Midterm Exam, Phys. Chem. I B (AY2022)

Periods 7-8, Friday, July 8, 2022: Total 45 points

Instructions:

(1) Closed-book exam: use pencils, erasers, and a ruler only.

(2) Work individually on the exam: testing YOUR knowledge. Cheating on the exam shall result in *failing grades* for *all* the specialized courses enrolled during the Semester (both the First and Second Terms). Such a violation leads to disciplinary action as stipulated in the Student Disciplinary Regulations.

(3) Answer the questions in the space provided after the questions. If you need more space to elaborate on your answer, use the blank side of the sheet also. The language for your answers is either *English* or *Japanese*. Write in print, please. Ensure that you include your student ID number and full name at the given spaces.

(4) Show all your process as you solve the problems. Correct but incomplete attempts will obtain partial points, whereas answers without showing your work will not receive points.

受験上の注意：

(1) 資料持込み不可。鉛筆と消しゴムと定規だけ使用する。(2) 個人で取り組む。あなたの知識をみるテストです。不正行為をおこなった者は，今期(第１・第２タームとも)履修しているすべての専門教育科目の評価が「不可」となり，学生懲戒指針に基づき懲戒処分を受けます。(3) 自分の解答は質問の後の与えられたスペースに書く。スペースが足りない場合は用紙の裏面も用いてよい。解答のための言語は「英語または日本語」とする。日本語は楷書で英語はブロック体で書く。自分の学生番号と名前を指定の場所に忘れず書く。(4) 解答プロセスも残す。途中まで正しい答案には部分点を与えるが，答えだけの場合は得点とならない。

Use $\hbar$ to denote Planck's constant divided by 2π. Possibly useful integrals are:

$$\int_0^\infty \exp(-\beta x^2)\,\mathrm{d}x = \frac{1}{2}\sqrt{\frac{\pi}{\beta}}; \quad \int_0^\infty x^{2n}\exp(-\beta x^2)\,\mathrm{d}x = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}}\sqrt{\frac{\pi}{\beta^{2n+1}}};$$

$$\int_0^\infty x^n \exp(-\beta x)\,\mathrm{d}x = \frac{n!}{\beta^{n+1}} \quad (\beta > 0; n, \text{positive integer})$$

where $\exp(x) = \mathrm{e}^x$.

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Problem 1: (14 points)

Read the sentences below and answer the questions that follow.

Consider a one-dimensional oscillating system of a particle with mass m attached to a spring with a force constant k_f. The Schrödinger equation for this quantum model of harmonic oscillation is written as

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+\frac{1}{2}k_f x^2\psi(x)=E\psi(x)$$

where x is the displacement from the equilibrium position, and E and $\psi(x)$ are the total energy and wavefunction, respectively. A solution of the equation has the form of

$$\psi_0(x)=N_0\exp(-\alpha x^2/2)$$

Here, the factor N_0 is the normalization constant, and the coefficient α is found as some positive value.

Question 1) Evaluate E and α for $\psi_0(x)$.

Question 2) The energy obtained in **Question 1** corresponds to the lowest energy possible for the oscillator. This implies that the particle is not completely at rest, even at 0 K. Give and explain another property which shows a striking distinction between the quantum and classical oscillators.

Question 3) Determine N_0 by normalizing $\psi_0(x)$.

Question 4) Calculate the expectation value of the potential energy $\langle V\rangle$ for $\psi_0(x)$.

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Problem 2: (5 points)

The Nobel Prize in Physics 2021 was awarded jointly to Syukuro Manabe, Klaus Hasselmann, and Giorgio Parisi for climate modeling and reliably predicting global warming. Our atmosphere contains greenhouse gases, which prevent heat (infrared light) from escaping into outer space. Computer-based climate models predict that an increase in atmospheric CO_2 should produce a rise in global temperature. Explain the reason from the viewpoint of infrared spectroscopy why N_2, the most abundant gas in our atmosphere, is NOT an offender in global warming.

Problem 3: (8 points)

Describe the way to determine the bond length r of diatomic molecules from their microwave spectra within the rigid rotor approximation. The rotational energy is given by

$$E_l = \frac{\hbar^2}{2I} l(l+1)$$

where l and I are the angular momentum quantum number and the moment of inertia of a diatomic molecule, respectively.

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Problem 4: (18 points)

Consider a rigid rotor model in two dimensions: a particle of mass m moving on a circular path of radius r in the xy-plane. It is better to choose the polar coordinates (r, ϕ) here because r is fixed. Taking the potential energy on the circle as zero ($V = 0$) and introducing the moment of inertia as $I = \boxed{\text{A}}$, one can write the Schrödinger equation as

$$-\frac{\hbar^2}{2I}\frac{\mathrm{d}^2\psi}{\mathrm{d}\phi^2} = E\psi$$

where E is the total energy. The solutions of the equation take the form

$$\psi(\phi) = N\exp(\mathrm{i}m_l\phi)$$

where N is the normalization constant. The quantity m_l is determined from (a)<u>a boundary condition which ψ must satisfy</u>. You see that (b)<u>the magnitude of the angular momentum is quantized in units of $\hbar$</u>.

Question 1) What is the math expression for the blank A? (Write your answer only.)

Question 2) Determine the normalization constant N.

Question 3) Concerning the underlined portion (a): write down the equation to represent the boundary condition, together with its physical basis.

Question 4) Find the allowed values of m_l from the relation you have answered in **Question 3**.

Question 5) Explain the underlined portion (b) by acting the angular momentum operator on $\psi(\phi)$.

Question 6) The lowest energy acceptable to the rotor is zero. Explain the reason why this does not violate the uncertainty principle.

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END OF QUESTIONS

Check your work before submission.