Hydrogen atom revisited

Consider again Schrödinger equation

$$i u_t = -\frac{1}{2}\Delta u + V\cdot u$$

where $u(x_1, x_2, x_3, t) \in \mathbb{C}$ $\quad V = \tilde{V}(r)$ $\quad r^2 = x_1^2 + x_2^2 + x_3^2$

Assume global boundary cond.

$$\int_{\mathbb{R}^3} |u(x,t)|^2 \, dx < \infty$$

Seperat. of Var.: $u(x_1, x_2, x_3, t) = v(x_1, x_2, x_3) \cdot e^{-i\lambda t/2}$

s.t. $\quad -\Delta v + V\cdot v = \lambda v \qquad \lambda \in \mathbb{R}, \; v(x_1, x_2, x_3) \in \mathbb{R}$

Another Sep. of Var. $\tilde{v}(r, \phi, \theta) = R(r)\, Y(\phi, \theta)$

$$\Longrightarrow \quad r^2 \lambda - 2 r^2 \cdot \tilde{V}(r) + \frac{r^2 R'' + 2 r R'}{R} = \gamma$$

$$= -\frac{1}{Y} \underbrace{\left\{ \frac{1}{\sin^2 \theta} Y_{\phi\phi} + \frac{1}{\sin\theta} (\sin\theta \, Y_\theta)_\theta \right\}}_{\text{Laplace operator on } \partial B_1(0)}$$

$\Longrightarrow$ EV equation for Laplace operator on $\partial B_1(0)$ in spherical coord.

$\Longrightarrow$ $\gamma = l \cdot (l+1) > 0$

$|m| \leq l$, $m \in \mathbb{Z}$, $l \in \mathbb{N}$

with eigenfct. $Y_l^m(\phi, \theta) = e^{im\phi} P_l^{|m|}(\cos\theta)$

$$\Longrightarrow \quad R'' + \frac{2}{r} R' + \left(\lambda - 2\tilde{V}(r) - \frac{l(l+1)}{r^2} \right) R = 0$$

BC: $R(0) < \infty$, $R(r) \to 0$, $r \to \infty$

For $\tilde{V}(r) = -\frac{1}{r}$ We assume that $\lambda < 0$.

We set $w(r) = e^{\beta r} R(r)$ with $\beta = \sqrt{-\lambda}$

$$\Rightarrow \quad w'' + 2\left(\frac{1}{r} - \beta\right) w' + \left[\frac{2(1-\beta)}{r} - \frac{\ell(\ell+1)}{r^2}\right] w = 0$$

Power series method: $w(r) = \sum_{k=0}^{\infty} a_k r^k$

$$\Rightarrow \sum_{k=0} k(k-1)\, a_k r^{k-2} + 2\sum_{k=0} k\, a_k r^{k-2} - 2\beta \sum_{k=0} k\, a_k r^{k-1}$$
$$+ 2(1-\beta)\sum_{k=0} a_k r^{k-1} - \ell(\ell+1)\sum_{k=0} a_k r^{k-2} = 0$$

$$\Rightarrow 0 = \sum_{k=0}^{\infty} \underbrace{\left[k(k-1) + 2k - \ell(\ell+1)\right]}_{k(k+1) - \ell(\ell+1)} a_k r^{k-2} + \sum_{k=1}^{\infty} \underbrace{\left[-2\beta k + 2(1-\beta)\right]}_{2(1-k\beta)} a_{k-1} r^{k-2}$$

$$\Rightarrow \left[k(k+1) - \ell(\ell+1)\right] a_k = 2(1-k\beta)\, a_{k-1} \qquad k \geq 1$$

$$-\ell(\ell+1)\, a_0 = 0$$

$\Longrightarrow$ for $k < \ell$ we have $a_k = 0$
and a_ℓ can be ~~a~~ arbitrary

If $\beta = \frac{1}{n}$ then $a_k = 0 \quad \forall k \geq n$

$\Longrightarrow$ w is a polynomial: $w = L_\ell^n(r)$

$$= \sum_{k=\ell}^{n-1} a_k r^k$$

$\Longrightarrow$ $\lambda = -\frac{1}{n^2}$ are EVs with eigenfct. ~~f~~ $v_{n\ell m}(r, \varphi, \theta)$

$$= e^{-r/n} L_\ell^n(r) \cdot Y_\ell^m(\varphi, \theta)$$

Remark: Again this set of eigenfct is not complete because we cannot solve the equ. for $\lambda \geq 0$.
(This corresponds to free electron)

Angular momentum in QM

In Newton mechanics: $\vec{x}(t) \in \mathbb{R}^3$ $\quad \vec{x}(t) \times \dot{\vec{x}}(t)$

$$\vec{L} = -i\,\vec{x} \times \nabla = (\ldots) = (L_1, L_2, L_3)$$

$$\Longrightarrow \quad |\vec{L}|^2 = -\text{ Laplace operator on } \partial B_1(0)$$

$$\left.\begin{array}{l} L_3 \\ L_1 \pm i L_2 \end{array}\right\} \text{ eigenfct. are spherical harmonic.}$$