Expansion of plane waves in spherical harmonics

Consider a free particle of mass $\mu$ in three dimension. The time-independent Schrödinger equation for the energy eigenstates in the coordinate representation is given by

$$\left(\nabla^2 + k^2\right)\psi_k(\vec{r}) = 0,$$

(1)
corresponding to an energy $E = \hbar^2k^2/(2\mu)$. The solution to eq. (1) is a plane wave,

$$\psi_k(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k} \cdot \vec{r}},$$

(2)
where the wave function is conventionally normalized such that

$$\int d^3x \psi^*_k(\vec{x}) \psi_k(\vec{x}) = \delta(\vec{k} - \vec{k}').$$

One can also solve eq. (1) in spherical coordinates. If we look for simultaneous eigenstates of the free particle Hamiltonian, and the angular momentum operators $L_z$ and $\vec{L}^2$, we obtain

$$\psi_{k}(r, \theta, \phi) = \langle r, \theta, \phi | E\ell m \rangle = i^\ell \left(\frac{2\mu k}{\pi \hbar^2}\right)^{1/2} \mathcal{A}_\ell(k) j_\ell(kr) Y_{\ell m}(\theta, \phi),$$

(3)
where the normalization factor has been chosen such that $\langle E'\ell' m' | E\ell m \rangle = \delta_{\ell\ell'}\delta_{mm'}\delta(E - E')$, and the factor of $i^\ell$ is conventional. In particular, since the free particle Hamiltonian commutes with the angular momentum operators $L_z$ and $\vec{L}^2$, it follows that any choice of $\ell$ and $m$ in eq. (3) yields an energy eigenstate of energy $E = \hbar^2k^2/(2\mu)$.

Hence, it must be possible to express the plane wave given in eq. (2) as a sum over spherical harmonics,

$$e^{i\vec{k} \cdot \vec{r}} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{\ell m}(\vec{k}) j_\ell(kr) Y_{\ell m}(\hat{r}).$$

(4)
The object of these notes is to determine the coefficients $c_{\ell m}(\vec{k})$.

It is always possible to choose the $z$-axis of our problem to lie along $\vec{k}$. For $\vec{k} = k\hat{z}$, $\vec{k} \cdot \vec{r} = kr \cos \theta$ (where $r \equiv |\vec{r}|$) and $\theta$ is the polar angle of the vector $\vec{r}$ with respect to the $z$-axis. Hence, the double sum in eq. (4) must be independent of the azimuthal angle $\phi$. This is possible only if $c_{\ell m}(k\hat{z}) = 0$ for all $m \neq 0$. That is, only the $m = 0$ term of eq. (4) survives and it follows that

$$e^{i kr \cos \theta} = \sum_{\ell=0}^{\infty} \left(\frac{2\ell + 1}{4\pi}\right)^{1/2} A_\ell(k) j_\ell(kr) P_\ell(\cos \theta),$$

(5)
where $A_\ell(k) \equiv c_{00}(k\hat{z})$, and we have employed the relation between $Y_{\ell 0}(\theta, \phi)$ and the Legendre polynomial, $P_\ell(\cos \theta)$.

\[^1\text{since } \hat{r} \equiv \hat{x} \sin \theta \cos \phi + \hat{y} \sin \theta \sin \phi + \hat{z} \cos \theta, \text{ it is convenient to write } Y_{\ell m}(\hat{r}) \text{ in place of } Y_{\ell m}(\theta, \phi).\]
We can extract the coefficient $A_\ell(k)$ by using the orthogonality relation of the Legendre polynomials,

$$\int_{-1}^{1} P_\ell(\cos \theta) P_\ell'(\cos \theta) \, d\cos \theta = \frac{2}{2\ell + 1} \delta_{\ell\ell'} . \tag{6}$$

Multiplying both sides of eq. (5) by $P_\ell'(\cos \theta)$ and then integrating over $\cos \theta$ with the help of eq. (6), we end up with

$$A_\ell(k) j_\ell(k r) = \sqrt{\pi} (2\ell + 1) \int_{-1}^{1} P_\ell(w) e^{ikrw} \, dw , \tag{7}$$

where $w \equiv \cos \theta$.

There are a number of different ways to obtain $A_\ell(k)$. One technique, which involves a direct evaluation of the integral on the right hand side of eq. (7), is given in Appendix A. The end result is obtained in eq. (19), which we repeat here,

$$\int_{-1}^{1} P_\ell(w) e^{ikrw} \, dw = 2i\ell j_\ell(k r) \tag{8}$$

Comparing eqs. (7) and (8), we conclude that

$$A_\ell(k) = i\ell \sqrt{4\pi(2\ell + 1)} . \tag{9}$$

However, one can obtain the same result by employing the following trick. Since $A_\ell(k)$ is independent of $r$, we can evaluate $A_\ell(k)$ by examining the $r \to \infty$ behavior of both sides of eq. (7). The large $r$ behavior of the left hand side is determined by the leading term of the asymptotic expansion of $j_\ell(k r)$,

$$j_\ell(k r) \sim \frac{1}{kr} \sin (kr - \frac{1}{2}\ell\pi) + O\left( \frac{1}{(kr)^2} \right) , \quad \text{as } r \to \infty. \tag{10}$$

We can determine the leading asymptotic behavior of the integral on the right hand side of eq. (7) by a repeated integration by parts,

$$\int_{-1}^{1} P_\ell(w) e^{ikrw} \, dw = \frac{1}{ikr} e^{ikr} P_\ell(w) \bigg|_{-1}^{1} - \frac{1}{ikr} \int_{-1}^{1} e^{ikrw} P'_\ell(w) \, dw$$

$$= \frac{1}{ikr} [e^{ikr} - e^{-ikr} e^{i\pi\ell}] + \frac{1}{(kr)^2} e^{ikrw} P'_\ell(w) \bigg|_{-1}^{1} - \frac{1}{(kr)^2} \int_{-1}^{1} e^{ikrw} P''_\ell(w) \, dw$$

$$= \frac{2i\ell}{kr} \sin (kr - \frac{1}{2}\pi\ell) + O\left( \frac{1}{(kr)^2} \right) , \tag{11}$$

where we have used $P_\ell(1) = 1$ and $P_\ell(-1) = (-1)^\ell = e^{i\pi\ell}$. Finally, in light of eqs. (10) and (11), it follows from eq. (7) that $A_\ell(k) = i\ell \sqrt{4\pi(2\ell + 1)}$, in agreement with eq. (9).

Inserting eq. (9) back into eq. (5), we end up with

$$e^{ikr \cos \theta} = \sum_{\ell=0}^{\infty} i\ell (2\ell + 1) j_\ell(k r) P_\ell(\cos \theta) . \tag{12}$$
Finally, we can relax the assumption that $\vec{k} = k\hat{z}$ by employing the addition theorem,

$$P_\ell(\cos \theta) = \frac{4\pi}{2\ell + 1} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{r}) Y_{\ell m}(\hat{k})^*, \quad \text{where } \cos \theta = \hat{k} \cdot \hat{r}.$$ 

Inserting the addition theorem for $P_\ell(\cos \theta)$ into eq. (12) yields our final result,

$$e^{i\vec{k} \cdot \vec{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell j_\ell(kr) Y_{\ell m}(\hat{k})^* Y_{\ell m}(\hat{r}).$$ (13)

That is, we have identified $c_{\ell m}(\vec{k}) = 4\pi i^\ell Y_{\ell m}(\hat{k})^*$ in eq. (4).

Eqs. (12) and (13) are both called the partial wave expansion of the plane wave. It is interesting to note that in light of eq. (10), which we can rewrite as

$$j_\ell(kr) \sim \frac{1}{2\ell+1} \left[ \frac{e^{ikr}}{kr} - \left( \frac{e^{-ikr}}{kr} \right) e^{i\pi \ell} \right] + O\left( \frac{1}{(kr)^2} \right), \quad \text{as } r \to \infty,$$

it follows from eq. (13) that a plane wave moving in the direction $\vec{k}$ can be decomposed into a linear combination of incoming and outgoing spherical waves.

**APPENDIX A: Evaluation of the integral appearing in eq. (7)**

The spherical Bessel function is given by the following formula,

$$j_\ell(\rho) = (-\rho)^\ell \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^\ell \left( \frac{\sin \rho}{\rho} \right).$$ (14)

Thus, we can write

$$j_0(\rho) = \frac{\sin \rho}{\rho} = \frac{1}{2} \int_{-1}^{1} e^{i\rho w} dw.$$ (15)

Next, we note that by an integration by parts,

$$\frac{1}{\rho} \frac{d}{d\rho} \int_{-1}^{1} e^{i\rho w} dw = \frac{i}{\rho} \int_{-1}^{1} w e^{i\rho w} dw = \frac{i}{2\rho} \int_{-1}^{1} e^{i\rho w} d(w^2 - 1) = -\frac{i}{2\rho} \int_{-1}^{1} (w^2 - 1)d(e^{i\rho w}) = \frac{1}{2} \int_{-1}^{1} (w^2 - 1)e^{i\rho w} dw.$$

Repeating this process $\ell$-times yields

$$\left( \frac{1}{\rho} \frac{d}{d\rho} \right)^\ell \int_{-1}^{1} e^{i\rho w} dw = \frac{1}{2^\ell \ell!} \int_{-1}^{1} (w^2 - 1)^\ell e^{i\rho w} dw.$$ (16)
Applying eq. (16) to eq. (15), it then follows from eq. (14) that

\[ j_\ell(\rho) = (-\rho)^\ell \left( \frac{1}{\rho} \frac{d}{d\rho} \right) ^\ell \frac{1}{2} \int_{-1}^{1} e^{i\rho w} dw = \frac{(-\rho)^\ell}{2^{\ell+1} \ell!} \int_{-1}^{1} (w^2 - 1)^\ell e^{i\rho w} dw \]

\[ = \frac{i^\ell}{2^{\ell+1} \ell!} \int_{-1}^{1} (w^2 - 1)^\ell \frac{d^\ell}{dw^\ell} (e^{i\rho w}) dw = \frac{(-i)^\ell}{2^{\ell+1} \ell!} \int_{-1}^{1} e^{i\rho w} \frac{d^\ell}{dw^\ell} (w^2 - 1)^\ell dw, \quad (17) \]

after integration by parts \( \ell \) times. Finally, we employ the Rodrigues formula for the Legendre polynomials,

\[ P_\ell(w) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dw^\ell} (w^2 - 1)^\ell. \]

Then, eq. (17) yields

\[ j_\ell(\rho) = \frac{(-i)^\ell}{2} \int_{-1}^{1} P_\ell(w) e^{i\rho w} dw. \quad (18) \]

We have thus succeeded in evaluating the integral that appears in eq. (7),

\[ \int_{-1}^{1} P_\ell(w) e^{ikrw} dw = 2i^\ell j_\ell(kr) \quad (19) \]

REFERENCE