INSTRUCTIONS:

- This exam contains four problems plus a bonus question (9 pages total). At the start of the exam make sure you have a complete set of problems.
- It is your responsibility to clearly show all steps in your derivations that might be necessary for judging your work fairly.
- Write legibly!!!
- Use the space on the back of the sheets if necessary.
- The equations sheet in on the last page. You can tear it off if this is more convenient for you. No need to turn in this page.
- Read the questions carefully, think about your answers, and make sure that you answer all parts of each question.
- Provide specific information that answers the question being asked.
- Always explain your reasoning.
- In problems 1-3 and the bonus question, if your answers contain *h* or *ħ* or other constants or physical characteristics with unspecified numeric values, keep them as letters, no need to substitute them with their numeric values.

Problem 1. (20 points) (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 $m_i = -1$ and $m_i = 2$.

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, $m_l = 2$.

Problem 2. (35 points) 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: $\Psi(\phi) = \frac{1}{\sqrt{2\pi}} \left[7e^{i\phi} - 2ie^{i4\phi} + 6e^{-i7\phi} \right]$. Answer the following four

questions (questions C and D are on the next page).

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. (20 points) 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. (25 points) 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 Å (1 Å=10⁻¹⁰ m), the transition from the ground state to the first excited state associated with its translational motion required 1.4169×10^{-23} J of energy. A transition between the ground state and the first excited vibrational state involved 4.3107×10^{-20} J of energy. The force (spring) constant characterizing vibrations in this molecule is 1902 N·m⁻¹ (1 N=1 kg·m·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.)

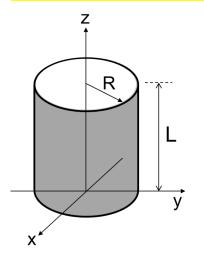
B. The quantum of energy required for a transition between the ground state and the first excited rotational state of the molecule in gas phase is 7.6785×10^{-23} J. From these data, determine the equilibrium bond length in the molecule. *Explain your assumptions*.

If you are done with the rest of the problems, you might want to answer the following conceptual question for an extra credit.

Bonus question. (15 points)

Consider a quantum mechanical particle of mass m moving on the outer surface of a hollow vertical cylinder (tube) of radius R and length L, see the drawing below. Ignore the gravitational force. Write the expressions for the energies and the wave functions that correspond to the stationary states of the particle. *Explain your reasoning*.

Hint: you can but don't need to write and solve the Schrödinger equation to answer these questions – just consider what motions the particle is involved in, try to decompose them into simple independent motions and use solutions to the respective problems that we already covered in this course.



Exam #1

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

$\Delta E = h\nu; \nu = \frac{c}{\lambda}; \lambda = \frac{h}{p}$	$h = 6.626 \times 10^{-34} \text{ J s}; h = h/(2\pi)$ $c = 3 \times 10^8 \text{ m/s}; k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$
$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}; E_{kinet} = K = \frac{p^2}{2m}$	$\Delta p_x \cdot \Delta x \ge \frac{\hbar}{2}$
$E = \frac{\hbar^2 k^2}{2m}; \ \Psi_+(x) = A e^{ikx}; \ \Psi(x) = A e^{-ikx}$	$m_{\rm e} = 9.1 \times 10^{-31} \rm kg$
$E_n = \frac{h^2 n^2}{8ma^2}; \ \Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a}x\right)$	$m_{\rm p}$ =1.67 ×10 ⁻²⁷ kg; 1 amu = 1.66 ×10 ⁻²⁷ kg
$E_{n} = (n + \frac{1}{2})h\nu; \Psi_{n}(x) = A_{n}H_{n}(\sqrt{\alpha}x)e^{-\alpha x^{2}/2}$ $\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}; \qquad A_{n} = \frac{1}{\sqrt{2^{n}n!}}\left(\frac{\alpha}{\pi}\right)^{1/4}$ $\alpha = \sqrt{k\mu}/\hbar; \mu = m_{1}m_{2}/(m_{1} + m_{2})$	$H_0(\sqrt{\alpha}x) = 1; H_1(\sqrt{\alpha}x) = 2\sqrt{\alpha}x$ $H_2(\sqrt{\alpha}x) = 2(2\alpha x^2 - 1)$ $H_3(\sqrt{\alpha}x) = 4\sqrt{\alpha}x(2\alpha x^2 - 3)$
$E_{m_l} = \frac{\hbar^2}{2I} m_l^2; \Psi_{m_l}(\phi) = \frac{1}{\sqrt{2\pi}} e^{im_l\phi}$	$\hat{l}_{z} = -i\hbar \frac{\partial}{\partial \phi}; \ l_{z} = m_{l}\hbar; \ I = \mu r^{2}$
$E_{l} = \frac{l(l+1)\hbar^{2}}{2I}; \Psi_{l.m_{l}} = Y_{l,m_{l}}(\theta,\phi);$ $\left \vec{l}\right ^{2} = l(l+1)\hbar^{2}; l_{z} = m_{l}\hbar$	$Y_{0,0}(\theta,\phi) = 1/\sqrt{4\pi} ; Y_{1,0}(\theta,\phi) = (3/4\pi)^{1/2} \cos\theta$ $Y_{1,\pm 1}(\theta,\phi) = \mp (3/8\pi)^{1/2} \sin\theta \ e^{\pm i\phi}$ $Y_{2,0}(\theta,\phi) = (5/16\pi)^{1/2} (3\cos^2\theta - 1)$ $Y_{2,\pm 1}(\theta,\phi) = \mp (15/8\pi)^{1/2} \cos\theta \sin\theta \ e^{\pm i\phi}$
$\begin{bmatrix} \hat{A}, \hat{B} \end{bmatrix} = \hat{A}\hat{B} - \hat{B}\hat{A}; \qquad \Delta A \times \Delta B \ge \frac{1}{2} \left \left\langle \begin{bmatrix} \hat{A}, \hat{B} \end{bmatrix} \right\rangle \right $	$Y_{2,\pm 2}(\theta,\phi) = (15/32\pi)^{1/2} \sin^2 \theta e^{\pm 2i\phi}$

Helpful Math:

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

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

 $\frac{\pi}{a}$

$$\int_{0}^{\infty} e^{-ax^{2}} x^{2n} dx = \sqrt{\frac{\pi}{a}} \frac{1 \cdot 3 \cdot 5 \cdot \dots \cdot (2n-1)}{2^{n+1} a^{n}} \text{ (for } n \ge 1\text{)}; \qquad \int_{0}^{\infty} e^{-ax^{2}} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}; \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty} e^{-ax^{2}} x^{2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}, \qquad \int_{0}^{\infty$$

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