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The Schrodinger equation describes the position of an electron as a wave. The wave function $\Psi(t, \mathbf{x})$ is interpreted as a probability density for the position of the electron. That is, the probability of the electron being in a region Ω in space at a time t_0 is

$$P(\text{electron in } \Omega \mid \text{at time } t_0) = \frac{\iiint_{\Omega} |\Psi(t = t_0)|^2 d\mathbf{x}}{\iiint_{\mathbb{R}^3} |\Psi(t = t_0)|^2 d\mathbf{x}}$$

The Schrodinger equation for the hydrogen atom describes how the probability distribution for the position of the electron in the atom evolves. It is

$$\begin{cases} i\partial_t \Psi = -\frac{1}{2}\Delta \Psi - \frac{1}{r}\Psi \\ \iiint |\Psi|^2 d\mathbf{x} \text{ finite} \end{cases} \quad (1)$$

where $r = |\mathbf{x}|$.

The first step in solving the equation is to separate variables: let

$$\Psi(\mathbf{x}, t) = T(t)v(\mathbf{x})$$

Plugging this into (1), we get

$$iT'v = -\frac{1}{2}T\Delta v - \frac{1}{r}Tv$$

Multiplying by 2 and dividing both sides by Tv ,

$$2i\frac{T'}{T} = -\frac{\Delta v}{v} - \frac{2}{r}$$

The left side of this equation depends only on t , and the right side depends only on \mathbf{x} . Therefore, both sides must equal a constant, λ .

The equation for $T(t)$ is

$$T' = \frac{\lambda}{2i}T \quad (2)$$

We can solve this simply by separating variables:

$$\begin{aligned}\frac{dT}{dt} &= \frac{\lambda}{2i}T \\ \frac{dT}{T} &= \frac{\lambda}{2i}dt \\ \int_0^t \frac{dT}{T} &= \int_0^t \frac{\lambda}{2i}dt \\ \log T - \log T(0) &= \frac{\lambda}{2i}t \\ T &= T(0)e^{-i\lambda t/2}\end{aligned}$$

Therefore, the $T(t)$ eigenfunction is

$$T(t) = e^{-i\lambda t/2} \quad (3)$$

The equation for $v(\mathbf{x})$ is

$$-\Delta v - \frac{2}{r}v = \lambda v \quad (4)$$

Thus, we have an eigenvalue problem for v . To solve it, we express v in spherical coordinates, and look for separable solutions of the form

$$v(\mathbf{x}) = v(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

Here, θ is the longitude coordinate and ϕ is the latitude coordinate. Therefore, we have $0 \leq \theta \leq 2\pi$ and $0 \leq \phi \leq \pi$. We also require that Y is periodic in θ : $Y(\theta, \phi) = Y(\theta + 2\pi, \phi)$ for all θ .

In spherical coordinates, the Laplacian operator is

$$\Delta = \partial_{rr} + \frac{2}{r}\partial_r + \frac{1}{r^2 \sin \phi} \partial_\phi(\sin \phi) \partial_\phi + \frac{1}{r^2 \sin^2 \phi} \partial_{\theta\theta}$$

Using this and $v = RY$, (4) becomes

$$\underbrace{\lambda RY}_{\lambda v} + \underbrace{\frac{2}{r}RY}_{\frac{2}{r}v} + \underbrace{R''Y + \frac{2}{r}R' + \frac{1}{r^2 \sin \phi} (\sin(\phi)RY_\phi)_\phi + \frac{1}{r^2 \sin^2 \phi} RY_{\theta\theta}}_{\Delta v} = 0$$

Multiplying both sides by r^2/R ,

$$\lambda r^2 + 2r + \frac{r^2 R''}{R} + \frac{2r R'}{R} + \frac{1}{Y} \left(\frac{1}{\sin \phi} (\sin(\phi)Y_\phi)_\phi + \frac{1}{\sin^2 \phi} Y_{\theta\theta} \right) = 0$$

and so

$$\lambda r^2 + 2r + \frac{r^2 R''}{R} + \frac{2r R'}{R} = -\frac{1}{Y} \left(\frac{1}{\sin \phi} (\sin(\phi)Y_\phi)_\phi + \frac{1}{\sin^2 \phi} Y_{\theta\theta} \right) \quad (5)$$

The left side of this equation depends only on r , while the right side depends only on θ and ϕ . Therefore, both sides must equal a constant. Call this constant γ . Setting the left side of (5) equal to γ and multiplying both sides by R/r^2 , we get

$$\left(\lambda + \frac{2}{r} - \frac{\gamma}{r^2}\right) R + R'' + \frac{2}{r} R' = 0 \quad (6)$$

Setting the right side of (5) equal to γ and multiplying both sides by Y , we get

$$\frac{1}{\sin \phi} (\sin(\phi) Y_\phi)_\phi + \frac{1}{\sin^2 \phi} Y_{\theta\theta} + \gamma Y = 0 \quad (7)$$

(6) is an ODE for R , and (7) is an eigenvalue problem for Y . Since we do not yet know the eigenvalues γ , our approach will be to find the eigenfunctions Y first, and then solve the equation for R . While solving the equation for R , we will also find the eigenvalues λ for v . Once we do all of this, we will have the eigenfunctions $v(r, \theta, \phi) = R(r)Y(\theta, \phi)$ for the entire problem.

To solve (7), we look for separable solutions $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$. Plugging this into (7), we get

$$\frac{1}{\sin \phi} (\sin(\phi)\Theta\Phi')_\phi + \frac{1}{\sin^2 \phi} \Theta''\Phi + \gamma\Theta\Phi = 0$$

Multiplying both sides by $\sin^2(\phi)/\Theta\Phi$,

$$\sin(\phi) \frac{(\sin(\phi)\Phi')'}{\Phi} + \frac{\Theta''}{\Theta} + \gamma \sin^2(\phi) = 0$$

and so

$$-\frac{\Theta''}{\Theta} = \sin(\phi) \frac{(\sin(\phi)\Phi')'}{\Phi} + \gamma \sin^2(\phi) \quad (8)$$

The left side of (8) is dependent only on θ , while the right side is dependent only on ϕ . Therefore, both sides must equal a constant. Call this constant α . Then by setting each side equal to α , we have

$$\Theta'' = -\alpha\Theta \quad (9)$$

and

$$\sin(\phi) (\sin(\phi)\Phi')' + \gamma \sin^2(\phi)\Phi = \alpha\Phi \quad (10)$$

We first solve the Θ equation, (9). $\alpha = 0$ is a degenerate solution, so we are only interested in the cases where $\alpha \neq 0$. First consider the case where $\alpha < 0$. Let $\alpha = -k, k > 0$. Then

$$\Theta'' = k\Theta$$

The general solution to this is

$$\Theta = Ae^{\sqrt{k}\theta} + Be^{-\sqrt{k}\theta} \quad (11)$$

Recall that we require Θ to be 2π periodic. However, (11) is not periodic, and so α cannot be less than 0. Now, consider the case where $\alpha > 0$. Let $\alpha = \omega^2$. Then the general solution to (9) is

$$\Theta = Ae^{i\omega\theta} + Be^{-i\omega\theta}$$

Using the condition that Θ has period 2π , we get that

$$Ae^{i\omega\theta} + Be^{-i\omega\theta} = Ae^{i\omega\theta+2\pi i\omega} + Be^{-i\omega\theta-2\pi i\omega}$$

This happens when $\omega = m, m \in \mathbb{Z}$. Therefore, we get that the eigenvalues are $\alpha = m^2$, and the eigenfunctions are

$$\Theta(\theta) = Ae^{im\theta} + Be^{-im\theta}$$

Note, however, that m can be negative. Thus, we can let $B = 0$ without losing any solutions. This is because at the end, we are going to linearly combine the eigenfunctions $\Psi = TR\Theta\Phi$. Letting $C_m = A_m + B_{-m}$, the part of the linear combination for Θ is

$$\begin{aligned} \sum_m A_m e^{im\theta} + B_m e^{-im\theta} &= (A_0 + B_0) + \sum_{m>0} (A_m + B_{-m})e^{im\theta} + (A_{-m} + B_m)e^{-im\theta} \\ &= C_0 + \sum_{m>0} C_m e^{im\theta} + C_{-m} e^{-im\theta} \\ &= \sum_m C_m e^{im\theta} \end{aligned}$$

Thus, we can say that the eigenfunctions are

$$\Theta(\theta) = C_m e^{im\theta} \tag{12}$$

so long as there are the same number of negative values for m as positive values for m . The corresponding eigenvalues are $\alpha = m^2$.

These eigenfunctions are orthogonal with respect to the inner product

$$(\Theta_m, \Theta_{m'}) = \int_0^{2\pi} \Theta_m(\theta) \bar{\Theta}_{m'}(\theta) d\theta = \int_0^{2\pi} e^{im\theta} e^{-im'\theta} d\theta$$

This is because for $m \neq m'$,

$$\int_0^{2\pi} e^{im\theta} e^{-im'\theta} d\theta = \int_0^{2\pi} e^{i(m-m')\theta} d\theta = \frac{e^{i(m-m')\theta}}{i(m-m')} \Big|_{\theta=0}^{2\pi} = 0$$

Now that we know $\alpha = m^2$, the Φ equation (10) becomes

$$\sin(\phi) (\sin(\phi)\Phi')' + \gamma \sin^2(\phi)\Phi = m^2\Phi$$

Bringing all the terms to one side and dividing by $\sin^2 \phi$,

$$\frac{(\sin(\phi)\Phi')'}{\sin \phi} + \left(\gamma - \frac{m^2}{\sin^2 \phi} \right) \Phi = 0 \tag{13}$$

Note there could be singularities at $\phi = 0$ or $\phi = \pi$. Since we require that the solution to the Schrodinger equation $\Psi = TR\Theta\Phi$ be finite everywhere, we have the condition that Φ is finite at $\phi = 0$ and $\phi = \pi$.

Now, make a change of variables $s = \cos \phi$. Then $ds = -\sin \phi d\phi$, and $d\phi = -\frac{ds}{\sin \phi}$. Also, $\sin^2 \phi = 1 - \cos^2 \phi = 1 - s^2$. Therefore,

$$\frac{(\sin(\phi)\Phi)'}{\sin \phi} = \frac{\frac{d}{d\phi} \left(\sin(\phi) \frac{d\Phi}{d\phi} \right)}{\sin \phi} = -\frac{d}{ds} \left(-\sin^2(\phi) \frac{d\Phi}{ds} \right) = \frac{d}{ds} \left((1 - s^2) \frac{d\Phi}{ds} \right)$$

Thus, (13) turns into

$$\frac{d}{ds} \left((1 - s^2) \frac{d\Phi}{ds} \right) + \left(\gamma - \frac{m^2}{(1 - s^2)} \right) \Phi = 0 \quad (14)$$

In addition, the condition that $\Phi(\phi)$ is finite at $\phi = 0$ and $\phi = \pi$ turns into the condition that $\Phi(s)$ is finite at $s = \pm 1$.

Equation (14) is called the associated Legendre equation, and its eigenfunctions are

$$\Phi(s) = P_l^{|m|}(s) = P_l^{|m|}(\cos \phi) \quad (15)$$

where l is an integer $\geq |m|$. $P_l^k(s)$ is defined for $l \geq k = |m|$ as the function

$$P_l^k(s) = \frac{(-1)^k}{2^l l!} (1 - s^2)^{k/2} \frac{d^{l+k}}{ds^{l+k}} (s^2 - 1)^l \quad (16)$$

The corresponding eigenvalues are $\gamma = l(l + 1)$.¹

This solution is finite at $s = \pm 1$. Since $l \geq k = |m|$, $(s^2 - 1)^l$ is a polynomial of degree $2l \geq l + k$. Thus, $(d^{l+k}/ds^{l+k})(s^2 - 1)^l$ is a polynomial of degree $2l - (l + k) = l - k$. So, $(d^{l+k}/ds^{l+k})(s^2 - 1)^l$ is finite at $s = \pm 1$. Furthermore, $(1 - s^2)^{k/2}$ is finite at $s = \pm 1$, and $(-1)^k/2^l l!$ is a finite constant. Therefore, all the factors are finite, and so this solution satisfies the condition that Φ is finite at $s = \pm 1$.

The eigenfunctions $P_l^{|m|}$ are orthogonal with respect to the inner product

$$(P_l^k, P_{l'}^k) = \int_{-1}^1 P_l^k(s) P_{l'}^k(s) ds$$

That is,

$$(P_l^k, P_{l'}^k) = \int_{-1}^1 P_l^k(s) P_{l'}^k(s) ds = 0 \quad \text{for } l \neq l'$$

¹I am actually not sure where the $(-1)^k$ in equation (16) comes from. The section in Strauss on Legendre functions seems to not have it. I was unable to derive this equation with the information in the section.

As an example, consider the case when $m = 0$, $l = 1$, and $l' = 3$. We have

$$\begin{aligned} P_1^0(s) &= \frac{1}{2} \frac{d}{ds}(s^2 - 1) = s \\ P_3^0(s) &= \frac{1}{48} \frac{d^3}{ds^3}(s^2 - 1)^3 \end{aligned}$$

The third derivative is

$$\begin{aligned} \frac{d^3}{ds^3}(s^2 - 1)^3 &= \frac{d^3}{ds^3}(s^6 - 3s^4 + 3s^2 - 1) \\ &= \frac{d^2}{ds^2}(6s^5 - 12s^3 + 6s) \\ &= \frac{d}{ds}(30s^4 - 36s^2 + 6) \\ &= 120s^3 - 72s \end{aligned}$$

Thus, the inner product is

$$\begin{aligned} \int_{-1}^1 P_1^0(s)P_3^0(s)ds &= \frac{1}{48} \int_{-1}^1 s(120s^3 - 72s)ds \\ &= \frac{1}{48} \int_{-1}^1 120s^4 - 72s^2 ds \\ &= \frac{1}{48} \left[\frac{120}{5}s^5 - \frac{72}{3}s^3 \right]_{-1}^1 \\ &= \frac{1}{48} [24s^5 - 24s^3]_{-1}^1 \\ &= 0 \end{aligned}$$

Recall that $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$. We can now put together an expression for Y :

$$Y_l^m(\theta, \phi) = \Theta_m(\theta)\Phi_l^m(\phi) = e^{im\theta} P_l^{|m|}(\cos \phi) \quad (17)$$

The relation $l \geq |m|$ puts a constraint on l and m . They must be in the range

$$l \geq 0 \quad , \quad -l \leq m \leq l$$

Also note that there are the same number of positive and negative values for m . This is exactly condition we needed earlier in order to use $\Theta(\theta) = e^{im\theta}$ instead of $\Theta(\theta) = e^{im\theta} + e^{-im\theta}$.

The functions Y_l^m are called spherical harmonics. They are orthogonal with respect to the inner product

$$(Y_l^m, Y_{l'}^{m'}) = (\Theta_m, \Theta_{m'}) \cdot (\Phi_l^m, \Phi_{l'}^{m'})$$

To see why this is true, consider the possible cases for the indices l, m, l' , and m' . We can split the cases up as follows:

- Case 1 : $m \neq m'$
- Case 2 : $m = m'$ and $l \neq l'$
- Case 3 : $m = m'$ and $l = l'$

For Case 1, since $m \neq m'$, we have $(\Theta_m, \Theta_{m'}) = 0$, and so $(Y_l^m, Y_{l'}^{m'}) = 0$. For Case 2, since $m = m'$ and $l \neq l'$, we have $(\Phi_l^m, \Phi_{l'}^{m'}) = (\Phi_l^m, \Phi_{l'}^m) = 0$, and so $(Y_l^m, Y_{l'}^{m'}) = 0$. Case 3 is the case where $Y_l^m = Y_{l'}^{m'}$, and so this case does not affect orthogonality. Thus, $(Y_l^m, Y_{l'}^{m'}) = 0$ if $m \neq m'$ or $l \neq l'$, and so the functions Y_l^m form an orthogonal set.

Note that the formula for the inner product is

$$(Y_l^m, Y_{l'}^{m'}) = \int_0^{2\pi} e^{im\theta} e^{-im'\theta} d\theta \int_{-1}^1 P_l^{|m|}(s) P_{l'}^{|m|}(s) ds = \int_0^{2\pi} \int_{-1}^1 e^{im\theta} e^{-im'\theta} P_l^{|m|}(s) P_{l'}^{|m|}(s) ds d\theta \quad (18)$$

Since $s = \cos \phi$, we have $ds = -\sin \phi d\phi$, and so

$$\begin{aligned} (Y_l^m, Y_{l'}^{m'}) &= \int_0^{2\pi} \int_{\pi}^0 e^{im\theta} e^{-im'\theta} P_l^{|m|}(\phi) P_{l'}^{|m|}(\phi) (-\sin \phi) d\phi d\theta \\ &= \int_0^{2\pi} \int_0^{\pi} e^{im\theta} e^{-im'\theta} P_l^{|m|}(\phi) P_{l'}^{|m|}(\phi) \sin(\phi) d\phi d\theta \end{aligned}$$

At this point, we have found the eigenfunctions Y_l^m , and have a solution for the time part $T(t)$. So the only part of the solution to $\Psi(t, r, \theta, \phi) = T(t)R(r)Y(\theta, \phi)$ that we do not know yet is $R(r)$. Recall that the equation for R is

$$\left(\lambda + \frac{2}{r} - \frac{\gamma}{r^2} \right) R + R'' + \frac{2}{r} R' = 0$$

Plugging in $\gamma = l(l+1)$ and rearranging terms, we get

$$R'' + \frac{2}{r} R' + \left(\lambda + \frac{2}{r} - \frac{l(l+1)}{r^2} \right) R = 0 \quad (19)$$

Because of the condition that $\iiint |\Psi|^2 d\mathbf{x}$ is finite, we require that $R(r)$ is finite for all r (in particular, $R(0)$ must be finite), and also that $R(\infty)$ is finite.

We can solve the ODE (19) for $\lambda < 0$ by doing a change of variables and then looking for solutions in the form of a power series.² Let $w(r) = e^{\beta r} R(r)$, where $\beta = \sqrt{-\lambda}$ for $\lambda < 0$. Then $R = e^{-\beta r} w$, and so

$$\begin{aligned} R' &= -\beta e^{-\beta r} w + e^{-\beta r} w' \\ &= e^{-\beta r} (-\beta w + w') \\ R'' &= -\beta e^{-\beta r} (-\beta w + w') + e^{-\beta r} (-\beta w' + w'') \\ &= e^{-\beta r} (\beta^2 w - 2\beta w' + w'') \end{aligned}$$

Substituting these for R , R' , and R'' in (19), as well as $\lambda = -\beta^2$, we get

$$e^{-\beta r} (\beta^2 w - 2\beta w' + w'') + \frac{2}{r} e^{-\beta r} (-\beta w + w') + \left(-\beta^2 + \frac{2}{r} - \frac{l(l+1)}{r^2} \right) e^{-\beta r} w = 0$$

²I tried to show that there are no solutions for $\lambda \geq 0$ satisfying the condition $R(0)$ finite, $R(\infty)$ finite, but can't yet — I actually haven't taken an ODE course and don't have much experience with ODEs.

Since $e^{-\beta r}$ is never 0, we can divide by it. Doing this and distributing,

$$\beta^2 w - 2\beta w' + w'' - \frac{2}{r}\beta w + \frac{2}{r}w' - \beta^2 w + \frac{2}{r}w - \frac{l(l+1)}{r^2}w = 0$$

Combining like terms,

$$w'' + 2\left(\frac{1}{r} - \beta\right)w' + \left(\frac{2(1-\beta)}{r} - \frac{l(l+1)}{r^2}\right)w = 0 \quad (20)$$

Now, consider the power series expansion of w , $w(r) = \sum_{k=0}^{\infty} a_k r^k$. Any analytic function can be expressed as a power series, so any (nice) solution is a solution of this form. We want to find the coefficients a_k . Plugging in the series into (20), we get

$$\sum_{k=0}^{\infty} k(k-1)a_k r^{k-2} + 2\left(\frac{1}{r} - \beta\right)\sum_{k=0}^{\infty} k a_k r^{k-1} + \left(\frac{2(1-\beta)}{r} - \frac{l(l+1)}{r^2}\right)\sum_{k=0}^{\infty} a_k r^k = 0$$

Note that we can say the sums for the derivatives start at $k = 0$. This is because all the coefficients before the constant term are zero. Thus, terms before the constant term are zero anyway, except possibly when $r = 0$. As we will soon see, however, we will find the coefficients by requiring the expression above to be zero *for all* r , and so the case when $r = 0$ will not affect our argument. Distributing the last two terms and bringing the factors of $1/r$ and $1/r^2$ into the sums,

$$\sum_{k=0}^{\infty} k(k-1)a_k r^{k-2} + 2\sum_{k=0}^{\infty} k a_k r^{k-2} - 2\beta\sum_{k=0}^{\infty} k a_k r^{k-1} + 2(1-\beta)\sum_{k=0}^{\infty} a_k r^{k-1} - l(l+1)\sum_{k=0}^{\infty} a_k r^{k-2} = 0$$

Now, change the indices in the third and fourth sums such that all sums are expressed in terms of factors of r^{k-2} . This gives us

$$\sum_{k=0}^{\infty} k(k-1)a_k r^{k-2} + 2\sum_{k=0}^{\infty} k a_k r^{k-2} - 2\beta\sum_{k=1}^{\infty} (k-1)a_{k-1} r^{k-2} + 2(1-\beta)\sum_{k=1}^{\infty} a_{k-1} r^{k-2} - l(l+1)\sum_{k=0}^{\infty} a_k r^{k-2} = 0$$

Combining the sums with the same indices,

$$\sum_{k=0}^{\infty} [k(k-1) + 2k - l(l+1)] a_k r^{k-2} + \sum_{k=1}^{\infty} [-2\beta(k-1) + 2(1-\beta)] a_{k-1} r^{k-2} = 0$$

Now, the left hand side must be identically zero. Therefore, the all the coefficients of r^{k-2} must be zero. Thus, for $k = 0$, we get

$$-l(l+1)a_0 = 0 \quad (21)$$

For all other k , we get

$$[k(k-1) + 2k - l(l+1)] a_k + [-2\beta(k-1) + 2(1-\beta)] a_{k-1} = 0$$

Bringing the a_{k-1} term to the other side of the equation and expanding products,

$$[k^2 - k + 2k - l(l+1)] a_k = -[-2\beta k + 2\beta + 2 - 2\beta] a_{k-1}$$

and so

$$[k(k+1) - l(l+1)] a_k = 2(\beta k - 1)a_{k-1} \quad (22)$$

Thus, (21) and (22) gives us a recursion relation for a_k .

Now, recall that l is an integer with $l \geq 0$. If $l = 0$, then a_0 is arbitrary. If not, then by (22) we get that $a_1 = 0$ if $l > 1$. If $l = 1$ then a_1 can be anything.

We can show by induction that all a_k are 0 until a_l , which is arbitrary. In the case where $k = 0$, (21) tells us that $a_0 = 0$ if $l > 0$, and that a_0 can be anything if $l = 0$. Now, assume $a_{k-1} = 0$ for $0 < k < l$. By (22), we get

$$[k(k+1) - l(l+1)] a_k = 0$$

And since $k < l$, $k(k+1) - l(l+1) \neq 0$ and so $a_k = 0$. In the case where $k = l$, (22) gives us

$$0 \cdot a_l = 2(\beta l - 1)a_{l-1} = 0$$

and so a_l can be anything.

Now, consider the case when $\beta = 1/n$, where n is an integer, $n > l$. Then (22) gives us

$$[n(n+1) - l(l+1)]a_n = 2\left(\frac{1}{n} \cdot n - 1\right) a_{n-1} = 2(1-1)a_{n-1} = 0$$

and so $a_n = 0$. Furthermore, once $a_n = 0$, (22) tells us that all $a_k = 0$ for $k > n$ as well. Thus, the power series $w(r) = \sum_k a_k r^k$ is a polynomial of degree $n-1$. Since $R(r) = e^{-\beta r} w(r)$, we get that $R(r)$ is a decreasing exponential times a polynomial. Thus, $R(r) \rightarrow 0$ as $r \rightarrow \infty$, and so the condition that $R(\infty) = 0$ is satisfied.

If β is not of the form $1/n$, then using (22) and the fact that all coefficients before a_l are 0, we get

$$a_k = a_l \prod_{j=l+1}^k \frac{2(\beta j - 1)}{j(j+1) - l(l+1)}$$

Thus, for very large k , we can say

$$a_k \approx a_l \prod_{j=l+1}^k \frac{2\beta j - 2}{j(j+1)} = 2a_l \prod_{j=l+1}^k \left(\frac{\beta}{j+1} - \frac{1}{j(j+1)} \right) \approx 2a_l \prod_{j=l+1}^k \frac{\beta}{j} = 2a_l \frac{\beta^{k-l}}{(k)_{k-l}}$$

where I used the notation $(p)_q = p(p-1)(p-2) \cdots (p-(q-1))$ for integers p and q . Now, for large r , the power series is dominated by the terms a_k for large k . Therefore, for large r , we can use the above approximation to get

$$w(r) = \sum_k a_k r^k \approx 2a_l \sum_k \frac{\beta^{k-l}}{(k)_{k-l}} r^k$$

So, $R(r) = e^{-\beta r} w(r)$ has the limit

$$\lim_{r \rightarrow \infty} R(r) = \lim_{r \rightarrow \infty} \frac{w(r)}{e^{\beta r}} = \lim_{r \rightarrow \infty} \frac{2a_l \sum_k (\beta^{k-l}/(k)_{k-l}) r^k}{\sum_k \beta^k r^k / k!}$$

Multiplying by 1 in the form $\frac{\beta^l/l!}{\beta^l/l!}$, we get that this is

$$\lim_{r \rightarrow \infty} R(r) = \lim_{r \rightarrow \infty} \frac{2a_l \sum_k (\beta^k/k!) r^k}{\beta^l/l! \sum_k \beta^k r^k / k!} = \frac{2a_l}{\beta^l/l!} \neq 0$$

Thus, the condition that $R(\infty) = 0$ is not satisfied, and so β must equal $1/n$ for an integer $n > l$.

Therefore, we get from the $\beta = 1/n$ case that the eigenfunctions are

$$R(r) = e^{-r/n} \sum_{k=l}^{n-1} a_k r^k \quad (23)$$

where the a_k satisfy

$$\begin{aligned} a_l &= 1 \\ a_k &= \frac{2(\beta k - 1)}{k(k+1) - l(l+1)} a_{k-1} \quad , \quad k > l \end{aligned}$$

and $n > l$. We can set $a_l = 1$ because all a_k are some constant number times a_l due to the recursion relation—thus, a_l is a constant factor. The corresponding eigenvalues are $\lambda = -\beta^2 = -1/n^2$.

Now, we know the eigenfunctions R and Y , as well as the solution for T . We can now put the whole problem together using (3), (23) and (17). The eigenfunctions are

$$\Psi_{lnm}(t, r, \theta, \phi) = T_n(t) R_{ln}(r) Y_l^m(\theta, \phi) = e^{it/2n^2} e^{-r/n} e^{im\theta} P_l^{|m|}(\cos \phi) \sum_{k=l}^{n-1} a_k r^k \quad (24)$$

Thus, using linearity we get the more general solution

$$\Psi(t, r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=l+1}^{\infty} A_{lmn} \left[e^{it/2n^2} e^{-r/n} e^{im\theta} P_l^{|m|}(\cos \phi) \sum_{k=l}^{n-1} a_k r^k \right] \quad (25)$$

Using an initial probability distribution $\Psi_0(r, \theta, \phi) = \Psi(t = 0, r, \theta, \phi)$ we should be able to compute the coefficients A_{lmn} . First, note that the plugging in $t = 0$ gets rid of the T eigenfunction, since $T(t = 0) = 1$. Thus,

$$\Psi_0 = \sum_l \sum_m \sum_n A_{lmn} R_{ln} Y_l^m$$

Now, recall that the functions $Y_l^m(\theta, \phi)$ are orthogonal with respect to the inner product (18). So for a particular l' and m' , taking the inner product with $Y_{l'}^{m'}$ makes all terms in the l and m sums zero except the l'^{th} and m'^{th} . Thus, taking the inner product gives us

$$\int_0^{2\pi} \int_0^\pi \Psi_0 Y_{l'}^{m'} d\phi d\theta = \left\| Y_{l'}^{m'} \right\|^2 \sum_{n=l'+1}^{\infty} A_{l'm'n} R_{l'n} \quad (26)$$

I wasn't able to find an inner product for the R functions that makes $R_{l'n}$ an orthogonal set (either through research or on my own—I did try to get one for a long time). I also actually haven't seen anything that suggests there is or isn't a such an inner product. However, since the degree of each of the polynomials in $R_{l'n}$ is different for each value of n , the functions $R_{l'n}$ seem like they would be orthogonal under some inner product. Even if they aren't orthogonal, though, they would at least be linearly independent. So even in the worst case, there should be some way to compute the coefficients $A_{l'm'n}$, even if it involves solving a linear system numerically.

If we do have that inner product in which the $R_{l'n}$ are orthogonal, we can use it to isolate the particular coefficient. That is, for a particular n' , we can take the inner product of both sides with $R_{l'n'}$ and get

$$\left(R_{l'n'}, \int_0^{2\pi} \int_0^\pi \Psi_0 Y_{l'}^{m'} d\phi d\theta \right) = \left\| Y_{l'}^{m'} \right\|^2 A_{l'm'n'} \left\| R_{l'n'} \right\|^2$$

This gives us

$$A_{l'm'n'} = \left(\left\| Y_{l'}^{m'} \right\|^2 \left\| R_{l'n'} \right\|^2 \right)^{-1} \left(R_{l'n'}, \int_0^{2\pi} \int_0^\pi \Psi_0 Y_{l'}^{m'} d\phi d\theta \right) \quad (27)$$

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