3D scattering continued.

Partial wave scattering

Consider a central potential $V(r)$ only — no angular dependence.

$$\psi_k(\vec{r}) = \psi_{0k}(\vec{r}) + \int d^3r' \, V(r') \, G_{0+}(\vec{r},\vec{r}';E) \, \psi_k(\vec{r}')$$

$$G_{0+}(\vec{r},\vec{r}';E) = -\frac{m}{2\pi\hbar^2} \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = \langle r| \frac{1}{E-H_0+i\delta} |\vec{r}'\rangle$$

define the z direction along $\vec{k}$.

Then $\qquad\qquad$ θ = angle of $\vec{r}$ to z axis

$$\psi_{0\vec{k}}(\vec{r}) = \frac{1}{\sqrt{(2\pi)^3}} e^{ikr\cos\theta}$$

$$= \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta)$$

expand $\psi_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} (2l+1) i^l A_l(r,k) P_l(\cos\theta)$

for G_{0+}, insert $\int dq \, |\psi_{0q}\rangle\langle\psi_{0q}|$ between $\langle r|$ and fraction

$$G_{0+}(\vec{r},\vec{r}';E) = \int d^3q \, \langle\vec{r}|\psi_{0q}\rangle\langle\psi_{0q}|\vec{r}'\rangle \frac{1}{E-\frac{\hbar^2q^2}{2m}+i\delta}$$

$$= \frac{1}{(2\pi)^3}\int d^3q \, e^{+i\vec{q}\cdot(\vec{r}-\vec{r}')} \frac{1}{E-\frac{\hbar^2q^2}{2m}+i\delta}$$

The problem is that $\vec{q}$ can point in any direction, it does not point along the z-axis.

Suppose a unit vector $\vec{e}_x$ points in the θ, ϕ direction. We use $Y_\ell^m(\vec{e}_x) = Y_\ell^m(\theta, \phi)$ denote the spherical harmonic in that direction. Then one can generalize our plane wave calculation to

$$e^{i\vec{q}\cdot\vec{r}} = 4\pi \sum_{\ell m} i^\ell j_\ell(qr)\, Y_\ell^{m*}(\vec{e}_{\vec{q}})\, Y_\ell^m(\vec{e}_{\vec{r}})$$

$$e^{-i\vec{q}\cdot\vec{r}\,'} = 4\pi \sum_{\ell' m'} (-i)^{\ell'} j_{\ell'}(qr')\, Y_{\ell'}^{m'}(\vec{e}_{\vec{q}})\, Y_{\ell'}^{m'*}(\vec{e}_{\vec{r}\,'})$$

and

$$G_{0+}(\vec{r},\vec{r}\,';E) = \frac{1}{(2\pi)^3}\cdot(4\pi)^2 \sum_{\ell m}\sum_{\ell' m'} \int d^3q \; i^\ell (-i)^{\ell'} j_\ell(qr)\, j_{\ell'}(qr')$$

$$Y_\ell^{m*}(\vec{e}_{\vec{q}})\, Y_{\ell'}^{m'}(\vec{e}_{\vec{q}})\, Y_\ell^m(\vec{e}_{\vec{r}})\, Y_{\ell'}^{m'*}(\vec{e}_{\vec{r}\,'}) \; \frac{1}{E - \frac{\hbar^2 q^2}{2m} + i\delta}$$

But $\int d\Omega_q \; Y_\ell^{m*}(\vec{e}_{\vec{q}})\, Y_{\ell'}^{m'}(\vec{e}_{\vec{q}}) = \delta_{mm'}\delta_{\ell\ell'} = \langle \ell m | \ell' m' \rangle$

due to orthogonality of the spherical harmonics.

So

$$G_{0+}(\vec{r},\vec{r}\,';E) = \frac{2}{\pi} \sum_{\ell m} \int_0^\infty dq\; \frac{q^2 j_\ell(qr)\, j_\ell(qr')\, Y_\ell^m(\vec{e}_{\vec{r}})\, Y_\ell^{m*}(\vec{e}_{r'})}{E - \frac{\hbar^2 q^2}{2m} + i\delta}$$

Note $j_\ell(-qr) = (-1)^\ell j_\ell(qr)$ so we can write

$$G_{0+}(\vec{r},\vec{r}\,';E) = \frac{1}{\pi}\,\frac{2m}{\hbar^2} \sum_{\ell m} Y_\ell^m(\vec{e}_r)\, Y_\ell^{m*}(\vec{e}_{r'}) \int_{-\infty}^{+\infty} dq\; \frac{q^2 j_\ell(qr)\, j_\ell(qr')}{k^2 - q^2 + i\delta}$$

Now use the fact that $P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^0(\vec{e}_{\vec{r}})$

To get

$$\sum_{\ell=0}^{\infty} \sqrt{2\ell+1}\, i^\ell A_\ell(r,k)\, Y_\ell^0(\vec{e}_{\vec{r}}) = \sum_{\ell=0}^{\infty} \sqrt{2\ell+1}\, i^\ell j_\ell(kr)\, Y_\ell^0(\vec{e}_{\vec{r}})$$

$$+ \int d^3r'\, V(r') \frac{1}{\pi}\frac{2m}{\hbar^2} \sum_{\ell' m'} Y_{\ell'}^{m'}(\vec{e}_{\vec{r}})\, Y_{\ell'}^{m'*}(\vec{e}_{\vec{r}'}) \int_{-\infty}^{+\infty} dq\, \frac{q^2 j_{\ell'}(qr)\, j_{\ell'}(qr')}{k^2 - q^2 + i\delta}$$

$$* \sum_\ell \sqrt{2\ell+1}\, i^\ell A_\ell(r',k)\, Y_\ell^0(\vec{e}_{\vec{r}'})$$

The integral over r' can be written $\int_0^\infty dr'\, r'^2 \int d\Omega_{\vec{e}_{\vec{r}'}}$

and $\int d\Omega_{\vec{e}_{\vec{r}'}}\, Y_{\ell'}^{m'*}(\vec{e}_{\vec{r}'})\, Y_\ell^0(\vec{e}_{\vec{r}'}) = \delta_{m'0}\,\delta_{\ell\ell'}$

so $RHS = \sum_{\ell=0}^{\infty} \sqrt{2\ell+1}\, i^\ell j_\ell(kr)\, Y_\ell^0(\vec{e}_r) + \int_0^\infty dr'\, r'^2\, V(r') \frac{2m}{\pi\hbar^2} \sum_{\ell=0}^{\infty} Y_\ell^0(\vec{e}_{\vec{r}})$

$$\int_{-\infty}^{+\infty} dq\, \frac{q^2 j_\ell(qr)\, j_\ell(qr')}{k^2 - q^2 + i\delta} \sqrt{2\ell+1}\, i^\ell A_\ell(r',k)$$

so we find

$$\boxed{A_\ell(r,k) = j_\ell(kr) + \frac{2m}{\pi\hbar^2}\int_0^\infty dr'\, r'^2\, V(r')\, A_\ell(r',k) \int_{-\infty}^{+\infty} dq\, \frac{q^2 j_\ell(qr)\, j_\ell(qr')}{k^2 - q^2 + i\delta}}$$

This is an integral equation for the partial wave amplitudes.

examine for large r $\qquad j_\ell(kr) \to \frac{1}{kr}\sin\left(kr - \frac{\ell\pi}{2}\right)$

the integral over q can be evaluated by contour integration using analytic properties of Bessel functions (done in Gottfried's book). we get

$$\int_{-\infty}^{+\infty} dq \, \frac{q^2 j_\ell(qr) j_\ell(qr')}{k^2 - q^2 + i\delta} \xrightarrow[\text{as } r\to\infty]{} \frac{-\pi i k e^{ikr}}{kr} \int_0^\infty dr' r'^2 j_\ell(kr') A_\ell(r',k)$$

so we find as $r \to \infty$

$$A_\ell(r,k) \to \frac{-1}{2ikr}\Big\{ \underbrace{e^{-i(kr - \frac{\ell\pi}{2})}}_{\text{incoming}} - e^{i(kr-\frac{\ell\pi}{2})} * \underbrace{\Big[1 - 2ik\int_0^\infty dr' r'^2 \, * \tfrac{2m}{\hbar^2}V(r') \, j_\ell(kr') A_\ell(r',k)\Big]}_{\text{outgoing}}\Big\}$$

let $$\boxed{e^{2i\delta_\ell(k)} = 1 - 2ik\int_0^\infty dr' r'^2 j_\ell(kr') A_\ell(r',k)} \quad * \tfrac{2m}{\hbar^2}V(r')$$

Then $$A_\ell(r,k) \to \frac{e^{i\delta_\ell(k)}}{kr} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(k)\right)$$

For large r. $\delta_\ell(k)$ = ℓth partial wave phase shift.
these are the important quantities to find.

Write $f(\vec{k}',\vec{k}) = f(k,\theta)$ $\quad \theta$ = angle $\vec{k}'$ makes to $\vec{k}$

~~then $f(k,\theta) = (A_\ell(r,k) - j_\ell(kr))$~~

$$f(k,\theta) = (2\pi)^{3/2} \lim_{r\to\infty} \left[(\psi_k(r) - \psi_{0k}(r)) \, r e^{-ikr} \right]$$

$$= \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) P_\ell(\cos\theta) \lim_{r\to\infty} \left[(A_\ell(r,k) - j_\ell(kr)) \, r e^{-ikr} \right]$$

$$= \sum_{l=0}^{\infty} \frac{i^l}{\cancel{i^l}} (2l+1) P_l(\cos\theta) \frac{e^{2i\delta_l(k)} - 1}{2ik\, i^l}$$

$$\boxed{f(k\theta) = \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) \frac{e^{i\delta_l(k)} \sin\delta_l(k)}{k}}$$

$$f_l(k\theta) = (2l+1) P_l(\cos\theta) \frac{e^{i\delta_l(k)} \sin\delta_l(k)}{k}$$

$$f_l(k) = \frac{e^{i\delta_l(k)} \sin\delta_l(k)}{k}$$ = partial wave scattering amplitude

$$f_l(k) = - \int_0^{\infty} dr\, r^2 j_l(kr) \frac{2m}{\hbar^2} V(r) A_l(r,k)$$

$$\boxed{\operatorname{Im} f_l(k) = \frac{1}{k} \sin^2\delta_l(k) = k\, |f_l(k)|^2}$$

like an optical theorem for each partial wave.

$$\boxed{\operatorname{Im}\left(f_l(k)^{-1}\right) = -k}$$

$$\sigma(k) = \int d\Omega_k\, |f(k,\cos\theta)|^2$$

$$= \sum_{ll'} (2l+1)(2l'+1) \int d\Omega_k\, P_l(\cos\theta) P_{l'}(\cos\theta)\, e^{i(\delta_l - \delta_{l'})} \frac{\sin\delta_l \sin\delta_{l'}}{k^2}$$

$$= \sum_l 2(2l+1) \frac{\sin^2\delta_l(k)}{k^2} \cdot 2\pi$$

$$\boxed{\sigma(k) = 4\pi \sum_{l=0}^{\infty} (2l+1) \frac{\sin^2\delta_l(k)}{k^2}}$$

determined by the phase shifts.

The Born approximation for the partial wave replaces $A_\ell(r,k)$ by $j_\ell(kr)$ so

$$e^{2i\delta_\ell^B(k)} - 1 \cong -2ik \int_0^\infty dr\, r^2 j_\ell^2(kr)\, \frac{2m}{\hbar^2} V(r)$$

$$\cong 2i\delta_\ell^B(k) \quad \text{since phase shift small when } V \text{ is small}$$

so

$$\boxed{\delta_\ell^B(k) \cong -k \frac{2m}{\hbar^2} \int_0^\infty dr\, r^2 j_\ell^2(kr)\, V(r)}$$

Attractive delta shell potential (example)

$$V(r) = -\frac{\hbar^2}{2m} \lambda\, \delta(r-a) \qquad a = \text{range}$$

$$\frac{1}{\pi}\int_{-\infty}^{\infty} dq \; \frac{q^2 j_\ell(qr)\, j_\ell(qr')}{k^2 - q^2 + i\delta} = -ik \begin{cases} j_\ell(kr)\left(j_\ell(kr') + i\eta_\ell(kr')\right) & r<r' \\ \left(j_\ell(kr) + i\eta_\ell(kr)\right) j_\ell(kr') & r'<r \end{cases}$$

so

$$A_\ell(r,k) - j_\ell(kr) = \frac{2m}{\hbar^2}\int_0^\infty dr'\, r'^2\, V(r')\, A_\ell(r',k)\,(-ik) \begin{cases} j_\ell(kr)\left(j_\ell(kr') + i\eta_\ell(kr')\right) & r<r' \\ \left(j_\ell(kr) + i\eta_\ell(kr)\right) j_\ell(kr') & r>r' \end{cases}$$

$$= +\lambda a^2 A_\ell(a,k)\, ik \begin{cases} j_\ell(kr)\left(j_\ell(ka) + i\eta_\ell(ka)\right) & r<a \\ \left(j_\ell(kr) + i\eta_\ell(kr)\right) j_\ell(ka) & r>a \end{cases}$$

$$A_\ell(a,k) = \frac{j_\ell(ka)}{1 - ik\lambda a^2 j_\ell(ka)\left(j_\ell(ka) + i\eta_\ell(ka)\right)}$$

so

$$A_\ell(r,k) = j_\ell(kr) + \frac{ik\lambda a^2 j_\ell(ka)\, \ast}{1 - ik\lambda a^2 j_\ell(ka)\left(j_\ell(ka) + i\eta_\ell(ka)\right)} \qquad \ast \begin{cases} j_\ell(kr)\left(j_\ell(ka) + i\eta_\ell(ka)\right) & r<a \\ \left(j_\ell(kr) + i\eta_\ell(kr)\right) j_\ell(ka) & r>a \end{cases}$$

$$f_\ell(k) = -\int_0^\infty dr\, r^2 j_\ell(kr) \frac{2m}{\hbar^2} V(r) A_\ell(r,k)$$

$$= \lambda a^2 j_\ell(ka) A_\ell(a,k)$$

$$\boxed{f_\ell(k) = \frac{\lambda a^2 j_\ell^2(ka)}{1 - ik\lambda a^2 j_\ell(ka)\left(j_\ell(ka) + i\eta_\ell(ka)\right)}}$$

$$\tan\delta_\ell(k) = \frac{\mathrm{Im}\, f_\ell(k)}{\mathrm{Re}\, f_\ell(k)} \qquad \text{but } f = \frac{\alpha}{\beta - i\gamma} = \frac{\alpha(\beta + i\gamma)}{\beta^2 + \gamma^2}$$

$$\tan\delta = \frac{\gamma}{\beta}$$

$$\boxed{\tan\delta_\ell(k) = \frac{k\lambda a^2 j_\ell^2(ka)}{1 + k\lambda a^2 j_\ell(ka)\eta_\ell(ka)}}$$

high energy

$$j_\ell(ka) \to \frac{1}{ka}\sin\left(ka - \frac{\ell\pi}{2}\right)$$

$$\eta_\ell(ka) \to -\frac{1}{ka}\cos\left(ka - \frac{\ell\pi}{2}\right)$$

$$f_\ell(k) \to \frac{\frac{\lambda}{k^2}\sin^2\left(ka - \frac{\ell\pi}{2}\right)}{1 - i\frac{\lambda}{k}\sin\left(ka - \frac{\ell\pi}{2}\right)\left(\sin\left(ka - \frac{\ell\pi}{2}\right) - i\cos\left(ka - \frac{\ell\pi}{2}\right)\right)}$$

$$= \frac{1}{k}\,\frac{\lambda\sin^2\left(ka - \frac{\ell\pi}{2}\right)}{k - i\lambda\sin\left(ka - \frac{\ell\pi}{2}\right)\left(\sin\left(ka - \frac{\ell\pi}{2}\right) - i\cos\left(ka - \frac{\ell\pi}{2}\right)\right)}$$

$\to 0$ as $k \to \infty$ $\Rightarrow$ phase shifts are small

$\Rightarrow$ first Born is good.

$$\tan\delta_\ell(k) \to \frac{\lambda\sin^2\left(ka - \frac{\ell\pi}{2}\right)}{k + \lambda\sin\left(ka - \frac{\ell\pi}{2}\right)\cos\left(ka - \frac{\ell\pi}{2}\right)} \to 0 \text{ as } k \to \infty$$

Now low energy $ka \ll 1$

$$j_\ell(ka) \to \frac{(ka)^\ell}{(2\ell+1)!!}\left[1 - \frac{(ka)^2}{2(2\ell+3)} + \cdots\right]$$

$$\eta_\ell(ka) \to -\frac{(2\ell-1)!!}{(ka)^{\ell+1}}\left[1 + \frac{(ka)^2}{2(2\ell-1)} + \cdots\right]$$

$$f_\ell(k) \to \frac{\lambda a^2 (ka)^{2\ell}}{\left((2\ell+1)!!\right)^2} \frac{1}{1 - ik\lambda a^2 \frac{(ka)^\ell}{(2\ell+1)!!}\left(\frac{(ka)^\ell}{(2\ell+1)!!} - i\frac{(2\ell-1)!!}{(ka)^{\ell+1}}\right)}$$

$$= \frac{\lambda a^2 (ka)^{2\ell}}{\left((2\ell+1)!!\right)^2} \frac{1}{1 + \frac{k\lambda a^2}{ka}\frac{1}{(2\ell+1)} - i\lambda a\frac{(ka)^{2\ell+1}}{[(2\ell+1)!!]^2}}$$

$$= a \frac{\lambda a (ka)^{2\ell}}{[(2\ell+1)!!]^2} \frac{1}{1 + \frac{\lambda a}{2\ell+1} - i\lambda a \frac{(ka)^{2\ell+1}}{[(2\ell+1)!!]^2}}$$

$$= O\left((ka)^{2\ell}\right)$$

$$\tan\delta_\ell(k) \to \frac{ka\,\lambda a\,(ka)^{2\ell}}{[(2\ell+1)!!]^2} \frac{1}{1 + ka\lambda a\frac{(ka)^\ell}{(2\ell+1)!!}\left(-\frac{(2\ell-1)!!}{(ka)^{\ell+1}}\right)}$$

$$\to \frac{\lambda a (ka)^{2\ell+1}}{[(2\ell+1)!!]^2} \frac{1}{1 - \frac{\lambda a}{2\ell+1}}$$

$$\boxed{\tan\delta_\ell(k) = O\left((ka)^{2\ell+1}\right)}$$

$\Rightarrow$ s wave dominates at low energies