Problem 2.4

Calculate $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, $\langle p^2\rangle$, σ_x, and σ_p, for the nth stationary state of the infinite square well. Check that the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

Solution

In Problem 2.3 the stationary states for the infinite square well potential,

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases},$$

were found to be

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

Calculate the expectation value of x at time t.

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \Psi_n^*(x,t)(x)\Psi_n(x,t)\,dx \\
&= \int_0^a \left[\sqrt{\frac{2}{a}} \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right) \sin\frac{n\pi x}{a}\right]^* (x) \left[\sqrt{\frac{2}{a}} \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right) \sin\frac{n\pi x}{a}\right] dx \\
&= \int_0^a \left[\sqrt{\frac{2}{a}} \exp\left(i\frac{\hbar\pi^2 n^2}{2ma^2}t\right) \sin\frac{n\pi x}{a}\right] (x) \left[\sqrt{\frac{2}{a}} \exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right) \sin\frac{n\pi x}{a}\right] dx \\
&= \frac{2}{a}\int_0^a x\sin^2\frac{n\pi x}{a}\,dx \\
&= \frac{2}{a}\int_0^a \frac{x}{2}\left(1-\cos\frac{2n\pi x}{a}\right) dx \\
&= \frac{1}{a}\left(\int_0^a x\,dx - \int_0^a x\cos\frac{2n\pi x}{a}\,dx\right) \\
&= \frac{1}{a}\left[\frac{a^2}{2} - \int_0^a \left(\frac{a}{2\pi}\frac{\partial}{\partial n}\sin\frac{2n\pi x}{a}\right) dx\right] \\
&= \frac{a}{2} - \frac{1}{2\pi}\frac{d}{dn}\int_0^a \sin\frac{2n\pi x}{a}\,dx \\
&= \frac{a}{2} - \frac{1}{2\pi}\frac{d}{dn}\left(-\frac{a}{2n\pi}\cos\frac{2n\pi x}{a}\right)\Big|_0^a \\
&= \frac{a}{2} + \frac{a}{4\pi^2}\frac{d}{dn}\left[\frac{1}{n}(\cos 2n\pi - 1)\right] \\
&= \frac{a}{2} + \frac{a}{4\pi^2}\left[-\frac{1}{n^2}(\cos 2n\pi - 1) + \frac{1}{n}(-2\pi\sin 2n\pi)\right] \\
&= \frac{a}{2} + \frac{a}{4\pi^2}\left[-\frac{1}{n^2}(1-1) + \frac{1}{n}(0)\right] \\
&= \frac{a}{2}
\end{aligned}$$

Calculate the expectation value of x^2 at time t.

$$\begin{aligned}
\langle x^2\rangle &= \int_{-\infty}^{\infty} \Psi_n^*(x,t)(x^2)\Psi_n(x,t)\,dx \\
&= \int_0^a \left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]^*(x^2)\left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]dx \\
&= \int_0^a \left[\sqrt{\frac{2}{a}}\exp\left(i\frac{\hbar\pi^2n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right](x^2)\left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]dx \\
&= \frac{2}{a}\int_0^a x^2\sin^2\frac{n\pi x}{a}\,dx \\
&= \frac{2}{a}\int_0^a \frac{x^2}{2}\left(1-\cos\frac{2n\pi x}{a}\right)dx \\
&= \frac{1}{a}\left(\int_0^a x^2\,dx - \int_0^a x^2\cos\frac{2n\pi x}{a}\,dx\right) \\
&= \frac{1}{a}\left[\frac{a^3}{3} - \int_0^a\left(-\frac{a^2}{4\pi^2}\frac{\partial^2}{\partial n^2}\cos\frac{2n\pi x}{a}\right)dx\right] \\
&= \frac{a^2}{3} + \frac{a}{4\pi^2}\frac{d^2}{dn^2}\int_0^a\cos\frac{2n\pi x}{a}\,dx \\
&= \frac{a^2}{3} + \frac{a}{4\pi^2}\frac{d^2}{dn^2}\left(\frac{a}{2n\pi}\sin\frac{2n\pi x}{a}\right)\bigg|_0^a \\
&= \frac{a^2}{3} + \frac{a^2}{8\pi^3}\frac{d^2}{dn^2}\left(\frac{1}{n}\sin 2n\pi\right) \\
&= \frac{a^2}{3} + \frac{a^2}{8\pi^3}\frac{d}{dn}\left(-\frac{1}{n^2}\sin 2n\pi + \frac{2\pi}{n}\cos 2n\pi\right) \\
&= \frac{a^2}{3} + \frac{a^2}{8\pi^3}\left(\frac{2}{n^3}\sin 2n\pi - \frac{2\pi}{n^2}\cos 2n\pi - \frac{2\pi}{n^2}\cos 2n\pi - \frac{4\pi^2}{n}\sin 2n\pi\right) \\
&= \frac{a^2}{3} + \frac{a^2}{8\pi^3}\left(-\frac{4\pi}{n^2}\right) \\
&= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}
\end{aligned}$$

The standard deviation in x at time t is then

$$\begin{aligned}
\sigma_x &= \sqrt{\langle x^2\rangle - \langle x\rangle^2} \\
&= \sqrt{\left(\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}\right) - \left(\frac{a}{2}\right)^2} \\
&= \sqrt{\frac{a^2}{12} - \frac{a^2}{2n^2\pi^2}} \\
&= \sqrt{\frac{a^2}{12n^2\pi^2}(n^2\pi^2 - 6)} \\
&= \frac{a}{2n\pi}\sqrt{\frac{n^2\pi^2-6}{3}}.
\end{aligned}$$

Now calculate the expectation value of p at time t.

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} \Psi_n^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi_n(x,t)\,dx \\
&= -i\hbar\int_0^a \left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]^* \frac{\partial}{\partial x}\left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]dx \\
&= -i\hbar\int_0^a \left[\sqrt{\frac{2}{a}}\exp\left(i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]\left[\sqrt{\frac{2}{a}}\frac{n\pi}{a}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\cos\frac{n\pi x}{a}\right]dx \\
&= -\frac{2i\hbar n\pi}{a^2}\int_0^a \sin\frac{n\pi x}{a}\cos\frac{n\pi x}{a}\,dx \\
&= -\frac{2i\hbar n\pi}{a^2}\int_0^a \frac{1}{2}\left[\sin\left(\frac{n\pi x}{a}+\frac{n\pi x}{a}\right)+\sin\left(\frac{n\pi x}{a}-\frac{n\pi x}{a}\right)\right]dx \\
&= -\frac{i\hbar n\pi}{a^2}\int_0^a \sin\frac{2n\pi x}{a}\,dx \\
&= -\frac{i\hbar n\pi}{a^2}\left(-\frac{a}{2n\pi}\cos\frac{2n\pi x}{a}\right)\Bigg|_0^a \\
&= -\frac{i\hbar n\pi}{a^2}\left[-\frac{a}{2n\pi}(\cos 2n\pi-\cos 0)\right] \\
&= 0
\end{aligned}$$

Calculate the expectation value of p^2 at time t.

$$\begin{aligned}
\langle p^2\rangle &= \int_{-\infty}^{\infty} \Psi_n^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)^2\Psi_n(x,t)\,dx \\
&= \int_0^a \left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]^*(-\hbar^2)\frac{\partial^2}{\partial x^2}\left[\sqrt{\frac{2}{a}}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]dx \\
&= -\hbar^2\int_0^a \left[\sqrt{\frac{2}{a}}\exp\left(i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]\left[-\sqrt{\frac{2}{a}}\frac{n^2\pi^2}{a^2}\exp\left(-i\frac{\hbar\pi^2 n^2}{2ma^2}t\right)\sin\frac{n\pi x}{a}\right]dx \\
&= \frac{2\hbar^2 n^2\pi^2}{a^3}\int_0^a \sin^2\frac{n\pi x}{a}\,dx \\
&= \frac{2\hbar^2 n^2\pi^2}{a^3}\int_0^a \frac{1}{2}\left(1-\cos\frac{2n\pi x}{a}\right)dx \\
&= \frac{\hbar^2 n^2\pi^2}{a^3}\left(x-\frac{a}{2n\pi}\sin\frac{2n\pi x}{a}\right)\Bigg|_0^a \\
&= \frac{\hbar^2 n^2\pi^2}{a^3}(a) \\
&= \frac{\hbar^2 n^2\pi^2}{a^2}
\end{aligned}$$

The standard deviation in p at time t is then

$$\sigma_p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\left(\frac{\hbar^2 n^2\pi^2}{a^2}\right)-(0)^2} = \frac{\hbar n\pi}{a}.$$

Notice that all calculated expectation values are independent of time (hence the name, "stationary state"). The uncertainty product at time t is

$$\sigma_x \sigma_p = \left(\frac{a}{2n\pi} \sqrt{\frac{n^2\pi^2 - 6}{3}} \right) \left(\frac{\hbar n\pi}{a} \right) = \frac{\hbar}{2} \sqrt{\frac{n^2\pi^2 - 6}{3}}.$$

which is consistent with the Heisenberg uncertainty principle ($\sigma_x \sigma_p \geq \hbar/2 = 0.5\hbar$) for all n. The ground state $n = 1$ comes closest to the uncertainty limit with

$$\sigma_x \sigma_p = \frac{\hbar}{2} \sqrt{\frac{\pi^2 - 6}{3}} \approx 0.568\hbar.$$