$$= \frac{a^2}{6\pi^2}\left(2\pi^2 - 15\right), \tag{4.202}$$

$$\begin{aligned}\langle \hat{P}^2 \rangle &= -h^2 \int_{-a}^{+a} \psi(x)\frac{d^2\psi(x)}{dx^2}\,dx = \frac{\pi^2 h^2}{a^2}A^2\int_{-a}^{a}\left[\cos\frac{\pi x}{a} + cos^2\left(\frac{\pi x}{a}\right)\right]dx \\ &= \frac{\pi^2 h^2}{3a^3}\int_{-a}^{a}\left[\frac{1}{2} + \cos\frac{\pi x}{a} + \frac{1}{2}\cos\frac{2\pi x}{a}\right]dx = \frac{\pi^2 h^2}{3a^2};\end{aligned} \tag{4.203}$$

hence $\Delta x = a\sqrt{1/3 - 5/(2\pi^2)}$ and $\Delta p = \pi h/(\sqrt{3}a)$. We see that the uncertainties product

$$\Delta x \Delta p = \frac{\pi h}{3}\sqrt{1 - \frac{15}{2\pi^2}} \tag{4.204}$$

satisfies Heisenberg's uncertainty principle, $\Delta x \Delta p > h/2$.

(d) Since $d\psi^2/dx^2$ is zero at the inflection points, we have

$$\frac{d^2\psi}{dx^2} = -\frac{\pi^2}{a^2}A\cos\frac{\pi x}{a} = 0. \tag{4.205}$$

This relation holds when $x = \pm a/2$; hence the classically allowed region is defined by the interval between the inflection points $-a/2 \le x \le a/2$. That is, since $\psi(x)$ decays exponentially for $x > a/2$ and for $x < -a/2$, the energy of the system must be smaller than the potential. Classically, the system cannot be found in this region.

**Problem 4.2**

Consider a particle of mass $m$ moving freely between $x = 0$ and $x = a$ inside an infinite square well potential.

(a) Calculate the expectation values $\langle \hat{X} \rangle_n$, $\langle \hat{P} \rangle_n$, $\langle \hat{X}^2 \rangle_n$, and $\langle \hat{P}^2 \rangle_n$, and compare them with their classical counterparts.

(b) Calculate the uncertainties product $\Delta x_n \Delta p_n$.

(c) Use the result of (b) to estimate the zero-point energy.

**Solution**

(a) Since $\psi_n(x) = \sqrt{2/a}\sin(n\pi x/a)$ and since it is a real function, we have $\langle \psi_n|\hat{P}|\psi_n\rangle = 0$ because for any real function $\phi(x)$ the integral $\langle \hat{P} \rangle = -ih\int \phi^*(x)(d\phi(x)/dx)\,dx$ is imaginary and this contradicts the fact that $\langle \hat{P} \rangle$ has to be real. On the other hand, the expectation values of $\hat{X}$, $\hat{X}^2$, and $\hat{P}^2$ are

$$\begin{aligned}\langle \psi_n|\hat{X}|\psi_n\rangle &= \int_0^a \psi_n^*(x)x\psi_n(x)\,dx = \frac{2}{a}\int_0^a x\sin^2\left(\frac{n\pi x}{a}\right)dx \\ &= \frac{1}{a}\int_0^a x\left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right]dx = \frac{a}{2},\end{aligned} \tag{4.206}$$

$$\begin{aligned}\langle \psi_n|\hat{X}^2|\psi_n\rangle &= \frac{2}{a}\int_0^a x^2\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{1}{a}\int_0^a x^2\left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right]dx \\ &= \frac{a^2}{3} - \frac{1}{a}\int_0^a x^2\cos\left(\frac{2n\pi x}{a}\right)dx\end{aligned}$$

$$= \frac{a^2}{3} - \frac{1}{2n\pi}x^2 \sin\left(\frac{2n\pi x}{a}\right)\Big|_{x=0}^{x=a} + \frac{1}{n\pi}\int_0^a x \sin\left(\frac{2n\pi x}{a}\right) dx$$

$$= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}, \tag{4.207}$$

$$\langle \psi_n | \hat{P}^2 | \psi_n \rangle = -\hbar^2 \int_0^a \psi_n^*(x) \frac{d^2\psi_n(x)}{dx^2} dx = \frac{n^2\pi^2\hbar^2}{a^2} \int_0^a |\psi_n(x)|^2 dx = \frac{n^2\pi^2\hbar^2}{a^2}. \tag{4.208}$$

In deriving the previous three expressions, we have used integrations by parts. Since $E_n = n^2\pi^2\hbar^2/(2ma^2)$, we may write

$$\langle \psi_n | \hat{P}^2 | \psi_n \rangle = \frac{n^2\pi^2\hbar^2}{a^2} = 2mE_n. \tag{4.209}$$

To calculate the classical average values $x_{av}$, $p_{av}$, $x_{av}^2$, $p_{av}^2$, it is easy first to infer that $p_{av} = 0$ and $p_{av}^2 = 2mE$, since the particle moves to the right with *constant* momentum $p = mv$ and to the left with $p = -mv$. As the particle moves at constant speed, we have $x = vt$, hence

$$x_{av} = \frac{1}{T}\int_0^T x(t)\,dt = \frac{v}{T}\int_0^T t\,dt = v\frac{T}{2} = \frac{a}{2}, \tag{4.210}$$

$$x_{av}^2 = \frac{1}{T}\int_0^T x^2(t)\,dt = \frac{v^2}{T}\int_0^T t^2 dt = \frac{1}{3}v^2T^2 = \frac{a^2}{3}, \tag{4.211}$$

where $T$ is half[5] of the period of the motion, with $a = vT$.

We conclude that, while the average classical and quantum expressions for $x$, $p$ and $p^2$ are identical, a comparison of (4.207) and (4.211) yields

$$\langle \psi_n | \hat{X}^2 | \psi_n \rangle = \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} = x_{av}^2 - \frac{a^2}{2n^2\pi^2}, \tag{4.212}$$

so that in the limit of large quantum numbers, the quantum expression $\langle \psi_n | \hat{X}^2 | \psi_n \rangle$ matches with its classical counterpart $x_{av}^2$: $\lim_{n\longrightarrow\infty}\langle \psi_n | \hat{X}^2 | \psi_n \rangle = a^2/3 = x_{av}^2$.

(b) The position and the momentum uncertainties can be calculated from (4.206) to (4.208):

$$\Delta x_n = \sqrt{\langle \psi_n | \hat{X}^2 | \psi_n \rangle - \langle \psi_n | \hat{X} | \psi_n \rangle^2} = \sqrt{\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} - \frac{a^2}{4}} = a\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}, \tag{4.213}$$

$$\Delta p_n = \sqrt{\langle \psi_n | \hat{P}^2 | \psi_n \rangle - \langle \psi_n | \hat{P} | \psi_n \rangle^2} = \sqrt{\langle \psi_n | \hat{P}^2 | \psi_n \rangle} = \frac{n\pi\hbar}{a}, \tag{4.214}$$

hence

$$\Delta x_n \Delta p_n = n\pi\hbar\sqrt{\frac{1}{12} - \frac{1}{2n^2\pi^2}}. \tag{4.215}$$

(c) Equation (4.214) shows that the momentum uncertainty for the ground state is not zero, but

$$\Delta p_1 = \frac{\pi\hbar}{a}. \tag{4.216}$$

[5]We may parameterize the other half of the motion by $x = -vt$, which when inserted in (4.210) and (4.211), where the variable $t$ varies between $-T$ and 0, the integrals would yield the same results, namely $x_{av} = a/2$ and $x_{av}^2 = a^2/3$, respectively.

This leads to a nonzero kinetic energy. Therefore, the lowest value of the particle's kinetic energy is of the order of $E_{min} \sim (\Delta p_1)^2/(2m) \sim \pi^2\hbar^2/(2ma^2)$. This value, which is in full agreement with the ground state energy, $E_1 = \pi^2\hbar^2/(2ma^2)$, is the zero-point energy of the particle.

**Problem 4.3**

An electron is moving freely inside a one-dimensional infinite potential box with walls at $x = 0$ and $x = a$. If the electron is initially in the ground state ($n = 1$) of the box and if we *suddenly* quadruple the size of the box (i.e., the right-hand side wall is moved instantaneously from $x = a$ to $x = 4a$), calculate the probability of finding the electron in:

(a) the ground state of the new box and

(b) the first excited state of the new box.

**Solution**

Initially, the electron is in the ground state of the box $x = 0$ and $x = a$; its energy and wave function are

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}, \qquad \phi_1(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right). \tag{4.217}$$

(a) Once in the new box, $x = 0$ and $x = 4a$, the ground state energy and wave function of the electron are

$$E_1' = \frac{\pi^2\hbar^2}{2m(4a)^2} = \frac{\pi^2\hbar^2}{32ma^2}, \qquad \psi_1(x) = \frac{1}{\sqrt{2a}}\sin\left(\frac{\pi x}{4a}\right). \tag{4.218}$$

The probability of finding the electron in $\psi_1(x)$ is

$$P(E_1') = |\langle\psi_1|\phi_1\rangle|^2 = \left|\int_0^a \psi_1^*(x)\phi_1(x)dx\right|^2 = \frac{1}{a^2}\left|\int_0^a \sin\left(\frac{\pi x}{4a}\right)\sin\left(\frac{\pi x}{a}\right)dx\right|^2; \tag{4.219}$$

the upper limit of the integral sign is $a$ (and not $4a$) because $\phi_1(x)$ is limited to the region between 0 and $a$. Using the relation $\sin a \sin b = \frac{1}{2}\cos(a-b) - \frac{1}{2}\cos(a+b)$, we have $\sin(\pi x/4a)\sin(\pi x/a) = \frac{1}{2}\cos(3\pi x/4a) - \frac{1}{2}\cos(5\pi x/4a)$; hence

$$\begin{aligned} P(E_1') &= \frac{1}{a^2}\left|\frac{1}{2}\int_0^a \cos\left(\frac{3\pi x}{4a}\right)dx - \frac{1}{2}\int_0^a \cos\left(\frac{5\pi x}{4a}\right)dx\right|^2 \\ &= \frac{128}{15^2\pi^2} = 0.058 = 5.8\%. \end{aligned} \tag{4.220}$$

(b) If the electron is in the first excited state of the new box, its energy and wave function are

$$E_2' = \frac{\pi^2\hbar^2}{8ma^2}, \qquad \psi_2(x) = \frac{1}{\sqrt{2a}}\sin\left(\frac{\pi x}{2a}\right). \tag{4.221}$$

The corresponding probability is

$$\begin{aligned} P(E_2') &= |\langle\psi_2|\phi_1\rangle|^2 = \left|\int_0^a \psi_2^*(x)\phi_1(x)dx\right|^2 = \frac{1}{a^2}\left|\int_0^a \sin\left(\frac{\pi x}{2a}\right)\sin\left(\frac{\pi x}{a}\right)dx\right|^2 \\ &= \frac{16}{9\pi^2} = 0.18 = 18\%. \end{aligned} \tag{4.222}$$