The Partial Wave Radial Equation PhL 12.19.08

These notes are ancillary to the non-relativistic QM scattering discussion of Schiff's Chapter 5.

Partial Wave Framework of the Radial Equation. 1
Theorem 1: The Cupping Theorem for $\chi(r)$ 2
Corollary 1. Beware near r=0. 2
Question: Are there boundary conditions implied for R(r) as $r \to 0$ for general V(r) ? 2
(a) Can R(r) diverge at r=0 ? If it can, then the slope at r=0 will be infinite. 2
(b) Can R have a non-zero slope at r=0, and can this slope be infinite ? 3
The Notion of "integrating in" from $r = \infty$ to find $R_\ell(r)$. 4
Theorem 2: The Large-r Sine Theorem. 4
Comment: 4
Review of the Partial Wave Expansion for the non-Coulomb case. 5
The Coulomb Scattering Situation 6
Non-coulomb review 6
Coulomb case: 7
What is a plane wave? 8
Conclusion: 9
Comments on the Coulomb Plane Wave 10
The Partial Wave Amplitude for Coulomb Scattering is $e^{2i\sigma_\ell}$ 12
Appendix A: Computing the partial wave expansion of the Coulomb Plane Wave 14

This is where some "missing information" lies in my QM pursuits.

Partial Wave Framework of the Radial Equation. In the partial wave expansion for a central potential V(r), *each* partial wave provides a solution to the full SE:

$$\psi_{\ell m}(r,\theta,\varphi) = R_\ell(r)\, Y_{\ell m}(\theta,\varphi)$$

The "radial SE" looks like this , from Schiff page 77 14.3

$$1/r^2 \partial_r(r^2 \partial_r R) + \{2\mu/\hbar^2[\, E\text{-}V(r)] - \ell(\ell+1)/r^2 \,\}\, R = 0$$

or for a Coulomb potential

$$1/r^2 \partial_r(r^2 \partial_r R) + \{\, k^2 - 2nk/r - \ell(\ell+1)/r^2 \,\}\, R = 0$$

where $nk = (\mu ZZ' e^2/\hbar^2)$ and $E = p^2/2\mu = (\hbar^2/2\mu)k^2$ and $V(r) = ZZ'e^2/r$. For other potentials, including no potential, we obviously replace the 1/r term above with something else.

If we write $R = \chi/r$, the equation for χ becomes (Schiff page 117 19.1)

$$\chi'' + [\, k^2 - (2\mu/\hbar^2)V(r) - \ell(\ell+1)/r^2]\, \chi = 0$$

I like this form because there is no first derivative and we can make this claim"

Theorem 1: The Cupping Theorem for χ(r) Assume that [...] in the χ equation just above has sign s at some value of r. There are two cases to consider:

(a) If s> 0, then χ"/χ < 0 => if χ is positive, it is cupping down toward the axis, meaning the solution is sinusoidal-like and is not going to blow up.

(b) If s<0, then χ"/χ > 0 => if χ is positive, it is cupping up, meaning expo like, not sinusoidal like, not stable, could blow up.

Corollary 1. Beware near r=0. In the case of V(r) = 0 or any V(r) that is repulsive, for small r you get case (b) and solution could blow up at r=0 so be careful. If V(r) is weaker than the centrifugal term, that centrifugal term will win as r→0 and put you into the dangerous expo-unstable situation near r=0.

Question: Are there boundary conditions implied for R(r) as r→ 0 for general V(r) ?

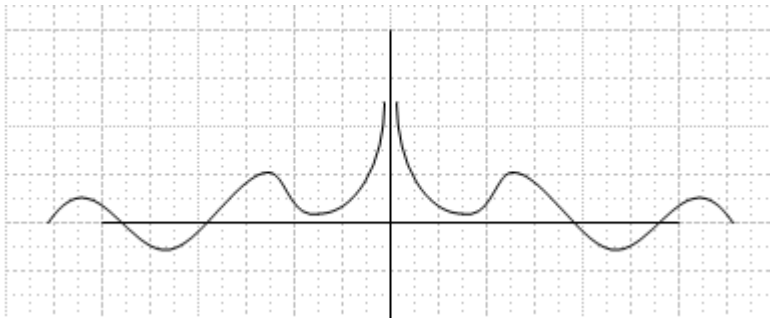
This is the question that I think Schiff has not remarked upon very well, though he does talk about the 1D case. Let's break this question down a bit:

(a) Can R(r) diverge at r=0 ? If it can, then the slope at r=0 will be infinite.

Consider first this fact:

$$Y_{\ell m}(\pi - \theta, \phi + \pi) = (-1)^{\ell} Y_{\ell m}(\theta, \phi)$$

Now assume that R blows up, so if we plot $\psi_\ell(r,\theta,\varphi)$ for even ℓ on a ray through the origin at angle θ,φ we see



As we cross through the origin, we jump instantly from $Y_{\ell m}(\theta,\varphi)$ to $Y_{\ell m}(\pi-\theta,\varphi+\pi)$ which for even ℓ causes no change at all. So our ψ for this partial wave is not differentiable at r=0 which sounds bad for an allowed "wave function" in QM. For the V=0 case, this would happen with an $n_\ell(kr)$ Bessel solution. For odd ℓ, we would flip the left side of the above picture, and things are even worse!

Schiff on page 86 above 15.11 says that "R must be finite at r=0" which would rule out the above situation, but he is working with a central well case where the potential V(r) is certainly smooth at r=0.

You might imagine that for a singular potential or just from the singular centrifugal term, a diverging ψ might be "legal" in some situations at r=0. Perhaps it just has to be integrable in a small ball around the origin so the probability doesn't diverge, though even that is questionable in a collision situation.

Let's see what various authors say about this in their "central potential radial equation" sections.

Saxon: Page 277 he says "*if* R is bounded at r=0, then $\chi = 0$ there" so he sidesteps the question.

Messiah: Page 350 he talks quite a lot about the origin situation. First he argues that $\chi(0) = 0$ (agreeing with Schiff) because only then is the radial momentum operator Hermitian, an argument detailed out on page 346. He then notes that, near r=0, if we assume the centrifugal term dominates, we have the spherical Bessel situation there where r=0 is a regular singular point so there are two solutions with the two indices, and the j solution goes with r^{ℓ} index and is regular there, while n goes with $r^{-\ell-1}$. Remember that j and n are solutions for function R (Schiff p 84 bottom), not χ. [Note that spherical Bessel is a special case where Δindices = integer, yet you don't get the log situation for the second solution.]

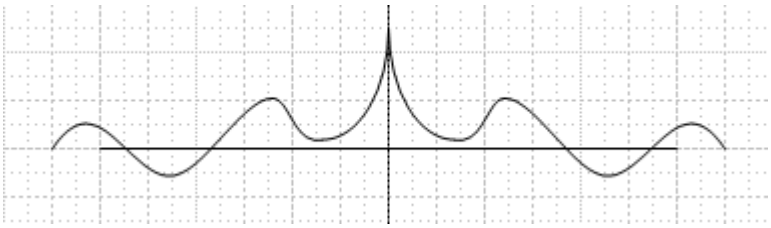
Comment: Suppose $R \sim r^{-k}$ is the form of the blow up at r=0. Then $\int r^2 dr\, r^{-2k}$ needs to be finite at least for a bound state problem. The integral of r^{-2k+2} is r^{-2k+1} so finite prob means $-2k+1 \geq 0$, $k \leq 1/2$. So even if k=1, your probability blows up. The $n_\ell \sim \rho^{-\ell-1}$ so even with ℓ=0, these must be excluded.

Messiah's conclusion is this: In order to prevent a divergent probability in a sphere around the origin, you just specify the boundary condition that R(0) = finite and $\chi(0) = 0$!

Answer to Question (a): No, R cannot diverge at the origin, it must be finite there so $\chi = rR = 0$ there. Thus, the picture I show above is not allowed.

(b) Can R have a non-zero slope at r=0, and can this slope be infinite ?

We have concluded that R cannot blow up at r=0, but can it look like this?



where there is a cusp at the origin. Recall from Schiff's 1D discussion that we ruled out such cusps there and this is what determined eigenvalues, see pictures on page 35 for example.

Well, again, let's assume that as $r \to 0$ the centrifugal term dominates, so our solutions are j-like. We then have that $j_\ell \sim \rho^{\ell}$ so that $(j_\ell)' \sim \ell\, \rho^{\ell-1}$. From the small ρ limit Schiff p 85 we see that

	R'(r)	R(r)
value of ℓ	slope of j_ℓ at r=0	j_ℓ itself at r=0
0	0	1

1	1/3	0
2,3,4...	0	0

and you see this in the A&S graphs on page 438, though the ℓ=0 case is not fully graphed.

Answer to question (b): We can never have infinite slope for R at r=0 just because the solution there is always a power and we have to rule out the diverging powers, so infinite slopes are ruled out with them. In fact, we can just think of the j_ℓ functions as the real behavior near r=0 for a soft potential like 1/r or for no potential, and with just two exceptions as noted in our table above, we always have R = 0 and R' = 0 at r=0!

The Notion of "integrating in" from r = ∞ to find $R_\ell(r)$.

Assuming a finite range potential, for large r the radial SE for χ is just this:

$$\chi'' + [\, k^2 - (2\mu/\hbar^2)V(r) - \ell(\ell+1)/r^2]\, \chi = 0 \qquad \rightarrow \qquad \chi'' + [\, k^2]\, \chi = 0$$

According to our theorem above, χ is sine-like, and in fact it is exactly sine and cosine! We could write the following general form

$$\chi = A\sin(kr + \varphi_\ell)$$

where we show two real constants for our entirely real ODE. Now suppose you start with this assumed form at large r, and you try to manually integrate the ODE in toward the origin. As you move along, $\chi(r)$ is some continuous function. Suppose V(r) = 0 or 1/r. Eventually as we get very close to the origin, we are going to get some linear combination of j_ℓ and n_ℓ functions, since these are the independent solutions there. If we have any n_ℓ, we are in trouble at the origin. It seems likely that there is only one value of δ_ℓ which will cause that n_ℓ contribution to vanish at the origin, so δ_ℓ is like an eigenvalue.

For example, suppose V(r) = 0 everywhere. We know from Schiff 86 top that $j_\ell \rightarrow \sin(kr - \ell\pi/2)/r$ which means that $\chi = rR \rightarrow \sin(kr - \ell\pi/2)$ and this means $\delta_\ell = -\ell\pi/2$. If we start with some slightly *different* phase shift at r=0 and "integrate in" toward the origin, when we get to the origin, our solution is going to blow up because it will have some n_ℓ component! We know this because had we started only with a j_ℓ component at r=0 and moved outward, we would get $\sin(kr - \ell\pi/2)$.

This suggests to me the following theorem:

Theorem 2: The Large-r Sine Theorem. For any potential V(r), we know that for large r our radial solution is $\chi = A\sin(kr + \varphi_\ell)$, and there is a unique value of φ_ℓ [within the obvious range] which will result in finite R at the origin, and will thus result in a legal radial wave function.

Comment: We should not be surprised to see that large r limits of solutions to radial SE's for χ always go like sine and cosine. This is because the large r equation is always $\chi'' + [\, k^2]\, \chi = 0$. So in some sense this sine and cosine asymptotic behavior is a "boundary condition".

Review of the Partial Wave Expansion for the non-Coulomb case.

Write the wavefunction which solves the scattering problem in two ways:

$$\psi_2 = \Sigma_\ell\, (2\ell+1)\, i^\ell\, R_\ell(r) P_\ell(z) \qquad \rightarrow\ \Sigma_\ell\, (2\ell+1)\, i^\ell\, A_\ell \sin [\, kr - \ell\pi/2 + \delta_\ell] \, P_\ell(z)\, /kr$$

NOTICE that we have added a factor i^ℓ which is not the usual thing one does, but of course the scale of R is arbitrary so we can so this.

Here we have used Theorem 2 but we set $\varphi_\ell = \delta_\ell - \ell\pi/2$ so that δ_ℓ will be the amount of phase shift *relative to* a j_ℓ function, *and* we have set $A = A_\ell/k$. We then expand the sin and get

$$\psi_2 \rightarrow (1/2ik)\, \Sigma_\ell\, (2\ell+1)\, i^\ell\, A_\ell\, [\, e^{ikr}\, e^{-in\ell/2}\, e^{+i\delta} \;-\; e^{-ikr}\, e^{+in\ell/2}\, e^{-i\delta}\,]\; P_\ell(z)/r$$

$$= (1/2ik)\, \{\; (e^{ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, i^\ell\, A_\ell\, e^{-in\ell/2}\, e^{+i\delta} \;-\; (e^{-ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, i^\ell\, A_\ell\, e^{+in\ell/2}\, e^{-i\delta}\;\}$$

$$= (1/2ik)\, \{\; (e^{ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, A_\ell\; e^{+i\delta} \;-\; (e^{-ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, i^\ell\, A_\ell\, e^{+in\ell/2}\, e^{-i\delta}\;\}$$

where we have completely separated are large-r ψ_2 into an outgoing and an incoming part.

Now we write

$$\psi_1 = e^{ikz} + (e^{ikr}/r) f(\theta)$$

We then expand each of these two factors on partial waves for large r

$$e^{ikz} = \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, i^\ell\, [\sin [\, kr - \ell\pi/2]/kr\,] \qquad \text{// expanding } j_\ell(kr) \text{ Schiff page 86}$$

$$= (1/2ik)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, i^\ell\, \{\; e^{ikr}\, e^{-in\ell/2} \;-\; e^{-ikr}\, e^{+in\ell/2}\;\}/r$$

$$= (1/2ik)\, \{\; (e^{ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, i^\ell\, e^{-in\ell/2} P_\ell(z) \;-\; (e^{-ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, i^\ell e^{+in\ell/2}\, P_\ell(z)\;\}$$

$$= (1/2ik)\, \{\; (e^{ikr}/r)\, \Sigma_\ell\, (2\ell+1)\; P_\ell(z) \;-\; (e^{-ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, i^\ell e^{+in\ell/2}\, P_\ell(z)\;\}$$

Finally, we expand our $f(\theta)$ as follows [defining f_ℓ in this way]

$$f(\theta) = (1/2ik)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z) f_\ell$$

Thus we can write ψ_1 as follows:

$$\psi_1 = (1/2ik)\, \{\; (e^{ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, [\, 1 + f_\ell\,] \;-\; (e^{-ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, i^\ell e^{+in\ell/2} P_\ell(z)\;\}$$

$$\psi_2 = (1/2ik)\, \{\; (e^{ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, A_\ell\; e^{+i\delta} \;-\; (e^{-ikr}/r)\, \Sigma_\ell\, (2\ell+1)\, P_\ell(z)\, i^\ell\, A_\ell\, e^{+in\ell/2}\, e^{-i\delta}\;\}$$

The incoming part of ψ_2 can only be balanced by that part of e^{ikz} and we get:

$$i^\ell e^{+i\pi\ell/2} = i^\ell A_\ell e^{+i\pi\ell/2} e^{-i\delta} \quad \Rightarrow 1 = A_\ell e^{-i\delta} \quad \Rightarrow A_\ell = e^{i\delta}$$

The outgoing part of ψ_2 is balanced by pieces of both the e^{ikz} term and the $f(\theta)$ term:

$$[\,1 + f_\ell\,] = A_\ell\ e^{+i\delta} = e^{2i\delta} \quad \Rightarrow \quad f_\ell = (e^{2i\delta} - 1) = e^{i\delta}\sin\delta/2i$$

and so we have reproduced the results on Schiff page 199 for the second time in notes, but I wanted to do it again. Notice that the "1" in $[\,1 + f_\ell\,]$ and in $(e^{2i\delta} - 1)$ is coming from e^{ikz} .

So, our basis for this simple form for $f_\ell = (e^{2i\delta} - 1)$ is Theorem 2 AND the set up of our scattering experiment in the form of ψ_1 where we know f is related to the cross section.

Question: How did we know that $\psi_1 = e^{ikz} + (e^{ikr}/r)f(\theta)$ satisfied the SE in the large-r limit?

Our only appeal was that for large r, we have no potential at all, and we know that e^{ikz} satisfies such a SE, and so does (e^{ikr}/r). For the Coulomb potential, this appeal fails so the logic of the above presentation fails.

The Coulomb Scattering Situation

Non-coulomb review. In the above non-coulomb case, the basic idea was that far away, you could ignore V(r) and you just got the usual spherical Bessel j_ℓ and n_ℓ functions which had the large-r limits $R = \chi/r$

$$R_1 = j_\ell(kr) \rightarrow \sin(kr - \ell\pi/2)/kr$$
$$R_2 = n_\ell(kr) \rightarrow -\cos(kr - \ell\pi/2)/kr$$

We knew that $\chi'' + [\,k^2]\,\chi = 0$ for large r, which had sin and cos solutions, so each χ_i is a linear combination of sin(kr) and cos(kr) and they just happen to fall out as shown above. We also knew that we wanted e^{ikz} as our incident beam, and we knew how to expand this in $j_\ell(kr)$ and thus for large-r, it make terms of the above form. Then by claiming that the experiment means $\psi = e^{ikz} + (e^{ikr}/r)f(\theta)$ and claiming that each term separately solves the large-r radial SE, we found a nice form for $f_\ell = (e^{2i\delta\ell} - 1)$ and we noted that the "1" comes from the e^{ikz} contribution to the outgoing wave.

One step in the above process involving looking at the full solution ψ in this way

$$\psi_2 = \Sigma_\ell\,(2\ell+1)\,i^\ell R_\ell(r)P_\ell(z) \rightarrow \Sigma_\ell\,(2\ell+1)\,i^\ell A_\ell \sin[\,kr - \ell\pi/2 + \delta_\ell]\,P_\ell(z)/kr$$

$$\rightarrow (1/2ik)\,\{\,(e^{ikr}/r)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z)\,A_\ell\ e^{+i\delta\ell} - (e^{-ikr}/r)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z)\,i^\ell A_\ell\,e^{+i\pi\ell/2}\,e^{-i\delta\ell}\,\}$$

$$\rightarrow \psi_2(e^{ikr}\text{ part}) + \psi_2(e^{-ikr}\text{ part})$$

where the exact $R_\ell(r)$ is some unknown combination of j_ℓ and n_ℓ in the intermediate region outside V(r) but not super far out. We then imposed the condition that ψ_2 be the same as $\psi_1 = e^{ikz} + (e^{ikr}/r)f(\theta)$ which we could write as $\psi_1 = e^{ikz}\,(e^{ikr}\text{part}) + e^{ikz}\,(e^{-ikr}\text{part}) + (e^{ikr}/r)f(\theta)$. Our balance then was

$\psi_2(e^{-ikr}\text{ part}) = e^{ikz}\,(e^{-ikr}\text{part})$
$\psi_2(e^{ikr}\text{ part}) = e^{ikz}\,(e^{ikr}\text{part}) + (e^{ikr}/r)f(\theta)$

Coulomb case: In the coulomb case, the exact χ large-r solutions are not those shown above, but are instead these

$F_\ell/kr \;\rightarrow\; \sin[kr - \eta\ln(2kr) - \ell\pi/2 + \sigma_\ell]/kr$ where $\sigma_\ell = \arg\Gamma(\ell+1+i\eta)$
$G_\ell/kr \;\rightarrow\; -\cos[kr - \eta\ln(2kr) - \ell\pi/2 + \sigma_\ell]/kr$

where I use the sign for G seen in GW, which is opposite that of A&S, but I use the normalization of A&S. We like the GW sign because it makes such a close analogy to the non-coulomb case. You see that we "pick up" two extra pieces in the phase. Note that F_ℓ is a χ solution, while $j_\ell(kr)$ is an R solution. The parameter $\eta = n = \text{constants}/k$.

In either case, the two functions are independent solutions of the radial SE.

Moreover, for the Coulomb potential everywhere, only the F_ℓ solution is allowed since it is the one regular at r=0, and we can then claim that

$$\psi_2 = \Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i^\ell\, B_\ell\, F_\ell(r)/kr$$

where B_ℓ are some partial wave amplitudes. Any set of them provides a SE solution. Our question is now this: what are the correct B_ℓ such that ψ_2 describes a scattering experiment? The answer is given in Schiff page 143 21.21 where he has written out

$$F_\ell(r)/kr = C_\ell(\eta)\,(kr)^\ell\, e^{+ikr}\, M(\ell+1+i\eta,\, 2\ell+2,\, -2ikr)$$

[In fact, this is really $F_\ell(r)^*$ not $F_\ell(r)$, a minor point, but we need to take note of it. The large-r behavior is unaltered since it is real.]

It seems pretty clear that the large-r behavior of the solutions can be separated into similar incoming and outgoing bins which we would use to form a ψ_2 solution for large r:

outgoing $\quad e^{i[kr - \eta\ln(2kr) - \ell\pi/2 + \sigma\ell]} = e^{i[kr - \eta\ln(2kr)]}\, e^{i[\sigma\ell - \ell\pi/2]}$

incoming $\quad e^{-i[kr - \eta\ln(2kr) - \ell\pi/2 + \sigma\ell]} = e^{-i[kr - \eta\ln(2kr)]}\, e^{-i[\sigma\ell - \ell\pi/2]}$

where we just ignore the log(r) terms in this regard.

We might be tempted to *try* something like this:

$$\psi_1 \rightarrow e^{ikz} + (e^{i[kr - \eta\ln(2kr)]}/r)f(\theta)$$

as our scattering problem "set up". This is the right thing to do for the second term, but the first term must be wrong because e^{ikz} is not a solution of the coulomb radial SE for large r. It turns out that the right thing to do is in fact this:

$$\psi_1 \rightarrow e^{i[kz+\eta\ln(kr-kz)]} + (e^{i[kr-\eta\ln(2kr)]}/r)f(\theta)$$

but right now I only know that by looking at Schiff page 140 where we cheated and used parabolic coordinates.

What is a plane wave?

This is supposed to be a surface of constant phase. I know that e^{ikz} is such a surface only because I know it in Cartesian coordinates! In spherical coordinates this thing is $e^{ikr\cos\theta}$. How do we know this solves the spherical SE which says $(\nabla^2+k^2)\psi = 0$. Well,

$$\nabla^2 e^{ikr\cos\theta} = 1/r^2\,\partial_r(r^2\partial_r e^{ikr\cos\theta}) + 1/[r^2\sin\theta] * \partial_\theta(\sin\theta\,\partial_\theta e^{ikr\cos\theta})$$

$$= ik\cos\theta/r^2\,\partial_r(r^2 e^{ikr\cos\theta}) - ikr/[r^2\sin\theta] * \partial_\theta(\sin^2\theta\, e^{ikr\cos\theta})$$

$$= ik\cos\theta/r^2\,\{r^2 ik\cos\theta + 2r\}\, e^{ikr\cos\theta} - ikr/[r^2\sin\theta]\,\{\sin^2\theta(-ikr\sin\theta) + 2\sin\theta\cos\theta\}\, e^{ikr\cos\theta}$$

$$= ik[\ \cos\theta\,\{ik\cos\theta + 2/r\} - 1/[r\sin\theta]\,\{\sin^2\theta(-ikr\sin\theta) + 2\sin\theta\cos\theta\}\ ]\ e^{ikr\cos\theta}$$

$$= ik[\ \cos\theta\,\{ik\cos\theta + 2/r\} - \{\sin\theta(-ik\sin\theta) + 2\cos/r\}\ ]\ e^{ikr\cos\theta}$$

$$= ik[\ ik\cos^2\theta + 2\cos\theta/r + ik\sin^2\theta - 2\cos/r\ ]\ e^{ikr\cos\theta}$$

$$= ik[\ ik\cos^2\theta + ik\sin^2\theta\ ]\ e^{ikr\cos\theta} = (ik)^2\, e^{ikr\cos\theta} = -k^2\, e^{ikr\cos\theta}$$

and THAT is why $e^{ikr\cos\theta} = e^{ikz}$ satisfies the SE in spherical coordinates when V(r) = 0. I did this out just to show that it is not totally obvious when you are in the wrong coordinate system.

Now, consider $\psi = e^{i[kz + nlnk(r-z)]}$. If we write this in parabolics, recall from Chap 4 Schiff notes that

$x = r\sin\theta\cos\varphi = \sqrt{\xi\eta}\cos\varphi$	$\xi = r - z$	$r = (\eta + \xi)/2$
$y = r\sin\theta\sin\varphi = \sqrt{\xi\eta}\sin\varphi$	$\eta = r + z$	$\cos\theta = z/r = (\eta - \xi)/(\eta + \xi)$
$z = r\cos\theta = (\eta - \xi)/2$	$\tan\varphi = y/x$	$\sin\theta = 2\sqrt{\xi\eta}\ /\ (\eta + \xi)$

So we have that

$$\psi = e^{ik(\eta-\xi)/2}\, e^{in\ln[k\xi]} = e^{ik(\eta-\xi)/2}\,(k\xi)^{in} = k^{in}\{e^{-ik\xi/2}\,\xi^{in}\}\{e^{ik\eta/2}\} = k^{in} f(\xi)\, g(\eta)$$

Does $g(\eta)$ satisfy the η equation shown in 16.30B for large η ? First compute:

$g = e^{ikη/2}$

$g' = ik/2\ g$

$g'' = (ik/2)^2 g$

$[ηg']' = ηg'' + g' = [\ η(ik/2)^2 + (ik/2)]\ g\ = -(k^2/4)ηg + (ik/2)g$

Then 16.30B, says [m = 0 on azimuthal]

$-(k^2/4)ηg + (ik/2)g + (k^2/4)ηg + νg = 0$

which is fine if we set ν = - (ik/2). If this ν value is right, then $e^{ikη/2}$ satisfies this equation for all η, not just large η.

So that is promising, but now we have to show that f(ξ) satisfies 16.30A and with the same value of ν .

$f = e^{-ikξ/2}\ ξ^{in}$

$f' = e^{-ikξ/2}\ in\ ξ^{in-1} - ik/2 * e^{-ikξ/2}\ ξ^{in} = [in\ ξ^{-1} - ik/2]\ ξ^{in}\ e^{-ikξ/2} = [in\ ξ^{-1} - ik/2]f$

$f'' = [in\ ξ^{-1} - ik/2]^2 f + [-in ξ^{-2}]\ f$

$[ξf']' = ξf'' + f' = [in - ikξ/2]\ [in\ ξ^{-1} - ik/2]f + [-in ξ^{-1}]f + [in\ ξ^{-1} - ik/2]f$

$= [in\ ξ^{-1} - ik/2]\ \{\ in - ikξ/2 + 1\ \}f + [-in ξ^{-1}]f$

$= (- ik/2)^2 ξf + [2(-ik/2)(in) - ik/2]\ f + [(in)(in+1) - in]\ ξ^{-1}f$

$= -(k^2/4)\ ξf + (-ik)\ [\ in + 1/2]\ f + (in)^2\ ξ^{-1}f$

$= -(k^2/4)\ ξf + \{\ kn - ik/2\}\ f - n^2\ ξ^{-1}f$ // keep all terms

Now with m azimuth = 0, equation 16.30A says

$[ξf']' - (\ - k^2ξ/4 + nk + ν)f = 0$

$-(k^2/4)\ ξf + \{\ kn - ik/2\}\ f - n^2\ ξ^{-1}f + k^2 f\ ξ/4 - nkf - νf = 0$

$\{- ik/2\}\ f - n^2\ ξ^{-1}f - νf = 0$

$\{\ ik/2\}\ f + n^2\ ξ^{-1}f + νf = 0$

Now if we use our previously found result that ν = - (ik/2), the first and third terms cancel. Then since we are in the large ξ limit, we throw out the second term, which is the ONLY approximation we have made!

Conclusion: The function

$$\psi = e^{ik(\eta-\xi)/2}\, e^{in\ln[k\xi]} = e^{ikz}\, e^{in\ln[k(r-z)]} = e^{i\{kz + n\ln[k(r-z)]\}}$$

satisfies the full Schrodinger equation (with Coulomb potential active) in parabolic coordinates, in the large ξ limit where we drop $1/\xi$ terms.

Comment: suppose we tried leaving out the ln(..) factor. Then we would have to show that $e^{ik\xi/2}$ satisfies the ξ equation with $\nu = -(ik/2)$, since that is what came from the η equation. But here is what we would get for our ξ equation in this case:

$[\xi f']' = -(k^2/4)\xi f + (ik/2)f$ // just copying the η result

$-(k^2/4)\xi f + (ik/2)f - (-k^2\xi/4 + nk + \nu)f = 0$?

$(ik/2)f - (nk + \nu)f = 0$?

$(ik/2)f - (nk - ik/2)f = 0$?

$ikf - nkf = 0$` => $(i-n)f = 0$ => $n = i$ = wrong!

This shows rather conclusively I think that $e^{ikz} = e^{ik(\eta-\xi)/2}$ does not solve the full SE with the Coulomb potential turned on, regardless of how we try to drop $1/\xi$ terms.

Comments on the Coulomb Plane Wave

This is what I would call the Coulomb Plane Wave incident beam function

$$\psi = e^{i\{kz + n\ln[k(r-z)]\}} = e^{i\{kr\cos\theta + n\ln[kr(1-\cos\theta)]\}}$$

If you try to go to the forward direction $\cos\theta = 1$, the ln blows up and we start winding phase like mad, so maybe better to think about the backward direction where our plane wave actually is coming in.

What is the appearance of a surface of constant phase?

$kr\cos\theta + n\ln[kr(1-\cos\theta)] = \text{constant} = kZ$

If we put the center of our "plane wave" centered at distance $r=z_1$ upstream, we can evaluate at $\theta = 180$ to get

$-kz_1 + n\ln[2kz_1] = kZ$

$e^{-kz_1}\, e^{n\ln[2kz_1]} = e^{kZ} = e^{-kz_1}\,(2kz_1)^n$

Then we can fiddle around:

$(kZ-krcos\theta) = \ln[kr(1-cos\theta)]^n$

$e^{(k[Z-rcos\theta])} = [kr(1-cos\theta)]^n$

$e^{kZ} = e^{+krcos\theta}\,[kr(1-cos\theta)]^n = e^{-kz_1}\,(2kz_1)^n$

Think of a scaled coordinate ρ where the plane wave is at $\rho_1 = kz_1$ upstream, then

$e^{+\rho cos\theta}\,(1-cos\theta)^n = e^{-\rho_1}\,(2\rho_1/\rho)^n$

Let's change to angle relative to the incoming axis, $\varphi = \pi - \theta$ and $cos\varphi = -cos\theta$ s0

$e^{-\rho cos\varphi}\,(1+cos\varphi)^n = e^{-\rho_1}\,(2\rho_1/\rho)^n$

$e^{-\rho cos\varphi}\,(2cos^2(\varphi/2))^n = e^{-\rho_1}\,(2\rho_1/\rho)^n$

$e^{-\rho cos\varphi}\,[cos(\varphi/2)]^n = e^{-\rho_1}\,(\rho_1/\rho)^n$

$e^{-\rho cos\varphi}\,[\rho\, cos(\varphi/2)]^n = e^{-\rho_1}\,(\rho_1)^n$

$e^{-\rho cos\varphi}\,(\rho+\rho cos\varphi)^n = e^{-\rho_1}\,(2\rho_1)^n$

$e^{-z}\,(\rho+z)^n = e^{-\rho_1}\,(2\rho_1)^n$

$e^{-z}\,(\sqrt{y^2+z^2}+z)^n = e^{-\rho_1}\,(2\rho_1)^n = C$

Here, if y=0 you are at $z = \rho_1$ and both sides are equal. As you move vertically in the y direction, z has to change, so you are not on the e^{ikz} type wavefront! If $n > 0$ then increasing y means you have to increase z, so the phase surface warps away from the Coulomb source. Vice versa if $n < 0$, and we are talking then about repulsive versus attractive Coulomb situations. If $n = 0$, you have turned off the Coulomb force and we get a flat wavefront as expected. At you go to large k, $n \to 0$ and front gets flat. So low energy means more curvature. If you go far away in z, the restrict y of interest, then front is sort of flat to first order.

Suppose $z >> y$ so we can say

$e^{-z}\,(\ 2z + 1/2\ y^2/z\ )^n \approx e^{-z}\,(2z)^n\,(\ 1 + n/8\ (y/z)^2\ ) = C$

$-z + n\ln(2z) + \ln(\ 1 + n/8\ (y/z)^2) = \ln C$

$-z + n\ln(2z) + n/8\ (y/z)^2 = \ln C$

$z = n/8\ (y/z)^2 - \ln C$

$dz \approx n/8 * 2ydy/z^2 \quad => \quad dz/dy \approx ny/4z^2$

But similar triangles in a little picture shows that

$$d\varphi = dy/R = dz/dy \;\Rightarrow\; dz/dy = y/R = ny/4z^2 \;\Rightarrow\; R = (4/n)z^2$$

If I did this dimly right, it suggests that the radius of curvature increases quadratically with z, so far from the target charge, the Coulomb Plane Wave is very flat and similar to e^{ikz}. As you move closer, I think it sort of folds around the target and morphs into an incoming spherical wave with no outgoing component, as indicated below in our partial wave expansion. This would be interesting to pursue, but let's not. Remember, this thing is only valid for large r, so you can't "watch it as it gets close". It then blends into the true closed form solution and you can't separate it from the scattered wave anymore.

So, this wavefront is a well defined animal as long as you stay away from the forward direction. I think of it as defining a slightly warped constant phase surface that is the incident beam approaching the scattering center. This is the Coulomb Plane Wave.

The Partial Wave Amplitude for Coulomb Scattering is $e^{2i\sigma_\ell}$

So, we now know that our correct "scattering setup" is this:

$$\psi_1 \;\rightarrow\; e^{i[kz+\eta\ln(r-z)]} + (e^{i[kr\,-\,\eta\ln(2kr)]}/r)f(\theta)$$

where the first term is our Coulomb Plane Wave, and the second term follows from the large-r limit of our Coulomb solutions, but outbound only. So maybe here is something we can use to balance things just as we did in the non-coulomb case, and then maybe we can find the form of f_ℓ in the expansion of $f(\theta)$.

$$\psi_2 = \Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i^\ell\,B_\ell\,F_\ell(r)/kr \rightarrow \Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i^\ell\,B_\ell \sin[kr - \eta\ln(2kr) - \ell\pi/2 + \sigma_\ell]/kr$$

since from above we had

$$F_\ell/kr \;\rightarrow\; \sin[kr - \eta\ln(2kr) - \ell\pi/2 + \sigma_\ell]/kr \qquad \text{where } \sigma_\ell = \arg\Gamma(\ell+1+i\eta)$$

But next, we will need a partial wave expansion of the Coulomb Plane Wave, which I do in Appendix A below. At first my confidence was low, now I think the result is exactly correct (large r)

$$e^{ikz+in\ln[k(r-z)]} \approx \Sigma_\ell\,(2\ell+1)\,P_\ell(w)\,\{\,i\;(-1)^\ell\;e^{-ikr}\;(2rk)^{in-1}\}$$

$$= \Sigma_\ell\,(2\ell+1)\,P_\ell(w)\,\{\,i\;(-1)^\ell\,e^{-i\{kr-n\ln(2kr)\}}\,\}/(2rk)$$

$$= \{\,i\;(-1)^\ell\,e^{-i\{kr-n\ln(2kr)\}}\,\}/(2rk)\,[\,\Sigma_\ell\,(2\ell+1)\,P_\ell(w)\,(-1)^\ell\,]$$

which looks promising. It seems to be an "incoming thing" only with e^{-ikr} which is good. This is different from what happened in the non-coulomb case where e^{ikz} had both incoming and outgoing. Maybe this is why we won't get that "1" in the result! Also, we will need:

$f(\theta) = (1/2ik)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z) f_\ell$

So here we go:

$\psi_1 = \psi_2$

$\Sigma_\ell\,(2\ell+1)\,P_\ell(w)\,\{\, i\,(-1)^\ell\, e^{-i\{kr-n\ln(2kr)\}}\,\}/2rk$

$+ (e^{i[kr\,-\,\eta\ln(2kr)]}/r)\,(1/2ik)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z) f_\ell$

$= \Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i^\ell B_\ell \sin[kr - n\ln(2kr) - \ell\pi/2 + \sigma_\ell]/kr$

Let's make this abbreviation:

$\varphi = kr - n\ln(2kr)$

so the above becomes

$\Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i\;\; (-1)^\ell\, e^{-i\varphi}/2rk \quad + (e^{i\varphi}/r)\,(1/2ik)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z) f_\ell$

$= \Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i^\ell B_\ell \sin[\varphi - \ell\pi/2 + \sigma_\ell]/kr$

$= \Sigma_\ell\,(2\ell+1)\,P_\ell(z)\;\; i^\ell B_\ell\,\{\, e^{i\varphi}\, e^{-i\ell\pi/2+i\sigma} - e^{-i\varphi}\, e^{+i\ell\pi/2-i\sigma}\,\}/(2ikr)$

Then our two equalities become:

$e^{-i\varphi}$: $\quad i\;(-1)^\ell/2 = -\,i^\ell B_\ell\, e^{+i\ell\pi/2-i\sigma}/(2i)$

$e^{+i\varphi}$: $\quad f_\ell = i^\ell B_\ell\, e^{-i\ell\pi/2+i\sigma}$

The first says

$(-1)^\ell = i^\ell B_\ell\, e^{i\ell\pi/2-i\sigma}$

$e^{+in\ell} = e^{in\ell/2}\, B_\ell\, e^{+i\ell\pi/2-i\sigma} = B_\ell\, e^{-i\sigma}\, e^{+in\ell}$

$\Rightarrow \quad B_\ell = e^{+i\sigma}$

$\Rightarrow \quad f_\ell = e^{in\ell/2}\,\{\, e^{+i\sigma}\,\}\, e^{-i\ell\pi/2+i\sigma} = e^{+2i\sigma\ell}$

and then we get

$f(\theta) = (1/2ik)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z) f_\ell = (1/2ik)\,\Sigma_\ell\,(2\ell+1)\,P_\ell(z)\; 2\, e^{+2i\sigma\ell}$

which agrees exactly with Schiff 21.22. I think we followed the same path really, but I think my words are more logical than his in making the comparison to the non-coulomb case. So yes, there is no "1" here because the incoming plane wave has no outgoing piece! We recall that it was exactly this outgoing piece that caused the "1" in the non-coulomb case. In other words, since nothing "comes out" from the Coulomb Plane Wave, there is no need to "subtract it off" in the partial wave amplitude using that "1".

Appendix A: Computing the partial wave expansion of the Coulomb Plane Wave

First, recall the expansion for the true plane wave for large r, which is this:

$$e^{ikz} = \Sigma_\ell \ (2\ell+1)\ i^\ell \ P_\ell(\cos\theta)\ (1/kr)\ \sin(kr - \tfrac{1}{2}\ \ell\ \pi)$$

We want to get a similar expansion for

$$e^{ikz+inln[k(r-z)]} = \Sigma_\ell \ (2\ell+1)\ P_\ell(w)\ H_\ell$$

and it is useful to first write the LHS as

$$e^{ikz+inln[k(r-z)]} = e^{ikrw}\ (rk)^{in}\ (1-w)^{in} \qquad \text{where } w = \cos\theta$$

$$\int dw\ P_\ell(w)\ \{\Sigma_{\ell'}\ (2\ell'+1)\ P_{\ell'}(w)\ H_{\ell'}\} \ = \ (rk)^{in}\ \{\ \int_{-1}^{1} dw\ P_\ell(w)\ e^{ikrw}\ (1-w)^{in}\ \} \ = 2\ H_\ell$$

Now as usual, convert to Gegenbauer so we have some hope of finding this integral.

$$I = \ \int_{-1}^{1} dw\ C^{1/2}_\ell\ (w)\ e^{ikrw}\ (1-w)^{in}$$

But I don't see this anywhere in the GR section, no such luck. So go back to

$$I = \ \int_{-1}^{1} dw\ P_\ell(w)\ (1-w)^{in}\ e^{ikrw} \ = \ \int_{-1}^{1} dw\ P_\ell(w)\ (1-w)^{in}\ \{\ 1/(ikr)\ \partial_w\ \}e^{ikrw}$$

$$= \ 1/(ikr)\ \ \int_{-1}^{1} dw\ [P_\ell(w)\ (1-w)^{in}]\ \partial_w\ e^{ikrw}$$

$$= 1/(ikr)\ \{\ P_\ell(w)\ (1-w)^{in}\ e^{ikrw}\ \}^{parts} \ - 1/(ikr)\ \ \int_{-1}^{1} dw\ e^{ikrw}\ \partial_w\ [P_\ell(w)\ (1-w)^{in}]$$

Now we argue as did Schiff on page 134 that if we continue doing parts on this second term, the entire second term is order $1/r^2$ so we *throw it out entirely* since we only want the large r limit of our integral. The first term is then all there is and we get [this is just the stationary phase method, see Math binder 4]

$$I = 1/(ikr)\ \{\ P_\ell(w)\ (1-w)^{in}\ e^{ikrw}\ \}^{parts}\ =\ 1/(ikr)\ \{\ \ P_\ell(1)\ 0^{in}\ e^{ikr}\ -\ P_\ell(-1)\ 2^{in}\ e^{-ikr}\ \}$$

$$= 1/(ikr)\ *\ (-1)^{\ell+1}\ 2^{in}\ e^{-ikr}$$

which tells us that

$$H_\ell = \ I\ (rk)^{in}/2 = i\ \ (-1)^\ell\ 2^{in-1}\ e^{-ikr}\ \ (rk)^{in-1}$$

which certainly has minimal dependence on ℓ. Do I believe this?

Suppose I were just doing the straight e^{ikz} . Then set n=0 in the above method and we would have gotten

$$I = 1/(ikr)\ \{\ P_\ell(w)\ e^{ikrw}\ \}^{parts}\ = 1/(ikr)\ \{\ P_\ell(1)\ e^{ikr}\ -\ P_\ell(-1)e^{-ikr}\ \} = 1/(ikr)\ \{e^{ikr}\ -\ (-1)^\ell\ \ e^{-ikr}\ \}$$

and I would be saying

$$H_\ell = (1/2)\ 1/(ikr)\ \{e^{ikr}\ -\ (-1)^\ell\ \ e^{-ikr}\ \}\ \ =\ \ (1/2)\ 1/(ikr)\ \{e^{ikr}\ -\ e^{i\pi\ell}\ \ e^{-ikr}\ \}$$

$$=\ \ (1/2)\ 1/(ikr)\ *\ e^{i\pi\ell/2}\{e^{ikr}\ e^{-i\pi\ell/2}\ -\ e^{i\pi\ell/2}\ \ e^{-ikr}\ \}$$

$$= (1/2)\ 1/(ikr)\ *\ e^{i\pi\ell/2}\{e^{i\,(kr-\ell\pi/2)}\ -\ e^{-i\,(kr-\ell\pi/2)}\ \}$$

$$= (1/2)\ 1/(ikr)\ *\ e^{i\pi\ell/2}\{2i\ \sin(kr-\ell\pi/2)\}\ \ = (1/kr)\ i^\ell\ \sin(kr-\ell\pi/2)$$

which amazingly is the right result!!! So maybe I do believe my integral above.

Then I claim to have shown this, valid only for very large r,

$$e^{ikz+inln[k(r-z)]}\ \ \approx\ \Sigma_\ell\ \ (2\ell+1)\ P_\ell(w)\ \{\ i\ \ (-1)^\ell\ 2^{in-1}\ e^{-ikr}\ \ (rk)^{in-1}\}$$

$$= \{\ i\ e^{-i\{kr-nln(2kr)}\ \ \}\ /(2rk)\ [\ \Sigma_\ell\ \ (2\ell+1)\ P_\ell(\cos\theta)\ (-1)^\ell\ ]$$

Is there a closed form for the [..] sum, which could be written using $P_\ell(\cos\theta)\ (-1)^\ell = P_\ell(-\cos\theta)$? I think I can argue this: (see Schiff notes for equation 21.23 in Chap 5)

$$\Sigma_\ell\ \ (2\ell+1)\ P_\ell(-\cos\theta) = 2\delta(1 + \cos\theta)$$

which means it is all at the backward direction where r = z so $e^{ikz+inln[k(r-z)]}$ blows up too. So my result is true in some sort of asymptotic distribution sense. In any event, when I use this expansion, I get what I want for the Coulomb partial wave shift!

Perhaps the following regulation method could be used: limit the partial wave sum to some large ℓ_{max} so that RHS does vanish for $z \neq -1$. Then carry through with the derivation of $f(\theta)$, then at the end take this to ∞.