Examination 2004
Quantum Mechanics PHYS3210
Time: 2 hours
Total number of questions 4. Answer all questions.
The questions are of equal value.
Calculators may be used.
This paper may be retained by the candidate.

$$\hbar = 1.054 \times 10^{-34} Js$$

$$1eV = 1.602 \times 10^{-19} J \quad .$$

Question 1

The first three rotational energy levels of the SiO molecule are

$$\begin{aligned}\epsilon_0 &= 0,\\ \epsilon_1 &= 1.8\times 10^{-4} eV,\\ \epsilon_2 &= 5.4\times 10^{-4} eV.\end{aligned}$$

The molecule consists of isotopes ^{28}Si and ^{16}O, $M_O = 26.5\times 10^{-27}kg$, $M_{Si} = 46.5\times 10^{-27}kg$.
1) (2mark) What is the degeneracy of each level? Write wave functions of all quantum states corresponding to these levels in terms of spherical harmonics Y_{lm}.

2) (4marks) Using the energy levels find the moment of inertia I of the molecule and the distance between the Silicon and the Oxygen nuclei.

3) (4marks) The molecule is injected into a region of uniform electric field directed along the z axis, $\vec{\mathcal{E}} = (0, 0, \mathcal{E})$. So the Hamiltonian is

$$H = \frac{\hat{l}^2}{2I} - d(\vec{\mathcal{E}}\cdot\vec{n}),$$

where $d = 1.0\times 10^{-29}Cm$ is the electric dipole moment of the molecule, and $\vec{n}$ is a unit vector directed along the axis of the molecule. Considering the electric interaction term in the Hamiltonian as a perturbation and using second order perturbation theory find an expression for the ground state energy. Using this expression calculate the energy in a field $\mathcal{E} = 100kV/m$. Express your answer in eV.

Question 2

1) (5marks) A quantum system has Hamiltonian $\hat{H} = \hat{H}_0 + \delta\hat{V}$, where $\delta\hat{V}$ represents a small perturbation. Energy levels and eigenstates of $\hat{H}_0$ are known

$$\hat{H}_0 \psi_n^{(0)} = \epsilon_n^{(0)} \psi_n^{(0)} \ .$$

Show that the energy ϵ_n corresponding to the Hamiltonian $\hat{H}$

$$\hat{H}\psi_n = \epsilon_n \psi_n$$

to first order in $\delta\hat{V}$ is

$$\epsilon_n = \epsilon_n^{(0)} + < n|\delta\hat{V}|n > \ .$$

2) (4marks) An electron in a Coulomb field is described by the Hamiltonian

$$\hat{H}_0 = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \ .$$

The ground state energy is $\epsilon_{1s}^{(0)} = -1 \times Ry$, where the Rydberg is $Ry = e^2/(8\pi\epsilon_0 a_B) \approx 13.606 eV$ and the Bohr radius is $a_B \approx 0.53 \times 10^{-10} m$. The corresponding wave function is

$$\psi_{1s} = \frac{1}{\sqrt{\pi a_B^3}} e^{-r/a_B} \ .$$

In a real Hydrogen atom the potential is slightly different from the Coulomb one because of the finite size of the nucleus. Considering the nucleus as a sphere of radius R ($R \approx 0.5 \times 10^{-15} m$) we conclude that

$$V(r) = \begin{cases} -e^2/(4\pi\epsilon_0 R) & , r < R \\ -e^2/(4\pi\epsilon_0 r) & , r > R \end{cases} \ , \tag{1}$$

Using first order perturbation theory find an expression for the shift of the 1s energy level due to the finite size of the nucleus. (Hint: you can simplify your calculations having in mind that $e^{-r/a_B} \approx 1$ at $r < R$.)

2a) (1mark) Calculate value of the energy shift. Express your answer in eV.

Question 3

The spin operator $\hat{\vec{s}}$ for a particle with spin 1/2 (for example an electron) can be expressed in terms of Pauli matrixes $\hat{\vec{\sigma}}$, $\hat{\vec{s}} = \frac{1}{2}\hat{\vec{\sigma}}$,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

1) (4marks) Calculate $\hat{s}^2 = \hat{s}_x^2 + \hat{s}_y^2 + \hat{s}_z^2$ and comment on the result.

2) (6marks) An electron is placed in a static magnetic field $\vec{B} = B(\sin\theta, 0, \cos\theta)$. The interaction of the electron spin with the magnetic field is given by the following Hamiltonian

$$\hat{H} = -\frac{e\hbar}{m_e}(\vec{B}\cdot\hat{\vec{s}}) = -\frac{e\hbar}{2m_e}\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{2}$$

Calculate the eigenvalues and corresponding eigenvectors and discuss the physical significance of your results.