Problem sheet 4: (Hilary Term, Weeks 1–2)

■ *Orbital angular momentum*

4.1 (a) Show explicitly using $\hat{L}_i = \epsilon_{ijk}\hat{x}_j\hat{p}_j$ that $[\hat{L}_i, \hat{x}_j] = \mathrm{i}\hbar\epsilon_{ijk}\hat{x}_k$ and $[\hat{L}_i, \hat{p}_j] = \mathrm{i}\hbar\epsilon_{ijk}\hat{p}_k$.

(b) Evaluate $[\hat{L}_x, \hat{L}_y]$ by writing $\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$ and using the results from part (a) of this question.

(c) You have now evaluated the commutation relation completely generally, but now let's just check that it is consistent with what you get from working in a coordinate representation. Write down expressions for $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ in terms of x, y, z and $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$ and $\frac{\partial}{\partial z}$. Show that for any differentiable function $f(x,y,z)$

$$(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x)f(x,y,z) = \mathrm{i}\hbar\hat{L}_z f(x,y,z).$$

Of course, since the above relation is true for any f, this can be written as an operator equation

$$[\hat{L}_x, \hat{L}_y] = \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x = \mathrm{i}\hbar\hat{L}_z,$$

as you will have found in part (b). Deduce similar expressions for $[\hat{L}_y, \hat{L}_z]$ and $[\hat{L}_z, \hat{L}_x]$.

(d) Defining $\hat{\boldsymbol{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$, show that

$$[\hat{L}_x, \hat{\boldsymbol{L}}^2] = [\hat{L}_y, \hat{\boldsymbol{L}}^2] = [\hat{L}_z, \hat{\boldsymbol{L}}^2] = 0.$$

(Hint: remember $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$.)

(e) What are the values of the components of $\hat{\boldsymbol{L}}$ that you would measure for a wave function given by $\psi(x,y,z) = \psi(|r|)$?

4.2 (a) Verify by brute force that the three functions $\cos\theta$, $\sin\theta\,\mathrm{e}^{\mathrm{i}\phi}$ and $\sin\theta\,\mathrm{e}^{-\mathrm{i}\phi}$ are all eigenfunctions of $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$.

(b) Find normalization constants N for each of the above functions so that

$$\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta\, \sin\theta\, N^2\, |\psi(\theta,\phi)|^2 = 1.$$

(c) Once normalized, these functions are called spherical harmonics and given the symbol $Y_{\ell m}(\theta,\phi)$. Hence deduce that your results are consistent with the functions:

$$Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta; \qquad Y_{11}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{\mathrm{i}\phi}; \qquad Y_{1-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{-\mathrm{i}\phi}.$$

(Note, you can't use this method to get the signs of Y_{10}, Y_{11} and Y_{1-1}. The minus sign in Y_{11} can be deduced by using a raising operator $\hat{L}_+$ on Y_{10}. This is not required.)

(d) Rewrite these functions in terms of spherical polar variables [$x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$] and then sketch $|Y_{10}|^2$, $|Y_{11}|^2$ and $|Y_{1-1}|^2$. (They are angular functions, so keep r fixed and look at the angle dependence. A cross section in the x–z plane will do. Why?)

4.3 The angular part of a system's wavefunction is

$$\langle\theta,\phi|\psi\rangle \propto (\sqrt{2}\cos\theta + \sin\theta\,\mathrm{e}^{-\mathrm{i}\phi} - \sin\theta\,\mathrm{e}^{\mathrm{i}\phi}).$$

What are the possible results of measurement of (a) $\hat{\boldsymbol{L}}^2$, and (b) $\hat{L}_z$, and their probabilities? What is the expectation value of $\hat{L}_z$?

4.4 A system's wavefunction is proportional to $\sin^2\theta\,\mathrm{e}^{2\mathrm{i}\phi}$. What are the possible results of measurements of (a) $\hat{L}_z$ and (b) $\hat{\boldsymbol{L}}^2$?

4.5 A system's wavefunction is proportional to $\sin^2\theta$. What are the possible results of measurements of (a) $\hat{L}_z$ and (b) $\hat{\boldsymbol{L}}^2$? Give the probabilities of each possible outcome.

4.6 A particle of mass m is described the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} - e\mathcal{E}\hat{x}.$$

(a) What is the physical origin of the last term in $\hat{H}$?

(b) Calculate the commutators $[\hat{L}_x, \hat{x}]$, $[\hat{L}_y, \hat{x}]$ and $[\hat{L}_z, \hat{x}]$.

(c) Which of the observables represented by the operators $\hat{\boldsymbol{L}}^2$, $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ are constants of the motion assuming (i) $\mathcal{E} = 0$; (ii) $\mathcal{E} \neq 0$

4.7 Show that $\hat{L}_i$ commutes with $\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{p}}$.

■ *Quantum rotor*

4.8 Explain why the rotational energy levels of a diatomic molecule are given by $E_\ell = \hbar^2\ell(\ell+1)/2I$ where I is the moment of inertia.

Show that for carbon monoxide (CO, in this case with the most common isotopes of carbon and oxygen, i.e. $^{12}\mathrm{C}^{16}\mathrm{O}$) the moment of inertia about the centre of mass is $I = \mu s^2$ where $\mu = 48m_\mathrm{p}/7$ is the reduced mass and s is the intra-nuclear distance. In the rotational spectrum of $^{12}\mathrm{C}^{16}\mathrm{O}$ the line arising from the transition $\ell = 4 \to 3$ is at 461.04077 GHz, while that arising from $\ell = 36 \to 35$ is at 4115.6055 GHz. Show from these data that in a non-rotating CO molecule the intra-nuclear distance is $s \sim 0.113\,\mathrm{nm}$, and that the electrons in the C—O bond act like a spring connecting the nuclei with a force constant $\sim 1904\,\mathrm{N\,m^{-1}}$. Hence show that the vibrational frequency of CO should lie near 6.47×10^{13} Hz (measured value is 6.43×10^{13} Hz).

[Hint: recall the classical relation $L = I\omega$. The centripetal force is $\mu s\omega^2$ (why?) and see how this force changes between the two transitions to estimate the spring constant.]

Quantum Mechanics: Problems

Problem sheet 5: (Hilary Term, Weeks 3–4)

■ *Spin*

5.1 Write down the expression for the commutator $[\sigma_i, \sigma_j]$ of two Pauli matrices. Show that the anticommutator of two Pauli matrices is

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}.$$

5.2 Let $\boldsymbol{n}$ be any unit vector and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ be the vector whose components are the Pauli matrices. Why is it physically necessary that $\boldsymbol{n} \cdot \boldsymbol{\sigma}$ satisfy $(\boldsymbol{n} \cdot \boldsymbol{\sigma})^2 = I$, where I is the 2×2 identity matrix? Let $\boldsymbol{m}$ be a unit vector such that $\boldsymbol{m} \cdot \boldsymbol{n} = 0$. Why do we require that the commutator $[\boldsymbol{m} \cdot \boldsymbol{\sigma}, \boldsymbol{n} \cdot \boldsymbol{\sigma}] = 2\mathrm{i}(\boldsymbol{m} \times \boldsymbol{n}) \cdot \boldsymbol{\sigma}$? Prove that these relations follow from the algebraic properties of the Pauli matrices. You should be able to show that $[\boldsymbol{m} \cdot \boldsymbol{\sigma}, \boldsymbol{n} \cdot \boldsymbol{\sigma}] = 2\mathrm{i}(\boldsymbol{m} \times \boldsymbol{n}) \cdot \boldsymbol{\sigma}$ for any two vectors $\boldsymbol{n}$ and $\boldsymbol{m}$.

5.3 Let $\boldsymbol{n}$ be the unit vector in the direction with polar coordinates (θ, ϕ). Write down the matrix $\boldsymbol{n} \cdot \boldsymbol{\sigma}$ and find its eigenvectors. Hence show that the state of a spin-half particle in which a measurement of the component of spin along $\boldsymbol{n}$ is certain to yield $\frac{1}{2}\hbar$ is

$$|+, \boldsymbol{n}\rangle = \sin(\theta/2)\, \mathrm{e}^{\mathrm{i}\phi/2}|-\rangle + \cos(\theta/2)\, \mathrm{e}^{-\mathrm{i}\phi/2}|+\rangle,$$

where $|\pm\rangle$ are the states in which $\pm\frac{1}{2}$ is obtained when s_z is measured. Obtain the corresponding expression for $|-, \boldsymbol{n}\rangle$. Explain physically why the amplitudes in the previous equation have modulus $2^{-1/2}$ when $\theta = \pi/2$ and why one of the amplitudes vanishes when $\theta = \pi$.

5.4 For a spin-half particle at rest, the operator $\boldsymbol{J}$ is equal to the spin operator $\boldsymbol{S}$. Use the properties of the Pauli spin matrices to show that in this case the rotation operator $U(\boldsymbol{\alpha}) \equiv \exp(-\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{J}/\hbar)$ is

$$U(\boldsymbol{\alpha}) = I \cos\left(\frac{\alpha}{2}\right) - \mathrm{i}\hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\sigma} \sin\left(\frac{\alpha}{2}\right),$$

where $\hat{\boldsymbol{\alpha}}$ is the unit vector parallel to $\boldsymbol{\alpha}$. Comment on the value this gives for $U(\boldsymbol{\alpha})$ when $\alpha = 2\pi$.

5.5 Explain why a spin-$\frac{1}{2}$ particle in a magnetic field $\boldsymbol{B}$ has a Hamiltonian given by

$$H = -\gamma \boldsymbol{S} \cdot \boldsymbol{B},$$

where γ is the gyromagnetic ratio which you should define.

In a coordinate system such that $\boldsymbol{B}$ lies along the z-axis, a proton is found to be in a eigenstate $|+, x\rangle$ of $\hat{S}_x$ at $t = 0$. Find $\langle \hat{S}_x \rangle$ and $\langle \hat{S}_y \rangle$ for $t > 0$.

■ $S > 1$ *systems*

5.6 Write down the 3×3 matrix that represents S_x for a spin-one system in the basis in which S_z is diagonal (i.e., the basis states are $|0\rangle$ and $|\pm\rangle$ with $S_z|+\rangle = |+\rangle$, etc.)

A beam of spin-one particles emerges from an oven and enters a Stern–Gerlach filter that passes only particles with $J_z = \hbar$. On exiting this filter, the beam enters a second filter that passes only particles with $J_x = \hbar$, and then finally it encounters a filter that passes only particles with $J_z = -\hbar$. What fraction of the particles stagger right through?

5.7 A system that has spin angular momentum $\sqrt{6}\hbar$ is rotated through an angle ϕ around the z-axis. Write down the 5×5 matrix that updates the amplitudes a_m that S_z will take the value m.

■ *Composite systems*

5.8 A system AB consists of two non-interacting parts A and B. The dynamical state of A is described by $|a\rangle$, and that of B by $|b\rangle$, so $|a\rangle$ satisfies the TDSE for A and similarly for $|b\rangle$. What is the ket describing the dynamical state of AB? In terms of the Hamiltonians $H_{\rm A}$ and $H_{\rm B}$ of the subsystems, write down the TDSE for the evolution of this ket and show that it is automatically satisfied. Do $H_{\rm A}$ and $H_{\rm B}$ commute? How is the TDSE changed when the subsystems are coupled by a small dynamical interaction $H_{\rm int}$? If A and B are harmonic oscillators, write down $H_{\rm A}$, $H_{\rm B}$. The oscillating particles are connected by a weak spring. Write down the appropriate form of the interaction Hamiltonian $H_{\rm int}$. Does $H_{\rm A}$ commute with $H_{\rm int}$? Explain the physical significance of your answer.

5.9 Explain what is implied by the statement that "the physical state of system A is correlated with the state of system B." Illustrate your answer by considering the momenta of cars on (i) London's circular motorway (the M25) at rush-hour, and (ii) the road over the Nullarbor Plain in southern Australia in the dead of night.

5.10 Consider a system of two particles of mass m that each move in one dimension along a given rod. Let $|1;x\rangle$ be the state of the first particle when it's at x and $|2;y\rangle$ be the state of the second particle when it's at y. A complete set of states of the pair of particles is $\{|xy\rangle\} = \{|1;x\rangle|2;y\rangle\}$. Write down the Hamiltonian of this system given that the particles attract one another with a force that's equal to C times their separation.

Suppose that the particles experience an additional potential $V(x,y) = \frac{1}{2}C(x+y)^2$. Show that the dynamics of the two particles is now identical with that of a single particle that moves in two dimensions in a particular potential $\Phi(x,y)$, and give the form of Φ.

5.11 In the lectures we derived Bell's inequality by considering measurements by Alice and Bob on an entangled pair of spins prepared in a singlet state. Bob measures the component of spin along an axis that is inclined by angle θ to that used by Alice. Given the expression

$$|-,\boldsymbol{b}\rangle = \cos(\theta/2)\,\mathrm{e}^{\mathrm{i}\phi/2}|-\rangle - \sin(\theta/2)\,\mathrm{e}^{-\mathrm{i}\phi/2}|+\rangle,$$

for the state of a spin-half particle in which it has spin $-\frac{1}{2}$ along the direction $\boldsymbol{b}$ with polar angles (θ,ϕ), with $|\pm\rangle$ the states in which there is spin $\pm\frac{1}{2}$ along the z-axis, calculate the amplitude that Bob finds the positron's spin to be $-\frac{1}{2}$ given that Alice has found $+\frac{1}{2}$ for the electron's spin. Hence show that the corresponding probability is $\cos^2(\theta/2)$.

Quantum Mechanics: Problems

Problem sheet 6: (Hilary Term, Weeks 5–6)

■ *The hydrogen atom*

6.1 Some things about hydrogen's gross structure that it's important to know (ignore spin throughout):

(a) What quantum numbers characterise stationary states of hydrogen?

(b) What combinations of values of these numbers are permitted?

(c) Give the formula for the energy of a stationary state in terms of the Rydberg $\mathcal{R}$. What is the value of $\mathcal{R}$ in eV?

(d) How many stationary states are there in the first excited level and in the second excited level?

(e) What is the wavefunction of the ground state?

(f) Write down an expression for the mass of the reduced particle.

(g) We can apply hydrogenic formulae to any two charged particles that are electrostatically bound. How does the ground-state energy then scale with (i) the mass of the reduced particle, and (ii) the charge Ze on the nucleus? (iii) How does the radial scale of the system scale with Z?

6.2 An electron is in the ground state of a hydrogen-like atom with nuclear charge $+Ze$.

(a) What is its average distance from the nucleus?

(b) At what distance from the nucleus is it most likely to be found?

(c) Show that the expectation value of the potential energy of the electron is the same as that given by the Bohr model, namely $-Ze^2/4\pi\epsilon_0 r_0$ where $r_0 = a_0/Z$.

(d) Show that the expectation value of the kinetic energy is equal to the value given by the Bohr model, namely $Ze^2/8\pi\epsilon_0 r_0$.

(e) Hence verify that the expectation value of the total energy agrees with the Bohr model.

6.3 Show that the speed of a classical electron in the lowest Bohr orbit is $v = \alpha c$, where $\alpha = e^2/4\pi\epsilon_0\hbar c$ is the fine-structure constant. What is the corresponding speed for a hydrogen-like Fe ion (atomic number $Z = 26$)? Given these results, what fractional errors must we expect in the energies of states that we derive from non-relativistic quantum mechanics.

6.4 Show that the electric field experienced by an electron in the ground state of hydrogen is of order $5 \times 10^{11}\,\mathrm{V\,m^{-1}}$. Why is it impossible to generate comparable macroscopic fields using charged electrodes. Lasers are available that can generate beam fluxes as big as $10^{22}\,\mathrm{W\,m^{-2}}$. Show that the electric field in such a beam is of comparable magnitude.

6.5 Positronium consists of an electron e^- and a positron e^+ (both spin-half and of equal mass) in orbit around one another. What are its energy levels? By what factor is a positronium atom bigger than a hydrogen atom?

6.6 Muonium consists of an electron e^- and a positive muon μ^+ (both spin-half particles but $m_\mu = 206.7m_\mathrm{e}$) in orbit around one another. What are its energy levels? By what factor is muonium atom bigger than a hydrogen atom?

6.7 The emission spectrum of the He^+ ion contains the Pickering series of spectral lines that is analogous to the Lyman, Balmer and Paschen series in the spectrum of hydrogen

Balmer $i = 1, 2, \ldots$	0.456806	0.616682	0.690685	0.730884
Pickering $i = 2, 4, \ldots$	0.456987	0.616933	0.690967	0.731183

The table gives the frequencies (in 10^{15} Hz) of the first four lines of the Balmer series and the first four even-numbered lines of the Pickering series. The frequencies of these lines in the Pickering series are almost coincident with the frequencies of lines of the Balmer series. Explain this finding. Provide a quantitative explanation of the small offset between these nearly coincident lines in terms of the reduced mass of the electron in the two systems. (In 1896 E.C. Pickering identified the odd-numbered lines in his series in the spectrum of the star ζ Puppis. Helium had yet to be discovered and he believed that the lines were being produced by hydrogen. Naturally he confused the even-numbered lines of his series with ordinary Balmer lines.)

6.8 Show that for hydrogen the matrix element $\langle 2, 0, 0|z|2, 1, 0\rangle = -3a_0$. On account of the non-zero value of this matrix element, when an electric field is applied to a hydrogen atom in its first excited state, the atom's energy is linear in the field strength.

Quantum Mechanics: Problems

Problem sheet 7: (Easter vacation)

■ *Hydrogen*

7.1 Tritium, ^{3}H, is highly radioactive and decays with a half-life of 12.3 years to ^{3}He by the emission of an electron from its nucleus. The electron departs with 16 keV of kinetic energy. Explain why its departure can be treated as sudden in the sense that the electron of the original tritium atom barely moves while the ejected electron leaves.

Calculate the probability that the newly formed ^{3}He atom is in an excited state. Hint: evaluate $\langle 1,0,0; Z=2|1,0,0; Z=1\rangle$

7.2 By writing $L^2 = (\boldsymbol{x}\times\boldsymbol{p})\cdot(\boldsymbol{x}\times\boldsymbol{p}) = \sum_{ijklm}\epsilon_{ijk}x_jp_k\,\epsilon_{ilm}x_lp_m$ show that

$$p^2 = \frac{L^2}{r^2} + \frac{1}{r^2}\left\{(\boldsymbol{r}\cdot\boldsymbol{p})^2 - \mathrm{i}\hbar\boldsymbol{r}\cdot\boldsymbol{p}\right\}.$$

By showing that $\boldsymbol{p}\cdot\hat{\boldsymbol{r}} - \hat{\boldsymbol{r}}\cdot\boldsymbol{p} = -2\mathrm{i}\hbar/r$, obtain $\boldsymbol{r}\cdot\boldsymbol{p} = rp_r + \mathrm{i}\hbar$. Hence obtain

$$p^2 = p_r^2 + \frac{L^2}{r^2}.$$

Give a physical interpretation of one over $2m$ times this equation.

■ *More on angular momentum*

7.3 An electron is in a magnetic field B along the z-axis. A measurement at time $t=0$ shows its spin to be in the x-direction. Find the probabilities that at a later time t the electron will be (i) in the x-direction, (ii) in the $-x$ direction, and (iii) in the z-direction.

7.4 Confirm, for the cases $\ell=1$ and $\ell=2$ that

$$\sum_{m=-\ell}^{\ell}|Y_\ell^m|^2 = \text{a constant.}$$

Discuss the significance of this result for the electron probability distributions in the hydrogen atom.

7.5 Show that $\langle j,j|\hat{J}_x|j,j\rangle = \langle j,j|\hat{J}_y|j,j\rangle = 0$ and that $\langle j,j|\hat{J}_x^2+\hat{J}_y^2|j,j\rangle = j\hbar^2$. Discuss the implications of these results for the uncertainty in the orientation of the classical angular momentum vector $\boldsymbol{J}$ for both small and large values of j.

7.6 A is a beam of atoms with spin-$\frac{1}{2}$ with the spin alined along the $+x$-axis. B is a beam of similar unpolarised atoms. A and B are separately passed through a Stern-Gerlach apparatus aligned along z. In each case you get two emerging beams coming out of the Stern-Gerlach experiment. Is there any difference between the two cases? If so, how could you detect that experimentally?

■ *Combining angular momentum*

7.7 When two angular momenta j_1 and j_2 are combined, the possible states of the resulting combination are descrived by $J = |j_1 - j_2|, |j_1 - j_2| + 1, \ldots j_1 + j_2$. Show (for the case $j_1 \geq j_2$, which you can choose without loss of generality) that the total degeneracy of the resulting states is given by

$$\sum_{J=j_1-j_2}^{j_1+j_2} (2J+1) = (2j_1+1)(2j_2+1),$$

and explain why this equal to the number of states of the two angular momenta before they were combined.

7.8 A box containing two spin-1 objects A and B is found to have angular-momentum quantum numbers $J = 2$, $M = 1$. Determine the probabilities that when J_z is measured for A (in units of $\hbar$), the values $m = \pm 1$ and 0 will be obtained.

7.9 The angular momentum of a hydrogen atom in its ground state is entirely due to the spins of the electron and proton. The atom is in the state $|1, 0\rangle$ in which it has one unit of angular momentum but none of it is parallel to the z-axis. Express this state as a linear combination of products of the spin states $|\pm, \mathrm{e}\rangle$ and $|\pm, \mathrm{p}\rangle$ of the proton and electron. Show that the states $|x\pm, \mathrm{e}\rangle$ in which the electron has well-defined spin along the x-axis are

$$|x\pm, \mathrm{e}\rangle = \frac{1}{\sqrt{2}} \left(|+, \mathrm{e}\rangle \pm |-, \mathrm{e}\rangle\right).$$

By writing

$$|1, 0\rangle = |x+, \mathrm{e}\rangle\langle x+, \mathrm{e}|1, 0\rangle + |x-, \mathrm{e}\rangle\langle x-, \mathrm{e}|1, 0\rangle,$$

express $|1, 0\rangle$ as a linear combination of the products $|x\pm, \mathrm{e}\rangle|x\pm, \mathrm{p}\rangle$. Explain the physical significance of your result.