221B Lecture Notes

Notes on Spherical Bessel Functions

1 Definitions

We would like to solve the free Schrödinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{d^2}{dr^2}r - \frac{l(l+1)}{r^2}\right]R(r) = \frac{\hbar^2 k^2}{2m}R(r). \tag{1}$$

$R(r)$ is the radial wave function $\psi(\vec{x}) = R(r)Y_l^m(\theta,\phi)$. By factoring out $\hbar^2/2m$ and defining $\rho = kr$, we find the equation

$$\left[\frac{1}{\rho}\frac{d^2}{d\rho^2}\rho - \frac{l(l+1)}{\rho^2} + 1\right]R(\rho) = 0. \tag{2}$$

The solutions to this equation are spherical Bessel functions. Due to some reason, I don't see the integral representations I use below in books on mathemtical formulae, but I believe they are right.

The behavior at the origin can be studied by power expansion. Assuming $R \propto \rho^n$, and collecting terms of the lowest power in ρ, we get

$$n(n+1) - l(l+1) = 0. \tag{3}$$

There are two solutions,

$$n = l \quad \text{or} \quad -l-1. \tag{4}$$

The first solution gives a positive power, and hence a regular solution at the origin, while the second a negative power, and hence a singular solution at the origin.

It is easy to check that the following integral representations solve the above equation Eq. (2):

$$h_l^{(\pm)}(\rho) = -i\frac{(\rho/2)^l}{l!}\int_{\pm 1}^{i\infty} e^{i\rho t}(1-t^2)^l dt. \tag{5}$$

By acting the derivatives in Eq. (2), one finds

$$\begin{aligned}
&\left[\frac{1}{\rho}\frac{d^2}{d\rho^2}\rho - \frac{l(l+1)}{\rho^2} + 1\right] h_l^{(\pm)}(\rho) \\
&= -i\frac{(\rho/2)^l}{l!}\int_{\pm 1}^{i\infty}(1-t^2)^l\left[\frac{l(l+1)}{\rho^2} + \frac{2(l+1)it}{\rho} - t^2 - \frac{l(l+1)}{\rho^2} + 1\right]dt \\
&= -i\frac{(\rho/2)^l}{l!}\frac{1}{i\rho}\int_{\pm 1}^{i\infty}\frac{d}{dt}\left[e^{i\rho t}(1-t^2)^{l+1}\right]dt. \qquad (6)
\end{aligned}$$

Therefore only boundary values contribute, which vanish both at $t = \pm 1$ and $t = i\infty$ for $\rho = kr > 0$. One can also easily see that $h_l^{(\pm)*}(\rho) = h_l^{\mp}(\rho^*)$ by taking the complex conjugate of the expression Eq. (5) and changing the variable from t to $-t$.

The integral representation Eq. (5) can be expanded in powers of $1/\rho$. For instance, for h_l^+, we change the variable from t to x by $t = 1 + ix$, and find

$$\begin{aligned}
h_l^{(+)}(\rho) &= -i\frac{(\rho/2)^l}{l!}\int_0^\infty e^{i\rho(1+ix)}x^l(-2i)^l\left(1-\frac{x}{2i}\right)^l idx \\
&= \frac{(\rho/2)^l}{l!}e^{i\rho}(-2i)^l\sum_{k=0}^{l} {}_lC_k\int_0^\infty e^{-x\rho}\left(-\frac{x}{2i}\right)^l x^l dx \\
&= \frac{e^{i\rho}}{\rho}\sum_{k=0}^{l}\frac{(-i)^{l-k}(l+k)!}{2^k k!(l-k)!}\frac{1}{\rho^k}. \qquad (7)
\end{aligned}$$

Similarly, we find

$$h_l^{(-)}(\rho) = \frac{e^{-i\rho}}{\rho}\sum_{k=0}^{l}\frac{i^{l-k}(l+k)!}{2^k k!(l-k)!}\frac{1}{\rho^k}. \qquad (8)$$

Therefore both $h_l^{(\pm)}$ are singular at $\rho = 0$ with power ρ^{-l-1}.

The combination $j_l(\rho) = (h_l^{(+)} - h_l^{(-)})/2i$ is regular at $\rho = 0$. This can be seen easily as follows. Because $h_l^{(-)}$ is an integral from $t = -1$ to $i\infty$, while $h_l^{(+)}$ from $t = +1$ to $i\infty$, the differencd between the two corresponds to an integral from $t = -1$ to $t = i\infty$ and coming back to $t = +1$. Because the integrand does not have a pole, this contour can be deformed to a straight integral from $t = -1$ to $+1$. Therefore,

$$j_l(\rho) = \frac{1}{2}\frac{(\rho/2)^l}{l!}\int_{-1}^{1} e^{i\rho t}(1-t^2)^l dt. \qquad (9)$$

In this expression, $\rho \to 0$ can be taken without any problems in the integral and hence $j_l \propto \rho^l$, *i.e.*, regular. The other linear combination $n_l = (h_l^{(+)} + h_l^{(-)})/2$ is of course singular at $\rho = 0$.

It is useful to see some examples for low l.

$$j_0 = \frac{\sin\rho}{\rho}, \qquad n_0 = \frac{\cos\rho}{\rho}, \qquad h_0^{(\pm)} = \frac{e^{\pm i\rho}}{\rho}, \tag{10}$$

$$j_1 = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}, \qquad n_1 = \frac{\cos\rho}{\rho^2} + \frac{\sin\rho}{\rho}, \qquad h_1^{(\pm)} = \left(\frac{1}{\rho^2} \mp \frac{i}{\rho}\right) e^{\pm i\rho}. \tag{11}$$

2 Asymptotic Behavior

Eqs. (7,8) give the asymptotic behaviors of $h_l^{(\pm)}$ for $\rho \to \infty$:

$$h_l^{(\pm)} \sim \frac{e^{\pm i\rho}}{\rho}(\mp i)^n = \frac{e^{\pm i(\rho - l\pi/2)}}{\rho}. \tag{12}$$

By taking linear combinations, we also find

$$j_l \sim \frac{\sin(\rho - l\pi/2)}{\rho}, \tag{13}$$

$$n_l \sim \frac{\cos(\rho - l\pi/2)}{\rho}. \tag{14}$$

3 Plane Wave Expansion

The non-trivial looking formula we used in the class

$$e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr) P_l(\cos\theta) \tag{15}$$

can be obtained quite easily from the integral representation Eq. (9). The point is that one can keep integrating it in parts. By integrating $e^{i\rho t}$ factor and differentiating $(1-t^2)^l$ factor, the boundary terms at $t = \pm 1$ always vanish up to l-th time because of the $(1-t^2)^l$ factor. Therefore,

$$j_l = \frac{1}{2}\frac{(\rho/2)^l}{l!}\int_{-1}^{1}\frac{1}{(i\rho)^l}\left(-\frac{d}{dt}\right)^l e^{i\rho t}(1-t^2)^l dt. \tag{16}$$

Note that the definition of the Legendre polynomials is

$$P_n(t) = \frac{1}{2}\frac{1}{n!}\frac{d^n}{dt^n}(t^2-1)^n. \tag{17}$$

Using this definition, the spherical Bessel function can be written as

$$j_l = \frac{1}{2}\frac{1}{i^l}\int_{-1}^{1} e^{i\rho t} P_l(t) dt. \tag{18}$$

Then we use the fact that the Legendre polynomials form a complete set of orthogonal polynomials in the interval $t \in [-1, 1]$. Noting the normalization

$$\int_{-1}^{1} P_n(t) P_m(t) dt = \frac{2}{2n+1}\delta_{n,m}, \tag{19}$$

the orthonormal basis is $P_n(t)\sqrt{(2n+1)/2}$, and hence

$$\sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(t) P_n(t') = \delta(t-t'). \tag{20}$$

By multipyling Eq. (18) by $P_l(t')(2l+1)/2$ and summing over n,

$$\sum_{n=1}^{\infty} \frac{2l+1}{2} P_l(t') j_n(\rho) = \frac{1}{2}\frac{1}{i^n}\int_{-1}^{1} e^{i\rho t} \sum_{n=0}^{\infty} P_l(t') P_l(t) dt = \frac{1}{2}\frac{1}{i^n} e^{i\rho t'}. \tag{21}$$

By setting $\rho = kr$ and $t' = \cos\theta$, we prove Eq. (15).

If the wave vector is pointing at other directions than the positive z-axis, the formula Eq. (15) needs to be generalized. Noting $Y_l^0(\theta, \phi) = \sqrt{(2l+1)/4\pi}\, P_l(\cos\theta)$, we find

$$e^{i\vec{k}\cdot\vec{x}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \sum_{m=-l}^{l} Y_l^{m*}(\theta_{\vec{k}}, \phi_{\vec{k}}) Y_l^m(\theta_{\vec{x}}, \phi_{\vec{x}}) \tag{22}$$

4 Delta-Function Normalization

An important consequence of the identity Eq. (22) is the innerproduct of two spherical Bessel functions. We start with

$$\int d\vec{x} e^{i\vec{k}\cdot\vec{x}} e^{-i\vec{k}'\cdot\vec{x}} = (2\pi)^3 \delta(\vec{k} - \vec{k}'). \tag{23}$$

Using Eq. (22) in the l.h.s of this equation, we find

$$\begin{aligned}
&\int d\vec{x} e^{i\vec{k}\cdot\vec{x}} e^{-i\vec{k}'\cdot\vec{x}} \\
&= \sum_{l,m}\sum_{l',m'}(4\pi)^2\int d\Omega_{\vec{x}} dr r^2 Y_l^{m*}(\Omega_{\vec{k}})Y_l^m(\Omega_{\vec{x}})Y_{l'}^{m'*}(\Omega_{\vec{x}})Y_{l'}^{m'}(\Omega_{\vec{k}'})j_l(kr)j_{l'}(k'r) \\
&= \sum_{l,m}(4\pi)^2\int dr r^2 j_l(kr)j_l(k'r)Y_l^{m*}(\Omega_{\vec{k}})Y_l^m(\Omega_{\vec{k}'}). \qquad (24)
\end{aligned}$$

On the other hand, the r.h.s of Eq. (23) is

$$(2\pi)^3\delta(\vec{k}-\vec{k}') = (2\pi)^3\frac{1}{k^2}\delta(k-k')\delta(\Omega_{\vec{k}}-\Omega_{\vec{k}'}) = (2\pi)^3\frac{1}{k^2\sin\theta}\delta(k-k')\delta(\theta-\theta')\delta(\phi-\phi'). \qquad (25)$$

Comparing Eq. (24) and (25) and noting

$$\sum_{l,m} Y_l^{m*}(\Omega_{\vec{k}})Y_l^m(\Omega_{\vec{k}'}) = \delta(\Omega_{\vec{k}}-\Omega_{\vec{k}'}), \qquad (26)$$

we find

$$\int_0^\infty dr r^2 j_l(kr)j_l(k'r) = \frac{\pi}{2k^2}\delta(k-k'). \qquad (27)$$