

1. We begin with the Klein-Gordon equation with potential $V = -Ze^2/r = -Z\alpha/r$:

$$\left(i\frac{\partial}{\partial t} + \frac{Z\alpha}{r}\right)^2 \Psi(\mathbf{x}, t) = (-\nabla^2 + m^2) \Psi(\mathbf{x}, t) \quad \text{where} \quad \Psi(\mathbf{x}, t) = e^{-iEt} \frac{u_l(r)}{r} Y_l^m(\theta, \phi) \quad (1)$$

which is

$$\left[\nabla^2 - \left(\frac{\partial}{\partial t}\right)^2 + \frac{2iZ\alpha}{r} \left(\frac{\partial}{\partial t}\right) + \frac{(Z\alpha)^2}{r^2} - m^2\right] \left[e^{-iEt} \frac{u_l(r)}{r} Y_l^m(\theta, \phi)\right] = 0 \quad (2)$$

Work on the time derivative first, and then cancel the factor e^{-iEt} ,

$$\left[\nabla^2 + E^2 + \frac{2Z\alpha E}{r} + \frac{(Z\alpha)^2}{r^2} - m^2\right] \left[\frac{u_l(r)}{r} Y_l^m(\theta, \phi)\right] = 0 \quad (3)$$

The Laplacian in the spherical coordinates is

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \quad (4)$$

Also recall $Y_l^m(\theta, \phi)$ satisfies the differential equation (see eq (3.237))

$$\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}\right] Y_l^m(\theta, \phi) = -l(l+1) Y_l^m(\theta, \phi) \quad (5)$$

This gives

$$\begin{aligned} \nabla^2 \left[\frac{u_l(r)}{r} Y_l^m(\theta, \phi)\right] &= \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr}\right) \left[\frac{u_l(r)}{r}\right] Y_l^m(\theta, \phi) - \frac{l(l+1)}{r^2} \frac{u_l(r)}{r} Y_l^m(\theta, \phi) \\ &= \left[\frac{1}{r^2} \frac{d}{dr} (ru'_l - u_l) - \frac{l(l+1)}{r^2} \frac{u_l}{r}\right] Y_l^m \\ &= \left[\frac{u''_l}{r} - \frac{l(l+1)}{r^2} \frac{u_l}{r}\right] Y_l^m \end{aligned} \quad (6)$$

Plug (6) back into (3) and cancel $Y_l^m(\theta, \phi)/r$, we obtain

$$u''_l + \left[E^2 - m^2 + \frac{2Z\alpha E}{r} + \frac{(Z\alpha)^2}{r^2} - \frac{l(l+1)}{r^2}\right] u_l = 0 \quad (7)$$

Divide by $\gamma^2 = 4(m^2 - E^2)$,

$$\frac{u''_l}{\gamma^2} + \left[-\frac{1}{4} + \frac{2Z\alpha E}{\gamma^2 r} - \frac{l(l+1) - (Z\alpha)^2}{\gamma^2 r^2}\right] u_l = 0 \quad (8)$$

With change of variable $\rho = \gamma r$, we have $u''_l = d^2 u_l / dr^2 = \gamma^2 d^2 u_l / d\rho^2$, we finally get

$$\frac{d^2 u_l}{d\rho^2} + \left[-\frac{1}{4} + \frac{2Z\alpha E}{\gamma \rho} - \frac{l(l+1) - (Z\alpha)^2}{\rho^2}\right] u_l = 0 \quad (9)$$

2. If $u_l(\rho)$ has the assumed form

$$u_l(\rho) = \rho^k (1 + c_1 \rho + c_2 \rho^2 + \dots) e^{-\rho/2} \quad (10)$$

we can insert (10) back to (9) and match the ρ^{k-2} term, which will produce

$$\begin{aligned} k(k-1) - l(l+1) + (Z\alpha)^2 &= 0 & \implies \\ \left(k - \frac{1}{2}\right)^2 - \left[\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2\right] &= 0 & \implies \\ k = k_{\pm} &= \frac{1}{2} \pm \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} \end{aligned} \quad (11)$$

In a physical situation, $u_l(\rho)$ is dominated by the leading term ρ^k , which makes the radial function $u_l/\rho \propto \rho^{k-1}$. Then the kinetic energy

$$K \propto \int \rho^2 d\rho \rho^{k-1} \frac{d^2 \rho^{k-1}}{d\rho^2} \propto \int \rho^{2k-2} d\rho \propto \rho^{2k-1} \quad (12)$$

which is divergent near origin for $k_- < 1/2$. For $Z\alpha \ll 1$, $k_+ \approx l+1$, so

$$R_l(\rho) \propto \frac{u_l(\rho)}{\rho} \approx \rho^l \quad (13)$$

agreeing with the Schrödinger solution (see eq (3.320)).

3. From (10),

$$\begin{aligned} u_l(\rho) &= \sum_i e^{-\rho/2} c_i \rho^{k+i} & \Rightarrow \\ \frac{du_l}{d\rho} &= \sum_i \left[e^{-\rho/2} c_i (k+i) \rho^{k+i-1} - \frac{1}{2} e^{-\rho/2} c_i \rho^{k+i} \right] & \Rightarrow \\ \frac{d^2 u_l}{d\rho^2} &= \sum_i \left[e^{-\rho/2} c_i (k+i)(k+i-1) \rho^{k+i-2} - e^{-\rho/2} c_i (k+i) \rho^{k+i-1} + \frac{1}{4} e^{-\rho/2} c_i \rho^{k+i} \right] \end{aligned} \quad (14)$$

Put this back into (9) and match the ρ^{k+i} term

$$c_{i+2}(k+i+2)(k+i+1) - c_{i+1}(k+i+1) + \frac{1}{4}c_i - \frac{1}{4}c_i + \frac{2Z\alpha E}{\gamma}c_{i+1} - [l(l+1) - (Z\alpha)^2]c_{i+2} = 0 \quad (15)$$

which gives the recurrence relation

$$\frac{c_{i+2}}{c_{i+1}} = \frac{(k+i+1) - 2Z\alpha E/\gamma}{(k+i+2)(k+i+1) - l(l+1) + (Z\alpha)^2} \rightarrow \frac{1}{i} \quad \text{as } i \rightarrow \infty \quad (16)$$

With this, the polynomial $\sum_i c_i \rho^i$ will approach e^ρ , which renders the whole $u_l(\rho)$ divergent for large ρ unless it terminates at some point, e.g., $c_{N+1} = 0$:

$$k + N = \frac{2Z\alpha E}{\gamma} \quad (17)$$

4. Combine (17) with (11), we have the restriction on E :

$$\begin{aligned} k &= \frac{2Z\alpha E}{\gamma} - N = \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} & \Rightarrow \\ 2Z\alpha E &= \left[N + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} \right] \gamma = \left[N + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} \right] 2\sqrt{m^2 - E^2} & \Rightarrow \\ E &= \frac{m}{\sqrt{1 + \frac{(Z\alpha)^2}{\left[N + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} \right]^2}}} \end{aligned} \quad (18)$$

By following the convention of equation (3.313), where $n = N + l + 1$ is called principal quantum number, E is rewritten as

$$E = \frac{m}{\sqrt{1 + \frac{(Z\alpha)^2}{\left[n - l - \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} \right]^2}}} \quad (19)$$

5. When $Z\alpha \ll 1$, (19) is reduced to

$$E \approx \frac{m}{\sqrt{1 + \frac{(Z\alpha)^2}{\left[n - l - \frac{1}{2} + \left(l + \frac{1}{2}\right)\right]^2}}} \approx m \left[1 - \frac{(Z\alpha)^2}{2n^2} \right] \quad (20)$$

which is manifestly the rest energy plus $E_n^{(0)}$.

Let's try to expand E to one more order of $Z\alpha$. Write

$$E = mA^{-1/2} \quad (21)$$

$$A = 1 + \frac{(Z\alpha)^2}{B^2} \quad (22)$$

$$\begin{aligned} B &= n - l - \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - (Z\alpha)^2} \\ &\approx n - l - \frac{1}{2} + \left(l + \frac{1}{2}\right) - \frac{(Z\alpha)^2}{2\left(l + \frac{1}{2}\right)} \\ &= n - \frac{(Z\alpha)^2}{2\left(l + \frac{1}{2}\right)} \end{aligned} \quad (23)$$

Then

$$\begin{aligned} E &\approx m \left[1 - \frac{1}{2} \frac{(Z\alpha)^2}{B^2} + \frac{1}{2!} \frac{3}{4} \frac{(Z\alpha)^4}{B^4} \right] \\ &\approx m \left\{ 1 - \frac{1}{2} (Z\alpha)^2 n^{-2} \left[1 + \frac{(Z\alpha)^2}{n\left(l + \frac{1}{2}\right)} \right] + \frac{3}{8} \frac{(Z\alpha)^4}{n^4} \right\} \\ &= m - \frac{m(Z\alpha)^2}{2n^2} - \frac{m(Z\alpha)^4}{2n^3\left(l + \frac{1}{2}\right)} + \frac{3}{8} \frac{(Z\alpha)^4}{n^4} \end{aligned} \quad (24)$$

whose third and fourth term match section 5.3.1 (*The Relativistic Correction to the Kinetic Energy*, in particular eq (5.104b)) perfectly.