Expansion of plane waves in spherical harmonics

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

$$(\vec{\boldsymbol{\nabla}}^{\boldsymbol{2}} + k^2)\psi_{\vec{\boldsymbol{k}}}(\vec{\boldsymbol{r}}) = 0\,, \tag{1}$$

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

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

where the wave function is conventionally normalized such that

$$\int d^3x\, \psi^*_{\vec{\boldsymbol{k}}}(\vec{x})\, \psi_{\vec{\boldsymbol{k}}'}(\vec{x}) = \delta^3(\vec{\boldsymbol{k}} - \vec{\boldsymbol{k}}')\,.$$

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 $\vec{\boldsymbol{L}}^{\boldsymbol{2}}$, we obtain

$$\psi_{\vec{\boldsymbol{k}}}(r,\theta,\phi) = \langle r,\theta,\phi|\, E\ell m\rangle = i^\ell \left(\frac{2\mu k}{\pi\hbar^2}\right)^{1/2} j_\ell(kr) Y_{\ell m}(\theta,\phi)\,, \tag{3}$$

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^ℓ is conventional. In particular, since the free particle Hamiltonian commutes with the angular momentum operators L_z and $\vec{\boldsymbol{L}}^{\boldsymbol{2}}$, it follows that any choice of ℓ and m in eq. (3) yields an energy eigenstate of energy $E = \hbar^2 k^2/(2\mu)$.

Hence, it must be possible to express the plane wave given in eq. (2) as a sum over spherical harmonics,[1]

$$e^{i\vec{\boldsymbol{k}}\cdot\vec{\boldsymbol{r}}} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} c_{\ell m}(\vec{\boldsymbol{k}}) j_\ell(kr) Y_{\ell m}(\hat{\boldsymbol{r}})\,. \tag{4}$$

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

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

$$e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty}\left(\frac{2\ell+1}{4\pi}\right)^{1/2} A_\ell(k) j_\ell(kr) P_\ell(\cos\theta)\,, \tag{5}$$

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

[1] since $\hat{\boldsymbol{r}} \equiv \hat{\boldsymbol{x}}\sin\theta\cos\phi + \hat{\boldsymbol{y}}\sin\theta\sin\phi + \hat{\boldsymbol{z}}\cos\theta$, it is convenient to write $Y_{\ell m}(\hat{\boldsymbol{r}})$ 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

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

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,

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

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 $j_\ell(kr)$,

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

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

$$\begin{aligned}
\int_{-1}^{1} P_\ell(w)e^{ikrw}\,dw &= \frac{1}{ikr}\,e^{ikrw}P_\ell(w)\bigg|_{-1}^{1} - \frac{1}{ikr}\int_{-1}^{1} e^{ikrw}P'_\ell(w) \\
&= \frac{1}{ikr}\bigl[e^{ikr} - e^{-ikr}e^{i\pi\ell}\bigr] + \frac{1}{(kr)^2}\,e^{ikrw}P'_\ell(w)\bigg|_{-1}^{1} - \frac{1}{(kr)^2}\int_{-1}^{1} e^{ikrw}P''_\ell(w) \\
&= \frac{2i^\ell}{kr}\sin\bigl(kr - \tfrac{1}{2}\pi\ell\bigr) + \mathcal{O}\left(\frac{1}{(kr)^2}\right)\,,
\end{aligned} \tag{11}$$

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

$$\boxed{e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} i^\ell(2\ell+1)j_\ell(kr)P_\ell(\cos\theta)\,.} \tag{12}$$

Finally, we can relax the assumption that $\vec{\boldsymbol{k}} = k\hat{\boldsymbol{z}}$ by employing the addition theorem,

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

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

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

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

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

it follows from eq. (13) that a plane wave moving in the direction $\vec{\boldsymbol{k}}$ 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,

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

Thus, we can write

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

Next, we note that by an integration by parts,

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

Repeating this process ℓ-times yields

$$\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell\int_{-1}^{1} e^{i\rho w}\,dw = \frac{1}{2^\ell\,\ell!}\int_{-1}^{1}(w^2-1)^\ell e^{i\rho w}\,dw\,. \tag{16}$$

Applying eq. (16) to eq. (15), it then follows from eq. (14) that

$$
\begin{aligned}
j_\ell(\rho) &= (-\rho)^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \frac{1}{2}\int_{-1}^{1} e^{i\rho w}\,dw = \frac{(-\rho)^\ell}{2^{\ell+1}\,\ell!}\int_{-1}^{1}(w^2-1)^\ell e^{i\rho w}\,dw \\
&= \frac{i^\ell}{2^{\ell+1}\,\ell!}\int_{-1}^{1}(w^2-1)^\ell \frac{d^\ell}{dw^\ell}\bigl(e^{i\rho w}\bigr)\,dw = \frac{(-i)^\ell}{2^{\ell+1}\,\ell!}\int_{-1}^{1} e^{i\rho w}\frac{d^\ell}{dw^\ell}\bigl(w^2-1\bigr)^\ell\,dw\,, \qquad (17)
\end{aligned}
$$

after integration by parts ℓ times. Finally, we employ the Rodrigues formula for the Legendre polynomials,

$$
P_\ell(w) = \frac{1}{2^\ell\,\ell!}\frac{d^\ell}{dw^\ell}\bigl(w^2-1\bigr)^\ell\,.
$$

Then, eq. (17) yields

$$
j_\ell(\rho) = \frac{(-i)^\ell}{2}\int_{-1}^{1} P_\ell(w)e^{i\rho w}\,dw\,. \qquad (18)
$$

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

$$
\int_{-1}^{1} P_\ell(w)e^{ikrw}\,dw = 2i^\ell j_\ell(kr) \qquad (19)
$$

REFERENCE

Kevin Cahill, *Physical Mathematics* (Cambridge University Press, Cambridge, UK, 2013)