

Problem 1. (This is a conceptual question.) Consider a quantum mechanical system in a superposition state in which the wave function $\Psi(x, t)$ is a linear combination of two wave functions each corresponding to a stationary state as specified below. Assume arbitrary nonzero projection coefficients (b_1 and b_2). *Is this superposition state a stationary state?* Answer this question for the following two cases. Explain your reasoning and support your answer by equations/calculations. *Reminder:* in the stationary state the probability density is time independent.

A. Particle on a ring (2D rigid rotor). The two wave functions describe rotational states with the quantum numbers $m_l = -1$ and $m_l = 2$.

B. Particle on a sphere (3D rigid rotor). The two wave functions describe rotational states with the quantum numbers: $l = 2, m_l = -1$ and $l = 2, m_l = 2$. *Note for Spring 2026: Ignore this question because we haven't covered the 3D rigid rotor yet.*

Problem 2. Consider a particle of mass μ moving on a ring of radius r . Assume the ring is placed in the x-y plane. The particle is prepared in a superposition state described by the following (unnormalized)

wave function: $\Psi(\phi) = \frac{1}{\sqrt{2\pi}} [7e^{i\phi} - 2ie^{i4\phi} + 6e^{-i7\phi}]$. Answer the following four questions.

A. List all values of the energy of the particle that one can obtain in a single measurement in this state and the corresponding probabilities.

B. Calculate the average value of the energy of the particle that would be obtained as a result of many measurements.

C. Calculate the average value of the angular momentum of the particle that would be obtained as a result of many measurements.

D. Is the particle more likely to be found moving in the counterclockwise direction (positive values of the angular momentum, l_z) or clockwise direction (negative l_z)? *Explain your reasoning and support it by calculations. Tip:* this is a probability question.

Problem 3. A quantum mechanical harmonic oscillator with mass μ and force (spring) constant k is in a state characterized by the quantum number $n = 3$. Do the following:

A. Write the expression for the wave function $\Psi(x, t)$ of the oscillator. Make sure the wave function is normalized and explicitly includes the time dependence.

B. Determine the values of coordinate x where you are unlikely to find the oscillator. *Explain your reasoning.*

Problem 4. Your task is to identify and characterize an unknown diatomic molecule X. Here is what you know. When the molecule was placed in a 3D box/cube of size $a = 5 \text{ \AA}$ ($1 \text{ \AA} = 10^{-10} \text{ m}$), the transition from the ground state to the first excited state associated with its translational motion required $1.4169 \times 10^{-23} \text{ J}$ of energy. A transition between the ground state and the first excited vibrational state involved $4.3107 \times 10^{-20} \text{ J}$ of energy. The force (spring) constant characterizing vibrations in this molecule is $1902 \text{ N} \cdot \text{m}^{-1}$ ($1 \text{ N} = 1 \text{ kg} \cdot \text{m} \cdot \text{s}^{-2}$). Answer the following two questions (see next page for question B)

A. Use this information to unambiguously identify the molecule. *Explain your assumptions.* (*Hint:* masses of the atoms in a diatomic molecule can be uniquely identified from the total mass and the reduced mass of the molecule. Consider how the energies of the transitions described above depend on these characteristics.)

B. The quantum of energy required for a transition between the ground state and the first excited rotational state of the molecule in gas phase is 7.6785×10^{-23} J. From these data, determine the equilibrium bond length in the molecule. *Explain your assumptions.*

Some equations and formulae that might or might not be useful:

$$\Delta E = h\nu; \nu = \frac{c}{\lambda}; \lambda = \frac{h}{p}$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}; E_{kinet} = K = \frac{p^2}{2m}$$

$$E = \frac{\hbar^2 k^2}{2m}; \Psi_+(x) = Ae^{ikx}; \Psi_-(x) = Ae^{-ikx}$$

$$E_n = \frac{\hbar^2 n^2}{8ma^2}; \Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a} x\right)$$

$$E_n = (n + \frac{1}{2})h\nu; \Psi_n(x) = A_n H_n(\sqrt{\alpha}x) e^{-\alpha x^2/2}$$

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}; A_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{\alpha}{\pi}\right)^{1/4}$$

$$\alpha = \sqrt{k\mu} / \hbar; \mu = m_1 m_2 / (m_1 + m_2)$$

$$E_{m_l} = \frac{\hbar^2}{2I} m_l^2; \Psi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}} e^{im_l \phi}$$

$$E_l = \frac{l(l+1)\hbar^2}{2I}; \Psi_{l,m_l} = Y_{l,m_l}(\theta, \phi);$$

$$|\vec{l}|^2 = l(l+1)\hbar^2; l_z = m_l \hbar$$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}; \Delta A \times \Delta B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right|$$

Helpful Math:

$$e^{i\alpha} = \cos \alpha + i \sin \alpha;$$

$$\cos \alpha = (e^{i\alpha} + e^{-i\alpha})/2; \sin \alpha = (e^{i\alpha} - e^{-i\alpha})/2i$$

$$\int_0^\infty e^{-ax^2} x^{2n} dx = \sqrt{\frac{\pi}{a}} \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)}{2^{n+1} a^n} \text{ (for } n \geq 1);$$

$$\int_0^a \sin^2\left(\frac{\pi n}{a} x\right) dx = \frac{a}{2}; \int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$h = 6.626 \times 10^{-34} \text{ J s}; \hbar = h/(2\pi)$$

$$c = 3 \times 10^8 \text{ m/s}; k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$$

$$\Delta p_x \cdot \Delta x \geq \frac{\hbar}{2}$$

$$m_e = 9.1 \times 10^{-31} \text{ kg}$$

$$m_p = 1.67 \times 10^{-27} \text{ kg}; 1 \text{ amu} = 1.66 \times 10^{-27} \text{ kg}$$

$$H_0(\sqrt{\alpha}x) = 1; H_1(\sqrt{\alpha}x) = 2\sqrt{\alpha}x$$

$$H_2(\sqrt{\alpha}x) = 2(2\alpha x^2 - 1)$$

$$H_3(\sqrt{\alpha}x) = 4\sqrt{\alpha}x(2\alpha x^2 - 3)$$

$$\hat{l}_z = -i\hbar \frac{\partial}{\partial \phi}; l_z = m_l \hbar; I = \mu r^2$$

$$Y_{0,0}(\theta, \phi) = 1/\sqrt{4\pi}; Y_{1,0}(\theta, \phi) = (3/4\pi)^{1/2} \cos \theta$$

$$Y_{1,\pm 1}(\theta, \phi) = \mp (3/8\pi)^{1/2} \sin \theta e^{\pm i\phi}$$

$$Y_{2,0}(\theta, \phi) = (5/16\pi)^{1/2} (3\cos^2 \theta - 1)$$

$$Y_{2,\pm 1}(\theta, \phi) = \mp (15/8\pi)^{1/2} \cos \theta \sin \theta e^{\pm i\phi}$$

$$Y_{2,\pm 2}(\theta, \phi) = (15/32\pi)^{1/2} \sin^2 \theta e^{\pm 2i\phi}$$

$$\sin 2\alpha = 2 \sin \alpha \cos \alpha; \cos 2\alpha = \cos^2 \alpha - \sin^2 \alpha;$$

$$2 \sin^2 \alpha = 1 - \cos 2\alpha; 2 \cos^2 \alpha = 1 + \cos 2\alpha$$

$$\int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}; \int_0^\infty e^{-ax^2} x^2 dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$$

$$n! = 1 \cdot 2 \cdot \dots \cdot n$$

Some atomic masses (in amu, rounded) of the most abundant isotopes:

H = 1; He = 4; Li = 7; Be = 9; B = 11; C = 12; N = 14; O = 16; F = 19; Ne = 20; Na = 23; Mg = 24; Al = 27; Si = 28; P = 31; S = 32; Cl = 35