5.2.6

The finite square well potential energy is

$$V(x)=\begin{cases} V_0 & x<-a \\ 0 & -a\le x\le a \\ V_0 & x>a \end{cases}$$

The energy eigenvalue equation is

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+0\right)\varphi_E(x)=E\varphi_E(x) \quad \textit{inside box}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\right)\varphi_E(x)=E\varphi_E(x) \quad \textit{outside box}$$

In the infinite well problem, we found it useful to use the wave vector k

$$k=\sqrt{\frac{2mE}{\hbar^2}}\ .$$

In this case, the wave vector outside the well is imaginary, so we define the decay constant q (κ in the text)

$$q=\sqrt{\frac{2m}{\hbar^2}\left(V_0-E\right)}\ .$$

Note that k and q are related by

$$k^2+q^2=\frac{2mV_0}{\hbar^2}\ .$$

For bound states, $0<E<V_0$, and therefore both k and q are real. We use these two constants to rewrite the energy eigenvalue equation:

$$\frac{d^2\varphi_E(x)}{dx^2}=-k^2\varphi_E(x) \quad \textit{inside box}$$

$$\frac{d^2\varphi_E(x)}{dx^2}=q^2\varphi_E(x) \quad \textit{outside box}$$

The energy eigenvalue equation inside the box is identical to the one we solved for the infinite well potential. The differential equation outside the box is similar except the constant is positive instead of negative, giving real exponential solutions rather than complex exponentials. Thus the solution outside the box is

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

This solution in the classically forbidden region is exponentially decaying, or growing, with a decay length, or growth length, of $1/q$.

The energy eigenstate must be constructed by connecting solutions in the three regions. We write the general solution as

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

The normalization condition (i.e. boundary condition at infinity) requires that $B = F = 0$. In the infinite well, we found that the solutions could be classified as having even or odd spatial symmetry. Let's do the same here. The even solutions are ($G = A$)

$$\varphi_{even}(x) = \begin{cases} Ae^{qx} & x < -a \\ D\cos(kx) & -a \le x \le a \\ Ae^{-qx} & x > a \end{cases}$$

The odd solutions are ($G = -A$)

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

Let's first do the even solutions. The boundary conditions at the right side of the well ($x = a$) give

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

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

The boundary conditions at the left side of the well ($x = -a$) yield the same equations, which must be true because of the symmetry. The two equations above have three unknowns: the amplitudes A and D and the energy E, which is contained in the parameters k and q. The normalization condition provides the third equation required to solve for all three unknowns. We find the energy condition rather simply by dividing the two equations, which eliminates the amplitudes and yields

$$k\tan(ka) = q$$

Now let's do the odd solutions. The boundary conditions at the right side of the well ($x = a$) give

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

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

Dividing the equations eliminates the normalization constants to yield

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

A graphical solution for the allowed energies using these two transcendental equations is most useful here. There are many ways of doing this. One way involves defining some new dimensionless parameters:

$$\alpha = ka = \sqrt{\frac{2mEa^2}{\hbar^2}}$$

$$\beta = qa = \sqrt{\frac{2m(V_0 - E)a^2}{\hbar^2}}$$

These definitions lead to the convenient expression

$$\alpha^2+\beta^2=\frac{2mV_0a^2}{\hbar^2}\equiv R^2$$

This allows us to write the transcendental equations in this form:

$$\alpha\tan(\alpha)=\beta \quad\rightarrow\quad \alpha\tan(\alpha)=\sqrt{R^2-\alpha^2}$$

$$-\alpha\cot(\alpha)=\beta \quad\rightarrow\quad -\alpha\cot(\alpha)=\sqrt{R^2-\alpha^2}$$

In each of these new transcendental equations, the left side is a modified trig function, while the right side is a circle with radius R. These functions are plotted below as a function of the parameter α. The intersection points of these curves determine the allowed values of α and hence the allowed energies E_n. Because the constant R is the radius of the circle, there are a limited number of allowed energies, and that number grows as R gets larger. The large circle below leads to four bound states, while the smaller circle leads to only one bound state. Note that there is always at least one bound state because the circle always intersects at least the first tangent curve (even state). To get at least one odd solution, we need the circle to be big enough that it intersects the first cotangent curve. Hence we require

$$R>\frac{\pi}{2} \quad\Rightarrow\quad \sqrt{\frac{2mV_0a^2}{\hbar^2}}>\frac{\pi}{2}$$

$$\Rightarrow\quad V_0>\frac{\pi^2\hbar^2}{8ma^2}$$

Note that the equality implied in the text is not allowed. A state with $R=\pi/2$ would lead to an odd state with $\alpha=\pi/2$ and $\beta=0$, yielding $E=V_0$ and $q=0$. However, that would imply a wave function outside the well that was constant ($e^{qx}=1$) and therefore not normalizable. Hence, the state with $E=V_0$ is not a physically allowed state. Thus, the way to interpret the text's question is: What is the energy of the ground state when the well is deep enough to just barely not allow an odd state. Now we use the equality $R=\pi/2$ and the ground state energy is given by the solution to the transcendental equation

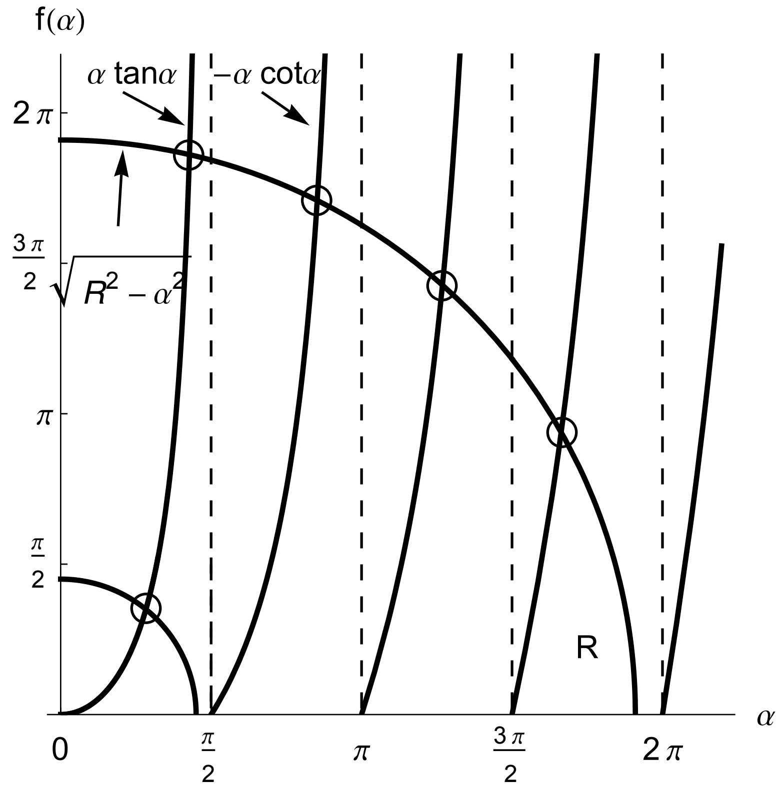
$$\alpha\tan(\alpha)=\sqrt{\frac{\pi^2}{4}-\alpha^2}$$

which yields

$$\alpha=0.934$$

giving an energy

$$E_{gnd\,state}=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2\alpha^2}{2ma^2}=0.872\frac{\hbar^2}{2ma^2}\,.$$


f(α)
α tanα
$-\alpha$ cotα
2 π
$\frac{3\pi}{2}$
$\sqrt{R^2-\alpha^2}$
π
$\frac{\pi}{2}$
R
α
0
$\frac{\pi}{2}$
π
$\frac{3\pi}{2}$
2 π

5.4.2 (a) For a delta function potential, we must reconsider the continuity equation for the derivative of the wave function. Above we found that

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

Start by solving the energy eigenvalue equation:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-aV_0\delta(x)\right)\varphi_E(x)=E\varphi_E(x)$$

Outside of the potential well, $V=0$, and $E>0$ so the solutions are complex exponentials. Assume a solution of form

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

with $k=\sqrt{2mE/\hbar^2}$ and we have assumed that there are particles incident from the left, but not from the right. The boundary condition on the continuity of the wave function at $x=0$ gives

$$A+B=C$$

The boundary condition on the wave function derivative from above gives

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

$$\lim_{\varepsilon\to 0}\left(ikCe^{ik\varepsilon}-ikAe^{-ik\varepsilon}+ikBe^{ik\varepsilon}\right)=-aV_0\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon}\delta(x)\varphi_E(x)dx$$

$$ik(C-A+B)=-aV_0\frac{2m}{\hbar^2}\varphi_E(0)$$

$$ik(C-A+B)=-aV_0\frac{2m}{\hbar^2}C$$

Solve these two equations for the ratios:

$$\frac{C}{A}=\frac{1}{1-i\dfrac{maV_0}{k\hbar^2}}$$

$$\frac{B}{A}=\frac{i\dfrac{maV_0}{k\hbar^2}}{1-i\dfrac{maV_0}{k\hbar^2}}$$

Now take the squares to get the transmission probability:

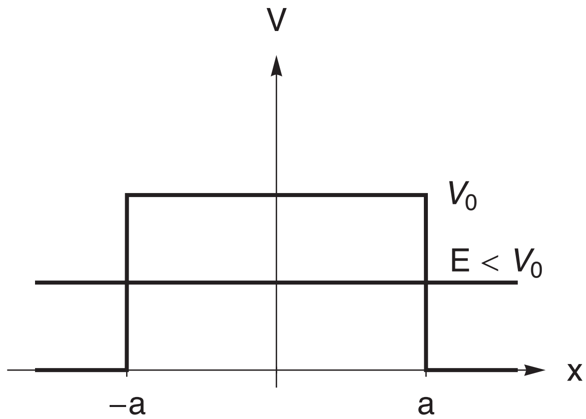
$$T=\frac{|C|^2}{|A|^2}=\frac{1}{1+\left(\dfrac{maV_0}{k\hbar^2}\right)^2}$$

and the reflection probability

$$R = \frac{|B|^2}{|A|^2} = \frac{\left(\frac{maV_0}{k\hbar^2}\right)^2}{1+\left(\frac{maV_0}{k\hbar^2}\right)^2}$$

Note that $T + R = 1$ as required by conservation of particle number or probability.

b)



A square potential energy barrier is shown above. The potential energy is described as

$$V(x) = \begin{cases} 0 & x < -a \\ V_0 & -a \le x \le a \\ 0 & x > a \end{cases}$$

If the energy E of the incident particle beam is less than the well height V_0, then the region $-a \le x \le a$ is classically forbidden. As in the previous well problems, there are separate eigenvalue equations in the different regions:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\varphi_E(x) = E\varphi_E(x); \;\; |x| < a$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 0\right)\varphi_E(x) = E\varphi_E(x); \;\; |x| > a$$

The energy E is less than the potential barrier height V_0, so the interior solutions must be real exponentials and the exterior solutions must be complex exponentials. It is useful to define a wave vector k outside the well and a decay constant q inside the well:

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Use these two constants to rewrite the energy eigenvalue equations as

$$\frac{d^2\varphi_E(x)}{dx^2} = q^2\varphi_E(x);\ |x| < a$$
$$\frac{d^2\varphi_E(x)}{dx^2} = -k^2\varphi_E(x);\ |x| > a$$

The general solutions to these equations are

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

where we have assumed that there are particles incident from the left, but not from the right. It is important that the wave function in the classically forbidden region contains *both* the exponentially decreasing *and* the exponentially growing terms. The growing term cannot vanish as it did in the case where the classically forbidden region extended to infinity. The boundary condition equations for continuity of the wave function and of the derivative of the wave function are

$$\varphi(-a): Ae^{-ika} + Be^{ika} = Ce^{-qa} + De^{qa}$$
$$\left.\frac{d\varphi(x)}{dx}\right|_{x=-a}: ikAe^{-ika} - ikBe^{ika} = qCe^{-qa} - qDe^{qa}$$
$$\varphi(a): Ce^{qa} + De^{-qa} = Fe^{ika}$$
$$\left.\frac{d\varphi(x)}{dx}\right|_{x=a}: qCe^{qa} - qDe^{-qa} = ikFe^{ika}$$

Solve the last two equations for *C* and *D* by addition and subtraction of the equations:

$$\begin{aligned} Ce^{qa} + De^{-qa} &= Fe^{ika} \\ Ce^{qa} - De^{-qa} &= (ik/q)Fe^{ika} \end{aligned} \quad \Rightarrow \quad \begin{aligned} 2Ce^{qa} &= Fe^{ika}(1+ik/q) \\ 2De^{-qa} &= Fe^{ika}(1-ik/q) \end{aligned}$$

Similarly rearrange (add and subtract) the first two equations:

$$2Ae^{-ika} = Ce^{-qa}(1+q/ik) + De^{qa}(1-q/ik)$$
$$2Be^{ika} = Ce^{-qa}(1-q/ik) + De^{qa}(1+q/ik)$$

and substitute from above to eliminate *C* and *D*:

$$4Ae^{-2ika} = Fe^{-2qa}(1+ik/q)(1+q/ik) + Fe^{2qa}(1-ik/q)(1-q/ik)$$
$$4B = Fe^{-2qa}(1+ik/q)(1-q/ik) + Fe^{2qa}(1-ik/q)(1+q/ik)$$

Simplify

$$4Ae^{-i2ka} = F\left[4\cosh 2qa - (ik/q + q/ik)2\sinh 2qa\right]$$
$$4B = F\left[-(ik/q - q/ik)2\sinh 2qa\right]$$

and solve for the ratios *B*/*A* and *F*/*A*

$$\frac{F}{A}=\frac{e^{-i2ka}}{\cosh 2qa+i\dfrac{q^2-k^2}{2kq}\sinh 2qa}$$

$$\frac{B}{A}=\frac{ie^{-i2ka}\dfrac{q^2+k^2}{2kq}\sinh 2qa}{\cosh 2qa+i\dfrac{q^2-k^2}{2kq}\sinh 2qa},$$

Now take the squares to get the transmission probability:

$$T=\frac{|F|^2}{|A|^2}=\frac{1}{\cosh^2(2qa)+\dfrac{(q^2-k^2)^2}{4k^2q^2}\sinh^2(2qa)}$$

$$=\frac{1}{1+\dfrac{(q^2+k^2)^2}{4k^2q^2}\sinh^2(2qa)}=\frac{1}{1+\dfrac{V_0^2}{4E(V_0-E)}\sinh^2(2qa)}$$

and the reflection probability

$$R=\frac{|B|^2}{|A|^2}=\frac{\dfrac{(q^2+k^2)^2}{4k^2q^2}\sinh^2(2qa)}{\cosh^2(2qa)+\dfrac{(q^2-k^2)^2}{4k^2q^2}\sinh^2(2qa)}$$

$$=\frac{\dfrac{(q^2+k^2)^2}{4k^2q^2}\sinh^2(2qa)}{1+\dfrac{(q^2+k^2)^2}{4k^2q^2}\sinh^2(2qa)}=\frac{\dfrac{V_0^2}{4E(V_0-E)}\sinh^2(2qa)}{1+\dfrac{V_0^2}{4E(V_0-E)}\sinh^2(2qa)}$$

Note that $T+R=1$ as required by conservation of particle number or probability.

3. a) The momentum probability density is

$$\mathcal{P}(p)=|\langle p|\psi\rangle|^2=|\psi(p)|^2$$

For a particle in the energy eigenstate $\psi_n(x)$, the momentum wave function is

$$\psi_n(p)=\langle p|n\rangle=\int_{-\infty}^{\infty}\langle p|x\rangle\langle x|n\rangle dx=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}e^{-ipx/\hbar}\psi_n(x)dx$$

Assuming that the state has an even number *n*, the spatial wave function $\psi_n(x)$ is

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

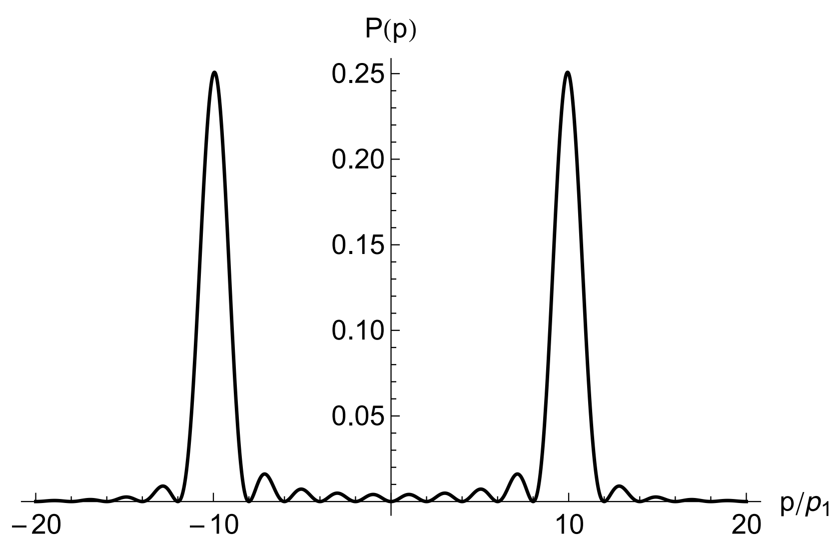
which yields

$$\begin{aligned}
\psi_n(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\psi_n(x)\,dx = \frac{1}{\sqrt{2\pi\hbar}}\int_{-L/2}^{L/2} e^{-ipx/\hbar}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)dx \\
&= \frac{1}{\sqrt{\pi\hbar L}}\int_{-L/2}^{L/2} e^{-ipx/\hbar}\left(\frac{e^{in\pi x/L}-e^{-in\pi x/L}}{2i}\right)dx \\
&= \frac{1}{2i\sqrt{\pi\hbar L}}\int_{-L/2}^{L/2}\left(e^{-i(p/\hbar-n\pi/L)x}-e^{-i(p/\hbar-n\pi/L)x}\right)dx \\
&= \frac{1}{2i\sqrt{\pi\hbar L}}\left[\frac{e^{-i(p/\hbar-n\pi/L)L/2}-e^{-i(p/\hbar-n\pi/L)L/2}}{-i(p/\hbar-n\pi/L)} - \frac{e^{-i(p/\hbar+n\pi/L)L/2}-e^{i(p/\hbar+n\pi/L)L/2}}{-i(p/\hbar+n\pi/L)}\right] \\
&= \frac{1}{i\sqrt{\pi\hbar L}}\left[\frac{\sin(pL/2\hbar-n\pi/2)}{(p-n\pi\hbar/L)/\hbar} - \frac{\sin(pL/2\hbar+n\pi/2)}{(p+n\pi\hbar/L)/\hbar}\right] \\
&= \frac{\hbar(-1)^{n/2}}{i\sqrt{\pi\hbar L}}\left[\frac{\sin(pL/2\hbar)}{(p-p_n)} - \frac{\sin(pL/2\hbar)}{(p+p_n)}\right] \\
&= \frac{\hbar(-1)^{n/2}}{i\sqrt{\pi\hbar L}}\frac{2p_n}{(p^2-p_n^2)}\sin(pL/2\hbar)
\end{aligned}$$

where we have defined $p_n \equiv n\pi\hbar/L$. The momentum probability density is

$$\begin{aligned}
\mathcal{P}_n(p) &= \left|\langle p|n\rangle\right|^2 = \left|\psi_n(p)\right|^2 \\
&= \frac{4\hbar}{\pi L}\frac{p_n^2}{(p^2-p_n^2)^2}\sin^2\left(p\frac{L}{2\hbar}\right) \\
&= \frac{4\pi n^2\hbar^3}{L^3}\frac{1}{(p^2-p_n^2)^2}\sin^2\left(p\frac{L}{2\hbar}\right)
\end{aligned}$$

b) Plot for n = 10:



c) The momentum probability density is peaked at the values $p = \pm p_n$. If we apply the de Broglie equation to the standing waves that we expect in an infinite square well, we find the momentum:

$$p = \frac{h}{\lambda}$$

$$L = n\frac{\lambda}{2} \Rightarrow \lambda_n = \frac{2L}{n} \Rightarrow p_n = \frac{h}{\left(\frac{2L}{n}\right)} = n\frac{h}{2L} = n\frac{\pi\hbar}{L}$$

We get peaks at positive and negative values because the standing wave comprises travelling waves moving in both directions.