QM II fall 2018

Exercise 1, discussed in the tutorial session Wed Sep 12th, return by Fri Sep 14th at 15h.

1. Show that you can write the eigenstates $|\uparrow / \downarrow\rangle$ of the spin operator S_z in terms of the eigenstates $|\leftarrow / \rightarrow\rangle$ of the spin operator S_y as

$$|\uparrow\rangle = (i|\leftarrow\rangle - |\rightarrow\rangle)/\sqrt{2}, \quad |\downarrow\rangle = (|\leftarrow\rangle - i|\rightarrow\rangle)/\sqrt{2} \tag{1}$$

Hint: Note that the phase of the eigenvectors can be chosen freely.

2. Assume that a particle initially in an eigenstate of S_z experiences a magnetic field in the y direction for a time τ. Calculate the final state of the particle and express it in the eigenbasis of S_z. Hint: The Hamiltonian describing a magnetic field of size B_0 in the direction j acting on a spin is of the form $H = -\gamma B_0 S_j$, where γ is the gyromagnetic ratio and the matrices $S_j = \hbar\sigma_j/2$ with

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2}$$

3. Suppose that the Hamiltonian $\hat{H}$ for some particular quantum system is a continuous function of some parameter λ. Let $E_n(\lambda)$ and $|\psi_n(\lambda)\rangle$ be the eigenvalues and eigenstates of $\hat{H}(\lambda)$. Prove the Feynman-Hellman theorem

$$\frac{\partial E_n}{\partial \lambda} = \langle\psi_n| \frac{\partial \hat{H}}{\partial \lambda} |\psi_n\rangle \tag{3}$$

Using the Feynman-Hellman theorem determine the expectation values of $1/r$ and $1/r^2$ for the hydrogen atom. Recall that for the radial wave function $u_{n\ell} \equiv rR_{n\ell}$ the effective Hamiltonian is

$$H = -\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{4}$$

and the energy levels are

$$E_n = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2(N+\ell+1)^2} \tag{5}$$

with $n = N + \ell + 1$.

4. Derive Kramer's relation

$$\frac{s+1}{n^2}\langle r^s\rangle - (2s+1)a\left\langle r^{s-1}\right\rangle + \frac{s}{4}\left[(2\ell+1)^2 - s^2\right]a^2\left\langle r^{s-2}\right\rangle = 0, \tag{6}$$

where $a_0 \equiv \frac{4\pi\varepsilon_0\hbar^2}{me^2}$ is the Bohr radius. This equation relates three different expectation values of powers of r for an electron in the Hydrogen atom state ψ_{nlm}. Hint: the radial equation can be written as

$$u''(r) = \left[\frac{\ell(\ell+1)}{r^2} - \frac{2}{a_0 r} + \frac{1}{n^2 a_0^2}\right]u(r) \tag{7}$$

Use it to express $\int \mathrm{d}r(ur^s u'')$ in terms of $\langle r^s\rangle$, $\left\langle r^{s-1}\right\rangle$, $\left\langle r^{s-2}\right\rangle$. Then integrate by parts to get rid of the second derivative. Show that $\int \mathrm{d}r(ur^s u') = -(s/2)\left\langle r^{s-1}\right\rangle$ and $\int \mathrm{d}r(u'r^s u') = -[2/(s+1)]\int \mathrm{d}r(u''r^{s+1}u')$.

5. The nucleus of a hydrogenlike atom is usually treated as a point charge Ze. Using first order perturbation theory, estimate the error due to this approximation by assuming that the nucleus is sphere of radius R with a uniform charge distribution. Calculate numerically the result for the ground state of an hydrogen atom taking $R = 0.9 \times 10^{-15}$m. Hint: the potential energy of the electron in the field of a homogenous sphere of radius R and total charge Ze is

$$V(r) = \frac{Ze^2}{4\pi\varepsilon_0}\begin{cases} \frac{1}{2R}\left(\frac{r^2}{R^2} - 3\right), & r \le R \\ -\frac{1}{r}, & r \ge R \end{cases} \tag{8}$$