

Department of Chemistry, Michigan State University

CEM 991, Fall 2021

Midterm Exam II

Deadline for Emailing Solutions to the Instructor: December 6, 2021, 8:00 pm Eastern Time

Name (Last, First, Middle Initial): **SOLUTIONS (Piecuch, Piotr)**

ID Number:

INSTRUCTIONS

- The maximum number of points that you can earn in this exam is 25. 25 points earned in this exam are equivalent to 250 points out of 1000 points constituting the final grade (i.e., 25 % of the final grade). In other words, 1 exam point earned in this exam is equivalent to 1 % of the final grade.
- Check that your booklet contains all 20 pages. The last page 20 contains a few potentially useful formulas.
- Write your name and student ID number in the spaces provided above.
- Answer in the spaces provided. Use the extra pages 18-20 for additional space, if necessary. If you have technical difficulties with directly using this exam booklet, write down and scan your solutions, as you normally do in the case of homework assignments, but do not forget to write your name and student ID number on the first page of your exam. Email your exam (this booklet or your own pages) to the instructor using the deadline described above. Late exams will not be accepted.
- Show ALL your work. Insufficient justification will result in a loss of points.
- Do not write anything in the score table given below.

Problem	Score
1	/8
2	/5
3	/6
4	/6
Total	/25

1. (8 pts.) Let $u_n(x)$ be the n -th eigenstate of the quantum harmonic oscillator,

$$u_n(x) = N_n H_n(\xi) e^{-\frac{1}{2}\xi^2} \quad (n = 0, 1, 2, \dots),$$

where

$$N_n = \left(\frac{\alpha}{2^n n! \pi^{\frac{1}{2}}} \right)^{\frac{1}{2}},$$

$$\xi = \alpha x, \quad \alpha = \left(\frac{m\omega_c}{\hbar} \right)^{\frac{1}{2}},$$

and H_n are the Hermite polynomials (ω_c is the angular frequency of the corresponding classical harmonic oscillator and m is its mass). It can be shown that

$$\langle u_n | \hat{x} | u_m \rangle = \begin{cases} \frac{1}{\alpha} \left(\frac{n+1}{2} \right)^{\frac{1}{2}} & \text{for } m = n+1 \\ \frac{1}{\alpha} \left(\frac{n}{2} \right)^{\frac{1}{2}} & \text{for } m = n-1 \\ 0 & \text{otherwise } (m \neq n \pm 1) \end{cases}. \quad (1)$$

- (a) (6 pts.) Use Eq. (1) and the generalized Parseval relation or the resolution of identity for eigenstates $|u_n\rangle$ to prove that

$$\langle u_n | \hat{x}^2 | u_n \rangle = \frac{1}{\alpha^2} (n + \frac{1}{2}),$$

$$\langle u_n | \hat{x}^2 | u_{n+1} \rangle = 0,$$

$$\langle u_n | \hat{x}^2 | u_{n+2} \rangle = \frac{1}{2\alpha^2} [(n+1)(n+2)]^{\frac{1}{2}}.$$

- (b) (2 pts.) Use Eq. (1), the above expressions for matrix elements of the $\hat{x}^2$ operator, the generalized Parseval relation or the resolution of identity for eigenstates $|u_n\rangle$, and the fact that one can write $\hat{x}^3$ as a product of $\hat{x}^2$ and $\hat{x}$ to show that

$$\langle u_n | \hat{x}^3 | u_{n+1} \rangle = \frac{3}{\alpha^3} \left(\frac{n+1}{2} \right)^{\frac{3}{2}}.$$

Solution

$$\begin{aligned} (a) \quad \langle u_n | \hat{x}^2 | u_n \rangle &= \langle u_n | \hat{x} \hat{x} | u_n \rangle \\ &= \sum_{k=0}^{\infty} \langle u_n | \hat{x} | u_k \rangle \langle u_k | \hat{x} | u_n \rangle. \end{aligned}$$

The only terms that enter the summation over k are, in this case, $k=n-1$ and $k=n+1$. For other

(solution of Problem 1 continued)

values of k , $\langle u_n | \hat{X} | u_k \rangle$ vanishes. We obtain,

$$\begin{aligned} \langle u_n | \hat{X}^2 | u_n \rangle &= \langle u_n | \hat{X} | u_{n-1} \rangle \langle u_{n-1} | \hat{X} | u_n \rangle \\ &+ \langle u_n | \hat{X} | u_{n+1} \rangle \langle u_{n+1} | \hat{X} | u_n \rangle \\ &\stackrel{\text{Eq. (1)}}{=} \frac{1}{\alpha} \left(\frac{n}{2}\right)^{\frac{1}{2}} \frac{1}{\alpha} \left(\frac{n}{2}\right)^{\frac{1}{2}} + \frac{1}{\alpha} \left(\frac{n+1}{2}\right)^{\frac{1}{2}} \frac{1}{\alpha} \left(\frac{n+1}{2}\right)^{\frac{1}{2}} \\ &= \frac{1}{\alpha^2} \left(\frac{n}{2} + \frac{n+1}{2}\right) = \frac{1}{\alpha^2} \left(\frac{2n+1}{2}\right) = \underline{\underline{\frac{1}{\alpha^2} \left(n + \frac{1}{2}\right)}}. \end{aligned}$$

$$\begin{aligned} \langle u_n | \hat{X}^2 | u_{n+1} \rangle &= \langle u_n | \hat{X} \hat{X} | u_{n+1} \rangle \\ &= \sum_{k=0}^{\infty} \langle u_n | \hat{X} | u_k \rangle \langle u_k | \hat{X} | u_{n+1} \rangle. \text{ Clearly,} \\ \langle u_n | \hat{X} | u_k \rangle &\neq 0 \text{ only if } k = n \pm 1. \text{ However,} \\ \langle u_{n-1} | \hat{X} | u_{n+1} \rangle &\text{ and } \langle u_{n+1} | \hat{X} | u_{n+1} \rangle = 0 \text{ (see Eq. (1))} \\ \text{Thus, } \underline{\underline{\langle u_n | \hat{X}^2 | u_{n+1} \rangle = 0.}} \end{aligned}$$

$$\begin{aligned} \langle u_n | \hat{X}^2 | u_{n+2} \rangle &= \langle u_n | \hat{X} \hat{X} | u_{n+2} \rangle \\ &= \sum_{k=0}^{\infty} \langle u_n | \hat{X} | u_k \rangle \langle u_k | \hat{X} | u_{n+2} \rangle. \text{ Once again,} \\ \langle u_n | \hat{X} | u_k \rangle &\neq 0 \text{ only if } k = n \pm 1. \text{ At the same} \\ \text{time, } \langle u_k | \hat{X} | u_{n+2} \rangle &\neq 0 \text{ only if } k = n+3 \text{ or } \\ n+1. \text{ The only value of } k &\text{ that satisfies both} \end{aligned}$$

(solution of Problem 1 continued)

conditions is $k=n+1$ (other k values result in either $\langle u_n | \hat{x} | u_k \rangle$ or $\langle u_k | \hat{x} | u_{n+2} \rangle$ being zero).

Thus,

$$\begin{aligned} \langle u_n | \hat{x}^2 | u_{n+2} \rangle &= \langle u_n | \hat{x} | u_{n+1} \rangle \langle u_{n+1} | \hat{x} | u_{n+2} \rangle \\ \text{Eq. (1)} \quad &= \frac{1}{\alpha} \left(\frac{n+1}{2} \right)^{\frac{1}{2}} \frac{1}{\alpha} \left(\frac{n+2}{2} \right)^{\frac{1}{2}} = \frac{1}{2\alpha^2} [(n+1)(n+2)]^{\frac{1}{2}}. \end{aligned}$$

$$\begin{aligned} (b) \quad \langle u_n | \hat{x}^3 | u_{n+1} \rangle &= \langle u_n | \hat{x}^2 \hat{x} | u_{n+1} \rangle \\ &= \sum_{k=0}^{\infty} \langle u_n | \hat{x}^2 | u_k \rangle \langle u_k | \hat{x} | u_{n+1} \rangle. \end{aligned}$$

Based on Eq. (1) and part (a), the only terms that enter the summation over k are $k=n$ and $k=n+2$. We obtain,

$$\begin{aligned} \langle u_n | \hat{x}^3 | u_{n+1} \rangle &= \langle u_n | \hat{x}^2 | u_n \rangle \langle u_n | \hat{x} | u_{n+1} \rangle \\ &+ \langle u_n | \hat{x}^2 | u_{n+2} \rangle \langle u_{n+2} | \hat{x} | u_{n+1} \rangle \\ &= \frac{1}{\alpha^2} \left(n + \frac{1}{2} \right) \frac{1}{\alpha} \left(\frac{n+1}{2} \right)^{\frac{1}{2}} + \frac{1}{2\alpha^2} [(n+1)(n+2)]^{\frac{1}{2}} \frac{1}{\alpha} \left(\frac{n+2}{2} \right)^{\frac{1}{2}} \\ &= \frac{1}{2^{3/2} \alpha^3} \left[(2n+1) \underbrace{(n+1)^{\frac{1}{2}}}_{\text{min}} + (n+2) \underbrace{(n+1)^{\frac{1}{2}}}_{\text{min}} \right] \\ &= \frac{(n+1)^{\frac{1}{2}}}{2^{3/2} \alpha^3} (3n+3) = \frac{3}{\alpha^3} \left(\frac{n+1}{2} \right)^{3/2}. \end{aligned}$$

(solution of Problem 1 continued)

2. (5 pts.) Let $u_n(x)$ be the n -th normalized eigenstate of the quantum harmonic oscillator,

$$u_n(x) = N_n H_n(\xi) e^{-\frac{1}{2}\xi^2} \quad (n = 0, 1, 2, \dots),$$

where

$$N_n = \left(\frac{\alpha}{2^n n! \pi^{\frac{1}{2}}} \right)^{\frac{1}{2}},$$

$$\xi = \alpha x, \quad \alpha = \left(\frac{m\omega_c}{\hbar} \right)^{\frac{1}{2}},$$

and H_n are the Hermite polynomials (ω_c is the angular frequency of the corresponding classical harmonic oscillator and m is its mass). Use the generating function for the Hermite polynomials,

$$S(\xi, s) = e^{-s^2 + 2s\xi},$$

to show that

$$\langle u_n | \hat{x}^3 | u_{n+3} \rangle = \frac{[(n+1)(n+2)(n+3)]^{\frac{1}{2}}}{2^{\frac{3}{2}} \alpha^3}.$$

Solution

$$\begin{aligned} \langle u_n | \hat{x}^3 | u_{n+3} \rangle &= \int_{-\infty}^{\infty} u_n^*(x) \hat{x}^3 u_{n+3}(x) dx \\ &\stackrel{\xi = \alpha x}{=} \frac{N_n N_{n+3}}{\alpha^4} \int_{-\infty}^{\infty} H_n(\xi) H_{n+3}(\xi) \xi^3 e^{-\xi^2} d\xi \\ &\stackrel{d\xi = \alpha dx}{=} \frac{N_n N_{n+3}}{\alpha^4} I_{n,n+3}, \text{ where, in general,} \\ I_{n,m} &= \int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) \xi^3 e^{-\xi^2} d\xi. \end{aligned}$$

Consider the following auxiliary integral:

(solution of Problem 2 continued)

$$A = \int_{-\infty}^{\infty} S(\xi, s) S(\xi, t) \xi^3 e^{-\xi^2} d\xi$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n! m!} I_{n,m}.$$

We obtain,

$$A = \int_{-\infty}^{\infty} e^{-s^2 + 2s\xi} e^{-t^2 + 2t\xi} e^{-\xi^2} \xi^3 d\xi$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-(s^2 + t^2 + \xi^2 - 2s\xi - 2t\xi + 2st)} \xi^3 d\xi$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-(\xi - s - t)^2} \xi^3 d\xi$$

$$\begin{aligned} \xi - s - t &= z \\ d\xi &= dz \end{aligned} \quad e^{2st} \int_{-\infty}^{\infty} e^{-z^2} (z + s + t)^3 dz$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-z^2} [z^3 + 3z^2(s+t) + 3z(s+t)^2 + (s+t)^3] dz$$

$$= e^{2st} \left[\int_{-\infty}^{\infty} z^3 e^{-z^2} dz + 3(s+t) \int_{-\infty}^{\infty} z^2 e^{-z^2} dz + 3(s+t)^2 \int_{-\infty}^{\infty} z e^{-z^2} dz + (s+t)^3 \int_{-\infty}^{\infty} e^{-z^2} dz \right]$$

(solution of Problem 2 continued)

$$+ (s+t)^3 \int_{-\infty}^{\infty} e^{-z^2} dz \Big]. \text{ We have,}$$

$$\int_{-\infty}^{\infty} z^3 e^{-z^2} dz = \int_{-\infty}^{\infty} z e^{-z^2} dz = 0, \text{ since } z^3 e^{-z^2} \text{ and } z e^{-z^2} \text{ are odd functions of } z.$$

Furthermore, from the formula on page 20,

$$\int_{-\infty}^{\infty} z^2 e^{-z^2} dz = \frac{2!}{2^2 1!} \sqrt{\pi} = \frac{1}{2} \sqrt{\pi},$$

$$\int_{-\infty}^{\infty} e^{-z^2} dz = \frac{0!}{2^0 0!} \sqrt{\pi} = \sqrt{\pi}.$$

$$\begin{aligned} \text{Thus, } A &= e^{2st} \sqrt{\pi} \left[\frac{3}{2}(s+t) + (s+t)^3 \right] \\ &= e^{2st} \sqrt{\pi} \left(\frac{3}{2}s + \frac{3}{2}t + s^3 + 3s^2t + 3st^2 + t^3 \right) \\ &= \sqrt{\pi} \left(\sum_n \frac{3 \cdot 2^{n-1} s^{n+1} t^n}{n!} + \sum_n \frac{3 \cdot 2^{n-1} s^n t^{n+1}}{n!} \right. \\ &\quad \left. + \sum_n \frac{2^n s^{n+3} t^n}{n!} + \sum_n \frac{3 \cdot 2^n s^{n+2} t^{n+1}}{n!} \right) \end{aligned}$$

(solution of Problem 2 continued)

$$+ \sum_n \frac{3 \cdot 2^n s^{n+1} t^{n+2}}{n!} + \sum_n \frac{2^n s^n t^{n+3}}{n!} \Bigg).$$

On the other hand, $A = \sum_{n,m=0}^{\infty} \frac{s^n t^m}{n! m!} I_{n,m}$.

We are interested in $I_{n,n+3}$, i.e., terms at $s^n t^{n+3}$.

We obtain,

$$\frac{I_{n,n+3}}{n! (n+3)!} = \sqrt{\pi} \frac{2^n}{n!},$$

or

$$I_{n,n+3} = \sqrt{\pi} 2^n (n+3)!.$$

Thus,

$$\begin{aligned} \langle u_n | \hat{x}^3 | u_{n+3} \rangle &= \frac{N_n N_{n+3}}{\alpha^4} I_{n,n+3} \\ &= \left(\frac{\alpha}{2^n n! \sqrt{\pi}} \right)^{\frac{1}{2}} \left(\frac{\alpha}{2^{n+3} (n+3)! \sqrt{\pi}} \right)^{\frac{1}{2}} \frac{1}{\alpha^4} \sqrt{\pi} 2^n (n+3)! \\ &= \frac{\cancel{\alpha}}{\alpha^4 \cancel{3}} \frac{1}{\cancel{2^n n! \sqrt{\pi}}} \left(\frac{1}{2^3 (n+1)(n+2)(n+3)} \right)^{\frac{1}{2}} \\ &\quad \times \cancel{\sqrt{\pi}} \cancel{2^n} (n+3)! = \frac{1}{2^{\frac{3}{2}} \alpha^3} \frac{(n+1)(n+2)(n+3)}{[(n+1)(n+2)(n+3)]^{\frac{1}{2}}} \\ &= \frac{[(n+1)(n+2)(n+3)]^{\frac{1}{2}}}{2^{\frac{3}{2}} \alpha^3}. \end{aligned}$$

3. (6 pts.) The angular momentum raising and lowering operators, $\hat{L}_+$ and $\hat{L}_-$, respectively, are defined as follows,

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y, \quad \hat{L}_- = \hat{L}_x - i\hat{L}_y.$$

One can easily prove that

$$[\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z.$$

One can also show that

$$\hat{L}_+ Y_{\ell,m}(\theta, \phi) = [(\ell - m)(\ell + m + 1)]^{\frac{1}{2}} \hbar Y_{\ell,m+1}(\theta, \phi), \quad (1)$$

$$\hat{L}_- Y_{\ell,m}(\theta, \phi) = [(\ell + m)(\ell - m + 1)]^{\frac{1}{2}} \hbar Y_{\ell,m-1}(\theta, \phi), \quad (2)$$

and

$$\hat{L}_z Y_{\ell,m}(\theta, \phi) = m\hbar Y_{\ell,m}(\theta, \phi), \quad (3)$$

where $Y_{\ell,m}(\theta, \phi)$ are the functions known as spherical harmonics.

(a) (3 pts.) Show that the operator $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ can be expressed in terms of $\hat{L}_+$, $\hat{L}_-$, and $\hat{L}_z$ in the following way,

$$\hat{L}^2 = \hat{L}_+ \hat{L}_- + \hat{L}_z(\hat{L}_z - \hbar). \quad (4)$$

(b) (3 pts.) Use Eqs. (1)–(4) to prove the well-known formula,

$$\hat{L}^2 Y_{\ell,m}(\theta, \phi) = \ell(\ell + 1)\hbar^2 Y_{\ell,m}(\theta, \phi).$$

Solution

(a) $\hat{L}_+ = \hat{L}_x + i\hat{L}_y, \quad \hat{L}_- = \hat{L}_x - i\hat{L}_y.$

Solving for $\hat{L}_x$ and $\hat{L}_y$,

$$\hat{L}_x = \frac{1}{2}(\hat{L}_+ + \hat{L}_-), \quad \hat{L}_y = \frac{1}{2i}(\hat{L}_+ - \hat{L}_-).$$

Thus,

$$\begin{aligned} \hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = \frac{1}{4}(\cancel{\hat{L}_+^2} + \hat{L}_+ \hat{L}_- \\ &\quad + \hat{L}_- \hat{L}_+ + \cancel{\hat{L}_-^2}) - \frac{1}{4}(\cancel{\hat{L}_+^2} - \hat{L}_+ \hat{L}_- \\ &\quad - \hat{L}_- \hat{L}_+ + \cancel{\hat{L}_-^2}) + \hat{L}_z^2, \quad \text{or} \end{aligned}$$

(solution of Problem 3 continued)

$$\begin{aligned}\hat{L}^2 &= \frac{1}{4} (2\hat{L}_+\hat{L}_- + 2\hat{L}_-\hat{L}_+) + \hat{L}_z^2 \\ &= \frac{1}{2} (\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+) + \hat{L}_z^2.\end{aligned}$$

Now, $[\hat{L}_+, \hat{L}_-] = \hat{L}_+\hat{L}_- - \hat{L}_-\hat{L}_+ = 2\hbar\hat{L}_z,$

so that $\hat{L}_-\hat{L}_+ = \hat{L}_+\hat{L}_- - 2\hbar\hat{L}_z.$

As a result,

$$\begin{aligned}\hat{L}^2 &= \frac{1}{2} (\hat{L}_+\hat{L}_- + \hat{L}_+\hat{L}_- - 2\hbar\hat{L}_z) + \hat{L}_z^2 \\ &= \hat{L}_+\hat{L}_- - \hbar\hat{L}_z + \hat{L}_z^2 \\ &= \underline{\underline{\hat{L}_+\hat{L}_- + \hat{L}_z(\hat{L}_z - \hbar)}}.\end{aligned}$$

$$(b) \quad \hat{L}^2 Y_{l,m} = \hat{L}_+\hat{L}_- Y_{l,m} + \hat{L}_z(\hat{L}_z - \hbar) Y_{l,m},$$

where $Y_{l,m} \equiv Y_{l,m}(\theta, \varphi).$

$$\hat{L}_+\hat{L}_- Y_{l,m} \stackrel{\text{Eq. (2)}}{=} \hat{L}_+ \left[(l+m)(l-m+1) \right]^{\frac{1}{2}} \hbar Y_{l,m-1}$$

(solution of Problem 3 continued)

$$\begin{aligned} &= [(\ell+m)(\ell-m+1)]^{\frac{1}{2}} \hbar \hat{L}_+ Y_{\ell, m-1} \\ &\stackrel{\text{Eq. (1)}}{=} [(\ell+m)(\ell-m+1)]^{\frac{1}{2}} \hbar [(\ell-m+1)(\ell+m)]^{\frac{1}{2}} \hbar Y_{\ell, m} \\ &= (\ell+m)(\ell-m+1) \hbar^2 Y_{\ell, m} . \end{aligned}$$

Thus,

$$\hat{L}^2 Y_{\ell, m} = [(\ell+m)(\ell-m+1) \hbar^2 + m(m-1) \hbar^2] Y_{\ell, m}$$

since

$$\hat{L}_z (\hat{L}_z - \hbar) Y_{\ell, m} = m(m-1) \hbar^2 Y_{\ell, m} .$$

We obtain,

$$\begin{aligned} \hat{L}^2 Y_{\ell, m} &= [(\ell+m)(\ell-m) + \cancel{\ell+m} + \cancel{m^2} - \cancel{m}] \hbar^2 Y_{\ell, m} \\ &= (\cancel{\ell^2} - \cancel{m^2} + \cancel{\ell} + \cancel{m^2}) \hbar^2 Y_{\ell, m} \\ &= \underline{\underline{\ell(\ell+1) \hbar^2 Y_{\ell, m}}} . \end{aligned}$$

(solution of Problem 3 continued)

4. (6 pts.) The normalized ground-state wave function for the particle in the one-dimensional square well potential

$$V(x) = \begin{cases} 0 & \text{for } -a < x < a \\ +\infty & \text{for } |x| > a \end{cases}$$

is given by the following formula:

$$u(x) = \begin{cases} \frac{1}{\sqrt{a}} \cos \frac{\pi}{2a} x & \text{for } -a < x < a \\ 0 & \text{for } |x| \geq a \end{cases} \quad (1)$$

Calculate the product of uncertainties $\Delta x \Delta p_x$ for the particle described by the wave function $u(x)$, Eq. (1). Compare the result with the lower-bound for $\Delta x \Delta p_x$ resulting from the Heisenberg relation, i.e., $\hbar/2$.

Solution

$$(\Delta x)^2 = \langle u | (\hat{x} - \langle u | \hat{x} | u \rangle)^2 | u \rangle,$$

$$(\Delta p_x)^2 = \langle u | (\hat{p}_x - \langle u | \hat{p}_x | u \rangle)^2 | u \rangle.$$

$$\begin{aligned} \langle u | \hat{x} | u \rangle &= \int_{-\infty}^{\infty} u(x)^* \hat{x} u(x) dx \\ &= \frac{1}{a} \int_{-a}^a \left(\cos \frac{\pi}{2a} x \right)^2 x dx = 0 \quad (\text{odd function}). \end{aligned}$$

$$\begin{aligned} \langle u | \hat{p}_x | u \rangle &= \int_{-\infty}^{\infty} u(x)^* \hat{p}_x u(x) dx \\ &= \frac{1}{a} \int_{-a}^a \left(\cos \frac{\pi}{2a} x \right) \frac{\hbar}{i} \frac{d}{dx} \left(\cos \frac{\pi}{2a} x \right) dx \\ &= -\frac{\hbar}{a i} \frac{\pi}{2a} \int_{-a}^a \left(\cos \frac{\pi}{2a} x \right) \left(\sin \frac{\pi}{2a} x \right) dx = 0, \\ &\quad (\text{odd function}) \end{aligned}$$

(solution of Problem 4 continued)

Thus,

$$(\Delta x)^2 = \langle u | \hat{x}^2 | u \rangle,$$

$$(\Delta p_x)^2 = \langle u | \hat{p}_x^2 | u \rangle.$$

$$(\Delta x)^2 = \int_{-\infty}^{\infty} u(x)^* \hat{x}^2 u(x) dx$$

$$= \frac{1}{a} \int_{-a}^a x^2 \left(\cos \frac{\pi}{2a} x \right)^2 dx$$

$$\stackrel{p.20}{=} \frac{1}{a} \int_{-a}^a x^2 \left(\frac{\cos \frac{\pi}{a} x + 1}{2} \right) dx$$

$$= \frac{1}{a} \left[\frac{1}{2} \int_{-a}^a x^2 \cos \frac{\pi}{a} x dx + \frac{1}{2} \int_{-a}^a x^2 dx \right]$$

$$\stackrel{p.20}{=} \frac{1}{2a} \left[\frac{\left(x^2 \left(\frac{\pi}{a} \right)^2 \sin \frac{\pi}{a} x - 2 \sin \frac{\pi}{a} x + 2 \frac{\pi}{a} x \cos \frac{\pi}{a} x \right)}{\left(\frac{\pi}{a} \right)^3} \right.$$

$$\left. + \frac{x^3}{3} \right]_{x=-a}^{x=+a} = \frac{1}{2a} \left[\frac{a^3}{\pi^3} \left(2 \frac{\pi}{a} \cancel{\cos \frac{\pi}{a}} \right) - 2 \frac{\pi}{a} \cancel{(-a)} \cos \frac{\pi}{a} \cancel{(-a)} + \frac{a^3}{3} - \frac{(-a)^3}{3} \right]$$

(solution of Problem 4 continued)

$$= \frac{1}{2a} \left[\frac{a^3}{\pi^3} (-4\pi) + \frac{2a^3}{3} \right]$$

$$= a^2 \left(\frac{1}{3} - \frac{2}{\pi^2} \right).$$

$$(\Delta p_x)^2 = \int_{-\infty}^{\infty} u(x)^* \hat{p}_x^2 u(x) dx$$

$$= \frac{1}{a} \int_{-a}^a \left(\cos \frac{\pi}{2a} x \right) \left(\frac{\hbar}{i} \right)^2 \frac{d^2}{dx^2} \left(\cos \frac{\pi}{2a} x \right) dx$$

$$= \frac{\hbar^2}{a} \left(\frac{\pi}{2a} \right)^2 \int_{-a}^a \left(\cos \frac{\pi}{2a} x \right)^2 dx$$

$$\stackrel{p.20}{=} \frac{\hbar^2 \pi^2}{4a^3} \int_{-a}^a \left(\frac{\cos \frac{\pi}{a} x + 1}{2} \right) dx$$

$$= \frac{\hbar^2 \pi^2}{4a^3} \left[\frac{1}{2} \int_{-a}^a \left(\cos \frac{\pi}{a} x \right) dx + \frac{1}{2} \int_{-a}^a dx \right]$$

$$= \frac{\hbar^2 \pi^2}{4a^3} \left[\frac{1}{2} \frac{a}{\pi} \left(\sin \frac{\pi}{a} x \right) + \frac{1}{2} x \right]_{x=-a}^{x=+a}$$

$$= \frac{\hbar^2 \pi^2}{4a^3} a = \frac{\hbar^2 \pi^2}{4a^2}.$$

(solution of Problem 4 continued)

Thus, $(\Delta x)^2 = a^2 \left(\frac{1}{3} - \frac{2}{\pi^2} \right),$

$$(\Delta p_x)^2 = \frac{\hbar^2 \pi^2}{4a^2},$$

and

$$\begin{aligned} (\Delta x)^2 (\Delta p_x)^2 &= \cancel{a^2} \left(\frac{1}{3} - \frac{2}{\pi^2} \right) \frac{\hbar^2 \pi^2}{\cancel{4a^2}} \\ &= \frac{\hbar^2}{4} \left(\frac{\pi^2}{3} - 2 \right), \end{aligned}$$

so that

$$\underline{(\Delta x)(\Delta p_x) = \frac{\hbar}{2} \sqrt{\frac{\pi^2}{3} - 2}}.$$

Since $\pi > 3$, $\frac{\pi^2}{3} > \frac{3^2}{3} = 3$, and

$$(\Delta x)(\Delta p_x) > \frac{\hbar}{2} \sqrt{3-2} = \frac{\hbar}{2}.$$

Potentially useful formulas

- $e^{-s^2+2s\xi} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n$
- $\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2} dx = \frac{(2n)!}{2^{2n} n!} \sqrt{\frac{\pi}{a^{2n+1}}}, \quad (a > 0, n = 0, 1, 2, \dots)$
- $\int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}, \quad (a > 0, n = 0, 1, 2, \dots)$
- $\int x^2 \cos(ax) dx = \frac{x^2 a^2 \sin(ax) - 2 \sin(ax) + 2ax \cos(ax)}{a^3}$
- $\cos 2x = 2 \cos^2 x - 1$