Central Force Scattering: Cons$^{\underline{x}}$n of ∡ Momentum.

Free Particle in 3D [Ref. Davydov Sec. 35]

1) For a free particle of mass m & energy E in 3D, the Schrodinger problem is:

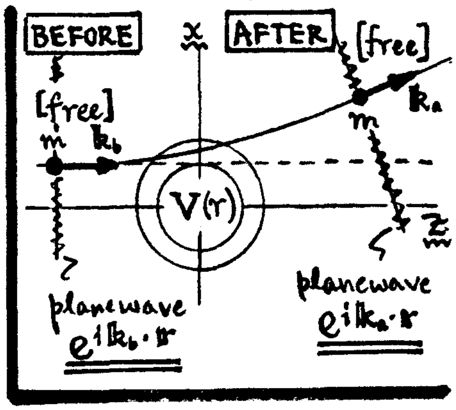
$$\rightarrow [\nabla^2 + k^2]\psi(\mathbf{r}) = 0, \text{ w/ } k^2 = 2mE/\hbar^2, \text{ and } E \geq 0. \qquad (1)$$

In rectangular cds, w/ $\mathbf{r} = (x, y, z)$ and $\mathbf{k} = (k_x, k_y, k_z)$, the elementary solutions are plane waves (or a superposition thereof), viz.

$$\rightarrow \underline{\psi_k(\mathbf{r}) = (1/2\pi)^{\frac{3}{2}} e^{i\mathbf{k}\cdot\mathbf{r}}} \longleftrightarrow \text{norm: } \int d^3x\, \psi_{k'}^*(\mathbf{r})\psi_k(\mathbf{r}) = \delta(\mathbf{k}-\mathbf{k}'). \qquad (2)$$

We have used such plane waves in our scattering analysis via Born Approxn. But such planewaves lack a useful feature: they are not eigenfcns of the ∡ momentum operator $\hat{\mathbb{L}} = \mathbf{r} \times \hat{\mathbf{p}}$, i.e.

$$\rightarrow \hat{\mathbb{L}}\,\psi_k(\mathbf{r}) = [\mathbf{r} \times \hbar\mathbf{k}]\,\psi_k(\mathbf{r}) \neq \text{cnst} \times \psi_k(\mathbf{r}). \qquad (3)$$



The reason this is a lack is: if the scattering potential $V(r)$ is spherically symmetric, then the particle's ∡ momentum must be conserved... and states with different values of (quantized) ∡ momentum will independently take part in the scattering, meanwhile retaining their identity. The planewave $e^{i\mathbf{k}\cdot\mathbf{r}}$ does not directly reflect this fact.

To prepare to bring ∡ momentum into the central force scattering problem, we will now find a way of expressing the free particle planewave $e^{i\mathbf{k}\cdot\mathbf{r}}$ in a series of terms, each of which is an eigenfcn of ∡ momentum. We will show:

$$\boxed{e^{ikz} = \sum_{l=0}^{\infty}(2l+1)\,i^l\, j_l(kr)\, P_l(\cos\theta)} \text{ w/ } z = r\cos\theta, \qquad (4)$$

for a planewave moving along the z-axis. j_l is the spherical Bessel fcn of order l, and P_l the Legendre polynomial of order l. This expression is the starting point for a scattering analysis called the "Partial Wave Method".

Schrödinger problem for free particle in 3D spherical cds (r, θ, φ).

2) The basic problem we want to do may be stated as follows...

["For a free particle with definite wave # k (i.e. energy $E = \hbar^2 k^2/2m$) and (quantized) ∡ momentum l, find the wavefcn ψ in spherical cds (r, θ, φ);"]

i.e. if// $\psi_{klm}(r, \theta, \varphi) = \frac{1}{r} u_{kl}(r) Y_{lm}(\theta, \varphi)$ ⎡ the $Y_{lm}(\theta, \varphi)$ are spherical harmonics,

... solve// $$\underline{\underline{\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] u_{kl}(r) = 0}},$$ RADIAL EQUATION with: $l = 0, 1, 2, \ldots$ (5)

The presence of the Y_{lm} in ψ_{klm} ensures that ψ will be an eigenfcn of ∡ momentum: $\hat{\mathbb{L}}^2 \psi_{klm} = [l(l+1)\hbar^2]\psi_{klm}$, etc. We will impose the norm...

$$\rightarrow \int_\infty d^3x\, \psi^*_{k'l'm'}(\mathbf{r})\, \psi_{klm}(\mathbf{r}) = \delta_{l'l}\, \delta_{m'm} \underbrace{\int_0^\infty u^*_{k'l'}(r)\, u_{kl}(r)\, dr}_{\text{set } = \delta(k'-k)}, \qquad (6)$$

essentially the same as in Eq. (2).

As for the RADIAL EQUATION in Eq. (5), we will impose the boundary conditions:

[**1.** As $r \to 0+$, $u_{kl}(r) \to 0$, at least as fast as $u_{kl} \sim r$ [so $\lim_{r\to 0+} \frac{1}{r} u_{kl}(kr) \to$ finite];

2. As $r \to \infty$, $u_{kl}(r)$ need <u>not</u> vanish [free particle <u>can</u> be found at ∞]. (7)

And we can solve Eq. (5) for $l = 0$ easily. Have...

$$\rightarrow l = 0 \Rightarrow \left[\frac{d^2}{dr^2} + k^2\right] u_{k0}(r) = 0 \Rightarrow u_{k0}(r) \propto \begin{cases} \sin kr, & \text{vanishes as } r \to 0; \\ \cos kr, & \text{finite as } r \to 0. \end{cases}$$

Choose: $u_{k0}(r) = \sqrt{\frac{2}{\pi}} \sin kr \longleftrightarrow$ norm: $\int_0^\infty u^*_{k'0}(r)\, u_{k0}(r)\, dr = \delta(k'-k)$

Soy $\underline{R_{k0}(r) = \frac{1}{r} u_{k0}(r) = \sqrt{\frac{2}{\pi}} \left(\frac{\sin kr}{r}\right)}$, is complete radial fcn for $l = 0$. (8)

For $l > 0$ and $r \to 0$, Eq. (5) is: $\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right] u_{kl} \simeq 0 \Rightarrow$ solutions $u_{kl} \sim r^{l+1}$.

Extract this asymptotic behavior by making the substitution:

$$\rightarrow u_{kl}(r) = C_l\, r^{l+1}\, v_{kl}(r)$$ ⎡ C_l = available norm cnst, $v_{kl}(r) \to$ cnst as $r \to 0+$. (9)

Solution to radial problem for a free particle in 3D.

With the substitution of Eq. (9), the RADIAL EQUATION -- Eq. (5) -- becomes:

$$\underline{\left[\frac{d^2}{dr^2} + 2\left(\frac{l+1}{r}\right)\frac{d}{dr} + k^2\right] v_{kl}(r) = 0.} \tag{10}$$

We can develop a recursion relation for the v_{kl}, as follows. Take $\frac{d}{dr} \times$ Eq. (10),

so $$\underline{\left[\frac{d^2}{dr^2} + 2\left(\frac{l+1}{r}\right)\frac{d}{dr} + \left(k^2 - 2\,\frac{l+1}{r^2}\right)\right]\frac{d}{dr}\, v_{kl}(r) = 0.} \tag{11}$$

Now let: $w_{kl} = \frac{1}{r}(dv_{kl}/dr)$. With this substitution, Eq. (11) reads:

$$\underline{\left[\frac{d^2}{dr^2} + 2\left(\frac{l+2}{r}\right)\frac{d}{dr} + k^2\right] w_{kl}(r) = 0,} \quad \text{w/} \quad w_{kl}(r) = \frac{1}{r}\,\frac{d}{dr}\, v_{kl}(r). \tag{12}$$

Comparison of (12) with (11) shows that $w_{kl}(r) = v_{k,l+1}(r)$. Thus, the recursion:

$$\rightarrow v_{k,l+1}(r) = \left(\frac{1}{r}\,\frac{d}{dr}\right) v_{kl}(r) \quad \Rightarrow \quad \underline{\underline{v_{kl}(r) = \left(\frac{1}{r}\,\frac{d}{dr}\right)^{l} v_{k0}(r)}} \;\Big/\; \underline{l = 0, 1, 2, \ldots} \tag{13}$$

But (from Eq. (9)): $u_{k0} = C_0\, r\, v_{k0} = \sqrt{\frac{2}{\pi}}\sin kr$, so $v_{k0}(r) = \sqrt{\frac{2}{\pi}}\left(\frac{\sin kr}{r}\right)$, for $C_0 = 1$.

Then the solutions $u_{kl}(r)$ to Eq. (5) are:

$$\underline{\underline{u_{kl}(r) = \sqrt{\frac{2}{\pi}}\, C_l\, r^{l+1}\left(\frac{1}{r}\,\frac{d}{dr}\right)^{l}\frac{\sin kr}{r}}} \tag{14}$$

For the norm in Eq. (6) [viz. $\int_0^\infty u^*_{k'l}(r)\, u_{kl}(r)\, dr = \delta(k'-k)$], need: $\underline{C_l = (-)^l/k^l}$.

Then the complete radial fcns for the free particle in 3D are...

$$\boxed{R_{kl}(r) \doteq \frac{1}{r}\, u_{kl}(r) = \frac{(-)^l}{k^l}\sqrt{\frac{2}{\pi}}\, r^l\left(\frac{1}{r}\,\frac{d}{dr}\right)^{l}\frac{\sin kr}{r}}\; ; \; \underline{l = 0, 1, 2, 3, \ldots} \tag{15}$$

The fcns on the RHS of (15) are called "spherical Bessel fcns", defined by:

$$\rightarrow j_l(x) = (-)^l x^l\left(\frac{1}{x}\,\frac{d}{dx}\right)^{l}\frac{\sin x}{x}, \quad \text{and} \quad j_l(x) = \sqrt{\frac{\pi}{2x}}\, J_{l+\frac{1}{2}}(x); \; \underline{l = 0, 1, 2, \ldots} \tag{16}$$

The $j_l(x)$ are related to the ordinary Bessel fcns $J_{l+\frac{1}{2}}(x)$ of half-integral order as shown. They are "well-known" (see, e.g. NBS Handbook, Ch. 10). So:

$$\boxed{R_{kl}(r) = \sqrt{\frac{2}{\pi}}\, k\, j_l(kr)}\; ; \; l = 0, 1, 2, \ldots \; ; \text{ in these terms.} \tag{17}$$

Characteristics of the $j_\ell(x)$. Asymptotic form for the radial fcns.

3) Since the $j_\ell(x)$ are among the "special fcns of physics", they have been thoroughly studied, and much is known about them. For example, the following facts:

$\boxed{1}$ $j_0(x) = \frac{\sin x}{x}$, $j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$, $j_2(x) = \left(\frac{3}{x^2} - 1\right)\frac{\sin x}{x} - \frac{3}{x^2}\cos x$, etc. (18)

$\boxed{2}$ The $j_\ell(x)$ satisfy the differential equation:

$$\rightarrow \left[\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} + \left(1 - \frac{\ell(\ell+1)}{x^2}\right)\right] j_\ell(x) = 0, \quad (19)$$

and they can be related to the confluent hypergeometric fcn $\Phi(\alpha, \gamma; z)$ by†:

$$\left[\!\left[j_\ell(x) = \left[\frac{\sqrt{\pi}/2^{\ell+1}}{\Gamma(\ell+\frac{3}{2})}\right] x^\ell e^{-ix}\, \Phi(\ell+1, 2\ell+2; 2ix) \right]\!\right]. \quad (20)$$

$\boxed{3}$ Asymptotic forms for $j_\ell(x)$ can be obtained from those for $\Phi(\alpha, \gamma; z)$, e.g.

$x \to 0$ $[\Rightarrow e^{-ix}\,\Phi(\alpha, \gamma; 2ix) \to 1]$.

$$\xrightarrow{\text{so}} j_\ell(x) \simeq \left[\frac{\sqrt{\pi}/2^{\ell+1}}{\Gamma(\ell+\frac{3}{2})}\right] x^\ell = x^\ell/(2\ell+1)!! \quad (21)$$

✓ after some Γ-fcn algebra, w/ $(2\ell+1)!! = 1\cdot 3\cdot 5\cdots(2\ell+1)$.

$x \to \infty$ $[\Rightarrow \Phi(\alpha, \gamma; z) \to [\Gamma(\gamma)/\Gamma(\gamma-\alpha)]\, e^{i\pi\alpha} z^{-\alpha}]$.

simple way } $j_\ell(x) = (-)^\ell x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x} \underset{x\to\infty}{\simeq} (-)^\ell \frac{1}{x}\frac{d^\ell}{dx^\ell}\sin x$ ✓ this is the leading term

... but: $\frac{d}{dx}\sin x = \cos x = (-)\sin(x - \frac{1}{2}\pi)$, and $\frac{d^\ell}{dx^\ell}\sin x = (-)^\ell \sin(x - \frac{\ell}{2}\pi)$ ...

$$\text{so } j_\ell(x) \simeq \frac{1}{x}\sin\left(x - \frac{\ell}{2}\pi\right), \text{ as } x \to \infty. \quad (22)$$

On the basis of (22), we can say that the radial wavefcn of (17) goes, for $r \to \infty$, as:

$$\rightarrow R_{k\ell}(r) \simeq \sqrt{\frac{2}{\pi}}\,\frac{1}{r}\sin\left(kr - \frac{\ell}{2}\pi\right), \text{ as } r \to \infty, \text{ for a free particle.} \quad (23)$$

This is for a completely free particle. But, suppose the particle has interacted with some finite-range potential $V(r)$ between its incoming period $(-\infty \leftarrow t)$ and

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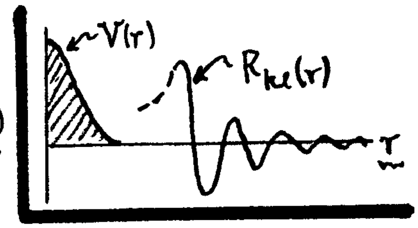
† S. Hassani "Foundations of Math. Physics" (Allyn & Bacon 1991), Sec. (9.5.5).

Notion of "phase shift" $\delta_\ell(k)$. Other solutions for $R_{k\ell}(r\to\infty)$.

outgoing period ($t\to+\infty$). Then $R_{k\ell}$ of Eq. (23) must be modified. Since $R_{k\ell}$ must still $\Rightarrow$ a particle free as $r\to\infty$, the r-dependence cannot change... $R_{k\ell}$ can at most be modified by a "phase shift" $\delta_\ell(k)$, as follows:

$$\rightarrow R_{k\ell}(r) \simeq \sqrt{\frac{2}{\pi}}\,\frac{1}{r}\sin\left[kr - \frac{\ell}{2}\pi + \delta_\ell(k)\right], \text{ as } r\to\infty, \tag{24}$$

particle having interacted w/ pot^l $V(r)$ at short range.



This asymptotic form of $R_{k\ell}(r)$ turns out to be OK for potentials that fall off fast enough so: $\lim_{r\to\infty} rV(r) = 0$. The phase shifts $\delta_\ell(k)$ are then sufficient to measure the residual (distorting) effects of V on $R_{k\ell}$; the $\delta_\ell(k)$ depend on the ∢ momentum state ℓ, and on energy: $k=\sqrt{2mE/\hbar^2}$.

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4) The $j_\ell(kr)$ are the only valid solutions for the free particle radial fcns $R_{k\ell}$ as $r\to 0$, because they are the only ones which remain finite at the origin [per boundary condition #1 in Eq. (7)]. When $r\to\infty$, where there are no special restrictions on $R_{k\ell}$, other solutions are possible. The full radial solution is:

$$\psi_{k\ell m}(\mathbf{r}) = R_{k\ell}(r)\,Y_{\ell m}(\theta,\varphi);\quad \ell=0,1,2,\ldots\ (-\ell\leq m\leq \ell),\ k=\text{free};$$

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)\right]R_{k\ell}(r) = 0; \tag{25}$$

$$\Rightarrow \text{solutions}: \quad R_{k\ell}(r) \propto \begin{cases} \underline{\underline{j_\ell(x)}} = \sqrt{\dfrac{\pi}{2x}}\,J_{+(\ell+\frac{1}{2})}(x),\ x=kr & \text{j_ℓ are SPHERICAL BESSEL FCNS} \\ \underline{\underline{n_\ell(x)}} = (-)^\ell\sqrt{\dfrac{\pi}{2x}}\,J_{-(\ell+\frac{1}{2})}(x) & \text{n_ℓ are SPHERICAL NEUMANN FCNS.} \end{cases}$$

These two forms of solution are directly related to the fact: if $J_{+\nu}$ is a solution to Bessel's eqtn, then so is $J_{-\nu}$. The $n_\ell(x)$ can be related to the confluent hypergeometric fcn, etc. [as in Eqs (18)-(22) above]. Key relations for the $n_\ell(x)$ are as follows...

Other solutions for $R_{k\ell}(r\to\infty)$. Spherical outgoing & incoming waves.

$$\left[\begin{array}{l} n_\ell(x) = (-)^{\ell+1}\, x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}\,; \\[2ex] n_0(x) = (-)\frac{\cos x}{x}\,,\quad n_1(x) = -\left(\frac{\cos x}{x^2} + \frac{\sin x}{x}\right),\ \text{etc.}; \\[2ex] \text{asymptopia}:\ n_\ell(x) \longrightarrow \begin{cases} -(2\ell-1)!!\,/\,x^{\ell+1}, & \text{as } x\to 0\ (n_\ell \text{ diverges}); \\ -\frac{1}{x}\cos\left(x - \frac{\ell}{2}\pi\right), & \text{as } x\to\infty. \end{cases} \end{array}\right] \tag{26}$$

Finally, we can use Spherical Hankel fcns, defined by:

$$\left[\begin{array}{l} h_\ell^{(1)}(x) = j_\ell(x) + i\,n_\ell(x) = i\,(-)^{\ell+1}\, x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{e^{+ix}}{x}\,, \\[2ex] h_\ell^{(2)}(x) = j_\ell(x) - i\,n_\ell(x) = \frac{1}{i}(-)^{\ell+1}\, x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{e^{-ix}}{x}\,; \end{array}\right. \tag{27}$$

$h_\ell^{(1)}(x)$ & $h_\ell^{(2)}(x)$ are linearly independent, just as e^{+ix} & e^{-ix}. The useful feature of Hankel fcns is that they behave like spherical waves* as $x = kr \to \infty$...

$$\left[\begin{array}{ll} h_\ell^{(1)}(kr) \simeq \frac{1}{kr}\, e^{+i\left(kr - \frac{\ell+1}{2}\pi\right)} & \leftarrow \text{spherical outgoing wave}; \\[2ex] h_\ell^{(2)}(kr) \simeq \frac{1}{kr}\, e^{-i\left(kr - \frac{\ell+1}{2}\pi\right)} & \leftarrow \text{spherical incoming wave}. \end{array}\right\}\ \text{as } r\to\infty. \tag{28}$$

We will use the $n_\ell(kr)$ later, in analyzing what's called "hard-core scattering".

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5) We do one more thing with the free-particle solutions, viz. develop an expansion of a planewave in spherical harmonics $Y_{\ell m}$. This will fill the lack (of $\measuredangle$ momentum eigenfcns) noted on p. "free 1", and will be useful in the Partial Wave Method of scattering analysis. Start by assuming the $R_{k\ell}(r)\,Y_{\ell m}(\theta,\varphi)$ are a complete set

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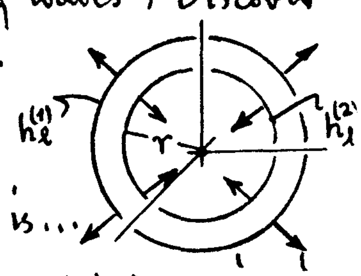
* Why are $h_\ell^{(1)}$ & $h_\ell^{(2)}$ of Eq. (28) called spherical outgoing & incoming waves? Discover this by looking at the probability current carried by ψ...



$$\mathbb{S} = (\hbar/2im)\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]$$

... for $\psi_{k\ell m} \sim \frac{1}{r} e^{\pm ikr}\, Y_{\ell m}(\theta,\varphi)$, comp$^{\underline{t}}$ of $\mathbb{S}$ along $\hat{r}$ is...

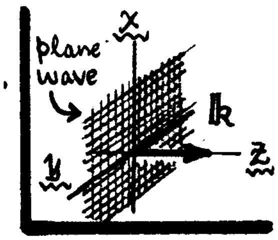
$\rightarrow S_r = \pm\frac{1}{r^2}(\hbar k/m)\left|Y_{\ell m}(\theta,\varphi)\right|^2$, as $r\to\infty$ ✓ (+) ⇒ moving out, (−) ⇒ moving in. wave $\propto \frac{1}{r^2}$ ⇒ spherical wave.

Expansion of a plane wave in spherical cds.

of eigenfcns for spherical symmetry, so that there exists a planewave expansion:

$$\rightarrow e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} a_{lm}\, R_{kl}(r)\, Y_{lm}(\theta,\varphi) \tag{29}$$

for suitable expansion coefficients a_{lm}. Specialize to $\mathbf{k} \parallel z$-axis...



$$e^{ikz} = \sum_{l=0}^{\infty} a_l\, j_l(kr)\, P_l(\cos\theta), \quad \text{w/ } z = r\cos\theta. \tag{30}$$

We need the coefficients a_l. Let $r \to 0$, and use: $j_l(kr) \simeq (kr)^l/(2l+1)!!$, so

$$\rightarrow \text{Eq (30)} \Rightarrow \underline{\sum_{l=0}^{\infty}\frac{1}{l!}(ikr\mu)^l \underset{r\to 0}{=} \sum_{l=0}^{\infty} a_l \frac{(kr)^l}{(2l+1)!!} P_l(\mu)}, \quad \text{w/ } \mu = \cos\theta, \tag{31}$$

after expanding e^{ikz} on the LHS in its Taylor series. PLAN: find the a_l by equating like powers of $(kr\mu)^l$ on LHS & RHS of Eq. (31). Note that:

$$\rightarrow P_l(\mu) = \frac{1}{2^l l!}\frac{d^l}{d\mu^l}(\mu^2-1)^l \quad \surd \text{ Rodrigues formula [p. 321 in Hassani's "... Math } \phi\text{"]} \tag{32}$$

... find the leading term in μ by imagining $\mu \to$ large...

$$\rightarrow P_l(\mu) \sim \frac{1}{2^l l!}\frac{d^l}{d\mu^l}\mu^{2l} = \frac{1}{2^l l!}\frac{(2l)!}{l!}\mu^l = \left[\frac{(2l+1)!!}{(2l+1)\,l!}\right]\mu^l + O(\mu^{l-2}), \tag{33}$$

[since $(2l)!/2^l = l!\,(2l+1)!!/(2l+1)$]. Use this result in (31) to identify terms:

$$\rightarrow \frac{1}{l!}(ikr\mu)^l = a_l \frac{(kr)^l}{\cancel{(2l+1)!!}} \cdot \left[\frac{\cancel{(2l+1)!!}}{(2l+1)\,l!}\right]\mu^l \Rightarrow \boxed{a_l = (i)^l(2l+1)}. \tag{34}$$

Using (34) in (30), we have the desired expansion of a plane wave in spherical cds:

$$\boxed{e^{ikz} = \sum_{l=0}^{\infty}(2l+1)\, i^l\, j_l(kr)\, P_l(\cos\theta)}, \quad \text{w/ } z = r\cos\theta. \tag{35}$$

The fcns in the sum are all eigenfcns of the ∡ momentum operator $\hat{\mathbb{L}}^2$, with eigenvalues $l(l+1)\hbar^2$. Notice that with the asymptotic form of Eq. (22):

$$e^{ikz} \simeq \frac{1}{kr}\sum_{l=0}^{\infty}(2l+1)\, i^l \sin\left(kr - \frac{l}{2}\pi\right) P_l(\cos\theta), \quad \text{as } r\to\infty; \quad \surd\ \text{use: } i^l = e^{i\frac{l}{2}\pi},\ \sin x = \frac{1}{2i}(e^{ix} - e^{-ix})$$

or/

$$e^{ikz} \simeq \frac{1}{2i}\sum_{l=0}^{\infty}(2l+1)\left[\underbrace{\left(\frac{e^{+ikr}}{kr}\right)}_{\text{spherical out}} - e^{il\pi}\underbrace{\left(\frac{e^{-ikr}}{kr}\right)}_{\text{spherical in}}\right] P_l(\cos\theta). \tag{36}$$

So a planewave at $r\to 0$ actually consists of a sum of incoming & outgoing spherical waves. Marvelous! We will exploit this curious fact in the near future.