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or

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta) \quad (7.24)$$

This is the expansion of a plane wave into partial waves. It is also called Bauer's formula.

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The expansion of plane wave can also be done in terms of spherical waves.

We write that k is represented by the $(\theta_k\ \phi_k)$ and r by the (θ_r, ϕ_r) coordinates, then the angle between the two is (θ, ϕ). Using addition theorem of spherical harmonics we can write that

$$P_l(\cos\theta) = \sum_{m=-l}^{+l} \frac{1}{2l+1} Y^*_{lm}(\theta_k \phi_k)\, Y_{lm}(\theta_r, \phi_r)$$

Let us use the asymptotic value of $j_l(kr)$ in (7.24)

$$j_l(kr) \underset{r\to\infty}{\sim} \frac{\sin(kr - l\pi/2)}{kr}$$

$$= \frac{1}{2ikr}\left[e^{i(kr - \frac{l\pi}{2})} - e^{-i(kr - \frac{l\pi}{2})}\right]$$

$$= \frac{1}{2ikr}\left[e^{ikr} e^{-\frac{il\pi}{2}} - e^{-ikr} e^{\frac{il\pi}{2}}\right]$$

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$$e^{\frac{il\pi}{2}} = \left(e^{\frac{i\pi}{2}}\right)^l = \left(\cos\frac{\pi}{2} + i\sin\frac{\pi}{2}\right)^l = i^l$$

and $e^{-\frac{il\pi}{2}} = \left(e^{-\frac{i\pi}{2}}\right)^l = (-i)^l$.

So $j_l(kr) \underset{kr\to\infty}{\sim} \frac{1}{2ikr}\left[(i)^{-l} e^{ikr} - (i)^l e^{-ikr}\right]$

∴ R.H.S. of (7.24) becomes

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

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

$$e^{ikr\cos\theta} = \frac{1}{2ikr} \sum_{l=0}^{\infty} \left[e^{ikr} + (-1)^{l+1} e^{-ikr}\right] P_l(\cos\theta) \quad (7.25)$$

The $\frac{e^{ikr}}{r}$ represents the outgoing spherical wave

and $\frac{e^{-ikr}}{r}$ " " incoming "

Differentiate (7.19B) w.r.t. ρ we get-

$$ixe^{i\rho x} = \sum_{l=0}^{\infty} C_l \frac{dJ_l(\rho)}{d\rho}\, P_l(x)$$

$$= \sum_{l=0}^{\infty} C_l\, P_l(x) \underbrace{\left[\frac{l\, J_{l-1}(\rho)}{(2l+1)} - \left(\frac{l+1}{2l+1}\right) J_{l+1}(\rho)\right]}_{= \frac{dJ_l(\rho)}{d\rho}} \quad (7.21A)$$

Now consider the R.H.S.

$$ixe^{i\rho x} = ix\, e^{i\rho x}$$

using (7.19B) $\quad ixe^{i\rho x} = \sum_{l=0}^{\infty} ixC_l J_l(\rho) P_l(x)$

$$= \sum_{l=0}^{\infty} iC_l J_l(\rho)\, xP_l(x) \quad (7.21B)$$

$$= \sum_{l=1}^{\infty} iC_l J_l(\rho) \underbrace{\left[\frac{l}{2l+1} P_{l-1}(x) + \frac{l+1}{2l+1} P_{l+1}(x)\right]}_{xP_l(x)}$$

In (7.21)B the index l now varies from $l=1$, because if l is zero the $P_{-1}(x)$ vanishes or not defined.

Compare (7.21A) and (7.21B) we get (coefficient of $P_l(x)$)

$$\left(\frac{l}{2l+1}\right) C_l J_{l-1}(\rho) - \frac{(l+1)}{(2l+1)} J_{l+1}(\rho) = i\,\frac{l+1}{2l+3}\, C_{l+1} J_{l+1}(\rho) + i\,\frac{l}{2l-1}\, C_{l-1} J_{l-1}(\rho) \quad (7.22)$$

Now compare the coefficients of the same order of J_l on both sides we get-

$$\frac{l}{2l+1}\, C_l J_{l-1}(\rho) = i\,\frac{l}{2l-1}\, C_{l-1} J_{l-1}(\rho)$$

$$\Rightarrow C_l = \frac{i(2l+1)}{(2l-1)}\, C_{l-1} \qquad l \geq 1$$

So $l=1$, $C_1 = i\,(3)\,C_0 = 3iC_0$

$l=2 \quad C_2 = i\,\frac{5}{3}\, C_1 = i\,\frac{5}{3}\cdot 3iC_0 = i^2\, 5C_0$

$l=3 \quad C_3 = i\,\frac{7}{5}\, C_2 = i\cdot\frac{7}{5}\cdot i^2\cdot 5\cdot C_0 = i^3\, 7C_0$

So in general $\quad C_l = i^l(2l+1)\,C_0 \qquad (7.23)$

Now C_0 can be found by putting $\rho = 0$ in (7.19B) so

$$e^{i\rho x} = \sum_{l=0}^{\infty} C_l J_l(\rho) P_l(x)$$

put $\rho = 0$, $l=0$, and $J_l(0) = \delta_{l0}$; so $J_0(\rho) = \delta_{00}$ and $P_0(x) = 1$

So $1 = C_0$ so.

$$\boxed{C_l = i^l(2l+1)} \qquad (7.23B)$$

So from 7.19B we find

$$e^{i\rho x} = \sum_{l=0}^{\infty} i^l(2l+1)\, J_l(\rho)\, P_l(x)$$

(3)

This is a second order differential equation so there are two independent solutions, the $j_\ell(kr)$ and $n_\ell(kr)$. At $r=0$ only $j_\ell(kr)$ is regular so

$$R_{k\ell}(r) = j_\ell(kr) \quad — (7.18)$$

So solution (7.16) is

$$\psi_{k\ell m}(r,\theta,\phi) = j_\ell(kr)\, Y_{\ell m}(\theta,\phi) \quad — (7.18A)$$

So the set $\{\psi_{k\ell m}\}_\infty$ of infinite orthonormal vectors with $\left\{\begin{matrix} \ell = 0 \text{ to } \infty \\ m = -\ell \text{ to } +\ell \\ k = 0 \text{ to } \infty \end{matrix}\right\}$ constitute a basis of the ∞-D Hilbert space of free particles. Each $\psi_{k\ell m}$ is called a spherical or partial wave. These are characterised by the angular momentum ℓ.

So the free particle wavefunctions can be described in two independent basis one is $\{\mathcal{V}_k\}_\infty$ and other is $\{\psi_{k\ell m}\}_\infty$. $\therefore$ using a Matrix one can switch from one basis to other.

So ~~for~~ a given vector $\mathcal{V}_k$ in $\{\mathcal{V}_k\}_\infty$ can be expanded in terms of a set of vectors in $\{\psi_{k\ell m}\}_\infty$ basis vectors. Therefore

$$e^{i\vec{k}\cdot\vec{r}} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} a_{\ell m}(r)\, j_\ell(kr)\, Y_{\ell m}(\theta,\phi) \quad (7.19)$$

In this expansion we need to determine $a_{\ell m}(r)$

(4)

To find $a_{\ell m}(r)$, we choose that wave is moving in the z direction so.

$$\vec{k}\cdot\vec{r} = kr\cos\theta = kz \quad \text{so.}$$

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikz}.$$

Because the R.H.S. of (7.19) does not contain x and y so the R.H.S should also be independent of ϕ or should not contain ϕ dependent terms. This can be ensured by choosing $m=0$, therefore we have to take

$$Y_{\ell 0}(\theta,\phi) = \sqrt{\frac{(2\ell+1)}{4\pi}}\cdot P_\ell(\cos\theta)$$

So (7.19) becomes

$$e^{ikz} = \sum_{\ell=0}^{\infty} a_{\ell 0}(r)\, j_\ell(kr) \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$$

$\rho = kr$

If we write $\cos\theta = x$, then $e^{ikz} = e^{ikr\cos\theta} = e^{i\rho x}$

or $$e^{i\rho x} = \sum_{\ell=0}^{\infty} C_\ell\, j_\ell(\rho)\, P_\ell(x) \quad — \cancel{7.20}\ (7.19B)$$

With $C_\ell = \sqrt{\frac{2\ell+1}{4\pi}}\, a_{\ell 0}$; $\rho = kr$; $x = \cos\theta$ (7.20)

1

Expansion of a plane wave into partial waves:

OR

Decomposition of a plane wave into partial waves:

We know that plane wave is a solution of a free particle Schrodinger equation. A free particle does not feel any potential so $V(r)=0$. Therefore the free particle Schrodinger Equation is

$$-\frac{\hbar^2 \nabla^2 \psi}{2M} = \frac{\hbar^2 k^2}{2M}\psi \qquad (7.10)$$

or $$(-\Delta - k^2)\psi(\vec{r}) = 0 \qquad (7.11)$$

where $\Delta = \nabla^2$, the Laplacian operator.

It's solution is given by $\nu_k(r)$, then

$$\nu_k(r) = (2\pi)^{-3/2} \cdot e^{i\vec{k}\cdot\vec{r}} \qquad -(7.12)$$

Thus the orthonormal set of vectors $\{\nu_k\}_{\infty}$ forms a basis (from $-\infty$ to $+\infty$) of the ∞-D Hilbert space of these free particles.

Eq^n (7.10) can be rewritten as

$$\hat{H}\psi(\vec{r}) = E\psi(\vec{r})$$

In spherical cardinale system we can write that $-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}\right]\psi = E\psi(\vec{r}) \quad -(7.13)$

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We can verify that $[\hat{H}, \hat{L}^2] = 0 \qquad -(7.14a)$

$[\hat{H}, \hat{L}_z] = 0 \qquad (7.14b)$

Because $[L^2, L_z] = 0$, so these operators can have simultaneous eigenfunctions. Because both L^2 and $\hat{L}_z$ have common eigenfunctions and these two commute with $\hat{H}$ so these are also eigenfunctions of $\hat{H}$.

Therefore

$$\hat{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi) \qquad -(7.15a)$$

$$\hat{L}_z Y_{lm}(\theta,\phi) = m\hbar\, Y_{lm}(\theta,\phi) \qquad -(7.15b)$$

and therefore

$$\psi(\vec{r}) \equiv \psi_{klm}(r,\theta,\phi) = R_{kl}(r)\, Y_{lm}(\theta,\phi) \qquad (7.16)$$

Use (7.16) in (7.13) we get

$$-\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}\right] R_{kl}(r) Y_{lm}(\theta,\phi) = E R_{kl}(r) Y_{lm}(\theta,\phi)$$

$$\Rightarrow \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial R_{k,l}}{\partial r}\right) Y_{lm}(\theta,\phi) - \frac{\hat{L}^2}{\hbar^2 r^2} R_{k,l}(r) Y_{lm}(\theta,\phi) = -k^2 R_{kl}(r) Y_{lm}(\theta,\phi)$$

$$\because \frac{2ME}{\hbar^2} = k^2$$

$$\Rightarrow \frac{1}{r^2}\left[2r\,\frac{\partial R_{kl}(r) Y_{lm}(\theta,\phi)}{\partial r} + r^2 \frac{\partial^2 R_{kl}(r) Y_{lm}(\theta,\phi)}{\partial r^2}\right] - \frac{l(l+1)\hbar^2}{\hbar^2 r^2} R_{kl}(r) Y_{lm}(\theta,\phi) = -k^2 R_{kl}(r) Y_{lm}(\theta,\phi)$$

Divide the entire equation by $Y_{lm}(\theta,\phi)$ we get

$$\frac{d^2 R_{kl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{kl}(r)}{dr} - \frac{l(l+1)}{r^2} R_{kl}(r) = -k^2 R_{kl}(r)$$

or $$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \left\{k^2 - \frac{l(l+1)}{r^2}\right\}\right] R_{k,l}(r) = 0 \qquad (7.17)$$