Problem 3.34

(a) Find the momentum-space wave function $\Phi_n(p,t)$ for the nth stationary state of the infinite square well.

(b) Find the probability density $|\Phi_n(p,t)|^2$. Graph this function, for $n = 1$, $n = 2$, $n = 5$, and $n = 10$. What are the most probable values of p, for large n? Is this what you would have expected?[40] Compare your answer to Problem 3.10.

(c) Use $\Phi_n(p,t)$ to calculate the expectation value of p^2, in the nth state. Compare your answer to Problem 2.4.

Solution

The position-space wave function of the infinite square well is

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right), \quad 0 \le x \le a,$$

where $n = 1, 2, \ldots$, and zero elsewhere. To find the momentum-space wave function, take the Fourier transform of $\Psi_n(x,t)$.

$$\begin{aligned}
\Phi_n(p,t) &= \mathscr{F}\{\Psi_n(x,t)\} \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi_n(x,t)\, dx \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_0^a e^{-ipx/\hbar} \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) dx \\
&= \frac{1}{\sqrt{\pi\hbar a}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) \int_0^a e^{-ipx/\hbar} \sin\frac{n\pi x}{a}\, dx \\
&= \frac{1}{\sqrt{\pi\hbar a}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) \int_0^a e^{-ipx/\hbar} \left(\frac{e^{in\pi x/a} - e^{-in\pi x/a}}{2i}\right) dx \\
&= \frac{1}{2i\sqrt{\pi\hbar a}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) \int_0^a \left\{\exp\left[i\left(-\frac{p}{\hbar} + \frac{n\pi}{a}\right)x\right] - \exp\left[-i\left(\frac{p}{\hbar} + \frac{n\pi}{a}\right)x\right]\right\} dx \\
&= \frac{1}{2i\sqrt{\pi\hbar a}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) \int_0^a \left[\exp\left(i\frac{n\pi\hbar - pa}{\hbar a}x\right) - \exp\left(-i\frac{n\pi\hbar + pa}{\hbar a}x\right)\right] dx \\
&= \frac{1}{2i\sqrt{\pi\hbar a}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right) \left[\int_0^a \exp\left(i\frac{n\pi\hbar - pa}{\hbar a}x\right) dx - \int_0^a \exp\left(-i\frac{n\pi\hbar + pa}{\hbar a}x\right) dx\right]
\end{aligned}$$

[40] See F. L. Markley, *Am. J. Phys.* **40**, 1545 (1972).

Evaluate the integrals and simplify the formula.

$$\begin{aligned}
\Phi_n(p,t) &= \frac{1}{2i\sqrt{\pi\hbar a}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left[\frac{\hbar a}{i(n\pi\hbar - pa)}\exp\left(i\frac{n\pi\hbar - pa}{\hbar a}x\right)\bigg|_0^a - \frac{\hbar a}{-i(n\pi\hbar + pa)}\exp\left(-i\frac{n\pi\hbar + pa}{\hbar a}x\right)\bigg|_0^a\right] \\
&= \frac{1}{2i^2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left\{\frac{1}{n\pi\hbar - pa}\left[\exp\left(i\frac{n\pi\hbar - pa}{\hbar}\right) - 1\right] + \frac{1}{n\pi\hbar + pa}\left[\exp\left(-i\frac{n\pi\hbar + pa}{\hbar}\right) - 1\right]\right\} \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left[\frac{\exp\left(i\frac{n\pi\hbar - pa}{\hbar}\right)}{n\pi\hbar - pa} - \frac{1}{n\pi\hbar - pa} + \frac{\exp\left(-i\frac{n\pi\hbar + pa}{\hbar}\right)}{n\pi\hbar + pa} - \frac{1}{n\pi\hbar + pa}\right] \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left[\frac{\exp\left(i\frac{n\pi\hbar - pa}{\hbar}\right)(n\pi\hbar + pa) - (n\pi\hbar + pa) + \exp\left(-i\frac{n\pi\hbar + pa}{\hbar}\right)(n\pi\hbar - pa) - (n\pi\hbar - pa)}{(n\pi\hbar - pa)(n\pi\hbar + pa)}\right] \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left\{\frac{n\pi\hbar\left[\exp\left(i\frac{n\pi\hbar - pa}{\hbar}\right) + \exp\left(-i\frac{n\pi\hbar + pa}{\hbar}\right)\right] + pa\left[\exp\left(i\frac{n\pi\hbar - pa}{\hbar}\right) - \exp\left(-i\frac{n\pi\hbar + pa}{\hbar}\right)\right] - 2n\pi\hbar}{n^2\pi^2\hbar^2 - p^2a^2}\right\} \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left[\frac{n\pi\hbar e^{-ipa/\hbar}\left(e^{in\pi} + e^{-in\pi}\right) + pae^{-ipa/\hbar}\left(e^{in\pi} - e^{-in\pi}\right) - 2n\pi\hbar}{n^2\pi^2\hbar^2 - p^2a^2}\right] \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left[\frac{n\pi\hbar e^{-ipa/\hbar}(2\cos n\pi) + pae^{-ipa/\hbar}(2i\sin n\pi) - 2n\pi\hbar}{n^2\pi^2\hbar^2 - p^2a^2}\right] \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left\{\frac{n\pi\hbar e^{-ipa/\hbar}[2(-1)^n] + pae^{-ipa/\hbar}[2i(0)] - 2n\pi\hbar}{n^2\pi^2\hbar^2 - p^2a^2}\right\} \\
&= -\frac{1}{2}\sqrt{\frac{\hbar a}{\pi}} \exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\left\{\frac{2n\pi\hbar\left[e^{-ipa/\hbar}(-1)^n - 1\right]}{n^2\pi^2\hbar^2 - p^2a^2}\right\} \\
&= -\sqrt{\pi\hbar^3 a}\exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\frac{ne^{-ipa/(2\hbar)}[e^{ipa/(2\hbar)} - (-1)^n e^{-ipa/(2\hbar)}]}{p^2a^2 - n^2\pi^2\hbar^2}
\end{aligned}$$

Simplify the formula even further by considering the cases where n is odd and even separately.

$$\Phi_n(p,t) = \begin{cases} -\sqrt{\pi\hbar^3 a}\exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\frac{ne^{-ipa/(2\hbar)}[e^{ipa/(2\hbar)} + e^{-ipa/(2\hbar)}]}{p^2a^2 - n^2\pi^2\hbar^2} & \text{if } n = 2k-1 \\ -\sqrt{\pi\hbar^3 a}\exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\frac{ne^{-ipa/(2\hbar)}[e^{ipa/(2\hbar)} - e^{-ipa/(2\hbar)}]}{p^2a^2 - n^2\pi^2\hbar^2} & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} -\sqrt{\pi\hbar^3 a}\exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\frac{ne^{-ipa/(2\hbar)}\left(2\cos\frac{pa}{2\hbar}\right)}{p^2a^2 - n^2\pi^2\hbar^2} & \text{if } n = 2k-1 \\ -\sqrt{\pi\hbar^3 a}\exp\left(-i\frac{n^2\pi^2\hbar}{2ma^2}t\right)\frac{ne^{-ipa/(2\hbar)}\left(2i\sin\frac{pa}{2\hbar}\right)}{p^2a^2 - n^2\pi^2\hbar^2} & \text{if } n = 2k \end{cases}$$

Now calculate $|\Phi_n(p,t)|^2$, the probability distribution for the particle's momentum in the nth stationary state of the infinite square well.

$$\begin{aligned} |\Phi_n(p,t)|^2 &= \Phi_n^*(p,t)\Phi_n(p,t) \\ &= \begin{cases} \pi\hbar^3 a\frac{4n^2\cos^2\frac{pa}{2\hbar}}{(p^2a^2 - n^2\pi^2\hbar^2)^2} & \text{if } n = 2k-1 \\ \pi\hbar^3 a\frac{4n^2\sin^2\frac{pa}{2\hbar}}{(p^2a^2 - n^2\pi^2\hbar^2)^2} & \text{if } n = 2k \end{cases} \\ &= \begin{cases} \frac{\pi a}{\hbar}\frac{4n^2\cos^2\frac{pa}{2\hbar}}{\left[\left(\frac{pa}{\hbar}\right)^2 - n^2\pi^2\right]^2} & \text{if } n = 2k-1 \\ \frac{\pi a}{\hbar}\frac{4n^2\sin^2\frac{pa}{2\hbar}}{\left[\left(\frac{pa}{\hbar}\right)^2 - n^2\pi^2\right]^2} & \text{if } n = 2k \end{cases} \end{aligned}$$

Check that it's normalized.

$$\int_{-\infty}^{\infty}|\Phi_n(p,t)|^2\,dp = \begin{cases} \frac{4\pi a n^2}{\hbar}\int_{-\infty}^{\infty}\frac{\cos^2\frac{pa}{2\hbar}}{\left[\left(\frac{pa}{\hbar}\right)^2 - n^2\pi^2\right]^2}\,dp & \text{if } n = 2k-1 \\ \frac{4\pi a n^2}{\hbar}\int_{-\infty}^{\infty}\frac{\sin^2\frac{pa}{2\hbar}}{\left[\left(\frac{pa}{\hbar}\right)^2 - n^2\pi^2\right]^2}\,dp & \text{if } n = 2k \end{cases}$$

Make the following substitution.

$$\frac{pa}{\hbar} = n\pi u \qquad \rightarrow \qquad \frac{pa}{2\hbar} = \frac{n\pi u}{2}$$

$$dp = \frac{n\pi\hbar}{a}\,du$$

Consequently, using partial fraction decomposition,

$$\int_{-\infty}^{\infty} |\Phi_n(p,t)|^2\,dp = \begin{cases} \dfrac{4\pi a n^2}{\hbar} \displaystyle\int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi u}{2}}{(n^2\pi^2 u^2 - n^2\pi^2)^2} \left(\frac{n\pi\hbar}{a}\,du\right) & \text{if } n = 2k-1 \\[2ex] \dfrac{4\pi a n^2}{\hbar} \displaystyle\int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi u}{2}}{(n^2\pi^2 u^2 - n^2\pi^2)^2} \left(\frac{n\pi\hbar}{a}\,du\right) & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{4}{\pi^2 n} \displaystyle\int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi u}{2}}{(u^2-1)^2}\,du & \text{if } n = 2k-1 \\[2ex] \dfrac{4}{\pi^2 n} \displaystyle\int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi u}{2}}{(u^2-1)^2}\,du & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{4}{\pi^2 n} \displaystyle\int_{-\infty}^{\infty} \left[\frac{1}{4(u+1)} + \frac{1}{4(u+1)^2} - \frac{1}{4(u-1)} + \frac{1}{4(u-1)^2}\right] \cos^2 \frac{n\pi u}{2}\,du & \text{if } n = 2k-1 \\[2ex] \dfrac{4}{\pi^2 n} \displaystyle\int_{-\infty}^{\infty} \left[\frac{1}{4(u+1)} + \frac{1}{4(u+1)^2} - \frac{1}{4(u-1)} + \frac{1}{4(u-1)^2}\right] \sin^2 \frac{n\pi u}{2}\,du & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{1}{\pi^2 n} \left[\displaystyle\int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi u}{2}}{u+1}\,du + \int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi u}{2}}{(u+1)^2}\,du - \int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi u}{2}}{u-1}\,du + \int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi u}{2}}{(u-1)^2}\,du\right] & \text{if } n = 2k-1 \\[2ex] \dfrac{1}{\pi^2 n} \left[\displaystyle\int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi u}{2}}{u+1}\,du + \int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi u}{2}}{(u+1)^2}\,du - \int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi u}{2}}{u-1}\,du + \int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi u}{2}}{(u-1)^2}\,du\right] & \text{if } n = 2k \end{cases}.$$

Make the substitutions, $v = u + 1$ and $w = u - 1$.

$$\int_{-\infty}^{\infty} |\Phi_n(p,t)|^2\,dp = \begin{cases} \frac{1}{\pi^2 n}\left[\int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi(v-1)}{2}}{v}\,dv + \int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi(v-1)}{2}}{v^2}\,dv - \int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi(w+1)}{2}}{w}\,dw + \int_{-\infty}^{\infty} \frac{\cos^2 \frac{n\pi(w+1)}{2}}{w^2}\,dw\right] & \text{if } n = 2k-1 \\ \frac{1}{\pi^2 n}\left[\int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi(v-1)}{2}}{v}\,dv + \int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi(v-1)}{2}}{v^2}\,dv - \int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi(w+1)}{2}}{w}\,dw + \int_{-\infty}^{\infty} \frac{\sin^2 \frac{n\pi(w+1)}{2}}{w^2}\,dw\right] & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \frac{1}{\pi^2(2k-1)}\left[\int_{-\infty}^{\infty} \frac{\cos^2\left(k\pi v - \frac{\pi v}{2} - k\pi + \frac{\pi}{2}\right)}{v}\,dv + \int_{-\infty}^{\infty} \frac{\cos^2\left(k\pi v - \frac{\pi v}{2} - k\pi + \frac{\pi}{2}\right)}{v^2}\,dv \right. \\ \qquad \left. - \int_{-\infty}^{\infty} \frac{\cos^2\left(k\pi w - \frac{\pi w}{2} + k\pi - \frac{\pi}{2}\right)}{w}\,dw + \int_{-\infty}^{\infty} \frac{\cos^2\left(k\pi w - \frac{\pi w}{2} + k\pi - \frac{\pi}{2}\right)}{w^2}\,dw\right] & \text{if } n = 2k-1 \\ \frac{1}{\pi^2(2k)}\left[\int_{-\infty}^{\infty} \frac{\sin^2(k\pi v - k\pi)}{v}\,dv + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi v - k\pi)}{v^2}\,dv - \int_{-\infty}^{\infty} \frac{\sin^2(k\pi w + k\pi)}{w}\,dw + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi w + k\pi)}{w^2}\,dw\right] & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \frac{1}{\pi^2(2k-1)}\left[\int_{-\infty}^{\infty} \frac{\left[-\sin\left(k\pi v - \frac{\pi v}{2} - k\pi\right)\right]^2}{v}\,dv + \int_{-\infty}^{\infty} \frac{\left[-\sin\left(k\pi v - \frac{\pi v}{2} - k\pi\right)\right]^2}{v^2}\,dv \right. \\ \qquad \left. - \int_{-\infty}^{\infty} \frac{\left[\sin\left(k\pi w - \frac{\pi w}{2} + k\pi\right)\right]^2}{w}\,dw + \int_{-\infty}^{\infty} \frac{\left[\sin\left(k\pi w - \frac{\pi w}{2} + k\pi\right)\right]^2}{w^2}\,dw\right] & \text{if } n = 2k-1 \\ \frac{1}{\pi^2(2k)}\left[\int_{-\infty}^{\infty} \frac{\sin^2(k\pi v - k\pi)}{v}\,dv + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi v - k\pi)}{v^2}\,dv - \int_{-\infty}^{\infty} \frac{\sin^2(k\pi w + k\pi)}{w}\,dw + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi w + k\pi)}{w^2}\,dw\right] & \text{if } n = 2k \end{cases}$$

Continue the simplification.

$$\int_{-\infty}^{\infty} |\Phi_n(p,t)|^2\,dp = \begin{cases} \dfrac{1}{\pi^2(2k-1)}\left[\displaystyle\int_{-\infty}^{\infty} \frac{\left[-(-1)^k \sin\left(k\pi v - \frac{\pi v}{2}\right)\right]^2}{v}\,dv + \int_{-\infty}^{\infty} \frac{\left[-(-1)^k \sin\left(k\pi v - \frac{\pi v}{2}\right)\right]^2}{v^2}\,dv \right. \\ \qquad \left. - \displaystyle\int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin\left(k\pi w - \frac{\pi w}{2}\right)\right]^2}{w}\,dw + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin\left(k\pi w - \frac{\pi w}{2}\right)\right]^2}{w^2}\,dw \right] & \text{if } n = 2k-1 \\ \dfrac{1}{\pi^2(2k)}\left[\displaystyle\int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi v\right]^2}{v}\,dv + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi v\right]^2}{v^2}\,dv \right. \\ \qquad \left. - \displaystyle\int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi w\right]^2}{w}\,dw + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi w\right]^2}{w^2}\,dw \right] & \text{if } n = 2k \end{cases}$$

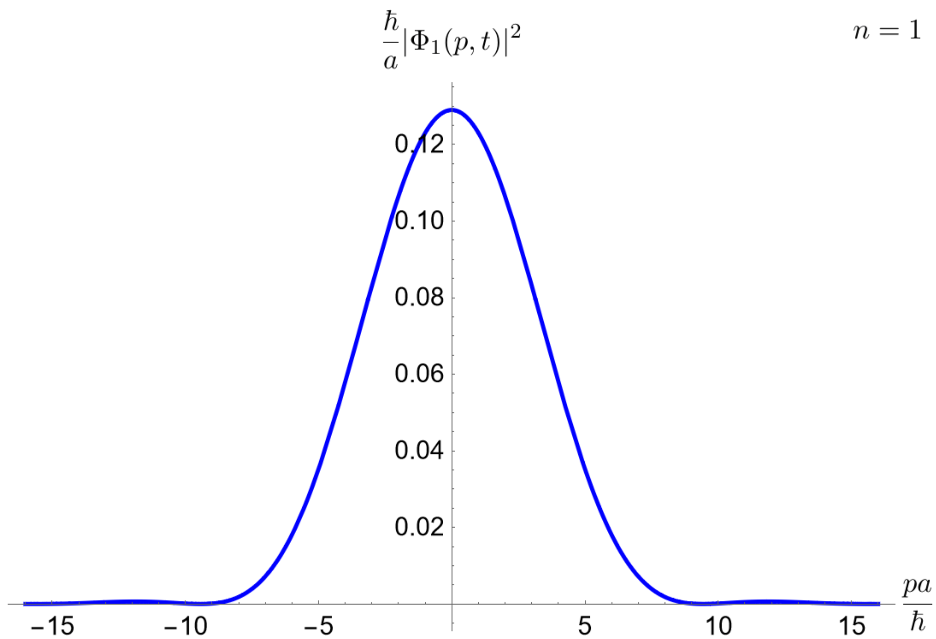
$$= \begin{cases} \dfrac{1}{\pi^2(2k-1)}\left[\cancel{\displaystyle\int_{-\infty}^{\infty} \frac{\sin^2\left(k\pi v - \frac{\pi v}{2}\right)}{v}\,dv} + \int_{-\infty}^{\infty} \frac{\sin^2\left(k\pi v - \frac{\pi v}{2}\right)}{v^2}\,dv \right. \\ \qquad \left. \cancel{- \displaystyle\int_{-\infty}^{\infty} \frac{\sin^2\left(k\pi w - \frac{\pi w}{2}\right)}{w}\,dw} + \int_{-\infty}^{\infty} \frac{\sin^2\left(k\pi w - \frac{\pi w}{2}\right)}{w^2}\,dw \right] & \text{if } n = 2k-1 \\ \dfrac{1}{\pi^2(2k)}\left(\cancel{\displaystyle\int_{-\infty}^{\infty} \frac{\sin^2 k\pi v}{v}\,dv} + \int_{-\infty}^{\infty} \frac{\sin^2 k\pi v}{v^2}\,dv - \cancel{\int_{-\infty}^{\infty} \frac{\sin^2 k\pi w}{w}\,dw} + \int_{-\infty}^{\infty} \frac{\sin^2 k\pi w}{w^2}\,dw \right) & \text{if } n = 2k \end{cases}$$

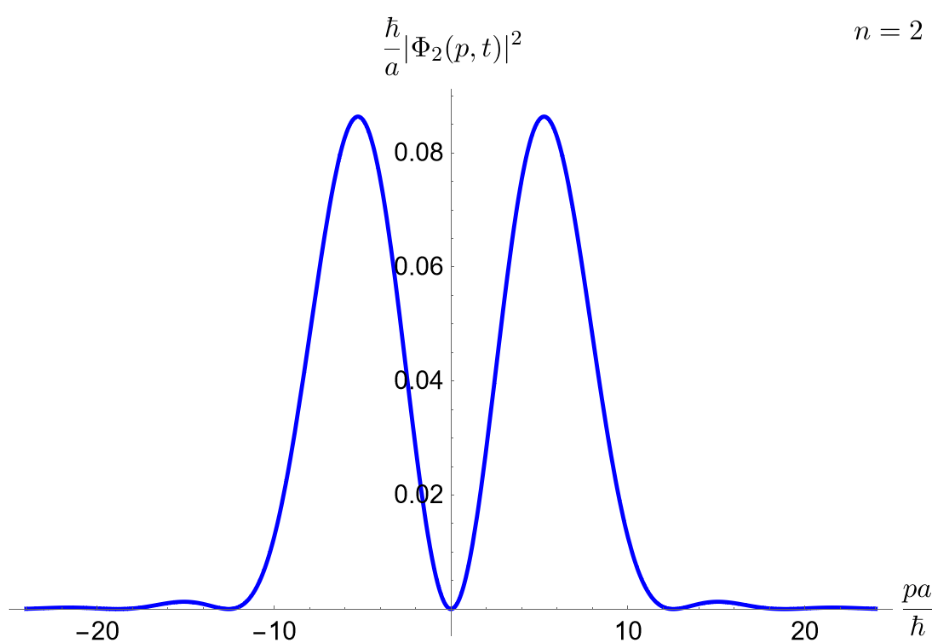
$$= \begin{cases} \dfrac{2}{\pi^2(2k-1)} \displaystyle\int_{-\infty}^{\infty} \frac{\sin^2\left(k - \frac{1}{2}\right)\pi w}{w^2}\,dw & \text{if } n = 2k-1 \\ \dfrac{2}{\pi^2(2k)} \displaystyle\int_{-\infty}^{\infty} \frac{\sin^2 k\pi w}{w^2}\,dw & \text{if } n = 2k \end{cases}$$

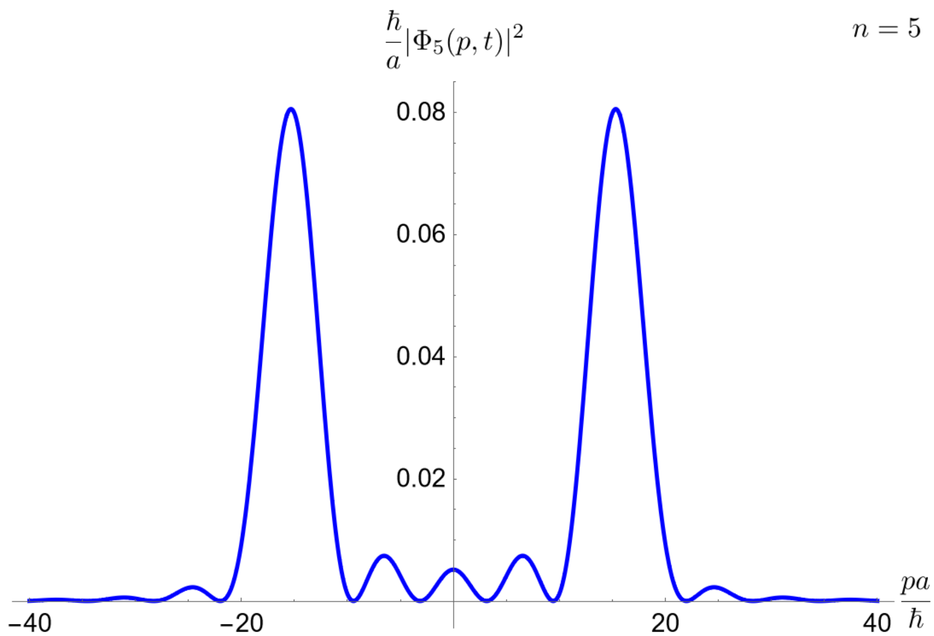
Evaluate the integrals and finally confirm that the momentum-space wave function is normalized.

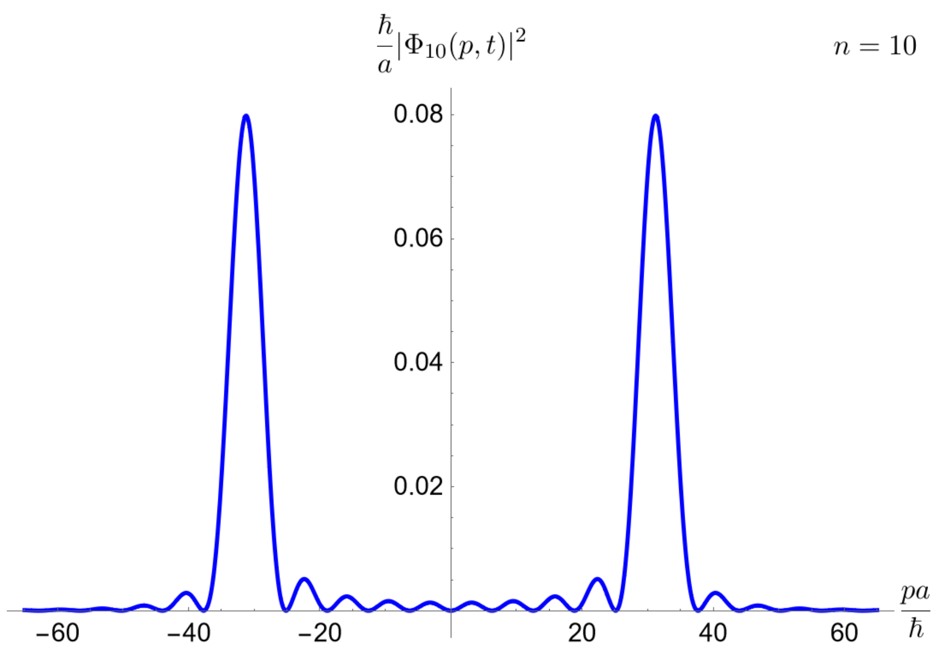
$$\int_{-\infty}^{\infty} |\Phi_n(p,t)|^2\, dp = \begin{cases} \dfrac{2}{\pi^2(2k-1)}\left[\left(k-\dfrac{1}{2}\right)\pi^2\right] & \text{if } n = 2k-1 \\ \\ \dfrac{2}{\pi^2(2k)}(k\pi^2) & \text{if } n = 2k \end{cases} = 1$$

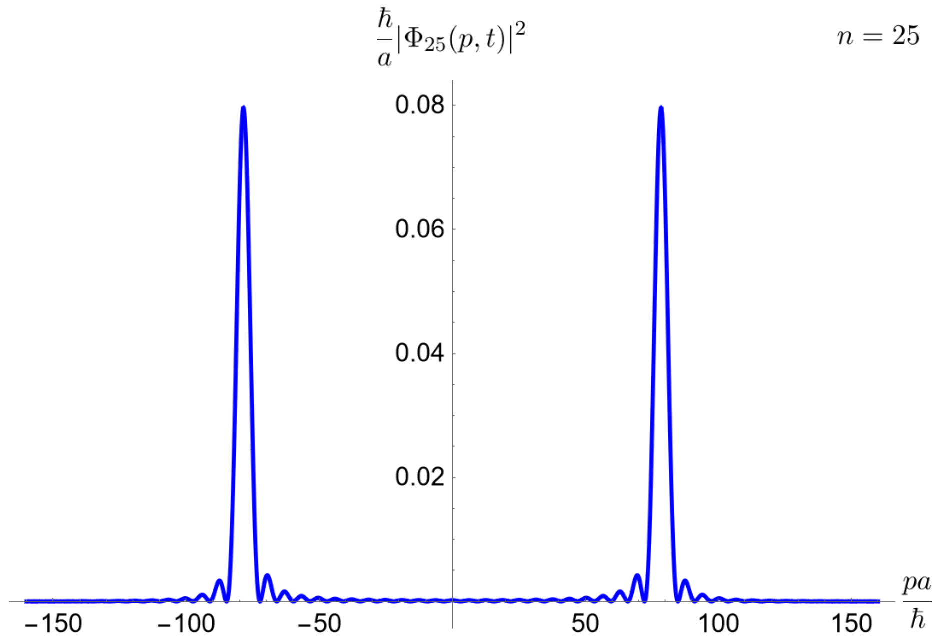
Below are plots of $(\hbar/a)|\Phi_n(p,t)|^2$ versus $pa/\hbar$ for various values of n.

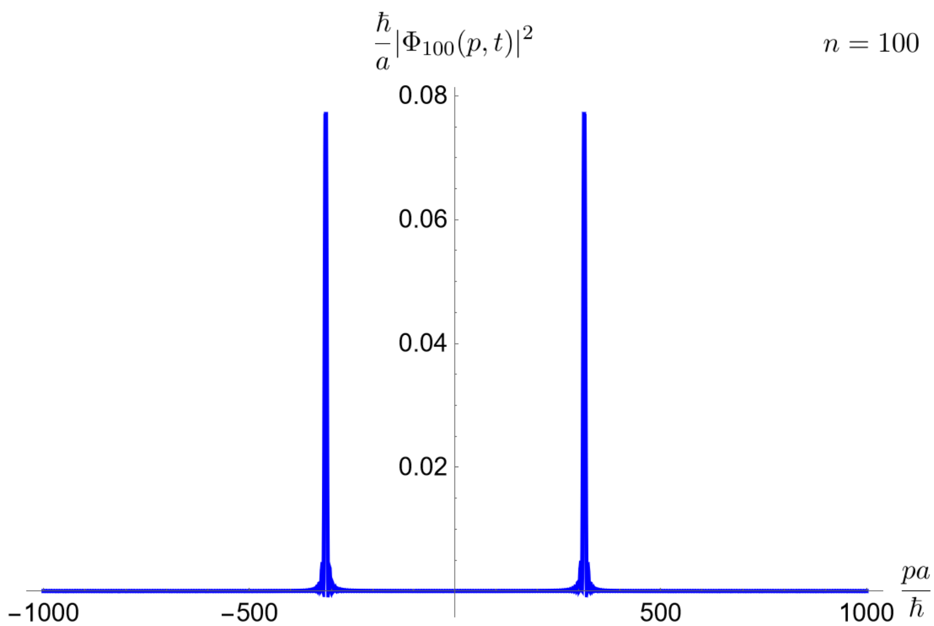





$\frac{\hbar}{a}|\Phi_5(p,t)|^2$
$n = 5$
0.08
0.06
0.04
0.02
−40
−20
20
40
$\frac{pa}{\hbar}$


$\frac{\hbar}{a}|\Phi_{10}(p,t)|^2$
$n = 10$
0.08
0.06
0.04
0.02
−60
−40
−20
20
40
60
$\frac{pa}{\hbar}$





The most probable values of p occur where the absolute maxima are in these graphs. Differentiate $|\Phi(p,t)|^2$ with respect to p and set it equal to zero.

$$\frac{\partial}{\partial p}|\Phi(p,t)|^2 = \begin{cases} \dfrac{2a^2n^2\pi\hbar^2\left[-(p^2a^2 - n^2\pi^2\hbar^2)\sin\frac{pa}{\hbar} - 4pa\hbar\left(1+\cos\frac{pa}{\hbar}\right)\right]}{(p^2a^2 - n^2\pi^2\hbar^2)^3} & \text{if } n = 2k-1 \\ \\ \dfrac{2a^2n^2\pi\hbar^2\left[(p^2a^2 - n^2\pi^2\hbar^2)\sin\frac{pa}{\hbar} - 4pa\hbar\left(1-\cos\frac{pa}{\hbar}\right)\right]}{(p^2a^2 - n^2\pi^2\hbar^2)^3} & \text{if } n = 2k \end{cases} = 0$$

The derivative vanishes when the quantities in square brackets do.

$$\begin{cases} -(p^2a^2 - n^2\pi^2\hbar^2)\sin\dfrac{pa}{\hbar} - 4pa\hbar\left(1+\cos\dfrac{pa}{\hbar}\right) = 0 & \text{if } n = 2k-1 \\ \\ (p^2a^2 - n^2\pi^2\hbar^2)\sin\dfrac{pa}{\hbar} - 4pa\hbar\left(1-\cos\dfrac{pa}{\hbar}\right) = 0 & \text{if } n = 2k \end{cases}$$

Divide both sides of each equation by $\hbar^2$.

$$\begin{cases} -\left(\dfrac{p^2a^2}{\hbar^2} - n^2\pi^2\right)\sin\dfrac{pa}{\hbar} - \dfrac{4pa}{\hbar}\left(1+\cos\dfrac{pa}{\hbar}\right) = 0 & \text{if } n = 2k-1 \\ \\ \left(\dfrac{p^2a^2}{\hbar^2} - n^2\pi^2\right)\sin\dfrac{pa}{\hbar} - \dfrac{4pa}{\hbar}\left(1-\cos\dfrac{pa}{\hbar}\right) = 0 & \text{if } n = 2k \end{cases}$$

Set $z = pa/\hbar$.

$$\begin{cases} -(z^2 - n^2\pi^2)\sin z - 4z(1+\cos z) = 0 & \text{if } n = 2k-1 \\ \\ (z^2 - n^2\pi^2)\sin z - 4z(1-\cos z) = 0 & \text{if } n = 2k \end{cases}$$

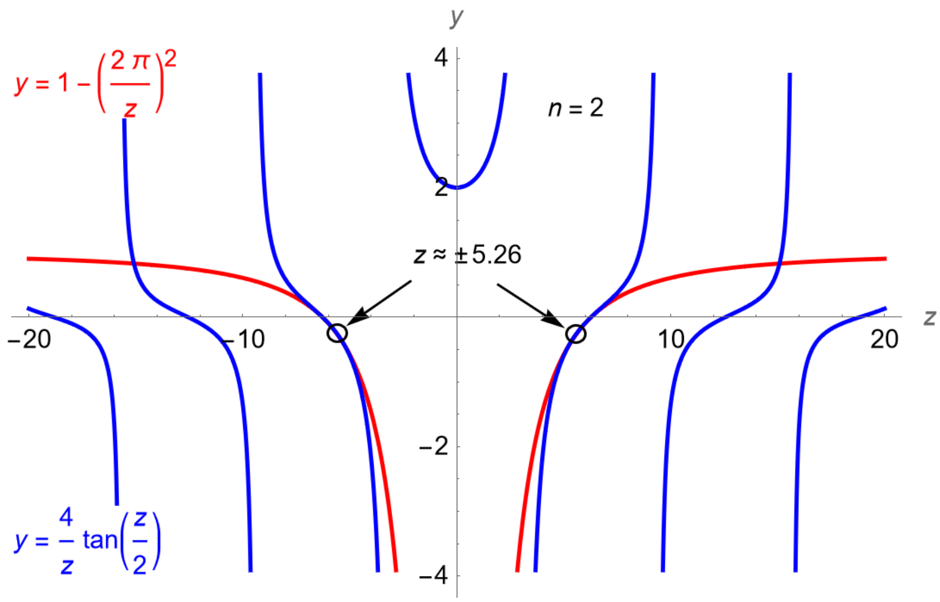
Rearrange the terms, assuming $z \neq n\pi$.

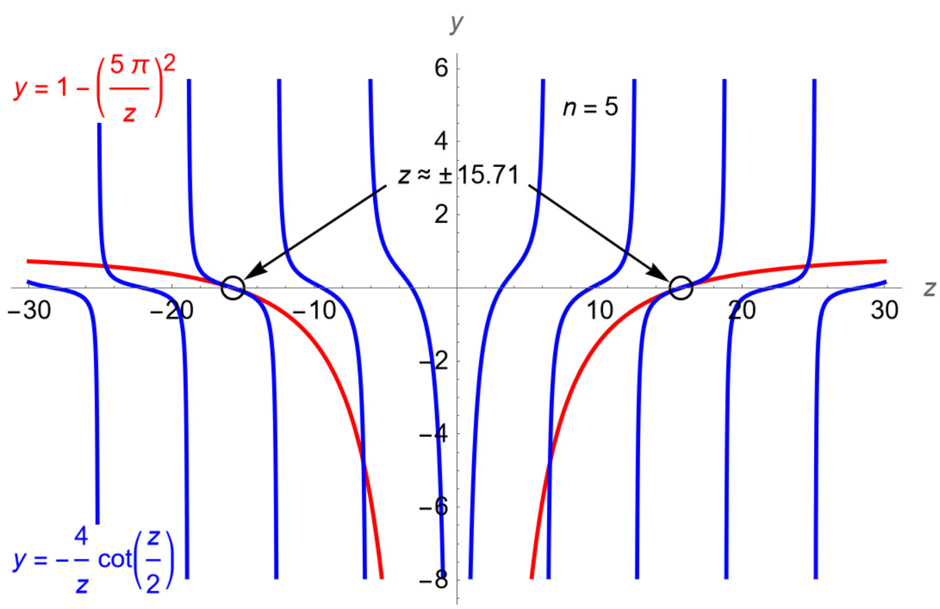
$$\begin{cases} z^2 - n^2\pi^2 = -4z\left(\dfrac{1+\cos z}{\sin z}\right) & \text{if } n = 2k-1 \\ \\ z^2 - n^2\pi^2 = 4z\left(\dfrac{1-\cos z}{\sin z}\right) & \text{if } n = 2k \end{cases}$$

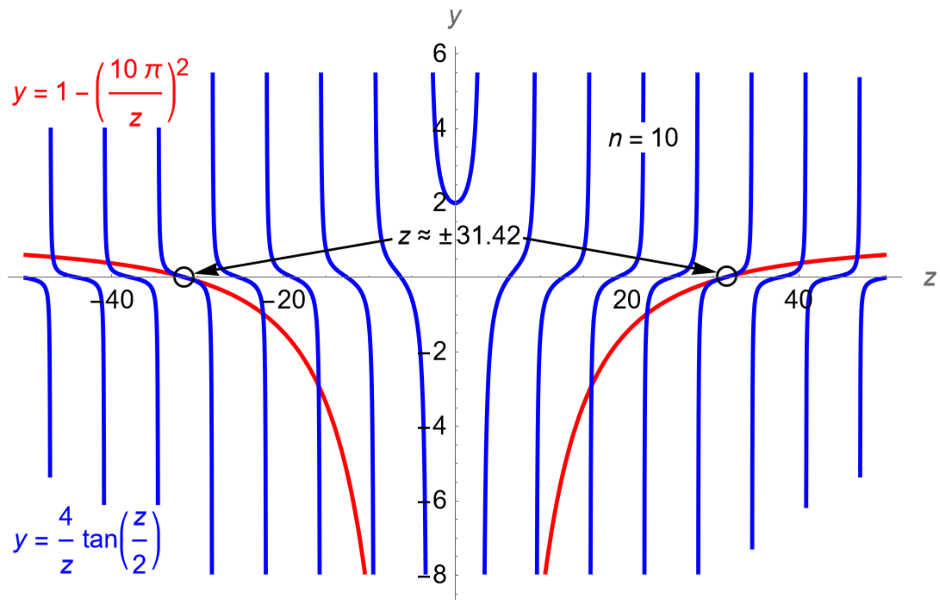
Divide both sides by z^2 and substitute the appropriate half-angle formulas.

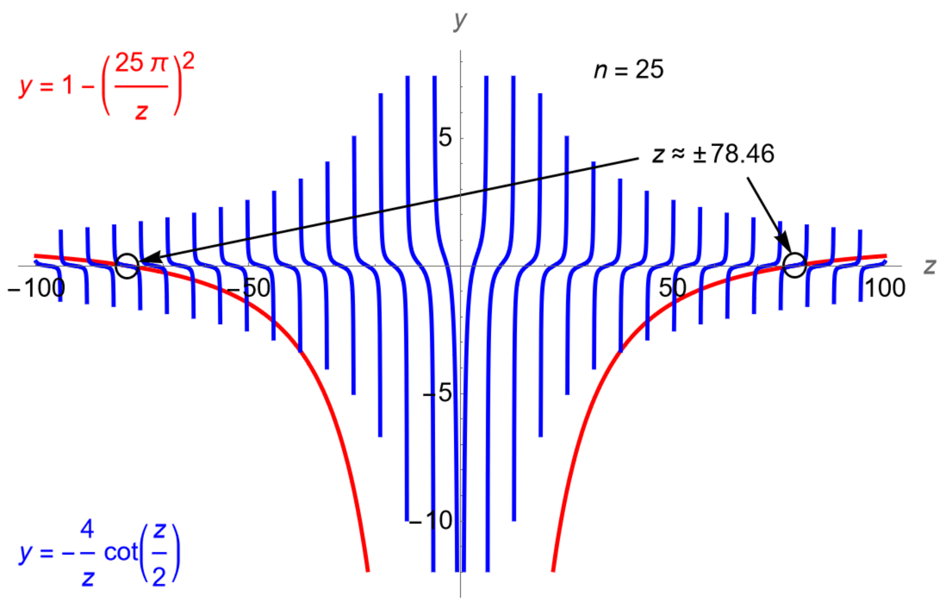
$$\begin{cases} 1 - \left(\dfrac{n\pi}{z}\right)^2 = -\dfrac{4}{z}\cot\dfrac{z}{2} & \text{if } n = 2k-1 \\ \\ 1 - \left(\dfrac{n\pi}{z}\right)^2 = \dfrac{4}{z}\tan\dfrac{z}{2} & \text{if } n = 2k \end{cases}$$

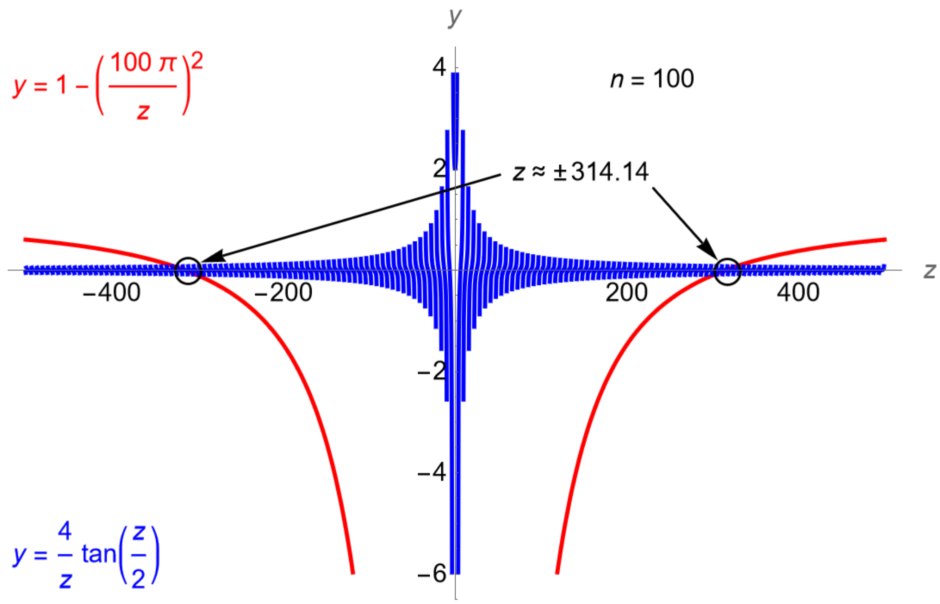
Graph the functions on both sides versus z for the values of n used previously and label the intersections where the absolute maxima are. For $n = 1$, the absolute maximum is at $z = 0$.


y
4
2
−2
−4
z
−20
−10
10
20
y = 1 − (2π/z)²
y = (4/z) tan(z/2)
n = 2
z ≈ ±5.26


y
6
4
2
−2
−4
−6
−8
z
−30
−20
−10
10
20
30
y = 1 − (5π/z)²
y = −(4/z) cot(z/2)
n = 5
z ≈ ±15.71


y
$y = 1 - \left(\frac{10\pi}{z}\right)^2$
n = 10
z ≈ ±31.42
$y = \frac{4}{z}\tan\left(\frac{z}{2}\right)$
z


y
$y = 1 - \left(\frac{25\pi}{z}\right)^2$
n = 25
z ≈ ±78.46
$y = -\frac{4}{z}\cot\left(\frac{z}{2}\right)$
z



Observe that the intersections where the absolute maxima are occur roughly on the z-axis when $n \geq 5$.

$$\begin{cases} 1 - \left(\frac{n\pi}{z}\right)^2 = -\frac{4}{z}\cot\frac{z}{2} \approx 0 & \text{if } n = 2k-1 \\ \\ 1 - \left(\frac{n\pi}{z}\right)^2 = \frac{4}{z}\tan\frac{z}{2} \approx 0 & \text{if } n = 2k \end{cases}$$

Solving for z yields $z \approx \pm n\pi$. Therefore, the most probable values of p for large n are

$$\frac{pa}{\hbar} \approx \pm n\pi \quad \rightarrow \quad p \approx \pm\frac{n\pi\hbar}{a}.$$

The Hamiltonian for a particle in the infinite square well is equal to the total mechanical energy.

$$H = T + V = \frac{p^2}{2m} + 0 = \frac{p^2}{2m} = E$$

Solve for p.

$$p = \pm\sqrt{2mE}$$

Plug in the formula for the energy of the nth stationary state.

$$p = \pm\sqrt{2m\left(\frac{n^2\pi^2\hbar^2}{2ma^2}\right)} = \pm\sqrt{\frac{n^2\pi^2\hbar^2}{a^2}} = \pm\frac{n\pi\hbar}{a}$$

In the limit as $n \rightarrow \infty$, then, the particle has the momenta predicted by classical mechanics.

The aim now is to calculate the expectation value of p^2 of the nth stationary state at time t using the momentum-space wave function.

$$\begin{aligned}
\langle p^2 \rangle &= \langle \Phi \,|\, \hat{p}^2 \,|\, \Phi \rangle \\
&= \int_{-\infty}^{\infty} \Phi_n^*(p,t) p^2 \Phi_n(p,t)\, dp \\
&= \int_{-\infty}^{\infty} p^2 |\Phi_n(p,t)|^2 \, dp \\
&= \begin{cases} \dfrac{4\pi a n^2}{\hbar} \displaystyle\int_{-\infty}^{\infty} \frac{p^2 \cos^2 \frac{pa}{2\hbar}}{\left[\left(\frac{pa}{\hbar}\right)^2 - n^2\pi^2\right]^2}\, dp & \text{if } n = 2k-1 \\ \dfrac{4\pi a n^2}{\hbar} \displaystyle\int_{-\infty}^{\infty} \frac{p^2 \sin^2 \frac{pa}{2\hbar}}{\left[\left(\frac{pa}{\hbar}\right)^2 - n^2\pi^2\right]^2}\, dp & \text{if } n = 2k \end{cases}
\end{aligned}$$

Make the following substitution.

$$\frac{pa}{\hbar} = n\pi u \qquad \rightarrow \qquad \frac{pa}{2\hbar} = \frac{n\pi u}{2} \qquad \rightarrow \qquad p = \frac{n\pi\hbar}{a} u$$

$$dp = \frac{n\pi\hbar}{a}\, du$$

Consequently, using partial fraction decomposition,

$$\langle p^2 \rangle = \begin{cases} \dfrac{4\pi a n^2}{\hbar} \displaystyle\int_{-\infty}^{\infty} \frac{\left(\frac{n\pi\hbar}{a} u\right)^2 \cos^2 \frac{n\pi u}{2}}{(n^2\pi^2 u^2 - n^2\pi^2)^2} \left(\frac{n\pi\hbar}{a}\, du\right) & \text{if } n = 2k-1 \\ \dfrac{4\pi a n^2}{\hbar} \displaystyle\int_{-\infty}^{\infty} \frac{\left(\frac{n\pi\hbar}{a} u\right)^2 \sin^2 \frac{n\pi u}{2}}{(n^2\pi^2 u^2 - n^2\pi^2)^2} \left(\frac{n\pi\hbar}{a}\, du\right) & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{4n\hbar^2}{a^2} \displaystyle\int_{-\infty}^{\infty} \frac{u^2 \cos^2 \frac{n\pi u}{2}}{(u^2-1)^2}\, du & \text{if } n = 2k-1 \\ \dfrac{4n\hbar^2}{a^2} \displaystyle\int_{-\infty}^{\infty} \frac{u^2 \sin^2 \frac{n\pi u}{2}}{(u^2-1)^2}\, du & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{4n\hbar^2}{a^2} \displaystyle\int_{-\infty}^{\infty} \left[-\frac{1}{4(u+1)} + \frac{1}{4(u+1)^2} + \frac{1}{4(u-1)} + \frac{1}{4(u-1)^2}\right] \cos^2 \frac{n\pi u}{2}\, du & \text{if } n = 2k-1 \\ \dfrac{4n\hbar^2}{a^2} \displaystyle\int_{-\infty}^{\infty} \left[-\frac{1}{4(u+1)} + \frac{1}{4(u+1)^2} + \frac{1}{4(u-1)} + \frac{1}{4(u-1)^2}\right] \sin^2 \frac{n\pi u}{2}\, du & \text{if } n = 2k \end{cases}.$$

Split up the integrals and then make the substitutions, $v = u + 1$ and $w = u - 1$.

$$\langle p^2\rangle = \begin{cases} \dfrac{n\hbar^2}{a^2}\left[-\displaystyle\int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi u}{2}}{u+1}\,du + \int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi u}{2}}{(u+1)^2}\,du + \int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi u}{2}}{u-1}\,du + \int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi u}{2}}{(u-1)^2}\,du\right] & \text{if } n = 2k-1 \\[2ex] \dfrac{n\hbar^2}{a^2}\left[-\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi u}{2}}{u+1}\,du + \int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi u}{2}}{(u+1)^2}\,du + \int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi u}{2}}{u-1}\,du + \int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi u}{2}}{(u-1)^2}\,du\right] & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{n\hbar^2}{a^2}\left[-\displaystyle\int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi(v-1)}{2}}{v}\,dv + \int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi(v-1)}{2}}{v^2}\,dv + \int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi(w+1)}{2}}{w}\,dw + \int_{-\infty}^{\infty}\frac{\cos^2\frac{n\pi(w+1)}{2}}{w^2}\,dw\right] & \text{if } n = 2k-1 \\[2ex] \dfrac{n\hbar^2}{a^2}\left[-\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi(v-1)}{2}}{v}\,dv + \int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi(v-1)}{2}}{v^2}\,dv + \int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi(w+1)}{2}}{w}\,dw + \int_{-\infty}^{\infty}\frac{\sin^2\frac{n\pi(w+1)}{2}}{w^2}\,dw\right] & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{(2k-1)\hbar^2}{a^2}\left[-\displaystyle\int_{-\infty}^{\infty}\frac{\cos^2\left(k\pi v - \frac{\pi v}{2} - k\pi + \frac{\pi}{2}\right)}{v}\,dv + \int_{-\infty}^{\infty}\frac{\cos^2\left(k\pi v - \frac{\pi v}{2} - k\pi + \frac{\pi}{2}\right)}{v^2}\,dv\right. \\ \qquad\qquad \left. + \displaystyle\int_{-\infty}^{\infty}\frac{\cos^2\left(k\pi w - \frac{\pi w}{2} + k\pi - \frac{\pi}{2}\right)}{w}\,dw + \int_{-\infty}^{\infty}\frac{\cos^2\left(k\pi w - \frac{\pi w}{2} + k\pi - \frac{\pi}{2}\right)}{w^2}\,dw\right] & \text{if } n = 2k-1 \\[2ex] \dfrac{(2k)\hbar^2}{a^2}\left[-\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2(k\pi v - k\pi)}{v}\,dv + \int_{-\infty}^{\infty}\frac{\sin^2(k\pi v - k\pi)}{v^2}\,dv + \int_{-\infty}^{\infty}\frac{\sin^2(k\pi w + k\pi)}{w}\,dw + \int_{-\infty}^{\infty}\frac{\sin^2(k\pi w + k\pi)}{w^2}\,dw\right] & \text{if } n = 2k \end{cases}$$

Use the facts that $\cos\left(x \pm \frac{\pi}{2}\right) = \mp \sin x$ and $\sin(x \pm k\pi) = \sin x \cos k\pi \pm \cos x \sin k\pi = (-1)^k \sin x$.

$$\langle p^2 \rangle = \begin{cases} \frac{(2k-1)\hbar^2}{a^2} \left[-\int_{-\infty}^{\infty} \frac{\left[-\sin\left(k\pi v - \frac{\pi v}{2} - k\pi\right)\right]^2}{v}\,dv + \int_{-\infty}^{\infty} \frac{\left[-\sin\left(k\pi v - \frac{\pi v}{2} - k\pi\right)\right]^2}{v^2}\,dv \right. \\ \qquad \left. + \int_{-\infty}^{\infty} \frac{\left[\sin\left(k\pi w - \frac{\pi w}{2} + k\pi\right)\right]^2}{w}\,dw + \int_{-\infty}^{\infty} \frac{\left[\sin\left(k\pi w - \frac{\pi w}{2} + k\pi\right)\right]^2}{w^2}\,dw \right] & \text{if } n = 2k-1 \\ \frac{(2k)\hbar^2}{a^2} \left[-\int_{-\infty}^{\infty} \frac{\sin^2(k\pi v - k\pi)}{v}\,dv + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi v - k\pi)}{v^2}\,dv + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi w + k\pi)}{w}\,dw + \int_{-\infty}^{\infty} \frac{\sin^2(k\pi w + k\pi)}{w^2}\,dw \right] & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \frac{(2k-1)\hbar^2}{a^2} \left[-\int_{-\infty}^{\infty} \frac{\left[-(-1)^k \sin\left(k\pi v - \frac{\pi v}{2}\right)\right]^2}{v}\,dv + \int_{-\infty}^{\infty} \frac{\left[-(-1)^k \sin\left(k\pi v - \frac{\pi v}{2}\right)\right]^2}{v^2}\,dv \right. \\ \qquad \left. + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin\left(k\pi w - \frac{\pi w}{2}\right)\right]^2}{w}\,dw + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin\left(k\pi w - \frac{\pi w}{2}\right)\right]^2}{w^2}\,dw \right] & \text{if } n = 2k-1 \\ \frac{(2k)\hbar^2}{a^2} \left[-\int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi v\right]^2}{v}\,dv + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi v\right]^2}{v^2}\,dv \right. \\ \qquad \left. + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi w\right]^2}{w}\,dw + \int_{-\infty}^{\infty} \frac{\left[(-1)^k \sin k\pi w\right]^2}{w^2}\,dw \right] & \text{if } n = 2k \end{cases}$$

v and w are just dummy variables, so the integrals can be cancelled and combined.

$$\langle p^2\rangle = \begin{cases} \dfrac{(2k-1)\hbar^2}{a^2}\left[\cancel{-\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\left(k\pi v-\frac{\pi v}{2}\right)}{v}\,dv} + \displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\left(k\pi v-\frac{\pi v}{2}\right)}{v^2}\,dv \right. \\ \qquad \left. \cancel{+\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\left(k\pi w-\frac{\pi w}{2}\right)}{w}\,dw} + \displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\left(k\pi w-\frac{\pi w}{2}\right)}{w^2}\,dw\right] & \text{if } n = 2k-1 \\ \dfrac{(2k)\hbar^2}{a^2}\left(\cancel{-\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2 k\pi v}{v}\,dv} + \displaystyle\int_{-\infty}^{\infty}\frac{\sin^2 k\pi v}{v^2}\,dv + \cancel{\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2 k\pi w}{w}\,dw} + \displaystyle\int_{-\infty}^{\infty}\frac{\sin^2 k\pi w}{w^2}\,dw\right) & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{2(2k-1)\hbar^2}{a^2}\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2\left(k\pi w-\frac{\pi w}{2}\right)}{w^2}\,dw & \text{if } n = 2k-1 \\ \dfrac{2(2k)\hbar^2}{a^2}\displaystyle\int_{-\infty}^{\infty}\frac{\sin^2 k\pi w}{w^2}\,dw & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{2(2k-1)\hbar^2}{a^2}\left[\left(k-\dfrac{1}{2}\right)\pi^2\right] & \text{if } n = 2k-1 \\ \dfrac{2(2k)\hbar^2}{a^2}(k\pi^2) & \text{if } n = 2k \end{cases}$$

$$= \begin{cases} \dfrac{(2k-1)^2\pi^2\hbar^2}{a^2} & \text{if } n = 2k-1 \\ \dfrac{(2k)^2\pi^2\hbar^2}{a^2} & \text{if } n = 2k \end{cases}$$

$$= \frac{n^2\pi^2\hbar^2}{a^2}$$

This is the result found in Problem 2.4 using the position-space wave function.