q}\right\}$$

Hence the wave function coefficients are

$$D=\frac{1}{\sqrt{a+\frac{1}{q}}}\qquad\qquad A=\frac{e^{qa}\cos(ka)}{\sqrt{a+\frac{1}{q}}}$$

Hence, the normalized even states are

$$\varphi_{even}(x)=\sqrt{a+\frac{1}{q}}\begin{cases}e^{qa}\cos(ka)e^{qx} & x<-a\\ \cos(kx) & -a\le x\le a\\ e^{qa}\cos(ka)e^{-qx} & x>a\end{cases}$$

For the odd states, the boundary condition (Problem 5.15) gives

$$A=-Ce^{qa}\sin(ka)$$

The normalization integral is

$$\begin{aligned}1=\langle E_n|E_n\rangle&=\int_{-\infty}^{\infty}|\varphi_n(x)|^2\,dx\\
&=\int_{-\infty}^{-a}\left|Ae^{qx}\right|^2dx+\int_{-a}^{a}|C\sin(kx)|^2\,dx+\int_{a}^{\infty}\left|-Ae^{-qx}\right|^2dx\\
&=\left|-Ce^{qa}\sin(ka)\right|^2\int_{-\infty}^{-a}e^{2qx}\,dx+|C|^2\int_{-a}^{a}\sin^2(kx)\,dx+\left|-Ce^{qa}\sin(ka)\right|^2\int_{a}^{\infty}e^{-2qx}\,dx\\
&=|C|^2\left\{e^{2qa}\sin^2(ka)\frac{e^{-2qa}}{2q}+a-\frac{\sin(2ka)}{2k}+e^{2qa}\sin^2(ka)\frac{e^{-2qa}}{2q}\right\}\\
&=|C|^2\left\{\sin^2(ka)\frac{1}{q}+a-\frac{\sin(2ka)}{2k}\right\}\end{aligned}$$

Using the quantization condition for odd states $-k\cot(ka)=q$ gives

$$1=|C|^2\left\{\sin^2(ka)\frac{-1}{k\cot(ka)}+a-\frac{\sin(2ka)}{2k}\right\}=|C|^2\left\{a-\frac{1}{k}\left(\frac{\sin^3(ka)}{\cos(ka)}+\frac{2\sin(ka)\cos(ka)}{2}\right)\right\}$$
$$=|C|^2\left\{a-\frac{\sin(ka)}{k}\left(\frac{\sin^2(ka)}{\cos(ka)}+\frac{\cos^2(ka)}{\cos(ka)}\right)\right\}=|C|^2\left\{a-\frac{1}{k\cot(ka)}\right\}=|C|^2\left\{a+\frac{1}{q}\right\}$$

Hence the wave function coefficients are

$$C = \frac{1}{\sqrt{a+\frac{1}{q}}} \qquad\qquad A = -\frac{e^{qa}\sin(ka)}{\sqrt{a+\frac{1}{q}}}$$

and the normalized odd states are

$$\varphi_{odd}(x) = \sqrt{a+\frac{1}{q}}\begin{cases} -e^{qa}\sin(ka)e^{qx} & x<-a \\ \sin(kx) & -a\le x\le a \\ e^{qa}\sin(ka)e^{-qx} & x>a \end{cases}$$

5.17 The probability of finding the particle outside the well for even states is

$$\mathcal{P}_{|x|>a} = 2\int_a^\infty |\varphi_n(x)|^2\,dx = 2\int_a^\infty \left|Ae^{-qx}\right|^2 dx = 2|A|^2\int_a^\infty e^{-2qx}\,dx = 2|A|^2\left\{\frac{e^{-2qa}}{2q}\right\}$$

Using the normalization result from Problem 5.16, we obtain

$$\mathcal{P}_{|x|>a} = 2\left|\frac{e^{qa}\cos(ka)}{\sqrt{a+\frac{1}{q}}}\right|^2\left\{\frac{e^{-2qa}}{2q}\right\} = \frac{\cos^2(ka)}{qa+1}$$

Using the quantization condition for even states $k\tan(ka) = q$, we get

$$\mathcal{P}_{|x|>a} = \frac{\cos^2(ka)}{1+qa} = \left(\frac{1}{1+qa}\right)\left(\frac{1}{1+\tan^2(ka)}\right) = \left(\frac{1}{1+qa}\right)\left(\frac{1}{1+q^2/k^2}\right) = \frac{k^2}{(1+qa)\left(k^2+q^2\right)}$$

Using the definitions $z = ka$ and $(ka)^2 + (qa)^2 = z_0^2$ gives

$$\mathcal{P}_{|x|>a} = \frac{z^2}{z_0^2\left(1+\sqrt{z_0^2-z^2}\right)}$$

For odd states, the result is

$$\mathcal{P}_{|x|>a} = \frac{\sin^2(ka)}{qa+1}$$

and using the quantization condition for odd states $-k\cot(ka) = q$ gives

$$\mathcal{P}_{|x|>a} = \frac{\sin^2(ka)}{1+qa} = \left(\frac{1}{1+qa}\right)\left(\frac{1}{1+\cot^2(ka)}\right) = \left(\frac{1}{1+qa}\right)\left(\frac{1}{1+q^2/k^2}\right) = \frac{k^2}{(1+qa)\left(k^2+q^2\right)}$$

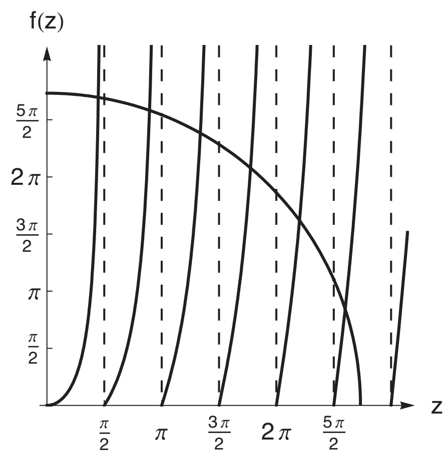
and hence the same general result.

Increasing energy corresponds to increasing z, with the limit being z_0. Increasing z causes the numerator of the probability expression to increase and the denominator to decrease, so the probability increases.

5.18 The well parameter z_0 is

$$z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}} = \sqrt{\frac{2(511keV)5eV(1.5nm/2)^2}{(1240eVnm/2\pi)^2}} = 8.59$$

which gives 6 bound states as shown below:



The bound states are determined by the roots of the quantization equations:

$$even \quad \rightarrow \quad z\tan(z) = \sqrt{z_0^2 - z^2}$$
$$odd \quad \rightarrow \quad -z\cot(z) = \sqrt{z_0^2 - z^2}$$

The Mathematica commands

```
Table[FindRoot[zTan[z]-Sqrt[z0^2-z^2],{z,(i-3/4)π,(i-1)π,(i-1/2)π}][[1,2]],{i,3}]
Table[FindRoot[zCot[z]+Sqrt[z0^2-z^2],{z,(i-1/3)π,(i-1/2)π,iπ}][[1,2]],{i,3}]
```

give the roots of z as

$$z = 1.40627, \quad 4.2011, \quad 6.91721, \quad 2.80837, \quad 5.5763, \quad 8.16747$$

Hence the allowed energies are

$$E = \frac{\hbar^2 z^2}{2ma^2} = \frac{z^2}{z_0^2}V_0 = 0.134\text{eV},\ 0.535\text{eV},\ 1.197\text{eV},\ 2.109\text{eV},\ 3.245\text{eV},\ 4.525\text{eV}$$

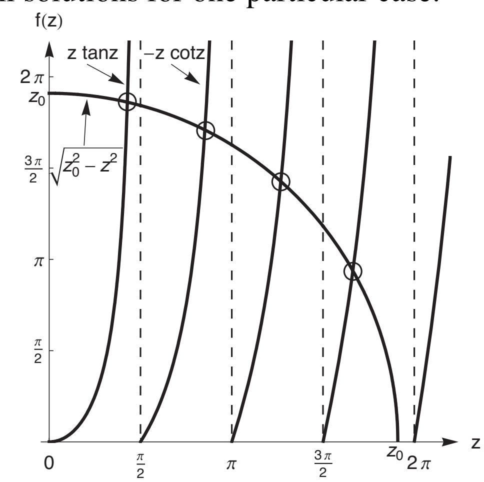
5.19 For the finite well, the allowed values of the parameter z are given by the transcendental equations

$$\textit{even parity (odd } n) \rightarrow \quad z\tan(z)=\sqrt{z_0^2-z^2}$$
$$\textit{odd parity (even } n) \rightarrow \quad -z\cot(z)=\sqrt{z_0^2-z^2}$$

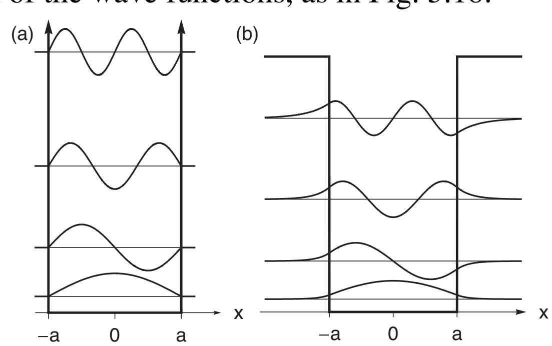
For the infinite well, the allowed values of the parameter z are

$$z_n = n\frac{\pi}{2}$$

Fig. 5.16 shows the finite well solutions for one particular case:



The dashed lines represent the allowed values of z for the infinite well case, with the corresponding value (same n) for the finite well case immediately to the left. It is clear from the plot that the difference between the allowed values of z for the finite and infinite well cases (same n) increases as z increases. The energy is given by $E_n = \hbar^2 z^2 / 2ma^2$, so the difference in energy eigenvalues is larger for higher energy states. This is also evident from consideration of the wave functions, as in Fig. 5.18:



The wavelength of a finite-well state is longer than the corresponding infinite-well state because the wave function leaks out of the well into the classically forbidden region (barrier penetration). The barrier penetration increases as the energy increases and so the difference in wavelengths and hence wave vectors and ultimately energies increases with increasing energy.

5.20 A "half-infinite" square well is a square well with infinite potential for $x \le 0$, finite potential with value V_0 for $x \ge a$, and zero potential in the well $0 < x < a$. The infinite potential for $x \le 0$ requires the wave function to be zero at the $x = 0$ boundary. At the $x = a$ boundary, the wave function and its derivative must match onto an exponentially decaying wave function. The odd parity states of the finite well solved in the text satisfy these boundary conditions, so the energy eigenstates are the $n = even$ states found before. The energies are (using $z_0 = \sqrt{2mV_0a^2/\hbar^2}$)

$$E = \frac{\hbar^2 z^2}{2ma^2} \qquad \textit{where} \qquad -z\cot(z) = \sqrt{z_0^2 - z^2}$$

The normalized states (Problem 5.16) are

$$\varphi(x) = \frac{1}{\sqrt{a + \frac{1}{q}}} \begin{cases} \sin(kx) & 0 < x < a \\ e^{qa}\sin(ka)e^{-qx} & x > a \end{cases}$$

where

$$ka = \sqrt{\frac{2mEa^2}{\hbar^2}}\ , \qquad qa = \sqrt{\frac{2m(V_0 - E)a^2}{\hbar^2}}$$

5.21 The probabilities are

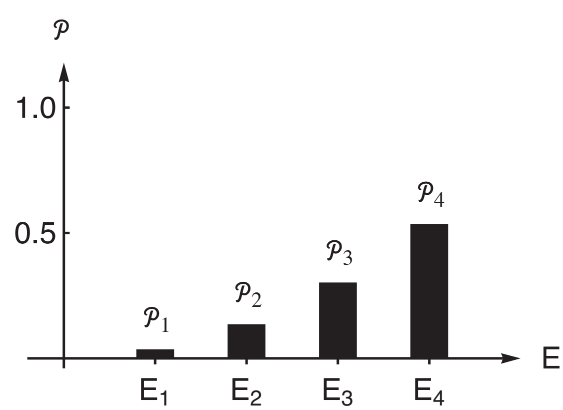
$$\mathcal{P}_{E_1} = \left|\langle E_1|\psi\rangle\right|^2 = \left|\langle E_1|\left(\tfrac{1}{\sqrt{30}}|E_1\rangle + \tfrac{2}{\sqrt{30}}|E_2\rangle + \tfrac{3}{\sqrt{30}}|E_3\rangle + \tfrac{4}{\sqrt{30}}|E_4\rangle\right)\right|^2 = \tfrac{1}{30}$$

$$\mathcal{P}_{E_2} = \left|\langle E_2|\psi\rangle\right|^2 = \left|\langle E_2|\left(\tfrac{1}{\sqrt{30}}|E_1\rangle + \tfrac{2}{\sqrt{30}}|E_2\rangle + \tfrac{3}{\sqrt{30}}|E_3\rangle + \tfrac{4}{\sqrt{30}}|E_4\rangle\right)\right|^2 = \tfrac{4}{30}$$

$$\mathcal{P}_{E_3} = \left|\langle E_3|\psi\rangle\right|^2 = \left|\langle E_3|\left(\tfrac{1}{\sqrt{30}}|E_1\rangle + \tfrac{2}{\sqrt{30}}|E_2\rangle + \tfrac{3}{\sqrt{30}}|E_3\rangle + \tfrac{4}{\sqrt{30}}|E_4\rangle\right)\right|^2 = \tfrac{9}{30}$$

$$\mathcal{P}_{E_4} = \left|\langle E_4|\psi\rangle\right|^2 = \left|\langle E_4|\left(\tfrac{1}{\sqrt{30}}|E_1\rangle + \tfrac{2}{\sqrt{30}}|E_2\rangle + \tfrac{3}{\sqrt{30}}|E_3\rangle + \tfrac{4}{\sqrt{30}}|E_4\rangle\right)\right|^2 = \tfrac{16}{30}$$

The histogram is



The average value of the energy is

$$\langle E\rangle=\sum_{n=1}^{\infty}\mathcal{P}_{E_n}E_n=\sum_{n=1}^{\infty}\left|\langle E_n|\psi\rangle\right|^2 nE_1=E_1\left(\tfrac{1}{30}1+\tfrac{4}{30}2+\tfrac{9}{30}3+\tfrac{16}{30}4\right)=\frac{10}{3}E_1$$

To find the uncertainty, we need the average of the squares:

$$\left\langle E^2\right\rangle=\sum_{n=1}^{\infty}\mathcal{P}_{E_n}E_n^2=\sum_{n=1}^{\infty}\left|\langle E_n|\psi\rangle\right|^2 n^2E_1^2=E_1^2\left(\tfrac{1}{30}1+\tfrac{4}{30}4+\tfrac{9}{30}9+\tfrac{16}{30}16\right)=\frac{59}{5}E_1$$

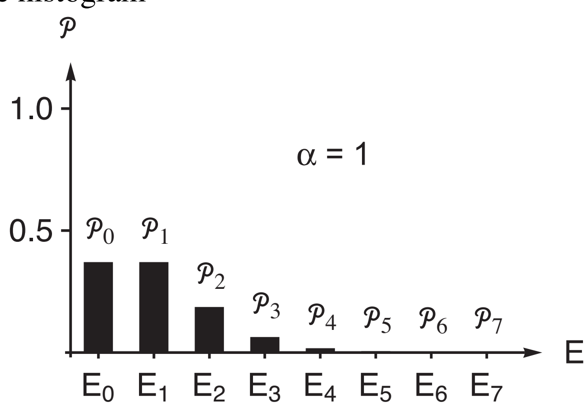
The uncertainty of the energy is

$$\Delta E=\sqrt{\left\langle E^2\right\rangle-\langle E\rangle^2}=E_1\sqrt{\left(\tfrac{59}{5}\right)-\left(\tfrac{10}{3}\right)^2}=E_1\sqrt{\tfrac{31}{45}}\cong 0.83\ E_1$$

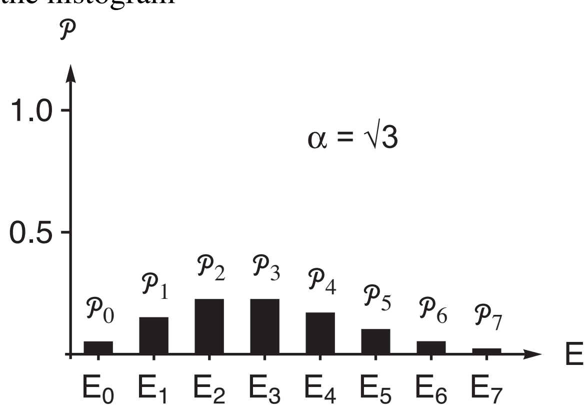
5.22 The probabilities are

$$\mathcal{P}_{E_n}=\left|\langle E_n|\psi\rangle\right|^2=\left|\langle E_n|\left(\sum_{m=0}^{\infty}\frac{\alpha^m e^{-\frac{\alpha^2}{2}}}{\sqrt{m!}}|E_m\rangle\right)\right|^2=\left|\sum_{m=0}^{\infty}\frac{\alpha^m e^{-\frac{\alpha^2}{2}}}{\sqrt{m!}}\delta_{nm}\right|^2=\left|\frac{\alpha^n e^{-\frac{\alpha^2}{2}}}{\sqrt{n!}}\right|^2=\frac{\alpha^{2n}e^{-\alpha^2}}{n!}$$

Assuming $\alpha=1$ gives the histogram



Assuming $\alpha=\sqrt{3}$ gives the histogram



The average value of the energy is

$$\langle E\rangle = \sum_{n=0}^{\infty}\mathcal{P}_{E_n}E_n = \sum_{n=0}^{\infty}\frac{\alpha^{2n}e^{-\alpha^2}}{n!}\left(n+\tfrac{1}{2}\right)\hbar\omega = \hbar\omega e^{-\alpha^2}\left(\sum_{n=1}^{\infty}\frac{\alpha^{2n}}{(n-1)!}+\tfrac{1}{2}\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!}\right)$$

$$= \hbar\omega e^{-\alpha^2}\left(\alpha^2\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!}+\tfrac{1}{2}\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!}\right) = \hbar\omega e^{-\alpha^2}\left(\alpha^2 e^{\alpha^2}+\tfrac{1}{2}e^{\alpha^2}\right) = \hbar\omega\left(\alpha^2+\tfrac{1}{2}\right)$$

To find the uncertainty, we need the average of the squares:

$$\langle E^2\rangle = \sum_{n=0}^{\infty}\mathcal{P}_{E_n}E_n^2 = \sum_{n=0}^{\infty}\frac{\alpha^{2n}e^{-\alpha^2}}{n!}\left(n+\tfrac{1}{2}\right)^2(\hbar\omega)^2$$

$$= (\hbar\omega)^2 e^{-\alpha^2}\left(\sum_{n=1}^{\infty}\frac{n\alpha^{2n}}{(n-1)!}+\sum_{n=1}^{\infty}\frac{\alpha^{2n}}{(n-1)!}+\tfrac{1}{4}\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!}\right)$$

$$= (\hbar\omega)^2 e^{-\alpha^2}\left(\alpha^2\sum_{m=0}^{\infty}\frac{(m+1)\alpha^{2m}}{m!}+\alpha^2\sum_{m=0}^{\infty}\frac{\alpha^{2m}}{m!}+\tfrac{1}{4}\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!}\right)$$

$$= (\hbar\omega)^2 e^{-\alpha^2}\left(\alpha^4\sum_{k=0}^{\infty}\frac{\alpha^{2k}}{k!}+2\alpha^2\sum_{m=0}^{\infty}\frac{\alpha^{2m}}{m!}+\tfrac{1}{4}\sum_{n=0}^{\infty}\frac{\alpha^{2n}}{n!}\right) = (\hbar\omega)^2\left(\alpha^4+2\alpha^2+\tfrac{1}{4}\right)$$

The uncertainty of the energy is

$$\Delta E = \sqrt{\langle E^2\rangle - \langle E\rangle^2} = \sqrt{(\hbar\omega)^2\left(\alpha^4+2\alpha^2+\tfrac{1}{4}\right)-\left(\hbar\omega\left(\alpha^2+\tfrac{1}{2}\right)\right)^2}$$

$$= \hbar\omega\sqrt{\left(\alpha^4+2\alpha^2+\tfrac{1}{4}\right)-\left(\alpha^4+\alpha^2+\tfrac{1}{4}\right)} = \hbar\omega\alpha$$

5.23 (i) For the 1st wave function, the normalization integral is

$$1 = \int_{-\infty}^{\infty}|\psi(x)|^2 dx = \int_{-\infty}^{\infty}\left|Ae^{-x^2/3}\right|^2 dx = |A|^2\int_{-\infty}^{\infty}e^{-2x^2/3}dx = 2|A|^2\frac{1}{2\sqrt{2/3}}\sqrt{\pi} = |A|^2\sqrt{\frac{3\pi}{2}}$$

yielding the normalized wave function

$$\psi(x) = \left(\frac{2}{3\pi}\right)^{1/4}e^{-x^2/3}$$

The probability that the particle is measured to be between 0 and 1 is

$$\mathcal{P}_{0<x<1} = \int_0^1|\psi(x)|^2 dx = \sqrt{\frac{2}{3\pi}}\int_0^1 e^{-2x^2/3}dx = \sqrt{\frac{2}{3\pi}}\sqrt{\frac{3}{2}}\int_0^{\sqrt{2/3}}e^{-t^2}dt = \frac{1}{\sqrt{\pi}}\int_0^{\sqrt{2/3}}e^{-t^2}dt$$

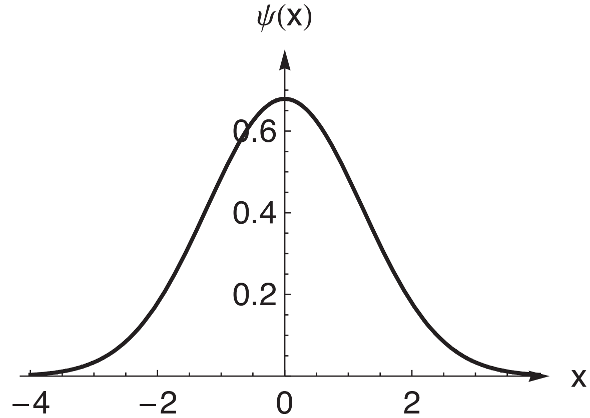
Recalling the definition of the error function:

$$erf(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt$$

the probability is

$$\mathcal{P}_{0<x<1} = \frac{1}{\sqrt{\pi}}\int_0^{\sqrt{2/3}} e^{-t^2}\,dt = \frac{1}{2}erf\left(\sqrt{2/3}\right) = 0.376$$

The plot of the wave function is shown below:



(ii) For the 2nd wave function the normalization integral is

$$1 = \int_{-\infty}^{\infty}\left|\psi(x)\right|^2 dx = \int_{-\infty}^{\infty}\left|B\frac{1}{x^2+2}\right|^2 dx = 2|B|^2\int_0^{\infty}\frac{1}{\left(x^2+2\right)^2}dx$$

$$= 2|B|^2\left[\frac{x}{4\left(x^2+2\right)} + \frac{\tan^{-1}\left(x/\sqrt{2}\right)}{4\sqrt{2}}\right]_0^{\infty} = 2|B|^2\frac{\pi/2}{4\sqrt{2}} = |B|^2\frac{\pi}{4\sqrt{2}}$$

yielding the normalized wave function

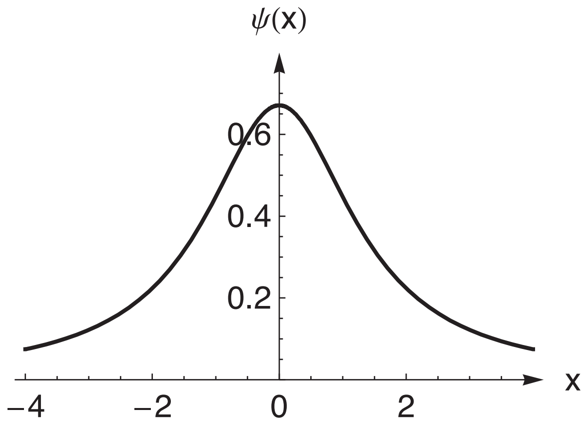
$$\psi(x) = \left(\frac{4\sqrt{2}}{\pi}\right)^{1/2}\frac{1}{x^2+2}$$

The probability that the particle is measured to be between 0 and 1 is

$$\mathcal{P}_{0<x<1} = \int_0^1\left|\psi(x)\right|^2 dx = \frac{4\sqrt{2}}{\pi}\int_0^1\frac{1}{\left(x^2+2\right)^2}dx = \frac{4\sqrt{2}}{\pi}\left[\frac{x}{4\left(x^2+2\right)} + \frac{\tan^{-1}\left(x/\sqrt{2}\right)}{4\sqrt{2}}\right]_0^1$$

$$= \frac{4\sqrt{2}}{\pi}\left[\frac{1}{12} + \frac{\tan^{-1}\left(1/\sqrt{2}\right)}{4\sqrt{2}}\right] = \frac{1}{\pi}\left[\frac{\sqrt{2}}{3} + \tan^{-1}\left(1/\sqrt{2}\right)\right] = 0.346$$

The plot of the wave function is shown below:



(iii) For the 3rd wave function the normalization integral is

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = \int_{-\infty}^{\infty} |C \ \mathrm{sech}(x/5)|^2 \, dx = 2|C|^2 \int_0^{\infty} \mathrm{sech}^2(x/5) dx$$
$$= 2|C|^2 \left[5 \ \tanh(x/5)\right]_0^{\infty} = 10|C|^2$$

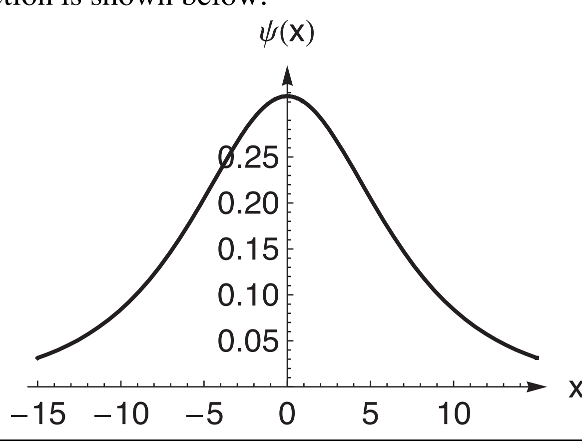
yielding the normalized wave function

$$\psi(x) = \frac{1}{\sqrt{10}} \mathrm{sech}(x/5)$$

The probability that the particle is measured to be between 0 and 1 is

$$\mathcal{P}_{0<x<1} = \int_0^1 |\psi(x)|^2 \, dx = \frac{1}{10} \int_0^1 \mathrm{sech}^2(x/5) dx = \frac{1}{10} \left[5 \ \tanh(x/5)\right]_0^1$$
$$= \frac{1}{2} \tanh(1/5) = 0.0987$$

The plot of the wave function is shown below:



5.24 The position representation of the energy eigenvalue equation is

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \varphi_E(x) = E \varphi_E(x)$$

Integrate from $-\varepsilon$ to ε to get

$$\int_{-\varepsilon}^{\varepsilon} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x)dx + \int_{-\varepsilon}^{\varepsilon} V(x)\varphi_E(x)dx = E\int_{-\varepsilon}^{\varepsilon}\varphi_E(x)dx$$

In the limit that $\varepsilon \to 0$, the integral on the right is zero. The first integral yields the wave function derivative, leaving

$$\left.\frac{d\varphi_E(x)}{dx}\right|_{\varepsilon} - \left.\frac{d\varphi_E(x)}{dx}\right|_{-\varepsilon} = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} V(x)\varphi_E(x)dx$$

If the potential energy is finite, then the integral on the right is zero, and the wave function derivative must be continuous. If the potential energy is infinite at the boundary, then the wave function derivative need not be continuous, as in the infinite square well problem and Prob. 5.25 with a delta function potential.

5.25 For a delta function potential, the position representation of the energy eigenvalue equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \beta\delta(x)\right)\varphi_E(x) = E\varphi_E(x)$$

Outside of the potential well, $V = 0$, so the solutions are real exponentials. Assume a solution of form

$$\varphi_E(x) = \begin{cases} Ae^{qx} + Be^{-qx}, & x < 0 \\ Ce^{qx} + De^{-qx}, & x > 0 \end{cases}$$

with $q = \sqrt{-2mE/\hbar^2}$. This boundary condition (normalizability) at infinity requires that $B = C = 0$. The boundary condition on the continuity of the wave function at $x = 0$ gives $A = D$, so

$$\varphi_E(x) = \begin{cases} Ae^{qx}, & x < 0 \\ Ae^{-qx}, & x > 0 \end{cases}$$

The boundary condition on the wave function derivative (Prob. 5.24) gives

$$\left.\frac{d\varphi_E(x)}{dx}\right|_{\varepsilon} - \left.\frac{d\varphi_E(x)}{dx}\right|_{-\varepsilon} = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} V(x)\varphi_E(x)dx$$

$$\lim_{\varepsilon\to 0}\left(-qAe^{-q\varepsilon} - qAe^{q\varepsilon}\right) = -\beta\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon}\delta(x)\varphi_E(x)dx$$

$$-2qA = -\beta\frac{2m}{\hbar^2}\varphi_E(0)$$

$$-2qA = -\beta\frac{2m}{\hbar^2}A$$

with the result

$$q = \frac{m\beta}{\hbar^2}$$

This yields the allowed energy

$$E = -\frac{\hbar^2 q^2}{2m} = -\frac{m\beta^2}{2\hbar^2}$$

Finally, we normalize the wave function:

$$1 = \langle E|E\rangle = \int_{-\infty}^{\infty} |\varphi_E(x)|^2 \, dx = 2|A|^2 \int_0^{\infty} e^{-2qx} \, dx = \frac{|A|^2}{q}$$

$$\Rightarrow A = \sqrt{q} = \frac{\sqrt{m\beta}}{\hbar}$$

The delta function potential energy well has only one bound state with solution

$$\varphi_E(x) = \frac{\sqrt{m\beta}}{\hbar} e^{-m\beta|x|/\hbar^2} \quad ; \quad E = -\frac{m\beta^2}{2\hbar^2}$$

5.26 Outside of the potential wells, $V = 0$, so the solutions are real exponentials. Assume a solution of form

$$\varphi_E(x) = \begin{cases} Ae^{qx}, & x < -a \\ Be^{qx} + Ce^{-qx}, & -a < x < a \\ De^{-qx}, & x > a \end{cases}$$

with $q = \sqrt{-2mE/\hbar^2}$. The boundary condition on the continuity of the wave function at $x = \pm a$ gives

$$Ae^{-qa} = Be^{-qa} + Ce^{qa}$$
$$De^{-qa} = Be^{qa} + Ce^{-qa}$$

The boundary condition on the wave function derivative (Prob. 5.24) at $x = a$ gives

$$\left.\frac{d\varphi_E(x)}{dx}\right|_{a+\varepsilon} - \left.\frac{d\varphi_E(x)}{dx}\right|_{a-\varepsilon} = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{a-\varepsilon}^{a+\varepsilon} V(x)\varphi_E(x)\,dx = -\beta\frac{2m}{\hbar^2}\varphi_E(a)$$

$$-qDe^{-qa} - \left(qBe^{qa} - qCe^{-qa}\right) = -\frac{2m\beta}{\hbar^2}De^{-qa}$$

$$qBe^{qa} - qCe^{-qa} = \left(\frac{2m\beta}{\hbar^2} - q\right)\left(Be^{qa} + Ce^{-qa}\right)$$

$$\left(2q - \frac{2m\beta}{\hbar^2}\right)Be^{qa} = \frac{2m\beta}{\hbar^2}Ce^{-qa}$$

$$e^{-2qa} = \frac{B}{C}\left(\frac{\hbar^2 q}{m\beta} - 1\right)$$

Likewise, the boundary condition on the wave function derivative at $x = -a$ gives

$$\left.\frac{d\varphi_E(x)}{dx}\right|_{-a+\varepsilon} - \left.\frac{d\varphi_E(x)}{dx}\right|_{-a-\varepsilon} = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-a-\varepsilon}^{-a+\varepsilon} V(x)\varphi_E(x)\,dx = -\beta\frac{2m}{\hbar^2}\varphi_E(a)$$

$$\left(qBe^{-qa} - qCe^{qa}\right) - qAe^{-qa} = -\frac{2m\beta}{\hbar^2}Ae^{-qa}$$

$$qBe^{-qa} - qCe^{qa} = \left(q - \frac{2m\beta}{\hbar^2}\right)\left(Be^{-qa} + Ce^{qa}\right)$$

$$\left(-2q + \frac{2m\beta}{\hbar^2}\right)Ce^{qa} = -\frac{2m\beta}{\hbar^2}Be^{-qa}$$

$$e^{-2qa} = \frac{C}{B}\left(\frac{\hbar^2 q}{m\beta} - 1\right)$$

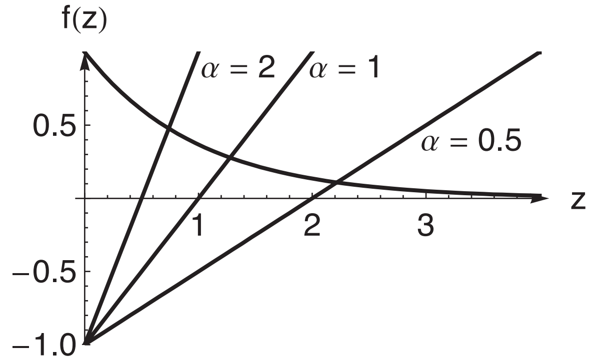
These two conditions are satisfied only if $C^2 = B^2$ or $C = \pm B$, which correspond to even and odd solutions, as one expects. For the even solution ($C = B = A\,e^{-2qa}/2\cosh 2qa$), we get $A = D$ and the quantization condition is

$$e^{-2qa} = \frac{\hbar^2 q}{m\beta} - 1$$

This transcendental equation can be solved graphically. Simplify the equation by letting $z = 2qa$ and $\alpha = \hbar^2/2ma\beta$, such that

$$e^{-z} = \alpha z - 1$$

Plot the two sides of this equation and identify the intersection as shown below:



There is only one allowed intersection point and therefore one allowed energy, which depends on the parameter $\alpha = \hbar^2/2ma\beta$. For example, for $\alpha = 1$, the allowed solution is $z = 2qa = 1.278$, which gives an energy

$$E = -\frac{\hbar^2 q^2}{2m} = -\frac{\hbar^2 (1.278)^2}{8ma^2} = -\,0.204\frac{\hbar^2}{ma^2}$$

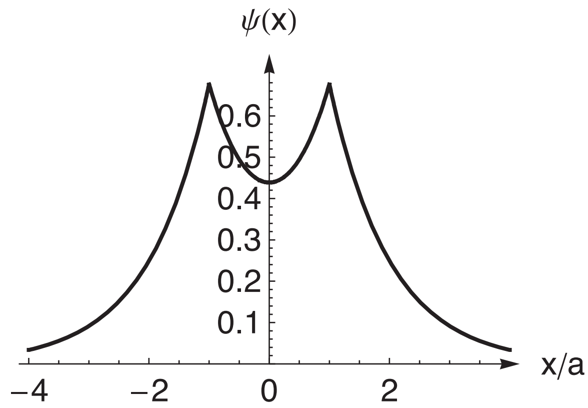
Normalizing the even wave function gives

$$\begin{aligned}
1 = \langle E|E\rangle &= \int_{-\infty}^{\infty} |\varphi_E(x)|^2\, dx = |A|^2 \int_{-\infty}^{-a} e^{2qx}\, dx + |B|^2 \int_{-a}^{a} 4\cosh^2 qx\, dx + |A|^2 \int_{a}^{\infty} e^{-2qx}\, dx \\
&= |A|^2 \frac{e^{-2qa}}{2q} + |A|^2 \frac{e^{-2qa}}{\cosh^2 qa}\left(\frac{1}{2q}\sinh 2qa + a\right) + |A|^2 \frac{e^{-2qa}}{2q} \\
&= |A|^2 \frac{e^{-2qa}}{q}\left(1 + \frac{2qa + \sinh 2qa}{2\cosh^2 qa}\right) = |A|^2 \frac{e^{-2qa}}{q}\left(\frac{4qa + \left(e^{qa} + e^{-qa}\right)^2 + \left(e^{2qa} - e^{-2qa}\right)}{\left(e^{qa} + e^{-qa}\right)^2}\right) \\
&= |A|^2 \frac{1}{q}\left(\frac{4qae^{-2qa} + \left(1 + e^{-2qa}\right)^2 + \left(1 - e^{-4qa}\right)}{\left(e^{qa} + e^{-qa}\right)^2}\right) = |A|^2 \frac{2}{q}\left(\frac{1 + 2qa + e^{2qa}}{\left(1 + e^{2qa}\right)^2}\right) \\
\Rightarrow A &= \sqrt{\frac{q}{2}}\frac{1 + e^{2qa}}{\sqrt{1 + 2qa + e^{2qa}}}
\end{aligned}$$

The even solution is

$$\varphi_{E,\,even}(x) = \begin{cases} Ae^{qx}, & x < -a \\ Ae^{-qa}\dfrac{\cosh qx}{2\cosh qa}, & -a < x < a \\ Ae^{-qx}, & x > a \end{cases} \qquad\qquad A = \sqrt{\frac{q}{2}}\frac{1 + e^{2qa}}{\sqrt{1 + 2qa + e^{2qa}}}$$

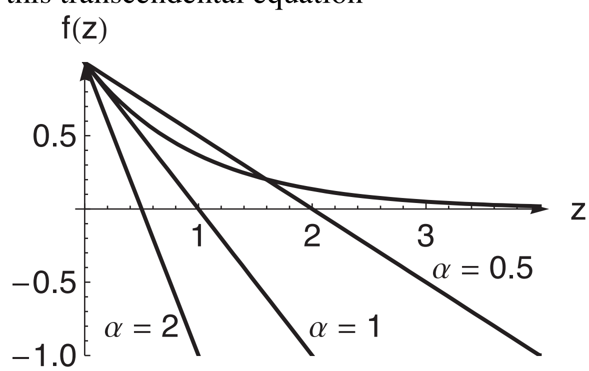
as shown below



For the odd solution ($C = -B = -De^{-2qa}/2\sinh 2qa$), we get $A = -D$ and the quantization condition is

$$e^{-2qa} = 1 - \frac{\hbar^2 q}{m\beta}$$

The graphical solution of this transcendental equation



shows that there is an odd solution only if

$$\alpha < 1 \quad \Rightarrow \quad \beta > \frac{\hbar^2}{2ma^2}$$

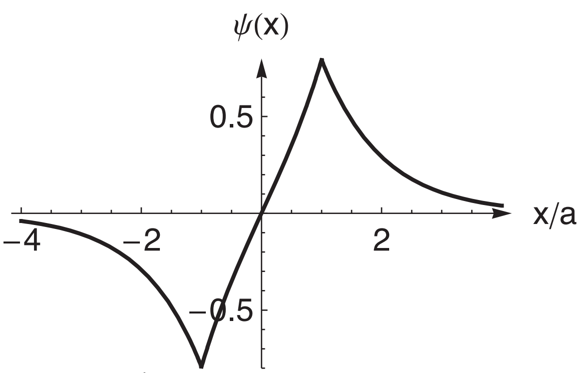
Normalizing the odd wave function gives

$$1=\langle E|E\rangle=\int_{-\infty}^{\infty}\left|\varphi_E(x)\right|^2dx=|D|^2\int_{-\infty}^{-a}e^{2qx}\,dx+|B|^2\int_{-a}^{a}4\sinh^2 qx\,dx+|D|^2\int_{a}^{\infty}e^{-2qx}\,dx$$
$$=|D|^2\frac{e^{-2qa}}{2q}+|D|^2\frac{e^{-2qa}}{\sinh^2 qa}\left(\frac{1}{2q}\sinh 2qa-a\right)+|D|^2\frac{e^{-2qa}}{2q}$$
$$=|D|^2\frac{e^{-2qa}}{q}\left(1+\frac{-2qa+\sinh 2qa}{2\sinh^2 qa}\right)=|D|^2\frac{e^{-2qa}}{q}\left(\frac{-4qa+\left(e^{qa}-e^{-qa}\right)^2+\left(e^{2qa}-e^{-2qa}\right)}{\left(e^{qa}-e^{-qa}\right)^2}\right)$$
$$=|D|^2\frac{1}{q}\left(\frac{-4qae^{-2qa}+\left(1-e^{-2qa}\right)^2+\left(1-e^{-4qa}\right)}{\left(e^{qa}-e^{-qa}\right)^2}\right)=|D|^2\frac{2}{q}\left(\frac{-1-2qa+e^{2qa}}{\left(-1+e^{2qa}\right)^2}\right)$$
$$\Rightarrow D=\sqrt{\frac{q}{2}}\frac{-1+e^{2qa}}{\sqrt{-1-2qa+e^{2qa}}}$$

The odd solution is

$$\varphi_{E,\,odd}(x)=\begin{cases}-De^{qx}, & x<-a\\ De^{-qa}\dfrac{\sinh qx}{2\sinh qa}, & -a<x<a\\ De^{-qx}, & x>a\end{cases}\qquad D=\sqrt{\frac{q}{2}}\frac{-1+e^{2qa}}{\sqrt{-1-2qa+e^{2qa}}}$$

as shown below



There are two bound states if $\beta>\hbar^2/2ma^2$, but only one bound state if $\beta<\hbar^2/2ma^2$

5.27 The superposition state is

$$|\psi(t)\rangle=\frac{1}{\sqrt{2}}|E_1\rangle e^{-iE_1t/\hbar}+\frac{1}{\sqrt{2}}|E_2\rangle e^{-iE_2t/\hbar}$$

The wave function representation is

$$\psi(x,t)=\frac{1}{\sqrt{2}}\varphi_1(x)e^{-iE_1t/\hbar}+\frac{1}{\sqrt{2}}\varphi_2(x)e^{-iE_2t/\hbar}$$
$$=\sqrt{\frac{1}{L}}\left[\sin\frac{\pi x}{L}e^{-iE_1t/\hbar}+\sin\frac{2\pi x}{L}e^{-iE_2t/\hbar}\right]$$

Now find the expectation value of the momentum:

$$\begin{aligned}
\langle p\rangle &= \langle\psi(t)|p|\psi(t)\rangle \\
&= \left\{\frac{1}{\sqrt{2}}\langle E_1|e^{iE_1t/\hbar}+\frac{1}{\sqrt{2}}\langle E_2|e^{iE_2t/\hbar}\right\}\ p\ \left\{\frac{1}{\sqrt{2}}|E_1\rangle e^{-iE_1t/\hbar}+\frac{1}{\sqrt{2}}|E_2\rangle e^{-iE_2t/\hbar}\right\} \\
&= \frac{1}{2}\Big[\langle E_1|p|E_1\rangle+\langle E_2|p|E_2\rangle+\langle E_1|p|E_2\rangle e^{i(E_1-E_2)t/\hbar}+\langle E_2|p|E_1\rangle e^{-i(E_1-E_2)t/\hbar}\Big]
\end{aligned}$$

The required integrals are:

$$\langle p\rangle_n = \langle E_n|p|E_n\rangle = \int_0^L \varphi_n^*(x)\left(-i\hbar\frac{d}{dx}\right)\varphi_n(x)\,dx = -i\hbar\int_0^L \varphi_n^*(x)\left(\frac{d\varphi_n(x)}{dx}\right)dx$$

$$\langle p\rangle_{nk} = \langle E_n|p|E_k\rangle = \int_0^L \varphi_n^*(x)\left(-i\hbar\frac{d}{dx}\right)\varphi_k(x)\,dx = -i\hbar\int_0^L \varphi_n^*(x)\left(\frac{d\varphi_k(x)}{dx}\right)dx$$

The first integral is just the expectation value of the momentum in an energy eigenstate:

$$\begin{aligned}
\langle p\rangle_n &= -i\hbar\int_0^L \varphi_n^*(x)\left(\frac{d\varphi_n(x)}{dx}\right)dx = -i\hbar\frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\left(\frac{n\pi}{L}\right)\cos\left(\frac{n\pi x}{L}\right)dx \\
&= -i\hbar\frac{2}{L}\left(\frac{n\pi}{L}\right)\left(\frac{L}{2n\pi}\right)\left[\sin^2\left(\frac{n\pi x}{L}\right)\right]_0^L = 0
\end{aligned}$$

which is zero as expected. The second integral is

$$\begin{aligned}
\langle p\rangle_{nk} &= -i\hbar\int_0^L \varphi_n^*(x)\left(\frac{d\varphi_k(x)}{dx}\right)dx = -i\hbar\frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\left(\frac{k\pi}{L}\right)\cos\left(\frac{k\pi x}{L}\right)dx \\
&= -i\hbar\frac{2}{L}\left(\frac{k\pi}{L}\right)\left(\frac{L}{\pi}\right)\int_0^\pi \sin(ny)\cos(ky)\,dy \\
&= -i\hbar\frac{2}{L}\left(\frac{k\pi}{L}\right)\left(\frac{L}{\pi}\right)\left[-\frac{\cos(n-k)y}{2(n-k)}-\frac{\cos(n+k)y}{2(n+k)}\right]_0^\pi \\
&= -i\hbar\frac{2}{L}\left(\frac{k\pi}{L}\right)\left(\frac{L}{\pi}\right)\left[-\frac{\cos(n-k)\pi}{2(n-k)}-\frac{\cos(n+k)\pi}{2(n+k)}+\frac{1}{2(n-k)}+\frac{1}{2(n+k)}\right] \\
&= -i\hbar\frac{2k}{L}\left[\frac{n}{n^2-k^2}-\frac{(-1)^{n-k}}{2(n-k)}-\frac{(-1)^{n+k}}{2(n+k)}\right] = -i\hbar\frac{2nk}{L(n^2-k^2)}\left[1-(-1)^{n+k}\right]
\end{aligned}$$

For the states in questions we get

$$\langle p\rangle_1 = \langle p\rangle_2 = 0$$

$$\langle p\rangle_{12} = -\langle p\rangle_{21} = i\frac{8\hbar}{3L}$$

and the result is

$$\langle p\rangle = \langle\psi(t)|p|\psi(t)\rangle = \frac{1}{2}\Big[\langle p\rangle_1 + \langle p\rangle_2 + \langle p\rangle_{12}\, e^{i(E_1-E_2)t/\hbar} + \langle p\rangle_{21}\, e^{-i(E_1-E_2)t/\hbar}\Big]$$
$$= \frac{1}{2}\left[i\frac{8\hbar}{3L}e^{i(E_1-E_2)t/\hbar} - i\frac{8\hbar}{3L}e^{-i(E_1-E_2)t/\hbar}\right] = i\frac{4\hbar}{3L}\Big[e^{-i3\pi^2\hbar t/2mL^2} - e^{+i3\pi^2\hbar t/2mL^2}\Big]$$
$$= \frac{8\hbar}{3L}\sin\left(\frac{3\pi^2\hbar}{2mL^2}t\right)$$

5.28 The boundary condition equations are

$$A\sin(k_1L/2) = B\sin(k_2L/2) + C\cos(k_2L/2)$$
$$k_1A\cos(k_1L/2) = k_2B\cos(k_2L/2) - k_2C\sin(k_2L/2)$$
$$B\sin k_2L + C\cos k_2L = 0$$

Solve the third equation for C and substitute into the other two:

$$C = -B\frac{\sin k_2L}{\cos k_2L}$$
$$A\sin(k_1L/2) = B\sin(k_2L/2) - B\frac{\sin k_2L}{\cos k_2L}\cos(k_2L/2)$$
$$k_1A\cos(k_1L/2) = k_2B\cos(k_2L/2) + k_2B\frac{\sin k_2L}{\cos k_2L}\sin(k_2L/2)$$

Solve the second equation for A and substitute into the third equation (for the moment, let $\alpha = k_1L/2$ and $\beta = k_2L/2$ to save ink):

$$A = B\frac{\sin\beta}{\sin\alpha} - B\frac{\sin 2\beta}{\cos 2\beta}\frac{\cos\beta}{\sin\alpha}$$
$$k_1\cos\alpha\left[\frac{\sin\beta}{\sin\alpha} - \frac{\sin 2\beta}{\cos 2\beta}\frac{\cos\beta}{\sin\alpha}\right] = k_2\cos\beta + k_2\frac{\sin 2\beta}{\cos 2\beta}\sin\beta$$

Factoring out some terms and cross multiplying gets

$$k_1\cos\alpha\sin\beta\left[1 - \frac{\sin 2\beta}{\cos 2\beta}\frac{\cos\beta}{\sin\beta}\right] = k_2\cos\beta\sin\alpha\left[1 + \frac{\sin 2\beta}{\cos 2\beta}\frac{\sin\beta}{\cos\beta}\right]$$

Now note that

$$\frac{\sin 2\beta}{\cos 2\beta}\frac{\cos\beta}{\sin\beta} = \frac{2\sin\beta\cos\beta}{\cos^2\beta - \sin^2\beta}\frac{\cos\beta}{\sin\beta} = \frac{2\cos^2\beta}{\cos^2\beta - \sin^2\beta}$$
$$\frac{\sin 2\beta}{\cos 2\beta}\frac{\sin\beta}{\cos\beta} = \frac{2\sin\beta\cos\beta}{\cos^2\beta - \sin^2\beta}\frac{\sin\beta}{\cos\beta} = \frac{2\sin^2\beta}{\cos^2\beta - \sin^2\beta}$$

so that

$$\left[1-\frac{\sin 2\beta}{\cos 2\beta}\frac{\cos\beta}{\sin\beta}\right]=1-\frac{2\cos^2\beta}{\cos^2\beta-\sin^2\beta}=\frac{-\cos^2\beta-\sin^2\beta}{\cos^2\beta-\sin^2\beta}=\frac{-1}{\cos^2\beta-\sin^2\beta}$$
$$\left[1+\frac{\sin 2\beta}{\cos 2\beta}\frac{\sin\beta}{\cos\beta}\right]=1+\frac{2\sin^2\beta}{\cos^2\beta-\sin^2\beta}=\frac{\cos^2\beta+\sin^2\beta}{\cos^2\beta-\sin^2\beta}=\frac{1}{\cos^2\beta-\sin^2\beta}$$

This simplifies the previous expression, and substituting back in the equations for α and β results in the resultant transcendental equation

$$k_1\cos\left(k_1L/2\right)\sin\left(k_2L/2\right)+k_2\cos\left(k_2L/2\right)\sin\left(k_1L/2\right)=0$$

5.29 For the case $E<V_0$, the solution in the right half of the well is a real exponential, so the full solution is

$$\varphi_E(x)=\begin{cases} A\sin k_1x, & 0<x<L/2 \\ B\sinh q_2x+C\cosh q_2x, & L/2<x<L \end{cases}$$

where $q_2=\sqrt{2m\left(V_0-E\right)/\hbar^2}$ is the decy length in the right side of the well. The three boundary conditions are

$$\varphi_E\left(L/2\right):A\sin\left(k_1L/2\right)=B\sinh\left(q_2L/2\right)+C\cosh\left(q_2L/2\right)$$
$$\left.\frac{d\varphi_E(x)}{dx}\right|_{x=L/2}:k_1A\cos\left(k_1L/2\right)=q_2B\cosh\left(k_2L/2\right)+q_2C\sinh\left(q_2L/2\right)$$
$$\varphi_E\left(L\right):B\sinh q_2L+C\cosh q_2L=0$$

Solve the third equation for *C* and substitute into the other two:

$$C=-B\frac{\sinh q_2L}{\cosh q_2L}$$
$$A\sin\left(k_1L/2\right)=B\sinh\left(q_2L/2\right)-B\frac{\sinh q_2L}{\cosh q_2L}\cosh\left(q_2L/2\right)$$
$$k_1A\cos\left(k_1L/2\right)=q_2B\cosh\left(q_2L/2\right)-q_2B\frac{\sinh q_2L}{\cosh q_2L}\sinh\left(q_2L/2\right)$$

Solve the second equation for *A* and substitute into the third equation (for the moment, let $\alpha=k_1L/2$ and $\beta=q_2L/2$ to save ink):

$$A=B\frac{\sinh\beta}{\sin\alpha}-B\frac{\sinh 2\beta}{\cosh 2\beta}\frac{\cosh\beta}{\sin\alpha}$$
$$k_1\cos\alpha\left[\frac{\sinh\beta}{\sin\alpha}-\frac{\sinh 2\beta}{\cosh 2\beta}\frac{\cosh\beta}{\sin\alpha}\right]=k_2\cosh\beta-k_2\frac{\sinh 2\beta}{\cosh 2\beta}\sinh\beta$$

Factoring out some terms and cross multiplying gets

$$k_1 \cos\alpha \sinh\beta \left[1 - \frac{\sinh 2\beta}{\cosh 2\beta}\frac{\cosh\beta}{\sinh\beta}\right] = k_2 \cosh\beta \sin\alpha \left[1 - \frac{\sinh 2\beta}{\cosh 2\beta}\frac{\sinh\beta}{\cosh\beta}\right]$$

Now note that

$$\frac{\sinh 2\beta}{\cosh 2\beta}\frac{\cosh\beta}{\sinh\beta} = \frac{2\sinh\beta\cosh\beta}{\cosh^2\beta + \sinh^2\beta}\frac{\cosh\beta}{\sinh\beta} = \frac{2\cosh^2\beta}{\cosh^2\beta + \sinh^2\beta}$$
$$\frac{\sinh 2\beta}{\cosh 2\beta}\frac{\sinh\beta}{\cosh\beta} = \frac{2\sinh\beta\cosh\beta}{\cosh^2\beta + \sinh^2\beta}\frac{\sinh\beta}{\cosh\beta} = \frac{2\sinh^2\beta}{\cosh^2\beta + \sinh^2\beta}$$

so that

$$\left[1 - \frac{\sinh 2\beta}{\cosh 2\beta}\frac{\cosh\beta}{\sinh\beta}\right] = 1 - \frac{2\cosh^2\beta}{\cosh^2\beta + \sinh^2\beta} = \frac{-\cosh^2\beta + \sinh^2\beta}{\cosh^2\beta + \sinh^2\beta}$$
$$\left[1 - \frac{\sinh 2\beta}{\cosh 2\beta}\frac{\sinh\beta}{\cosh\beta}\right] = 1 - \frac{2\sinh^2\beta}{\cosh^2\beta + \sinh^2\beta} = \frac{\cosh^2\beta - \sinh^2\beta}{\cosh^2\beta + \sinh^2\beta}$$

This simplifies the previous expression, and substituting back in the equations for α and β results in the resultant transcendental equation

$$k_1 \cos(k_1 L/2)\sinh(q_2 L/2) + q_2 \cosh(q_2 L/2)\sin(k_1 L/2) = 0$$

Note that this is similar to Eq. (5.145), for the case $E > V_0$, with the change that the trig functions of the second wave number are changed to hyperbolic trig functions because the wave is a real exponential in that region. This can be done formally with the change $k_2 \to iq_2$.

5.30 The update equations are

$$\varphi_E(x+\Delta x) = \varphi_E(x) + \left(\frac{d\varphi_E}{dx}\right)_x \Delta x + \frac{1}{2}\left(\frac{d^2\varphi_E}{dx^2}\right)_x (\Delta x)^2$$
$$\left(\frac{d\varphi_E}{dx}\right)_{x+\Delta x} = \left(\frac{d\varphi_E}{dx}\right)_x + \frac{1}{2}\left[\left(\frac{d^2\varphi_E}{dx^2}\right)_x + \left(\frac{d^2\varphi_E}{dx^2}\right)_{x+\Delta x}\right]\Delta x$$

where the second derivative comes from the energy eigenvalue equation:

$$\frac{d^2\varphi_E(x)}{dx^2} = -\frac{2m}{\hbar^2}\left[E - V(x)\right]\varphi_E(x)$$

For a finite square well, we defined the dimensionless parameter

$$z_0 = \sqrt{\frac{2mV_0 a^2}{\hbar^2}}$$

Using this parameter, we recast the second derivative in a dimensionless fashion for use on the computer:

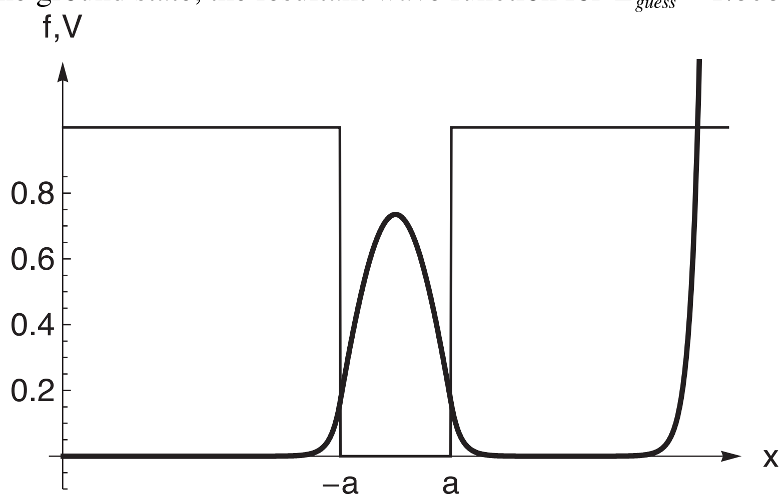
$$\frac{d^2\varphi_E(x)}{dx^2} = -\frac{z_0^2}{a^2V_0}\left[E - V(x)\right]\varphi_E(x) = -\frac{z_0^2}{a^2}\left[\frac{E}{V_0} - \frac{V(x)}{V_0}\right]\varphi_E(x)$$

$$\frac{d^2\varphi_E(x)}{d(x/a)^2} = -z_0^2\left[\frac{E}{V_0} - \frac{V(x)}{V_0}\right]\varphi_E(x)$$

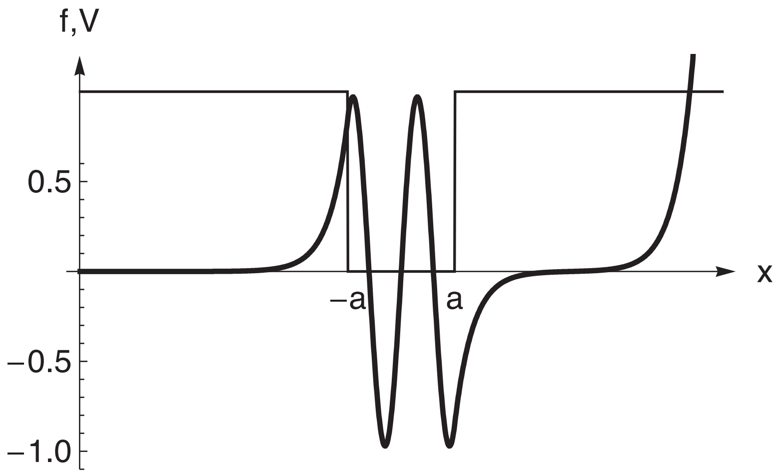
The Mathematica code to implement this with dimensionless position and energy ($E_{guess} = E/V_0 = E\big/\left(z_0^2\left(\hbar^2/2ma^2\right)\right)$) is

```
np = 100; (* choose density of points *)
V = Join[Table[1,{np*5}],Table[0,{np*2}],Table[1,{np*5}]];   (* define potential well *)
z0 = 6;                                                          (* set well parameter *)
Eguess = 1.8081064296/36;                                    (* choose guess for energy *)
dx = 1/np;                                                     (* set position density *)
f = Table[0, {i, 12*np}];                        (*initialize array for wave function *)
fp =  Table[0, {i, 12*np}];           (*initialize array for wave function derivative *)
f[[1]] = 0;                                 (* set wave function to zero far from well *)
fp[[1]] =  4*10^-13;              (* set derivative to finite value far from well *)
Do[                                                                         (* do loop *)
  fpp1 = -z0^2*(Eguess - V[[i]])*f[[i]];           (* calculate 2nd derivative at x *)
  f[[i+1]]=f[[i]]+fp[[i]]*dx +1/2*fpp1*dx^2;        (* update wave function at x +dx *)
  fpp2 = -z0^2*(Eguess - V[[i+1]])*f[[i+1]];     (* calculate 2nd derivative at x +dx *)
  fp[[i+1]] = fp[[i]] + 1/2*(fpp1 + fpp2)*dx,       (* update 1st derivative at x +dx *)
{i, 1,  Length[f] - 1}]                                                 (* end do loop *)
ListPlot[{f, V}, PlotRange -> {-0.1, 1.2}]                          (* plot wave function *)
```

The energy parameter E_{guess} is our guess for the energy of a desired energy eigenstate. In this program, we change the value of E_{guess} manually and look at the output plot to decide what to do next. If the energy guess is close to the right value, then the wave function will decay to zero outside the well and then diverge far from the well. By adjusting our guess, we can move the divergence point farther away to get a better estimate, as in Fig. 5.29. The initial derivative value is adjusted to make the resultant wave function of order unity. For the ground state, the resultant wave function for $E_{guess} = 1.8081.../z_0^2$ is



This result matches the 1.81 in Eq. (5.89). For the $n = 4$ state, we choose $E_{guess} = 27.30456/z_0^2$ and get the wave function



as in Fig. 5.29(c).

5.31 The well parameter z_0 is

$$z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}} = \sqrt{\frac{2(511keV)5eV(1.5nm/2)^2}{(1240eVnm/2\pi)^2}} = 8.59$$

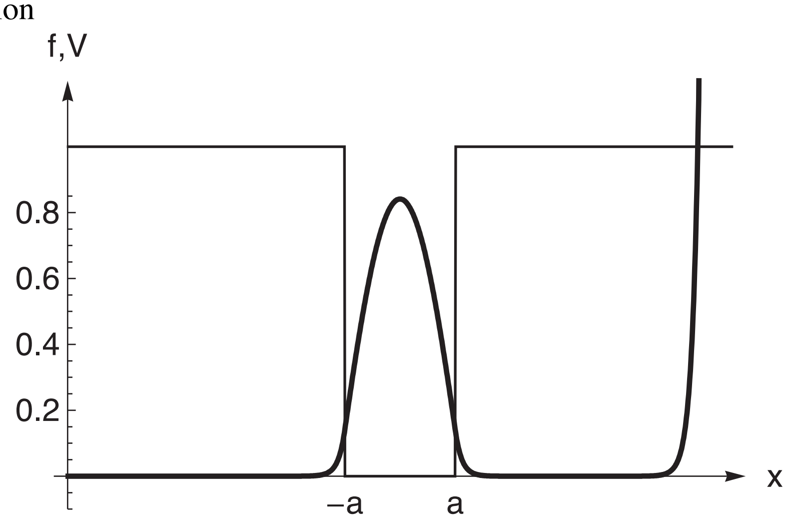
which gives 6 bound states as we found in Problem 5.18. Using the Mathematica code from Problem 5.30, we get the ground state function and energy

$$E_{guess} = 1.977/z_0^2$$

This gives an energy

$$E_1 = E_{guess}V_0 = E_{guess}\frac{z_0^2\hbar^2}{2ma^2} = 1.977\frac{\hbar^2}{2ma^2} = 1.977\frac{(1240eVnm/2\pi)^2}{2(511keV)(1.5nm/2)^2} = 0.134eV$$

and a wave function



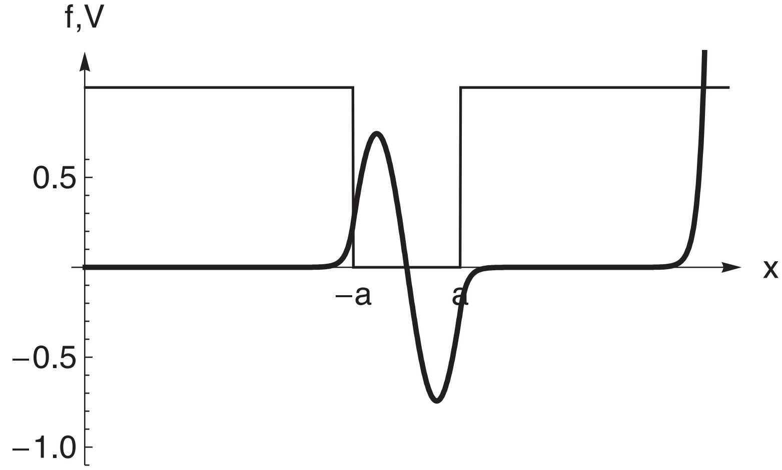
For the first excited state, the numerical integration gives

$$E_{guess} = 7.885/z_0^2$$

an energy

$$E_1 = E_{guess}V_0 = E_{guess}\frac{z_0^2\hbar^2}{2ma^2} = 7.885\frac{\hbar^2}{2ma^2} = 7.885\frac{\left(1240eVnm/2\pi\right)^2}{2\left(511keV\right)\left(1.5nm/2\right)^2} = 0.534eV$$

and a wave function



In Problem 5.18, we found that the transcendental equation gave the allowed energies

$$E = 0.134\text{eV},\ 0.535\text{eV},\ 1.197\text{eV},\ 2.109\text{eV},\ 3.245\text{eV},\ 4.525\text{eV}$$

so there is good agreement.

5.32 The well parameter z_0 is (note that the well width $d = 2a$)

$$z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}} = \sqrt{\frac{2\left(0.067\times 511keV\right)0.1eV\left(d\left(nm\right)/2\right)^2}{\left(1240eVnm/2\pi\right)^2}} = 0.2096\ d\left(nm\right)$$

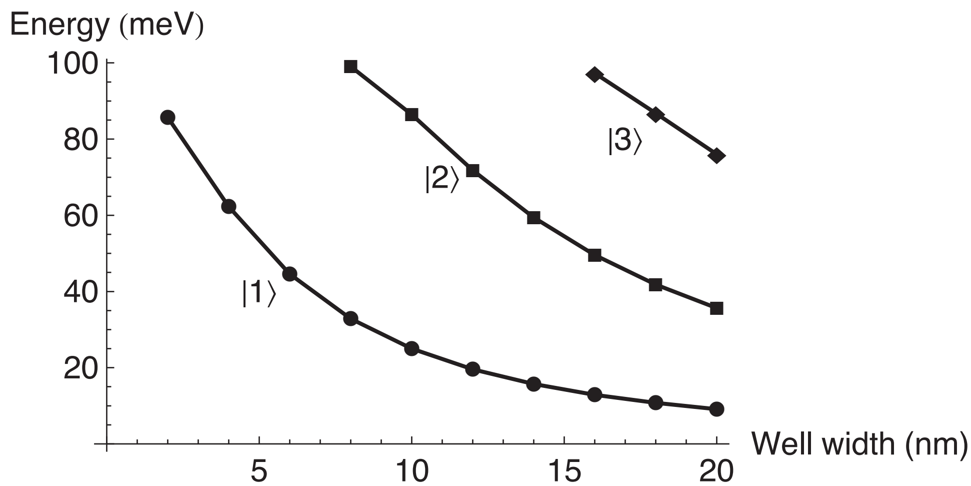
For example, when the well width is 20 nm, $z_0 = 4.193$. This gives three solutions to the transcendental equations

$$z\tan\left(z\right) = \sqrt{z_0^2 - z^2} \quad \rightarrow \quad z = 1.264,\ 3.653$$
$$-z\cot\left(z\right) = \sqrt{z_0^2 - z^2} \quad \rightarrow \quad z = 2.502$$

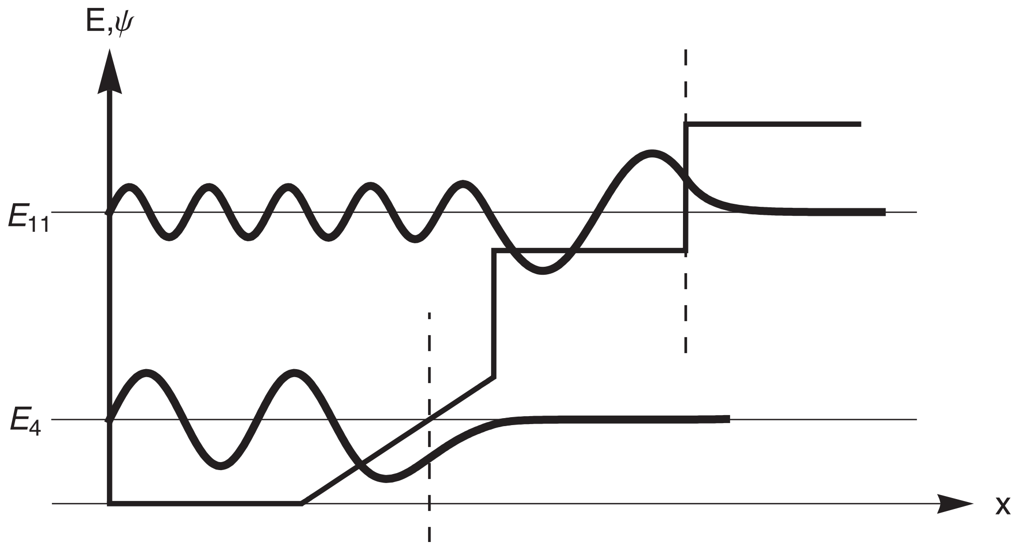
and energies

$$E = \frac{\hbar^2z^2}{2ma^2} = 9.1\text{ meV},\ 35.6\text{ meV},\ 76.0\text{ meV}$$

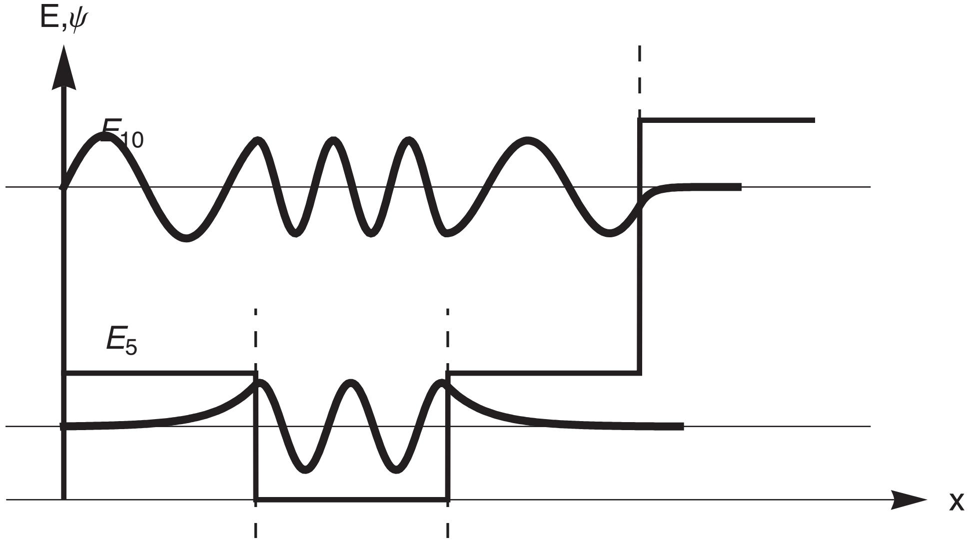
Using well sizes from 2 to 20 nm gives the resultant plot:



5.33 The plots are shown below:

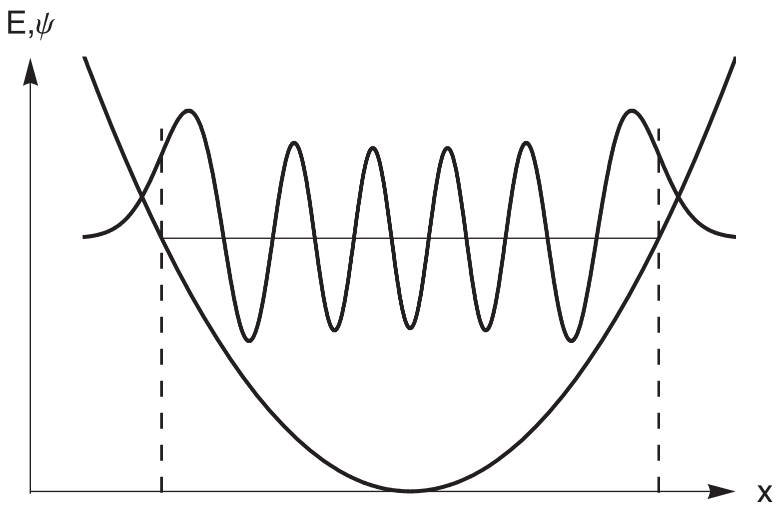


The wave function is oscillatory in the classically allowed regions and exponentially decaying in the forbidden regions, demarcated by the dashed lines. In each case, the number of antinodes in the wave function equals the principal quantum number *n*. For *n*= 11, the wavelength in the right part is longer because the potential is higher, and the amplitude is increased there also.

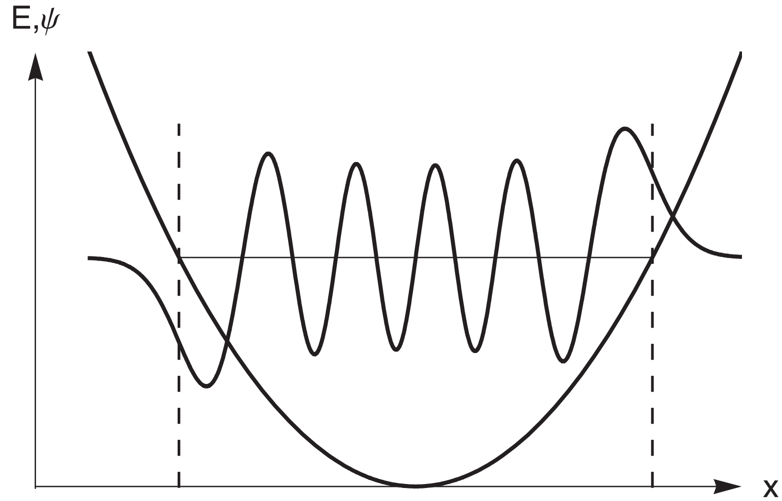


The wave function is oscillatory in the classically allowed regions and exponentially decaying in the forbidden regions, demarcated by the dashed lines. In each case, the number of antinodes in the wave function equals the principal quantum number n. For n= 10, the wavelength in the central part is shorter because the potential is lower, and the amplitude is decreased there also (only slightly in this case).

5.34 Plots below



Classically allowed and forbidden regions are demarcated by the dashed lines where the energy of the state equals the potential energy (hence kinetic energy is zero). The state above has 11 antinodes so is the n = 11 state. The n = 10 state is shown below.


E,ψ
x