Spring 2013

FYST530 Quantum Mechanics II

Return by Wed 23.1. at 16.00 to the box labeled FYST530

Problem set 1 — Discussed Thu 24.1. at **14.00** in FYS5

1. (a) Suppose the Hamiltonian H, for some particular quantum system, is a function of some parameter λ. Let $E_n(\lambda)$ and $\psi_n(\lambda)$ be the eigenvalues and eigenfunctions of $H(\lambda)$. Prove the **Feynman-Hellman theorem**:

$$\frac{\partial E_n}{\partial \lambda} = \left\langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \right\rangle .$$

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

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

   and the eigenvalues are

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

   Here N refers to the largest power of the Laguerre polynomial associated with the solution of $u_{n\ell}$ and it's related to the principal quantum n and to the angular momentum quantum number ℓ via $n = N + \ell + 1$.

2. Derive the **Kramer's relation**

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

   where $a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2}$ is the Bohr radius. This relation relates the three different expectation values of r for an electron in the Hydrogen atom state ψ_{nlm}. What are the formulas for $\langle r^{-1}\rangle$, $\langle r\rangle$, $\langle r^2\rangle$ and $\langle r^3\rangle$?

   Hint: The radial equation can be written as

$$u'' = \left[\frac{\ell(\ell+1)}{r^2} - \frac{2}{ar} + \frac{1}{n^2a^2}\right]u.$$

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

3. The nucleus of an hydrogen-like atom is usually treated as a point charge Ze. Using the first order perturbation theory, estimate the error due to this approximation by assuming that the nucleus is a sphere of radius R with a uniform charge distribution. Calculate the numerical 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 homogenous sphere of radius R and total charge Ze is

$$V(r) = \frac{Ze^2}{4\pi\epsilon_0} \begin{cases} \frac{1}{2R}\left(\frac{r^2}{R^2} - 3\right), & r \leq R \\ -\frac{1}{r}, & r \geq R \end{cases} .$$

   Can you derive this, too? It comes out from Maxwell's first equation.

4. Consider a free, non-relativistic particle (in one dimension) with mass m located in $x = a$ at $t = 0$, that is, the particle is described by the wave function

$$\Psi(t = 0, x) = \langle x|\Psi(t = 0)\rangle = \delta(x - a)$$

   in coordinate space. Find the time evolution of Ψ for $t > 0$. In other words, compute $\langle x|\Psi(t)\rangle$. The result is known as the free particle **propagator**.

   Hint: Recall that the time evolution of a state $|\Psi\rangle$ is given by $|\Psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\Psi(t = 0)\rangle$.