Department of Chemistry, Michigan State University

CEM 991, Fall 2023

Midterm Exam II

Deadline for Submitting Solutions to the Instructor: December 6, 2023, 4:10 pm EST

Name (Last, First, Middle Initial):
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 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. Return 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,

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

where

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

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

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

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

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

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

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

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

(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

(*solution of Problem 1 continued*)

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

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

where

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

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

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

(solution of Problem 2 continued)

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

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

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

and

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

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,

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

(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

(*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:

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

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

Potentially useful formulas

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