

Department of Chemistry, Michigan State University

CEM 991, Fall 2021

Midterm Exam I

Deadline for Emailing Solutions to the Instructor: November 8, 2021, 8:00 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 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	/7
2	/5
3	/4
4	/5
5	/4
Total	/25

1. (7 pts.) Consider a classical particle with mass m under the influence of a force derived from the potential $V(\rho, t) = \frac{1}{2}K\rho^2$, where $\rho = \sqrt{x^2 + y^2}$ and K is a constant. Let us assume that the motion of the particle is constrained by the condition $z = 0$, i.e., the particle is forced to remain on the (x, y) plane, and let ρ and ϕ designate the polar coordinates, so that

$$\begin{aligned}x &= \rho \cos \phi, \\y &= \rho \sin \phi.\end{aligned}$$

- (a) Derive the formula for the kinetic energy of the particle in polar coordinates and write the corresponding Lagrange function (Lagrangian). (3 pts.)
- (b) Derive the explicit form of the Lagrange equations in terms of ρ and ϕ and their time derivatives. (2 pts.)
- (c) Derive the explicit formula for the Hamilton function (Hamiltonian) in terms of ρ , ϕ , p_ρ , and p_ϕ . (2 pts.)

Solution

(solution of Problem 1 continued)

(solution of Problem 1 continued)

2. (5 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.) Let A be a linear operator whose domain is the entire Hilbert space $\mathcal{H}$.
- (a) Assuming that operator A represents a one-to-one mapping of $\mathcal{H}$ onto itself, i.e., the domain and range of A are $\mathcal{H}$ and the inverse operator A^{-1} exists, prove that $(A^{-1})^\dagger = (A^\dagger)^{-1}$. (2 pts.)
Hint: Consider the following inner product expression: $(f, A^{-1}Ag) = (f, g)$ for all $f, g \in \mathcal{H}$.
- (b) Assuming that operator A is unitary, i.e., $(Af, Ag) = (f, g)$ for every $f, g \in \mathcal{H}$, show that it is also bounded, i.e., that there exists a real number $M > 0$ such that $\|Af\| \leq M\|f\|$ for every $f \in \mathcal{H}$. What is the smallest value of M in the last inequality? (2 pts.)

Solution

(solution of Problem 5 continued)

