Radial wave functions of free particles

a) Basic spherical Bessel functions and their asymptotics.

The radial wave functions of free particles obey the radial Schrödinger equation for the particle with the orbital moment $l$ reads:

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{d R_l}{dr} + \left( k^2 - \frac{l (l + 1)}{r^2} \right) R_l = 0,$$  \hspace{1cm} (1)

where $k = \sqrt{2mE/\hbar}$ is the modulus of the wave vector. Replacing the variable $r$ by $z = kr$ the equation (1) is transformed to the following dimensionless form:

$$\frac{d^2 R_l}{dz^2} + 2 \frac{d R_l}{dz} + \left( 1 - \frac{l (l + 1)}{z^2} \right) R_l = 0$$  \hspace{1cm} (2)

The two independent solutions of this equation will be denoted as $j_l(z)$ (Spherical Bessel functions) and $n_l(z)$ (Spherical Neumann functions). They are determined by their asymptotic behavior at $z \to \infty$:

$$j_l(z) \approx \frac{\sin \left( z - \frac{l \pi}{2} \right)}{z}; \quad n_l(z) \approx \frac{\cos \left( z - \frac{l \pi}{2} \right)}{z}; \quad z \to \infty \quad \text{(3)}$$

At $l = 0$ the two independent solutions of equation (2) are $j_0(z) = \frac{\sin z}{z}$ and $n_0(z) = \frac{\cos z}{z}$. We will show that $j_l(z)$ is regular at $z \to 0$ (more accurately, it behaves as $z^l$), whereas $n_l(z)$ diverges as $z^{-l-1}$. To prove these statements and find explicitly these functions at $l \neq 0$, we introduce a new function $\chi_l(z)$ instead of $j_l(z)$ by the relation:

$$j_l(z) = z^l \chi_l(z) \quad \text{(4)}$$

Substituting (4) into (2), we find differential equation for $\chi_l(z)$:

$$z\chi''_l + 2(l + 1) \chi'_l + z \chi_l = 0,$$ \hspace{1cm} (5)

where prime means differentiation by $z$ (please, check). Let us first differentiate equation (5), eliminate $\chi_l$ from the resulting equation using the same equation (5) and then substitute $\chi_l' = -z \chi_{l+1}$. The equation for $\chi_{l+1}$ has the required form, i.e. it is similar to the equation (5) with the only difference that the coefficient $2 (l + 1)$ at the first derivative is replaced by $2 (l + 2)$. Thus, the functions $\chi_l$ obey the recurrent relation $\chi_{l+1} = -\frac{1}{z} \frac{d}{dz} \chi_l$. From here it follows:

$$j_l(z) = (-1)^l z^l \left( \frac{1}{z} \frac{d}{dz} \right)^l j_0(z) = (-1)^l z^l \left( \frac{1}{z} \frac{d}{dz} \right)^l \frac{\sin z}{z} \quad \text{(6)}$$
In analogous way substituting \( n_l(z) = z^l \chi_l(z) \) and so far, we arrive at an equation:

\[
 n_l(z) = (-1)^l z^l \left( \frac{1}{z} \frac{d}{dz} \right)^l n_0(z) = (-1)^l z^l \left( \frac{1}{z} \frac{d}{dz} \right)^l \frac{\cos z}{z} \tag{7}
\]

To check that the functions \( j_l(z) \), \( n_l(z) \) defined by equations (6,7) have required asymptotics (3), we note that at \( z \to \infty \) all differentiation should be performed with sine or cosine only, other terms are much smaller. Each differentiation changes sign to cosine, i.e. adds \(-\pi/2\) to the argument and changes sign, which is compensated by the factor \((-1)^l\).

The asymptotics of \( j_0(z) \) at \( z \to 0 \) can be found if one takes in account that

\[
 \frac{1}{z} \frac{d}{dz} = 2 \pi i z \tag{10}
\]

where \( f(s) \) is a function turning into zero in the points \( s = \pm 1 \). It is straightforward to check the following properties of the integral representation:

\[
 j_l(z) \approx \frac{2^l l! z^l}{(2l + 1)!}; \quad z \to 0 \tag{8}
\]

In the case of \( n_l(z) \) at \( z \to 0 \) the dominant term can be obtained by differentiation of \( \frac{1}{z} \). It gives:

\[
 n_l(z) \approx (2l - 1)!! z^{-l-1}; \quad z \to 0 \tag{9}
\]

b) Integral representation

The function \( \chi_l(z) \) allows an integral representation of the following form:

\[
 \chi_l(z) = \int_1^{-1} e^{isz} \varphi_l(s) \, ds, \tag{10}
\]

where \( f(s) \) is a function turning into zero in the points \( s = \pm 1 \). It is straightforward to check the following properties of the integral representation:

\[
 \frac{d}{dz} \chi_l(z) = \int_1^{-1} e^{isz} i s \varphi_l(s) \, ds; \quad z \chi_l(z) = \int_1^{-1} e^{isz} i \frac{d}{ds} \varphi_l(s) \, ds \tag{11}
\]

or in the operator form:

\[
 \frac{d}{dz} = i s; \quad z = \frac{d}{ds} \tag{12}
\]

Thus equation (5) for the function \( \chi_l(z) \) results in the following equation for the function \( \varphi_l(s) \):

\[
 (1 - s^2) \frac{d\varphi_l}{ds} + 2ls \varphi_l = 0 \tag{13}
\]
Its solution turning into zero at \( s = \pm 1 \) is \( \varphi_l(s) = A \left(1 - s^2\right)^l \), where \( A \) is a constant. Substituting it into integral representation (10), we find:

\[
\chi_l(z) = A \int_{-1}^{1} e^{i z s} \left(1 - s^2\right)^l \, ds
\]  
(14)

The constant \( A \) can be found from comparison of the values \( \chi_l(0) \) found by two different ways. Putting \( z = 0 \) in equation (14), we find:

\[
\chi_l(0) = A \int_{-1}^{1} (1 - s^2)^l \, ds
\]  
(15)

The integral in the right-hand side by the change of variable \( t = s^2 \) can be transformed into the integral representation of the Beta-function:

\[
\int_{-1}^{1} (1 - s^2)^l \, ds = \int_{0}^{1} (1 - t)^{l/2} t^{-1/2} \, dt = B(l + 1, 1/2) = \frac{\Gamma(l + 1) \Gamma(1/2)}{\Gamma(l + 3/2)}
\]  
(16)

We employ well known properties of the Euler Gamma-functions: \( \Gamma(l + 1) = l! \) (for integer \( l \)); \( \Gamma(x + 1) = x\Gamma(x) \). The latter property allows expressing

\[
\Gamma(l + 3/2) = (l + 1/2) \Gamma(l + 1/2) = (l + 1/2)(l - 1/2)\Gamma(l - 1/2) = \ldots = (l + 1/2)(l - 1/2) \ldots 1/2\Gamma(1/2)
\]  
(17)

Collecting all factors and substituting them in (15), we find:

\[
\chi_l(0) = A \frac{2^{l+1} \Gamma}{(2l + 1)!!}
\]  
(18)

On the other hand from the definition of \( \chi_l(z) \) (4) and the asymptotic (8) we find \( \chi_l(0) = 1/(2l + 1)!! \). Comparing this value to equation (18), we find \( A = \frac{1}{2^{l+1} \Gamma} \) and

\[
\chi_l(z) = \frac{1}{2^{l+1} \Gamma} \int_{-1}^{1} e^{i z s} \left(1 - s^2\right)^l \, ds
\]  
(19)

Substituting this value in equation (4) we find the integral representation for the spherical Bessel function:

\[
j_l(z) = \frac{z^l}{2^{l+1} \Gamma} \int_{-1}^{1} e^{i z s} \left(1 - s^2\right)^l \, ds
\]  
(20)

Employing the second operator equation (12) and the equation for Legendre polynomials:

\[
P_l(x) = \frac{1}{2^l \Gamma} \left( \frac{d}{dx} \right)^l (x^2 - 1)^l,
\]  
(21)
we arrive at integral representation of the Spherical Bessel function in terms of Legendre polynomials:

\[ j_l(z) = \frac{(-i)^l}{2} \int_{-1}^{1} e^{isz} P_l(s) \, ds \]  

(22)

It is convenient to rewrite the latter equality as the Fourier representation of the Legendre polynomial:

\[ \int_{-1}^{1} e^{isz} P_l(s) \, ds = 2i^l j_l(z) \]  

(23)

**Expansion of the plane wave into spherical harmonics**

The expansion must have a form:

\[ e^{ikz} = \sum_{l=0}^{\infty} C_l(r) P_l(\cos \theta) \]  

(24)

The coefficients \( C_l(r) \) can be found multiplying equation (24) by a Legendre polynomial, integrating it with \( \sin \theta \) over \( \theta \) and using the ortho-normalization condition:

\[ \int_{-1}^{1} P_l(x) P_{l'}(x) \, dx = \frac{2}{2l + 1} \delta_{ll'} \]  

(25)

The result reads:

\[ C_l(r) = \frac{2l + 1}{2} \int_{-1}^{1} e^{ikrx} P_l(x) \, dx = (2l + 1) i^l j_l(kr) \]  

(26)

Thus, the expansion of the plane wave into spherical harmonics reads:

\[ e^{ikz} = \sum_{l=0}^{\infty} (2l + 1) i^l j_l(kr) P_l(\cos \theta) \]  

(27)

Asymptotically at \( kr \gg 1 \), equation (27) takes form:

\[ e^{ikz} = \frac{e^{ikr}}{2ikr} \sum_{l=0}^{\infty} (2l + 1) P_l(\cos \theta) - \frac{e^{-ikr}}{2ikr} \sum_{l=0}^{\infty} (-1)^l (2l + 1) P_l(\cos \theta) \]  

(28)

The first sum is equal to \( 2\delta (1 - \cos \theta) \), the second one to \( 2\delta (1 + \cos \theta) \).