Homework 2

Due: February 2 at 11:59 PM. Submit on Canvas.

Problem 1: Let $k \geq 0$ be an integer. Consider a quantum harmonic oscillator, with angular frequency ω, in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} \left[|2k\rangle + |2k+1\rangle \right]. \tag{1}$$

10   **A:** What is $|\psi(t)\rangle$? Is this state stationary?

15   **B:** Evaluate the expectation value of the momentum: $\langle \psi(t)|p|\psi(t)\rangle$.

10   **C:** Suppose that we measure the energy H at time $t = \pi/\omega$.

     C1. What are the possible outcomes we can get? What is the probability of each?

     C2. For $t > \pi/\omega$, what can you say about $\langle \psi(t)|p|\psi(t)\rangle$?

Problem 2 (Quantum optics): The electric field of a monochromatic plane wave can be written as

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}^-(\mathbf{x}, t) + \mathbf{E}^+(\mathbf{x}, t), \tag{2a}$$

$$\mathbf{E}^-(\mathbf{x}, t) = \mathbf{C} e^{i\mathbf{k} \cdot \mathbf{x} - i\omega t} a, \tag{2b}$$

$$\mathbf{E}^+(\mathbf{x}, t) = \mathbf{C} e^{-i\mathbf{k} \cdot \mathbf{x} + i\omega t} a^\dagger, \tag{2c}$$

with $\omega = c|\mathbf{k}|$. The constant spatial vector $\mathbf{C}$ will not be important to us in this problem. The a and $a^\dagger$ in these formulas represent raising and lowering operators of a quantum harmonic oscillator, obeying $[a, a^\dagger] = 1$. The intensity operator is given by

$$I = \mathbf{E}^+ \cdot \mathbf{E}^-. \tag{3}$$

10   **A:** Suppose we look at the relative strength of fluctuations in the instantaneous intensity,

$$g = \frac{\langle \psi|I^2|\psi\rangle}{\langle \psi|I|\psi\rangle^2} = \frac{\left\langle \psi \left| \left(a^\dagger a\right)^2 \right| \psi \right\rangle}{\langle \psi|a^\dagger a|\psi\rangle^2}. \tag{4}$$

Explain why $g \geq 1$, in quantum mechanics.

10   **B:** In quantum optics, your photodetector will not measure g. Instead, you measure

$$g' = \frac{\left\langle \psi \left| \left(a^\dagger\right)^2 a^2 \right| \psi \right\rangle}{\langle \psi|a^\dagger a|\psi\rangle^2}. \tag{5}$$

In classical physics, a and $a^\dagger$, which are related to the amplitudes of the electric field $\mathbf{E}^\pm$, commute, so $g = g'$. Show however that in quantum mechanics, $g \neq g'$, by finding a state $|\psi\rangle$ in which $g' < 1$, while $g \geq 1$. The experimental observation $g' < 1$ confirmed the quantum nature of light in the 1960s.

Problem 3 (Atom in a harmonic trap): In this problem we will describe atoms in a harmonic trap. This qualitative type of experiment is routinely done locally here at JILA, and relies on the angular momentum of the atom to couple to a magnetic field (as we will detail a little more later in the class). For now, you can think that the Hamiltonian of the atom is

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \alpha B \tag{6}$$

where $m \approx 10^{-26}$ kg is the atomic mass (here we assume that the atom is Li), and $\alpha \approx 10^{-23}$ J/T is a constant. B represents the modulus of the local magnetic field. An atom trap can be made by combining a large, uniform, rotating magnetic field

$$\mathbf{B}_{\text{rot}} = B_1 \left(\cos(\omega t)\hat{\mathbf{x}} + \sin(\omega t)\hat{\mathbf{y}} \right) \tag{7}$$

with a "quadrupole" magnetic field

$$\mathbf{B}_{\text{quad}} = \frac{B_2}{L} \left(x\hat{\mathbf{x}} + y\hat{\mathbf{y}} - 2z\hat{\mathbf{z}} \right). \tag{8}$$

You can check that both fields obey $\nabla \cdot \mathbf{B} = 0$, so are physical.

10 **A:** Let us begin by showing that H is approximately a three-dimensional harmonic oscillator.

    A1. Evaluate $B = |\mathbf{B}_{\text{rot}} + \mathbf{B}_{\text{quad}}|$ by taking the length of the combined vector.

    A2. Assume that B_1 is very large, so that you can do a Taylor expansion in B_2. Show that

$$B \approx B_1 + \frac{B_2}{L} \left(x\cos(\omega t) + y\sin(\omega t) \right) + \frac{B_2^2}{2L^2 B_1} \left(x^2 + y^2 + 4z^2 - (x\cos(\omega t) + y\sin(\omega t))^2 \right). \tag{9}$$

    A3. An effective time-independent H can be found by averaging over the t variable. By evaluating the integrals over $\sin(\omega t)$, $\cos(\omega t)$ and their appropriate powers, show that this time-independent H is given by

$$H \approx \alpha B_1 + \frac{p_x^2 + p_y^2 + p_z^2}{2m} + \frac{\alpha B_2^2}{4L^2 B_1} \left(x^2 + y^2 + 8z^2 \right). \tag{10}$$

    The first term in H adds an overall constant to your later answers - feel free to ignore it.

    A4. In a real experiment, one might take $B_1 = 15$ mT, $B_2 = 5$ T, $L = 0.5$ m. Based on these numbers, and the harmonic approximation to H given in (10), estimate the size R of the wave function in its ground state (you can take, e.g. the width of the Gaussian wave function to be R). Confirm that $B_1 \gg B_2 R/L$, and therefore that our approximation from A2 is appropriate.

20 **B:** Now we turn to the quantum problem.

    B1. For the Hamiltonian in (10), find the four lowest eigenvalues of H, and all corresponding eigenvectors (you can keep them in bra-ket notation, without finding the position-space answer, as long as you explain conceptually what's going on). As part of your answer describe the degeneracy of these energy levels.

    B2. What is the frequency scale of oscillations of the atom in this harmonic ptotential?

15 **Problem 4:** Numerically solve the differential equation

$$\frac{d^2\psi}{dx^2} + \left(2E - x^2\right)\psi = 0, \tag{11}$$

fixing initial conditions $\psi(0) = 1$ and $\frac{d\psi}{dx}(0) = 0$.[1] This is the harmonic oscillator's Schrödinger equation in units where $\hbar = m = \omega = 1$. Describe what you find for the numerical solutions for E in the domain $0 < E < 3$, and explain what is going on.

Problem 5 (Carbon dioxide): The CO_2 molecule is a linear molecule with a central carbon atom surrounded by two oxygen atoms. Assuming for simplicity that the molecule moves in one spatial dimension, approximating that the only degrees of freedom are the atomic positions, and approximating each covalent bond with a harmonic oscillator, the Hamiltonian describing this molecule's dynamics is

$$H = \frac{p_1^2}{2m_O} + \frac{p_2^2}{2m_C} + \frac{p_3^2}{2m_O} + \frac{k}{2}\left(x_1 - x_2\right)^2 + \frac{k}{2}\left(x_2 - x_3\right)^2. \tag{12}$$

10 **A:** There is a general strategy (that you may have learned in classical mechanics) for solving *coupled harmonic oscillators*. Let us denote $p_i = (p_1, p_2, p_3)$ as the three momenta, and $x_i = (x_1, x_2, x_3)$ as the three coordinates. We look for an invertible matrix S_{ij} such that we can define coordinates

$$P_i = \sum_{j=1}^{3} S_{ij}p_j, \tag{13a}$$

$$X_i = \sum_{j=1}^{3} S_{ji}^{-1}x_j, \tag{13b}$$

and that in these coordinates,

$$H = \sum_{j=1}^{3} \frac{1}{2}\left[P_j^2 + \omega_j^2 X_j^2\right]. \tag{14}$$

A1. To show why this is a good idea, begin by evaluating the commutators $[X_i, P_j]$.

A2. Explain how to find the eigenvalues and eigenfunctions of H, as given in (14). You do not need to, as of yet, actually find ω_j for CO_2 – we'll do that next.

10 **B:** Now we turn to the CO_2 molecule. We'll need the matrix S_{ij}. To do this, we look for a matrix $S = R \cdot \tilde{S}$ (a product of two matrices). Define $\tilde{P}_i$ and $\tilde{X}_i$ as in (13), but using $\tilde{S}$.

B1. Find a simple (diagonal) matrix $\tilde{S}$ such that

$$H = \sum_{j=1}^{3} \frac{\tilde{P}_j^2}{2} + \sum_{i,j=1}^{3} \frac{1}{2}\tilde{X}_i\tilde{K}_{ij}\tilde{X}_j. \tag{15}$$

The matrix $\tilde{K}$ does not need to be diagonal, but it should be symmetric.

B2. Describe qualitatively how to find ω_j^2 in (14), given the matrix $\tilde{K}$.

B3. Find the matrix R, and/or deduce expressions for X_i in terms of the original x_j coordinates. The X_i are called *normal mode* (coordinates): describe the physical motion of the CO_2 molecule in each of your three normal modes.

B4. What are the eigenvalues of H for the CO_2 molecule? Qualitatively describe the eigenfunctions.

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[1] *Hint:* I suggest using `NDSolve` in `Mathematica`. You should be able to modify the example given in the documentation to solve this problem using about one line of code (for each E).