

Department of Chemistry, Michigan State University

CEM 991, Fall 2023

Midterm Exam I

Deadline for Submitting Solutions to the Instructor: November 13, 2023, 4:10 pm EDT

Name (Last, First, Middle Initial):

Student 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 point earned in this exam is equivalent to 1 % of the final grade.
- Check that your booklet contains all 18 pages.
- Write your name and student ID number in the spaces provided above.
- Answer in the spaces provided. Use the extra pages 16-18 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	/6
2	/6
3	/4
4	/5
5	/4
Total	/25

1. (6 pts.) Consider a classical particle with mass m under the influence of a force derived from the potential $V(\mathbf{r}, t)$ (no constraints). Let x_1 , x_2 , and x_3 define the Cartesian components of the radius vector $\mathbf{r}$ from the origin to the particle and let ρ , ϕ , and z designate the cylindrical components of $\mathbf{r}$, so that

$$\begin{aligned}x_1 &= \rho \cos \phi, \\x_2 &= \rho \sin \phi, \\x_3 &= z.\end{aligned}$$

- (a) Derive the formula for the kinetic energy of the particle in cylindrical coordinates (3 pts.).
- (b) Derive the explicit formula for the Hamilton function (Hamiltonian) of the particle in cylindrical coordinates assuming that $V = \frac{1}{2}K\rho^2$ (K is a constant) (3 pts.).

Solution

(solution of Problem 1 continued)

(solution of Problem 1 continued)

2. (6 pts.) Consider a normalized one-dimensional wave packet $\psi = \psi(x, t)$ under the influence of a force derived from the real potential $V = V(x, t)$. The mass of the corresponding classical particle is designated by m . Use the time-dependent Schrödinger equation to show that

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{1}{m}\langle\hat{p}_x\rangle, \quad (1)$$

where $\hat{x}$ and $\hat{p}_x$ are the coordinate and momentum operators, respectively, and

$$\langle\hat{F}\rangle = \int_{-\infty}^{+\infty} \psi^* \hat{F} \psi dx$$

represents the expectation value of operator $\hat{F}$. Briefly comment on Eq. (1).

Hints: Use the equations

$$\int_{-\infty}^{+\infty} \psi^* \frac{\partial^2 \phi}{\partial x^2} dx = \int_{-\infty}^{+\infty} \left(\frac{\partial^2 \psi^*}{\partial x^2} \right) \phi dx$$

and

$$\frac{\partial^2 fg}{\partial x^2} = \frac{\partial^2 f}{\partial x^2} g + 2 \frac{\partial f}{\partial x} \frac{\partial g}{\partial x} + f \frac{\partial^2 g}{\partial x^2},$$

where ψ and ϕ are functions that vanish at $x = \pm\infty$ and f and g are arbitrary functions.

Solution

(solution of Problem 2 continued)

(solution of Problem 2 continued)

(solution of Problem 2 continued)

3. (4 pts.) Let $\hat{H}$, $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$, $\hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z})$, and $\hat{V}$ designate the Hamiltonian, momentum, coordinate, and potential energy operators, respectively, for a single particle in three dimensions. Use the following commutator relationships:

$$[\hat{x}, \hat{H}] = \frac{i\hbar}{m} \hat{p}_x,$$

$$[\hat{p}_x, \hat{H}] = -i\hbar \frac{\partial \hat{V}}{\partial x},$$

and analogous formulas for $[\hat{y}, \hat{H}]$ and $[\hat{p}_y, \hat{H}]$ to show that

$$[\hat{L}_z, \hat{H}] = i\hbar \hat{D}_z,$$

where $\hat{L}_z$ and $\hat{D}_z$ are the operators representing the z components of the angular momentum ($\mathbf{L} = \mathbf{r} \times \mathbf{p}$) and torque ($\mathbf{D} = \mathbf{r} \times \mathbf{F}$). Can you tell, without performing any additional calculations, what would the formulas for the Poisson brackets of x and H , p_x and H , and L_z and H be? If you can tell this, please write down these formulas.

Auxiliary formula: $[\hat{F}_1 \hat{F}_2, \hat{G}] = \hat{F}_1 [\hat{F}_2, \hat{G}] + [\hat{F}_1, \hat{G}] \hat{F}_2$.

Solution

(solution of Problem 3 continued)

4. (5 pts.) The ground and first-excited eigenstates of the one-dimensional harmonic oscillator are described by the following normalized wave functions:

$$u_0(x) = \sqrt{\frac{\alpha}{\pi^{\frac{1}{2}}}} e^{-\frac{1}{2}\alpha^2 x^2},$$

and

$$u_1(x) = \sqrt{\frac{2\alpha^3}{\pi^{\frac{1}{2}}}} x e^{-\frac{1}{2}\alpha^2 x^2},$$

respectively. Here, $\alpha = (\frac{m\omega}{\hbar})^{\frac{1}{2}}$, where m is the oscillator's mass and ω is the angular frequency.

- (a) Show that u_0 and u_1 are orthogonal. (1 pt.)
- (b) The energy eigenvalue E_0 corresponding to the ground eigenstate u_0 is $\frac{1}{2}\hbar\omega$. Calculate the expectation value $\langle \hat{V} \rangle_0$ of the potential energy operator $\hat{V} = \frac{1}{2}m\omega^2 \hat{x}^2$ in the state described by u_0 . Compare $\langle \hat{V} \rangle_0$ with E_0 . (2 pts.)
- (c) Based on the relationship between $\langle \hat{V} \rangle_0$ and E_0 obtained in part (b), determine the expectation value of the kinetic energy operator $\hat{T} = \frac{\hat{p}_x^2}{2m}$ in the state described by u_0 . (2 pts.)

Auxiliary formula: $\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2} dx = \frac{(2n)!}{2^{2n}n!} \sqrt{\frac{\pi}{a^{2n+1}}}, a > 0, n = 0, 1, 2, \dots$

Solution

(solution of Problem 4 continued)

(solution of Problem 4 continued)

5. (4 pts.) Operator U is called *unitary* if (i) its domain is the entire Hilbert space ($D(U) = \mathcal{H}$) (ii) its range is the entire Hilbert space ($\Delta(U) = \mathcal{H}$), and (iii) for every $f, g \in \mathcal{H}$ we can write

$$(Uf, Ug) = (f, g). \quad (1)$$

The above definition of a unitary operator does not mention that unitary operators are also linear operators, and yet it can be shown that they are linear. In particular,

$$U(f + g) = Uf + Ug \quad (2)$$

for all $f, g \in \mathcal{H}$. Use the inner product expression $(U(f + g) - Uf - Ug, U(f + g) - Uf - Ug)$, the bilinearity and positive-definiteness of the inner product, and the property represented by Eq. (1) to show that Eq. (2) is indeed true.

Solution

(solution of Problem 5 continued)

