

Problem sheet - HT tutorial 2

Self-assessed questions

Q1. Describing spin- $\frac{1}{2}$ angular momentum

The Pauli sigma matrices are given by

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

(a) Verify that the operators

$$S_x = \frac{\hbar}{2}\sigma_x, \quad S_y = \frac{\hbar}{2}\sigma_y, \quad S_z = \frac{\hbar}{2}\sigma_z$$

satisfy the commutation rules for angular momentum and that

$$\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2 I,$$

where

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(b) Find the eigenvalues (which are real), and corresponding normalised eigenvectors (which may be complex), of S_x , S_y , and S_z .

If you've done this right you should find that the matrices therefore have all the properties required to represent an angular momentum-like degree of freedom, with total angular momentum quantum number $j = \frac{1}{2}\hbar$. So just explain how it all fits with the answers you've got.

[JMR QM HT Q3.1]

Q2. Measurement of spin angular momentum

Measuring spin- $\frac{1}{2}$ Let $|\uparrow z\rangle$ and $|\downarrow z\rangle$ denote the eigenstates of \mathbf{S}^2 and S_z

$$\mathbf{S}^2|\uparrow z\rangle = \frac{1}{2}(\frac{1}{2} + 1)\hbar^2|\uparrow z\rangle, \quad S_z|\uparrow z\rangle = +\frac{1}{2}\hbar|\uparrow z\rangle$$

$$\mathbf{S}^2|\downarrow z\rangle = \frac{1}{2}(\frac{1}{2} + 1)\hbar^2|\downarrow z\rangle, \quad S_z|\downarrow z\rangle = -\frac{1}{2}\hbar|\downarrow z\rangle$$

and similarly $|\uparrow x\rangle$ and $|\downarrow x\rangle$ denote the eigenstates of \mathbf{S}^2 and S_x .

- (a) express $|\uparrow x\rangle$ and $|\downarrow x\rangle$ as linear combinations of $|\uparrow z\rangle$ and $|\downarrow z\rangle$ and vice versa.
- (b) A system is prepared in the state $|\uparrow x\rangle$. Then a measurement of S_z is made. What are the possible outcomes and their probabilities?
- (c) Suppose that the outcome is in fact $\frac{1}{2}\hbar$. What is now the state of the system? If we now measure S_x what do we find?

[JMR QM HT Q3.2]

Q3. Measurement of the spin angular momentum along some axis

Consider a spin- $\frac{1}{2}$ particle whose spin state was

$$|\Psi\rangle = \frac{1}{\sqrt{5}}(2|\uparrow_z\rangle + |\downarrow_z\rangle),$$

where $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$ are the $\pm\frac{1}{2}\hbar$ eigenstates of S_z , respectively. Suppose we now measure the projection of the particle's angular momentum along an axis defined by the unit vector $\mathbf{n} = \frac{1}{5}(3, 4, 0)$. What is probability that a result of $-\frac{1}{2}\hbar$ is obtained?

Q4. Analysis of the Stern-Gerlach measurement

Stern-Gerlach experiment A spin- $\frac{1}{2}$ particle of charge e has an intrinsic magnetic dipole moment $\boldsymbol{\mu} = g_s \frac{e}{2m} \mathbf{S}$. The combination $\mu_B = \frac{e\hbar}{2m}$ is called the *Bohr magneton* and has value $9.3 \times 10^{-24} \text{ JT}^{-1}$. The number g_s is not determined by non-relativistic QM; Dirac's relativistic wave equation tells us that $g_s = 2$. In fact, it is not exactly 2 but the deviation can be calculated in Quantum Electrodynamics which tells us that we expect $g_s/2 = 1.001\,159\,652\,153(28)$. The best experimental measurement is $g_s/2 = 1.001\,159\,652\,188(4)$. See V.W. Hughes and T. Kinoshita, *Rev. Mod. Phys.* **71** S133 (1999).

- What is the net *force* on a magnetic dipole in a uniform \mathbf{B} field?
- Explain why there *is* a net force in a non-uniform \mathbf{B} field. (Because it's more familiar you may find it easier to explain why there is a net force on an electric dipole in a non-uniform \mathbf{E} field.)
- The only contribution to the magnetic moment of a silver atom comes from the valence electron so its magnetic moment behaves just like the electron's. Silver atoms with a kinetic energy of about $3 \times 10^{-20} \text{ J}$ each travel a distance of 0.03 m through a non-uniform magnetic field of gradient $2.3 \times 10^3 \text{ Tm}^{-1}$. Explain why the beam splits into two and calculate the separation of the two beams at a distance of 0.25 m downstream from the magnet.

[JMR QM HT Q3.3]

Q5. Expectation values of an electron

An electron in the Coulomb field of a proton is in a state described by the wave function

$$\Psi(\mathbf{r}) = \frac{1}{6} \left[4\psi_{100}(\mathbf{r}) + 3\psi_{211}(\mathbf{r}) - \psi_{210}(\mathbf{r}) + \sqrt{10}\psi_{21-1}(\mathbf{r}) \right],$$

where $\psi_{nlm}(\mathbf{r})$ are the eigenstates of hydrogen. (a) Confirm that $\Psi(\mathbf{r})$ is normalized properly. (b) What is the expectation value of the energy? (c) What is the expectation value of L^2 ? (d) What is the expectation value of L_z ?

Main questions

Q1. The spherical box potential

The free particle stationary state Schrödinger equation in 3-D, separated in polar coordinates $\psi(r, \theta, \phi) = R_\ell(r)Y_{\ell m}(\theta, \phi)$, leads to the radial equation

$$-\frac{\hbar^2}{2mr^2} \frac{d}{dr} \left(r^2 \frac{dR_\ell}{dr} \right) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} R_\ell = ER_\ell$$

(a) Verify that

$$R_0(r) = A_0 \frac{\sin kr}{r}$$

$$R_1(r) = \frac{A_1}{r} \left(\frac{\sin kr}{kr} - \cos kr \right)$$

where A_0 and A_1 are constants, are solutions of the R_ℓ equation for $\ell = 0$ and $\ell = 1$ respectively.

- (b) The spherical box potential is defined by $V(r) = 0$ for $r \leq a$, $V(r) = \infty$ for $r > a$. This will force the boundary condition $R_\ell(r = a) = 0$. Give approximate numerical values, in units of $\frac{\hbar^2}{2ma^2}$, for the lowest *two* energy eigenvalues in each of the cases (a) $\ell = 0$ (b) $\ell = 1$. [$\ell = 0$ is easy; for $\ell = 1$ you need to solve the equation $\tan x = x$.]
- (c) ††What is wrong with the solution $R_0(r) = B_0 \frac{\cos kr}{r}$ in the $\ell = 0$ case? N.B. This has nothing to do with normalization of the wavefunction. This function is normalizable in three dimensions.

[JMR QM HT Q2.1]

Q2. The Coulomb potential

- (a) What quantum numbers are needed to describe the state of an electron (neglecting spin) in hydrogen? Why is it possible to obtain states with simultaneously well defined eigenvalues of H , L^2 and of L_z ? Draw a diagram of the spectrum up to and including second excited states and label it carefully with all the quantum numbers of the states.
- (b) The ground state wavefunction in hydrogen is proportional to $e^{-r/a}$, where $a = 4\pi\epsilon_0\hbar^2/m\epsilon^2$. Check that this satisfies the time independent Schrödinger equation and normalise it (N.B. get the volume element right!).
- (c) $|\psi(x, y, z)|^2 dx dy dz$ is the probability for finding a particle between (x, y, z) and $(x + dx, y + dy, z + dz)$. In r, θ, ϕ this becomes $|\psi(r, \theta, \phi)|^2 r^2 \sin \theta d\theta d\phi dr$. So the probability of finding the particle between r and $r + dr$, without caring about its angular position, is

$$P(r) dr = \left[\int_0^\pi d\theta \int_0^{2\pi} d\phi |\psi(r, \theta, \phi)|^2 \sin \theta \right] r^2 dr.$$

Writing $\psi = R_{n\ell}(r)Y_{\ell m}(\theta, \phi)$ show that

$$P(r) dr = r^2 |R_{n\ell}(r)|^2 dr.$$

- (d) Sketch $P(r)$ for the ground state wavefunction. Find the value of r for which it is a maximum and calculate the average value of r in this state.

[JMR QM HT Q2.3]

Q3. The 3D harmonic potential

A particle moves in 3-D subject to the potential $V = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$.

- (a) Writing $\psi(x, y, z) = X(x)Y(y)Z(z)$ show that the time-independent Schrödinger equation can be solved in terms of the solutions for the 1-D oscillator.
 (b) Assuming the 1-D results, show that the energy eigenvalues are

$$E(n_x, n_y, n_z) = \hbar\omega \left(\frac{3}{2} + n_x + n_y + n_z \right)$$

where the n 's are integers ≥ 0 . What is the degeneracy of the levels with (i) $E = 3\hbar\omega/2$, (ii) $E = 5\hbar\omega/2$, and (iii) $E = 7\hbar\omega/2$? Compare the energy spectrum and degeneracies for the Coulomb problem and the 3-D oscillator problem.

- (c) †To save you looking them up the ground and first excited states for the 1-D oscillator have wavefunctions

$$\begin{aligned}\phi_0(x) &= A_0 e^{-x^2/2a^2} \\ \phi_1(x) &= A_1 x e^{-x^2/2a^2}.\end{aligned}$$

Write down the wavefunctions for the ground and first excited states of the 3-D oscillator.

- (d) †Rewrite the potential in polar coordinates. Are the eigenvalues of \mathbf{L}^2 and L_z good quantum numbers for this Hamiltonian?
 (e) †Using (3) rewrite the 3-D oscillator wavefunctions you found in part (b) in terms of the spherical harmonics and functions of r . What are the \mathbf{L}^2 eigenvalues of your wavefunctions? What are the L_z eigenvalues of your wavefunctions?

[JMR QM HT Q2.4]

Q4. Mathematical tricks with Pauli matrices

The Pauli matrices we can be formed into a 3D vector operator $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Given two scalar 3D vectors \mathbf{a} and \mathbf{b} prove that

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}).$$

Use this result to show that for any vector \mathbf{a} with magnitude a we have

$$\exp(i\boldsymbol{\sigma} \cdot \mathbf{a}) = \cos(a) + i \left(\boldsymbol{\sigma} \cdot \frac{\mathbf{a}}{a} \right) \sin(a).$$

Q5. Hamiltonians of rotating systems

The Hamiltonian for an axially symmetric rotator is

$$H = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_3},$$

where I_1 and I_3 are moments of inertia. (a) What are the eigenvalues of H ? (b) Sketch the spectrum assuming that $I_1 > I_3$. (c) What is the spectrum in the limit that I_1 is much larger than I_3 ? Suppose we have another system described by the Hamiltonian

$$H = \frac{L^2}{2I} + \alpha L_z,$$

where I is a moment of inertia and α is a coupling constant. (d) What are the eigenstates and associated energy eigenvalues of this system?