Problem sheet - HT tutorial 3

Self-assessed questions

Q1. Practise at adding up angular momenta

Addition of angular momenta All pairs of angular momenta, whether integer or half-integer, combine according to exactly the same rules: if we combine states of angular momentum quantum numbers j_1 and j_2 then the possible total angular momentum quantum numbers are $J = j_1 + j_2$ down to $J = |j_1 - j_2|$ in integer steps. The electron and proton both have intrinsic spin-$\frac{1}{2}$.

(a) The ground state of hydrogen has no orbital angular momentum so its total angular momentum, quantum number I, comes entirely from the electron and proton spins. What are the possible values of I?

(b) Now consider an $\ell = 1$ state of the hydrogen atom. Work out the possible values of I by first combining the spins and then combining the results with the orbital angular momentum.

(c) Repeat but this time first combine the electron spin with the orbital angular momentum and thn combine the results with the proton spin. You should find the same list of possible values for I.

[JMR QM HT Q4.3]

Q2. Singlet and triplet state of two spin-$\frac{1}{2}$ particles

Consider two spin-$\frac{1}{2}$ particles, whose spins are described by the vector Pauli operators σ_1 and σ_2, respectively. Let $\mathbf{e}$ be the unit vector along the direction connecting the two particles and define the operator

$$S_{12} = 3(\sigma_1 \cdot \mathbf{e})(\sigma_2 \cdot \mathbf{e}) - \sigma_1 \cdot \sigma_2.$$

Show that if the two particles are in an $S = 0$ state (singlet) then

$$S_{12}\psi_{\text{singlet}} = 0.$$

Show that for an $S = 1$ state (triplet) we have

$$(S_{12} - 2)(S_{12} + 4)\psi_{\text{triplet}} = 0.$$

Q3. Spin dependent potentials

In a low energy neutron-proton system, possessing zero orbital angular momentum, the potential energy of the pair of particles is given by

$$V(r) = V_1(r) + V_2(r)\left(3\frac{(\sigma_1 \cdot \mathbf{r})(\sigma_2 \cdot \mathbf{r})}{r^2} - \sigma_1 \cdot \sigma_2\right) + V_3(r)\sigma_1 \cdot \sigma_2,$$

where $\mathbf{r}$ is the vector connecting the particles with magnitude r, while $V_1(r), V_2(r)$ and $V_3(r)$ are three potential functions. Calculate the potential for the neutron-proton when it is (a) in a spin singlet state, and (b) in a spin triplet state.

Q4. Measurements of spin for a two-particle system

Consider two electrons in a spin singlet state

$$|\psi_{\text{singlet}}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2\right),$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the $s_z = \pm\frac{1}{2}\hbar$ eigenstates of S_z, respectively for each electron. (a) If a measurement of the spin of one electron shows that it is in a state with $s_z = \frac{1}{2}\hbar$, what is the probability that a measurement of the z-component of the spin of the other electron also yields $s_z = \frac{1}{2}\hbar$? (b) If a measurement of the spin of one of the electrons shows that it is in a state $s_y = \frac{1}{2}\hbar$, what is the probability that a measurement of the x-component of the spin yields $s_x = \frac{1}{2}\hbar$ for the second electron? (c) Now suppose that the two electrons are in the product state

$$|\psi_{\text{prod}}\rangle = \left(\cos(\alpha_1)|\uparrow\rangle_1 + \sin(\alpha_1)e^{i\beta_1}|\downarrow\rangle_1\right)\left(\cos(\alpha_2)|\uparrow\rangle_2 + \sin(\alpha_2)e^{i\beta_2}|\downarrow\rangle_2\right).$$

What is the probability that the two electrons are in a spin triplet state?

Main questions

Q1. A first approximate attempt to solve the Helium atom - non-interacting electrons

Independent motion. Write down, but do not try to solve, the time-independent Schrödinger equation for the Helium atom (assuming the nucleus is infinitely heavy). Now suppose you neglect the potential which acts between the electrons. Solve the resulting approximate equation by an appropriate "separation of variables" i.e. write $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_1(\mathbf{r}_1)\psi_2(\mathbf{r}_2)$ where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the electrons. Identify the separate equations for $\psi_1(\mathbf{r}_1)$ and $\psi_2(\mathbf{r}_2)$ as hydrogen - like Schrödinger equations with e^2 replaced by $2e^2$. Hence calculate the energy of the ground state of the He atom in this approximation, relative to the ground state of the He^{++} ion. The real value is -79 eV; the large discrepancy is due to the electrostatic repulsion between the two electrons.

[JMR QM HT Q4.1]

Q2. Treating the two-body problem properly

Relative and centre-of-mass separation. Consider two particles with masses m_1 and m_2, in 1-D, with the potential energy $V(x_1 - x_2)$. The stationary state Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V(x_1 - x_2)\right]\Psi(x_1, x_2) = E\Psi(x_1, x_2).$$

(a) Why can this equation *not* be separated in the coordinates x_1 and x_2 ?

(b) Define the centre of mass coordinate $X = (m_1x_1 + m_2x_2)/M$ where $M = m_1 + m_2$, and the relative coordinate

$$x = x_1 - x_2.$$

By using the chain rule in the form

$$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial X}\frac{\partial X}{\partial x_1} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial x_1}$$

(or, better, in the operator form

$$\frac{\partial}{\partial x_1} = \frac{\partial X}{\partial x_1}\frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1}\frac{\partial}{\partial x},$$

and similarly for $\frac{\partial}{\partial x_2}$) show that the Schrödinger equation can be re-written as

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial X^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x, X) = E\Psi$$

where the *reduced mass* μ is equal to $m_1m_2/(m_1 + m_2)$.

(c) Show that this equation can be separated in the coordinates x and X i.e. solutions can be found of the form

$$\Psi(x, X) = \psi_{rel}(x)\psi_{CM}(X).$$

Obtain the equation satisfied by $\psi_{rel}(x)$.

(d) What is the solution of the equation for $\psi_{CM}(X)$? Explain the answer physically.

[JMR QM HT Q4.2]

Q3. Angular momenta of two spin-$\frac{1}{2}$ particles (c.f. with qubits)

Two spin-$\frac{1}{2}$ particles, let's call them a and b. Independent of whether they interact or not the combined system has a basis set of spin state functions which are formed as products of the single spin-$\frac{1}{2}$ states. In particular consider the states

$$\begin{aligned} |1\rangle &= |\uparrow\rangle_a|\uparrow\rangle_b \\ |2\rangle &= |\uparrow\rangle_a|\downarrow\rangle_b \\ |3\rangle &= |\downarrow\rangle_a|\uparrow\rangle_b \\ |4\rangle &= |\downarrow\rangle_a|\downarrow\rangle_b, \end{aligned}$$

where, for example, $|1\rangle$ describes the state in which both particles have spin-up along the z-axis. The spin angular momentum operators for the two particles are $\boldsymbol{S}^a$ and $\boldsymbol{S}^b$ respectively and the total angular momentum operator is now

$$\boldsymbol{S} = \boldsymbol{S}^a + \boldsymbol{S}^b.$$

(a) Show that $S_z|1\rangle = \hbar|1\rangle$ and $S_z|2\rangle = 0$; find the result of acting with S_z on the other two states.

(b) How many states do we expect to find with total angular momentum quantum number $S = 1$, and how many with $S = 0$?

(c) Which of the states *must* have total angular momentum quantum number $S = 1$, and which *may* have $S = 0$?

(d) In fact the states with total angular momentum quantum number $S = 1$ are symmetric under exchange of a and b whereas those with $S = 0$ are anti-symmetric. Write down the corectly identified states.

[JMR QM HT Q4.4]

Q4. Adding up angular momenta

More addition of angular momenta

Considering a system of two non-interacting particles with orital angular momentum operators $\boldsymbol{L}^{(1)}$ and $\boldsymbol{L}^{(2)}$ respectively; the total angular momentum operator is

$$\boldsymbol{L} = \boldsymbol{L}^{(1)} + \boldsymbol{L}^{(2)}.$$

We denote the eigenvalues of $\boldsymbol{L}^{(1)}.\boldsymbol{L}^{(1)}$ and $L_z^{(1)}$ by $\ell_1(\ell_1+1)\hbar^2$ and $m_1\hbar$ respectively (and similarly for particle 2). We denote the eigenvalues of $\boldsymbol{L}.\boldsymbol{L}$ and L_z by $L(L+1)\hbar^2$ and $M\hbar$ respectively.

(a) Consider the angular momenta of two particles which are each in $\ell = 1$ states. How many states of the form $\phi_{\ell_1=1,m_1}(\boldsymbol{r}_1)\phi_{\ell_2=1,m_2}(\boldsymbol{r}_2)$ have L_z quantum number $M = 2$? Repeat the exercise for $M = 1, 0, -1, -2$ and comment on any symmetry in the results; how many states do you get altogether? According to the triangle rule the total angular momentum quantum number could be $L = 2, 1$, or 0; how many of these states are there altogether? Now make sure you have the same number of states in the (L, M) labelling as in the $(\ell_1, m_1, \ell_2, m_2)$ labelling.

(b) How many states of the form $\phi_{\ell_1,m_1}(\boldsymbol{r}_1)\phi_{\ell_2,m_2}(\boldsymbol{r}_2)$ have L_z quantum number $M = \ell_1 + \ell_2$? How many have L_z quantum number $M = \ell_1 + \ell_2 - 1$? Carry on until you get to "How many have L_z quantum number $M = 0$?" – why is it not necessary to go any further? Now explain how these results are consistent with the possible L values being $\ell_1 + \ell_2, \ell_1 + \ell_2 - 1, \ldots, |\ell_1 - \ell_2|$ which is what the triangle rule of addition tells us. Why can we not have $L > \ell_1 + \ell_2$?

[JMR QM HT Q4.5]