Course 624-07, Quantum Mechanics 2

Mathematical Appendix 1

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 $l\hbar$ reads:

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

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:

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

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 $z\to\infty$:

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

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:

$$j_l\,(z)=z^l\chi_l\,(z) \tag{4}$$

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

$$z\chi_l''+2\,(l+1)\,\chi_l'+z\chi_l=0, \tag{5}$$

where prime means differentiation by z (please, check). Let us first differentiate equation (5), eliminate χ_l from the resulting equation using the same equation (5) and then substitute $\chi_l'=-z\chi_{l+1}$. The equation for χ_{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 χ_l obey the recurrent relation $\chi_{l+1}=-\frac{1}{z}\frac{d}{dz}\chi_l$. From here it follows:

$$j_l\,(z)=(-1)^l\,z^l\left(\frac{1}{z}\frac{d}{dz}\right)^l j_0\,(z)=(-1)^l\,z^l\left(\frac{1}{z}\frac{d}{dz}\right)^l\frac{\sin z}{z} \tag{6}$$

In analogues way substituting $n_l(z) = z^l \varkappa(z)$ 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 $\frac{1}{z}\frac{d}{dz} = 2\frac{d}{d(z^2)}$ and that

$$\frac{\sin z}{z} = \sum_{n=0}^{\infty} \frac{(-1)^n \left(z^2\right)^n}{(2n+1)!}$$

The first non vanishing term after differentiation of this sum l times over z^2 is $\frac{(-1)^l l!}{(2l+1)!}$. Substituting it to the equation (6), we find the asymptotic:

$$j_l(z) \simeq \frac{2^l l! z^l}{(2l+1)!} = \frac{z^l}{(2l+1)!!};\ z \to 0 \tag{8}$$

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:

$$n_l(z) \simeq (2l-1)!! z^{-l-1};\ z \to 0 \tag{9}$$

b) *Integral representation*

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

$$\chi_l(z) = \int_{-1}^{1} e^{izs} \varphi_l(s)\, ds, \tag{10}$$

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

$$\frac{d}{dz}\chi_l(z) = \int_{-1}^{1} e^{izs} is\varphi_l(s)\, ds;\ z\chi_l(z) = \int_{-1}^{1} e^{izs} i\frac{d}{ds}\varphi_l(s)\, ds \tag{11}$$

or in the operator form:

$$\frac{d}{dz} = is;\ z = i\frac{d}{ds} \tag{12}$$

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

$$\left(1 - s^2\right)\frac{d\varphi_l}{ds} + 2ls\varphi_l = 0 \tag{13}$$

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:

$$\chi_l(z) = A\int_{-1}^{1} e^{izs}\left(1-s^2\right)^l ds \tag{14}$$

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:

$$\chi_l(0) = A\int_{-1}^{1} \left(1-s^2\right)^l ds \tag{15}$$

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:

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

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

$$\begin{aligned} \Gamma(l+3/2) &= (l+1/2)\Gamma(l+1/2) = (l+1/2)(l-1/2)\Gamma(l-1/2) = \\ ... &= (l+1/2)(l-1/2)...1/2\Gamma(1/2) \end{aligned} \tag{17}$$

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

$$\chi_l(0) = A\frac{2^{l+1}l!}{(2l+1)!!} \tag{18}$$

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 $A = \frac{1}{2^{l+1}l!}$ and

$$\chi_l(z) = \frac{1}{2^{l+1}l!}\int_{-1}^{1} e^{izs}\left(1-s^2\right)^l ds \tag{19}$$

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

$$j_l(z) = \frac{z^l}{2^{l+1}l!}\int_{-1}^{1} e^{izs}\left(1-s^2\right)^l ds \tag{20}$$

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

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l \left(x^2-1\right)^l, \tag{21}$$

we arrive at integral representation of the Spherical Bessel function in terms of Legendre polynomials:

$$j_l(z) = \frac{(-i)^l}{2} \int_{-1}^{1} e^{izs} P_l(s)\, ds \tag{22}$$

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

$$\int_{-1}^{1} e^{izs} P_l(s)\, ds = 2i^l j_l(z) \tag{23}$$

Expansion of the plane wave into spherical harmonics

The expansion must have a form:

$$e^{ikz} = \sum_{l=0}^{\infty} C_l(r)\, P_l(\cos\theta) \tag{24}$$

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

$$\int_{-1}^{1} P_l(x)\, P_{l'}(x)\, dx = \frac{2}{2l+1}\delta_{ll'} \tag{25}$$

The result reads:

$$C_l(r) = \frac{2l+1}{2} \int_{-1}^{1} e^{ikrx} P_l(x)\, dx = (2l+1)\, i^l j_l(kr) \tag{26}$$

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

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(kr)\, P_l(\cos\theta) \tag{27}$$

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

$$e^{ikz} = \frac{e^{ikr}}{2ikr} \sum_{l=0}^{\infty} (2l+1)\, P_l(\cos\theta) - \frac{e^{-ikr}}{2ikr} \sum_{l=0}^{\infty} (-1)^l (2l+1)\, P_l(\cos\theta) \tag{28}$$

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