11/23/16 Lecture 17 outline

• Last time: Coulomb potential: $V = -Ze^2/r$, so $\psi_{E,\ell,m} = R_{E,\ell}(r)Y_{\ell m}(\theta\phi)$ with $R_{E,\ell} \equiv u_{E,\ell}/r$ and the radial ODE (taking $E = -|E| < 0$) is

$$(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} - \frac{Ze^2}{r} + |E|)u = 0.$$

Define $\rho \equiv \kappa r$ where $\hbar\kappa \equiv \sqrt{2m|E|}$ and $\rho_0 \equiv \sqrt{2m/|E|}(Ze^2/\hbar)$ and use $\alpha \equiv e^2/\hbar c \approx 1/137$. Then $u_{E,\ell} \equiv \rho^{\ell+1}e^{-\rho}w(\rho)$ solves the radial S.E. if $w(\rho)$ satisfies an ODE. Again, the $\rho \to 0$ behavior is determined by the angular momentum term in V_{eff}, i.e. $\ell(\ell+1)\hbar^2/2mr^2$. Because $V(r) \to 0$ for $r \to \infty$, the leading behavior in that limit is what we would get for a free particle with $E < 0$, which gives the $e^{-\rho}$ term; the Coulomb term corrects this with power-law behavior for $r \to \infty$, which is similar to the similar to the WKB correction at order $\hbar$. The solutions can be written in terms of hypergeometric functions. If we write $w(\rho) = \sum a_\ell \rho^\ell$, the recursion relation is

$$\frac{a_{k+1}}{a_k} = \frac{-\rho_0 + 2(k+\ell+1)}{(k+\ell+2)(k+\ell+1) - \ell(\ell+1)}$$

which has $a_{k+1}/a_k \to 2/k$, consistent with $e^{2\rho}$ for large ρ for generic E. As usual for bound state problems, we find that E has to be quantized or the solution would be badly behaved for $r \to \infty$, would get $w(\rho) \to e^\rho$ for generic E. To avoid this, the series for $w(\rho)$ must truncate at finite order N. This requires $\rho_0 = 2(N + \ell + 1)$. Note degeneracy.

Upshot: Find that the radial equation gives $E_n = -\frac{1}{2}mc^2Z^2\alpha^2/n^2$ where $n = N+\ell+1$, with $N = 0, 1, 2\ldots$, i.e. $\ell = 0, 1, \ldots, n-1$. The degeneracy for fixed n is $\sum_{\ell=0}^{n-1}(2\ell+1) = n^2$. Taking $a_0 \equiv \hbar^2/me^2$, (with F a Hypergometric function)

$$R_{n,\ell}(r) \propto r^\ell e^{-Zr/na_0}F(-n+\ell+1; 2\ell+2; 2Zr/na_0).$$

• The degeneracy of the Coulomb potential is related to a special symmetry associated with $V = -k/r$. Classically it conserves the Runge-Lenz vector $\vec{N}_{cl} = \vec{p}\times\vec{L}/m - k\vec{x}/r$. In QM we define

$$\vec{N} = \frac{1}{2m}(\vec{p}\times\vec{L} - \vec{L}\times\vec{p}) - \frac{k\vec{x}}{\sqrt{x^2+y^2+z^2}}.$$

which is conserved: $[N, H] = 0$. Since it is a vector, we can write $N_{\ell,m}$, with $\ell = 1$ and $m = 1, 0, -1$. Can use it to change ℓ of the E eigenstates without changing E, so degeneracy in ℓ. The way it changes ℓ is related to addition of angular momentum.

• The total angular momentum of a particle is $\vec{J} = \vec{L} + \vec{S}$. This is a special case of the topic of addition of angular momentum. The total angular momentum can come from adding that of two systems, $\vec{J} = \vec{J}_1 + \vec{J}_2$, with a system with $|j_1, m_1\rangle$ and another with $|j_2, m_2\rangle$. For example, the two systems can be two electrons, and we want to find their combined total spin. We tensor product together all the $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$. Note $\vec{J}^2 = \vec{J}_1^2 + \vec{J}_2^2 + 2\vec{J}_1 \cdot \vec{J}_2 = \vec{J}_1^2 + \vec{J}_2^2 + 2J_{1,z}J_{2,z} + J_{1+}J_{2-} + J_{1-}J_{2+}$. Find that the tensor product has j that can run from $j = |j_1 - j_2|$ to $j = j_1 + j_2$, differing by integer values, and $m = m_1 + m_2$. The total dimension is indeed the product $(2j_1 + 1)(2j_2 + 1)$, check.

• Example of combining two spin 1/2s.

• $|j_1 j_2; m_1 m_2\rangle \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle$. Also $|j_1 j_2; jm\rangle$. Clebsch-Gordon coefficients $\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle$. Using $J_z = J_{1z} + J_{2z}$, show $m = m_1 + m_2$. Recipe: start with case $j = j_1 + j_2$, $m = j_1 + j_2$, where the only possibility is $|j_1 j_1\rangle \otimes |j_2 j_2\rangle$. Now use $J_- = J_{1-} + J_{2-}$ to get all m values for $j = j_1 + j_2$. Now get $j = m = j_1 + j_2 - 1$ by orthogonality:

$$|j_1 + j_2; j_1 + j_2 - 1\rangle = \sqrt{\frac{j_1}{j_1 + j_2}}|j_1, j_1 - 1\rangle |j_2 j_2\rangle + \sqrt{\frac{j_2}{j_1 + j_2}}|j_1 j_1\rangle |j_2 j_2 - 1\rangle,$$

$$|j_1 + j_2 - 1; j_1 + j_2 - 1\rangle = -\sqrt{\frac{j_2}{j_1 + j_2}}|j_1, j_1 - 1\rangle |j_2 j_2\rangle + \sqrt{\frac{j_1}{j_1 + j_2}}|j_1 j_1\rangle |j_2 j_2 - 1\rangle.$$

Now lower m to get all $j = j_1 + j_2 - 1$ cases. Now get $j = m j_1 + j_2 - 2$, by imposing orthogonality with the known (from previous steps) vectors with $j_1 + j_2$ and $j_1 + j_2 - 1$ and $m = j_1 + j_2 - 2$. Keep going until done.

Ended here

• Example of combining spin 1 and spin 1/2. Clebsch Gordon coefficients.

• Consider the case $j_1 = \ell$ an integer, and $j_2 = \frac{1}{2}$. This is of use for Hydrogen etc where the electron has both orbital and spin angular momentum. Get $j = \ell \pm \frac{1}{2}$ for $\ell > 0$, and $j = \frac{1}{2}$ for $\ell = 0$. Note that $\vec{L} \cdot \vec{S} = \frac{1}{2}(\vec{J}^2 - \vec{L}^2 - \vec{S}^2)$ is $(\hbar^2/2)(j(j+1) - \ell(\ell+1) - 3/4)$ is $\ell\hbar^2/2$ for $j = \ell + \frac{1}{2}$ and $-(\ell+1)\hbar^2/2$ for $j = \ell - \frac{1}{2}$.

• Atomic notation: ${}^{2S+1}L_J$, with $L = 0, 1, 2, 3, \ldots$ denoted by $S, P, D, F, \ldots$ e.g. ${}^2P_{3/2}$ means $\ell = 1$, $s = 1/2$, $j = 3/2$. The ground state of He is ${}^1S_0$.

• Wigner-Eckart theorem. Let $T_q^{(k)}$ be an operator with $\ell = k$ and $m = q$. For example, $T_0^{(2)} = U_+ V - +2U_0 V_0 + U_- U_+$ where $\vec{U}$ and $\vec{V}$ are two vectors and $U\pm = \mp(U_x \pm iU_y)/\sqrt{2}$ and $U_0 = U_z$. They have $[J_z, T_q^{(k)}] = \hbar q T_q^{(k)}$ and $[J_\pm, T_q^{(k)}] = \hbar\sqrt{(k \pm q)(k \pm q + 1)} T_{q\pm 1}^{(k)}$, i.e. $T_q^{(k)}$ transform like $|k, q\rangle$.

The theorem says that

$$\langle \alpha', j'm' | T_q^{(k)} | \alpha, jm \rangle = (2j+1)^{-1/2} \langle jk; mq | jk; j'm' \rangle \langle \alpha' j' || T^{(k)} || \alpha j \rangle.$$

The first term is a CG coefficient, which is zero unless $m' = q + m$ and $|j-k| \le j' \le j+k$. The last term is independent of m and m'; this is where the symmetry gives some helpful mileage.