Chemistry 432
Problem Set 3
Spring 2019
Solutions

1. Consider a particle of mass m with quantum number n moving in a one-dimensional box of length L.

   (a) Find the probability of finding the particle in the left two-thirds of the box.
   Answer:

$$p = \frac{2}{L}\int_0^{2L/3} \sin^2 \frac{n\pi x}{L} dx$$

$$y = \frac{n\pi x}{L} \qquad dx = \frac{L}{n\pi} dy$$

$$p = \frac{2}{L}\frac{L}{n\pi}\int_0^{2n\pi/3} \sin^2 y dy$$

$$= \frac{2}{n\pi}\left[\frac{y}{2} - \frac{1}{4}\sin 2y\right]_0^{2n\pi/3}$$

$$= \frac{2}{3} - \frac{1}{2n\pi}\sin\frac{4n\pi}{3}$$

   (b) For what value of n is this probability a maximum?
   Answer:

n	p
1	.804
2	.598
3	.667
4	.701
5	.639
6	.667
7	.686
8	.649
9	.667
10	.680

   Maximum at $n = 1$.

(c) What is the probability as $n \to \infty$?

Answer:

$$\lim_{n\to\infty} p = \frac{2}{3}$$

the classical result.

2. For a particle of mass m in a box of length L in quantum state n, find:

(a) $< x >$;

Answer:

$$\langle x \rangle = \frac{2}{L}\int_0^L \sin\frac{n\pi x}{L} x \sin\frac{n\pi x}{L} dx$$

$$y = \frac{n\pi x}{L} \qquad x = \frac{Ly}{n\pi} \qquad dx = \frac{L}{n\pi}dy$$

$$\langle x \rangle = \frac{2}{L}\left(\frac{L}{n\pi}\right)^2 \int_0^{n\pi} y\sin^2 y dy$$

$$= \frac{2L}{(n\pi)^2}\left[\frac{y^2}{4} - \frac{y\sin 2y}{4} - \frac{\cos 2y}{8}\right]_0^{n\pi}$$

$$= \frac{2L}{(n\pi)^2}\frac{(n\pi)^2}{4} = \frac{L}{2}$$

(b) $< p >$;

Answer:

$$\langle p \rangle = \frac{2}{L}\int_0^L \sin\frac{n\pi x}{L}\frac{\hbar}{i}\frac{d}{dx}\sin\frac{n\pi x}{L}dx$$

$$= \frac{\hbar}{i}\frac{2}{L}\frac{n\pi}{L}\int_0^L \sin\frac{n\pi x}{L}\cos\frac{n\pi x}{L} = 0$$

(c) $< K = p^2/2m >$.

$$\langle K \rangle = \frac{2}{L}\int_0^L \sin\frac{n\pi x}{L}\left(\frac{-\hbar^2}{2m}\right)\frac{d^2}{dx^2}\sin\frac{n\pi x}{L}dx$$

$$= -\frac{2}{L}\frac{\hbar^2}{2m}\int_0^L \sin\frac{n\pi x}{L}\left[-\left(\frac{n\pi}{L}\right)^2\right]\sin\frac{n\pi x}{L}$$

$$= \frac{\hbar^2}{mL}\frac{(n\pi)^2}{L^2}\int_0^L \sin^2\frac{n\pi x}{L}dx$$

$$= \frac{\hbar^2 n^2\pi^2}{mL^3}\frac{L}{2}$$

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

3. Consider a one-dimensional particle of mass m confined to move in a box of length L on a coordinate system defined so that the potential energy is given by

$$V(x) = \begin{cases} 0 & -\frac{L}{2} \le x \le \frac{L}{2} \\ \infty & \text{elsewhere} \end{cases}$$

(a) Show that the normalized wavefunctions

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left[n\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right] \qquad n = 1, 2, 3, \ldots$$

satisfy the Schrödinger equation for the particle within the box.
Answer:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d\psi}{dx} = \left(\frac{2}{L}\right)^{1/2} \frac{n\pi}{L} \cos\left[n\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right]$$

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2}{L}\right)^{1/2} \left(\frac{n\pi}{L}\right)^2 \sin\left[n\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right] = -\left(\frac{n\pi}{L}\right)^2\psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \frac{n^2\pi^2\hbar^2}{2mL^2}\psi = E\psi$$

(b) Give the appropriate boundary conditions for the system defined in part "a," and show that the wavefunctions given in part 'a" satisfy the boundary conditions.
Answer:

$$\psi(-L/2) = \psi(L/2) = 0$$

$$\psi(-L/2) = \left(\frac{2}{L}\right)^{1/2} \sin\left[n\pi\left(-\frac{L}{2L} + \frac{1}{2}\right)\right] = \left(\frac{2}{L}\right)^{1/2} \sin(0) = 0$$

$$\psi(L/2) = \left(\frac{2}{L}\right)^{1/2} \sin\left[n\pi\left(\frac{L}{2L} + \frac{1}{2}\right)\right] = \left(\frac{2}{L}\right)^{1/2} \sin(n\pi) = 0$$

(c) For a particle in the first excited state with associated wavefunction

$$\psi_2(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left[2\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right]$$

determine at what point or points in space the particle is most likely to be found.
Answer:

$$p_2(x) = \frac{2}{L}\sin^2\left[2\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right]$$

$$p_2'(x) = \frac{4}{L}\frac{2\pi}{L}\sin\left[2\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right]\cos\left[2\pi\left(\frac{x}{L} + \frac{1}{2}\right)\right]$$

$$= 0 \qquad \text{at}$$

$$2\pi\left(\frac{x}{L}+\frac{1}{2}\right)=\frac{\pi}{2} \qquad \text{or} \qquad \frac{3\pi}{2}$$

Then

$$x=-\frac{L}{4},\frac{L}{4}$$

(d) For a particle represented by the first excited state wavefunction given in part "c," calculate the probability that a measurement of the position of the particle will give a result in the interval $-L/2 \leq x \leq 0$.

Answer:

$$p=\frac{2}{L}\int_{-L/2}^{0}\sin^2\left[2\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]dx$$

$$\text{Let} \qquad y=\frac{2\pi x}{L}+\pi \qquad dx=\frac{L}{2\pi}dy$$

$$p=\frac{2}{L}\frac{L}{2\pi}\int_0^{\pi}\sin^2 y\ dy=\frac{1}{\pi}\left[\frac{y}{2}-\frac{1}{4}\sin 2y\right]_0^{\pi}$$

$$=\frac{1}{2}$$

4. The wavefunction for a particle of mass m in a box of length L defined on the interval $-L/2 \leq x \leq L/2$ is given by

$$\psi(x)=N\sin\left[\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]$$

where N is the normalization factor. Derive an expression for the expectation value of the kinetic energy of the particle.

Answer:

$$N^2\int_{-L/2}^{L/2}\sin^2\left[\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]dx=1$$

$$y=\pi\left(\frac{x}{L}+\frac{1}{2}\right) \qquad dy=\frac{\pi}{L}dx \qquad dx=\frac{L}{\pi}dy$$

$$N^2\frac{L}{\pi}\int_0^{\pi}\sin^2 y\ dy=N^2\frac{L}{\pi}\left[\frac{y}{2}-\frac{1}{4}\sin 2y\right]_0^{\pi}=N^2\frac{L}{2}=1$$

or

$$\psi(x)=\left(\frac{2}{L}\right)^{1/2}\sin\left[\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]$$

$$\langle T\rangle=\int_D\psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi(x)dx$$

$$=-\frac{2\hbar^2}{2mL}\int_{-L/2}^{L/2}\sin\left[\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]\frac{d^2}{dx^2}\sin\left[\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]\ dx$$

$$=\left(\frac{2\hbar^2}{2mL}\right)\left(\frac{\pi^2}{L^2}\right)\int_{-L/2}^{L/2}\sin^2\left[\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]\ dx$$

$$= \left(\frac{2\hbar^2}{2mL}\right)\left(\frac{\pi^2}{L^2}\right)\left(\frac{L}{2}\right) = \frac{\pi^2\hbar^2}{2mL^2}$$

5. A particle of mass m is confined to a one-dimensional box of length L in the domain $-L/4 < x < 3L/4$. Show that the wavefunction

$$\psi(x) = \sin\left(\frac{\pi x}{L} + \frac{\pi}{4}\right)$$

satisfies the time-independent Schrödinger equation for the system as well as the appropriate boundary conditions.
Answer:

$$\hat{H}\psi = E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$$

$$\psi'(x) = \frac{\pi}{L}\cos\left(\frac{\pi x}{L} + \frac{\pi}{4}\right) \qquad \psi''(x) = -\frac{\pi^2}{L^2}\sin\left(\frac{\pi x}{L} + \frac{\pi}{4}\right)$$

$$\hat{H}\psi = \frac{\hbar^2\pi^2}{2mL^2}\sin\left(\frac{\pi x}{L} + \frac{\pi}{4}\right) \qquad E = \frac{\hbar^2\pi^2}{2mL^2}$$

$$\psi(-L/4) = \psi(3L/4) = 0$$

$$\psi(-L/4) = \sin\left(\frac{\pi}{L}\frac{-L}{4} + \frac{\pi}{4}\right) = \sin 0 = 0$$

$$\psi(3L/4) = \sin\left(\frac{\pi}{L}\frac{3L}{4} + \frac{\pi}{4}\right) = \sin\pi = 0$$

6. The normalized wavefunction for a particle of mass m in a one-dimensional box of length L on the domain $0 < x < L$ in its 4^{th} excited energy state is given by

$$\psi_5(x) = \left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{5\pi x}{L}\right).$$

Calculate the probability that a measurement of the position of the particle will give a result in the region between $x = 0$ and the first node of the wavefunction.
Answer:
The first node occurs at

$$\frac{5\pi x}{L} = \pi \qquad \text{or} \qquad x = \frac{L}{5}$$

$$p = \int_0^{L/5}\psi^*(x)\psi(x)\ dx = \frac{2}{L}\int_0^{L/5}\sin^2\left(\frac{5\pi x}{L}\right)dx$$

$$y = \frac{5\pi x}{L} \qquad dx = \frac{L}{5\pi}dy$$

$$p = \left(\frac{2}{L}\right)\left(\frac{L}{5\pi}\right)\int_0^{\pi}\sin^2 y\ dy$$

$$= \frac{2}{5\pi}\left(\frac{y}{2} - \frac{1}{4}\sin 2y\right)\Big|_0^{\pi} = \frac{1}{5}$$

7. The normalized wavefunction for a particle of mass m in a one-dimensional box in quantum state n on the domain $-L/2 \leq x \leq L/2$ is given by

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(n\pi\left[\frac{x}{L} + \frac{1}{2}\right]\right).$$

Calculate the probability the particle is found on the interval between $-L/2$ and the first node of the wavefunction.

Answer:

The first node is found at

$$n\pi\left(\frac{x}{L} + \frac{1}{2}\right) = \pi \qquad \frac{x}{L} + \frac{1}{2} = \frac{1}{n} \qquad x = L\left(\frac{1}{n} - \frac{1}{2}\right)$$

$$p = \frac{2}{L}\int_{-L/2}^{L(1/n-1/2)} \sin^2\left(n\pi\left[\frac{x}{L} + \frac{1}{2}\right]\right) dx$$

$$y = n\pi\left(\frac{x}{L} + \frac{1}{2}\right) \qquad dx = \frac{L}{n\pi} dy$$

$$p = \left(\frac{2}{L}\right)\left(\frac{L}{n\pi}\right)\int_0^{\pi} \sin^2 y\ dy$$

$$= \frac{2}{n\pi}\left[\frac{y}{2} - \frac{1}{4}\sin 2y\right]_0^{\pi} = \frac{1}{n}$$

8. A particle of mass m is confined to move in a box of length L on the domain $-L/10 \leq x \leq 9L/10$ by action of potential energy

$$V(x) = \begin{cases} 0 & -\frac{L}{10} \leq x \leq \frac{9L}{10} \\ \infty & \text{elsewhere} \end{cases}$$

The particle is in the state with quantum number $n = 2$ and associated normalized wavefunction

$$\psi_2(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left[\frac{2\pi}{L}\left(x + \frac{L}{10}\right)\right].$$

Show that $\psi_2(x)$ satisfies the appropriate boundary conditions for the system, and find the points in space that the particle is most likely to be found.

Answer:

$$\psi_2(-L/10) = \psi_2(9L/10) \text{ should} = 0$$

$$\psi_2(-L/10) = \left(\frac{2}{L}\right)^{1/2} \sin\left[\frac{2\pi}{L}\left(-\frac{L}{10} + \frac{L}{10}\right)\right] = \left(\frac{2}{L}\right)^{1/2} \sin 0 = 0$$

$$\psi_2(9L/10) = \left(\frac{2}{L}\right)^{1/2} \sin\left[\frac{2\pi}{L}\left(\frac{9L}{10} + \frac{L}{10}\right)\right] = \left(\frac{2}{L}\right)^{1/2} \sin 2\pi = 0$$

$$p(x) = \frac{2}{L}\sin^2\left[\frac{2\pi}{L}\left(x + \frac{L}{10}\right)\right]$$

$$p'(x) = \frac{4}{L}\frac{2\pi}{L}\sin\left[\frac{2\pi}{L}\left(x+\frac{L}{10}\right)\right]\cos\left[\frac{2\pi}{L}\left(x+\frac{L}{10}\right)\right] = 0$$

at

$$\frac{2\pi}{L}\left(x+\frac{L}{10}\right) = \frac{\pi}{2}, \frac{3\pi}{2}$$

or

$$x = \frac{3L}{20}, \frac{13L}{20}$$

9. A particle of mass m in a box of length L, defined on the domain $-L/5 \leq x \leq 4L/5$, occupies its first excited energy state with associate normalized wavefunction

$$\psi_2(x) = \left(\frac{2}{L}\right)^{1/2}\sin\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right].$$

Let x_n be the coordinate of the node of the wavefunction, x_L and x_U be the coordinates where the particle is most likely to be found such that $x_L < x_U$. Determine the locations x_n, x_L and x_U, and calculate the probability that a measurement of the coordinate of the particle gives a result in the range $x_L \leq x \leq x_n$.

Answer:

$$\sin\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right] = 0$$

when

$$\frac{2\pi}{L}\left(x_n+\frac{L}{5}\right) = \pi \qquad \text{or} \qquad x_n = \frac{3L}{10}$$

Now

$$p(x) = \left(\frac{2}{L}\right)\sin^2\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right]$$

and

$$p'(x) = \left(\frac{8\pi}{L^2}\right)\sin\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right]\cos\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right]$$

$$p'(x) = 0 \quad \text{when} \quad \cos\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right] = 0$$

or

$$\frac{2\pi}{L}\left(x+\frac{L}{5}\right) = \frac{\pi}{2}, \frac{3\pi}{2}$$

and

$$x_L = \frac{L}{20} \qquad x_U = \frac{11L}{20}$$

$$p = \frac{2}{L}\int_{L/20}^{3L/10}\sin^2\left[\frac{2\pi}{L}\left(x+\frac{L}{5}\right)\right]dx$$

$$y = \frac{2\pi}{L}\left(x+\frac{L}{5}\right) \qquad dy = \frac{2\pi}{L}dx$$

$$p = \frac{2}{L}\frac{L}{2\pi}\int_{\pi/2}^{\pi}\sin^2 y\; dy = \frac{1}{\pi}\left[\frac{y}{2} - \frac{1}{4}\sin 2y\right]_{\pi/2}^{\pi} = \frac{1}{4}$$

10. A quantum particle of mass m is confined to a one-dimensional box on the domain $-L/2 \le x \le L/2$. The normalized solutions to the Schrödinger equation for the particle are given by

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left[n\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right], n = 1, 2, \ldots$$

Let x_1 be the first node of the wavefunction for $n = 3$ and x_2 be the second node of the wavefunction for $n = 3$. Calculate the probability that a measurement of the position of the particle in the state defined by $n = 3$ gives a result in the range $x_1 \le x \le x_2$.

Answer:

$$x_1 : 3\pi\left(\frac{x_1}{L}+\frac{1}{2}\right) = \pi \qquad x_1 = -\frac{L}{6}$$

$$x_2 : 3\pi\left(\frac{x_2}{L}+\frac{1}{2}\right) = 2\pi \qquad x_2 = \frac{L}{6}$$

$$p = \frac{2}{L}\int_{-L/6}^{L/6} \sin^2\left[3\pi\left(\frac{x}{L}+\frac{1}{2}\right)\right]\, dx$$

$$y = 3\pi\left(\frac{x}{L}+\frac{1}{2}\right) \qquad dy = \frac{3\pi}{L}dx$$

$$p = \frac{2}{L}\frac{L}{3\pi}\int_{\pi}^{2\pi} \sin^2 y\; dy$$

$$= \frac{2}{3\pi}\left[\frac{y}{2}-\frac{1}{4}\sin 2y\right]_{\pi}^{2\pi} = \frac{2}{3\pi}\frac{\pi}{2} = \frac{1}{3}$$

11. The first-excited state normalized wavefunction for a particle of mass m confined to move in a one-dimensional box on the domain $-L/7 \le x \le 6L/7$ is given by

$$\psi_2(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left[\frac{2\pi}{L}\left(x+\frac{L}{7}\right)\right].$$

Show that the wavefunction satisfies the proper boundary conditions for the system, find the first node of the wavefunction, and calculate the probability that a measurement of the position of the particle lies in the range from $x = -L/7$ to the first node of the wavefunction.

Answer:

Boundary conditions

$$\sin\left[\frac{2\pi}{L}\left(-\frac{L}{7}+\frac{L}{7}\right)\right] = \sin 0 = 0$$

$$\sin\left[\frac{2\pi}{L}\left(\frac{6L}{7}+\frac{L}{7}\right)\right] = \sin 2\pi = 0$$

Node

$$\frac{2\pi}{L}\left(x+\frac{L}{7}\right) = \pi \text{ at } x = \frac{5L}{14}$$

Probability

$$p = \frac{2}{L}\int_{-L/7}^{5L/14} \sin^2\left[\frac{2\pi}{L}\left(x+\frac{L}{7}\right)\right]$$

$$y = \frac{2\pi}{L}\left(x+\frac{L}{7}\right) \qquad dx = \frac{L}{2\pi}dy$$

$$p = \frac{2}{L}\frac{L}{2\pi}\int_0^{\pi}\sin^2 y\ dy = \frac{1}{\pi}\left[\frac{y}{2}-\frac{1}{4}\sin 2y\right]_0^{\pi} = \frac{1}{2}$$

12. Calculate $< xy^2 >$ for a particle of mass m having quantum numbers n_x and n_y in a two-dimensional box whose sides have lengths L_x and L_y.
Answer:

$$\langle xy^2\rangle = \frac{2}{L_x}\frac{2}{L_y}\int_0^{L_x} dx\int_0^{L_y} dy\ xy^2\sin^2\frac{n_x\pi x}{L_x}\sin^2\frac{n_y\pi y}{L_y}$$

$$= \frac{2}{L_x}\frac{2}{L_y}\int_0^{L_x} dx\ x\sin^2\frac{n_x\pi x}{L_x}\int_0^{L_y} dy\ y^2\sin^2\frac{n_y\pi y}{L_y}$$

$$\frac{L_x}{2}\frac{2}{L_y}\int_0^{L_y} dy\ y^2\sin^2\frac{n_y\pi y}{L_y}$$

where we have used the result found in Problem 2a. Using

$$z = \frac{n_y\pi y}{L_y} \qquad dy = \frac{L_y}{n_y\pi}dz$$

Then

$$\langle xy^2\rangle = \frac{L_x}{2}\frac{2}{L_y}\left(\frac{L_y}{n_y\pi}\right)^3\int_0^{n_y\pi} dz z^2\sin^2 z$$

$$= \frac{L_x}{2}\frac{2L_y^2}{(n_y\pi)^3}\left[\frac{z^3}{6}-\left(\frac{z^2}{4}-\frac{1}{8}\right)\sin 2z - \frac{z\cos 2z}{4}\right]_0^{n_y\pi}$$

$$= L_xL_y^2\frac{1}{2}\left[\frac{1}{3}-\frac{1}{2(n_y\pi)^2}\right]$$

13. The normalized wavefunctions for a particle of mass m in a one-dimensional box of length L on the domain $0 \le x \le L$ are given by the set

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2}\sin\frac{n\pi x}{L} \quad n = 1, 2, 3, \ldots$$

Calculate $< xyz >$ for a particle of mass m having quantum numbers n_x, n_y and n_z in a three-dimensional box whose sides have lengths L_x, L_y and L_z.
Answer:
In one dimension

$$\langle x\rangle = \frac{2}{L}\int_0^L x\sin^2\frac{n\pi x}{L}\ dx$$

$$y = \frac{n\pi x}{L} \qquad x = \frac{Ly}{n\pi} \qquad dx = \frac{L}{n\pi} dy$$

$$\langle x \rangle = \frac{2}{L} \left(\frac{L}{n\pi}\right)^2 \int_0^{n\pi} y \sin^2 y \; dy$$

$$= \frac{2L}{(n\pi)^2} \left[\frac{y^2}{4} - \frac{1}{4} y \sin(2y) - \frac{1}{8}\cos(2y)\right]_0^{n\pi} = \frac{L}{2}$$

In three dimensions

$$\Psi_{n_x,n_y,n_z}(x,y,z) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$$

so that

$$\langle xyz \rangle = \langle x \rangle \langle y \rangle \langle z \rangle = \frac{L_x L_y L_z}{8}$$

14. The normalized wavefunction for a quantum particle of mass m in a one-dimensional box of length L on the domain $0 \leq x \leq L$ with quantum number n is given by

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin \frac{n\pi x}{L}$$

Consider a particle of mass m in a two-dimensional box whose sides are of lengths L_x and L_y; i.e. the domain is $0 \leq x \leq L_x$ and $0 \leq y \leq L_y$. Suppose the quantum state of the particle is defined by the quantum numbers in the x and y Cartesian directions by $n_x = 1$ and $n_y = 2$. Calculate $\langle x^2 y \rangle$ for the particle.

Answer:

$$\langle x^2 y \rangle = \langle x^2 \rangle \langle y \rangle$$

$$\langle x^2 \rangle = \int_0^{L_x} \left(\frac{2}{L_x}\right)^{1/2} \sin \frac{\pi x}{L_x} x^2 \left(\frac{2}{L_x}\right)^{1/2} \sin \frac{\pi x}{L_x} \; dx = \frac{2}{L_x} \int_0^{L_x} x^2 \sin^2 \frac{\pi x}{L_x} \; dx$$

$$z = \frac{\pi x}{L_x} \qquad x = \frac{L_x}{\pi} z \qquad dx = \frac{L_x}{\pi} \; dz$$

$$\langle x^2 \rangle = \frac{2}{L_x} \left(\frac{L_x}{\pi}\right)^3 \int_0^{\pi} z^2 \sin^2 z \; dz = \frac{L_x^2}{6\pi^3}[2\pi^3 - 3\pi]$$

$$\langle y \rangle = \frac{2}{L_y} \int_0^{L_y} y \sin^2 \frac{2\pi y}{L_y} \; dy$$

$$z = \frac{2\pi y}{L_y} \qquad y = \frac{L_y}{2\pi} z \qquad dy = \frac{L_y}{2\pi} \; dz$$

$$\langle y \rangle = \frac{2}{L_y} \left(\frac{L_y}{2\pi}\right)^2 \int_0^{2\pi} z \sin^2 z \; dz = \frac{2}{L_y} \left(\frac{L_y}{2\pi}\right)^2 \frac{4\pi^2}{4} = \frac{L_y}{2}$$

$$\langle x^2 y \rangle = \frac{L_y}{2} \frac{L_x^2}{6\pi^3} [2\pi^3 - 3\pi]$$