Phys 506 lecture 23: 3D scattering continued

1 Partial wave scattering

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

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

$$G_{0+}\left(\mathbf{r}', \mathbf{r}'; E\right) = -\frac{m}{2\pi\hbar^2} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = \langle r | \frac{1}{E - \hat{H}_0 + i\delta} \left|\mathbf{r}'\right\rangle$$

define the z direction to lie along $\mathbf{k}$. Then

$$\psi_{0\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{(2\pi)^3}} e^{ikr\cos\theta} \quad \text{with} \quad \theta = \text{ angle of } \mathbf{r} \text{ to } z \text{ axis}$$

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

Expand

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

with yet to be determined constants $A_l(r,k)$. For G_{0+} insert $\int dq |\psi_{0q}\rangle\langle\psi_{0q}|$ between $\langle r|$ and the fraction

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

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

The challenge with evaluating this is that $\mathbf{q}$ can point in any direction—it does not necessarily point along the z-axis.

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

$$e^{i\mathbf{q}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(qr) Y_l^{m*}(\mathbf{e}_{\mathbf{q}}) Y_l^m(\mathbf{e}_{\mathbf{r}})$$

$$e^{-i\mathbf{q}'\mathbf{r}'} = 4\pi \sum_{lm'} (-i)^l j_{l'}\left(q_r'\right) Y_{l'}^{m'}(\mathbf{e}_{\mathbf{q}}) Y_{l'}^{m'*}\left(\mathbf{e}_{\mathbf{r}}\right)$$

and

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

$$\times Y_l^{m*}\left(\mathbf{e}_{\mathbf{q}}\right) Y_{l'}^{m'}\left(\mathbf{e}_{\mathbf{q}}\right) Y_l^m\left(\mathbf{e}_{\mathbf{r}}\right) Y_{l'}^{m'*}\left(\mathbf{e}_{\mathbf{r}'}\right) \frac{1}{E - \frac{\hbar^2 q^2}{2m} + i\delta}$$

But

$$\int d\Omega_q Y_l^{m*}\left(\mathbf{e_q}\right) Y_{l'}^{m'}\left(\mathbf{e_q}\right) = \delta_{mm'}\delta_{ll'} = \left\langle lm \mid l'm' \right\rangle$$

due to orthogonality of the spherical harmonics. So

$$G_{0+}\left(\mathbf{r},\mathbf{r}';E\right) = \frac{2}{\pi}\sum_{lm}\int_0^\infty dq \quad q^2 \frac{j_l(qr)j_l(qr')Y_l^m\left(\mathbf{e_r}\right)Y_l^{m*}\left(\mathbf{e_r}\right)}{E-\frac{\hbar^2q^2}{2m}+i\delta}.$$

Note that $j_l\left(-qr\right) = (-1)^l j_l\left(qr\right)$, so we can write

$$G_{0+}\left(\mathbf{r},\mathbf{r}';E\right) = \frac{1}{\pi}\frac{2m}{\hbar^2}\sum_{lm} Y_l^m(\mathbf{e_r})Y_l^{m*}(\mathbf{e_{r'}})\int_0^\infty dq \quad q^2\frac{j_l(qr)j_l(qr')}{k^2-q^2+i\delta}$$

Now use the fact that $P_l(\cos\theta) = \sqrt{\frac{4\pi}{2(l+1)}}Y_l^0\left(\mathbf{e_r}\right)$ to get

$$\begin{aligned}
&\sum_{l=0}^\infty \sqrt{2l+1}i^l A_l(r,k)Y_l^0\left(\mathbf{e_r}\right) = \sum_{l=0}^\infty \sqrt{2l+1}i^l j_l(kr)Y_l^0\left(\mathbf{e_{r'}}\right)\\
&+\int d^3r' V\left(r'\right)\frac{1}{\pi}\frac{2m}{\hbar^2}\sum_{l'm'} Y_{l'}^{m'}\left(\mathbf{e_r}\right)Y_{l'}^{m'*}\left(\mathbf{e_{r'}}\right)\int_{-\infty}^{+\infty} dq \quad q^2\frac{j_{l'}\left(qr\right)j_{l'}\left(qr'\right)}{k^2-q^2+i\delta}\\
&\times\sum_l \sqrt{2l+1}i^l A_l\left(r',k\right)Y_l^0\left(\mathbf{e_{r'}}\right)
\end{aligned}$$

The integral over r' can be written as $\int_0^\infty dr' r'^2\int d\Omega_{\mathbf{e_{r'}}}$, and $\int d\Omega_{\mathbf{e_{r'}}} Y_{l'}^{m'*}\left(\mathbf{e_{r'}}\right)Y_l^0\left(\mathbf{e_{r'}}\right) = \delta_{m'0}\delta_{ll'}$, so, the right hand side becomes

$$\begin{aligned}
=&\sum_{d=0}^\infty \sqrt{2l+1}i^l j_l(kr)Y_l^0\left(\mathbf{e_r}\right) + \int_0^\infty dr' r'^2 V\left(r'\right)\frac{2m}{\pi\hbar^2}\sum_{l=0}^\infty Y_l^0\left(\mathbf{e_r}\right)\\
&\times\int_{-\infty}^{+\infty} dq\frac{q^2 j_l(qr)j_l\left(qr'\right)}{k^2-q^2+i\delta}\sqrt{2l+1};i^l A_l\left(r',k\right),
\end{aligned}$$

so we find

$$\boxed{A_l(r,k) = j_l(kr) + \frac{2m}{\pi\hbar^2}\int_0^\infty dr' r'^2 V\left(r'\right)A_l\left(r',k\right)\int_{-\infty}^{+\infty} dq\frac{q^2 j_l(qr)j_l\left(qr'\right)}{k^2-q^2+i\delta}.}$$

This is an integral equation for the partial wave amplitudes.

2 Behavior far from the scattering center

Let us examine it for large r : $j_l(kr) \to \frac{1}{kr}\sin\left(kr-\frac{l\pi}{2}\right)$ The integral over q can be evaluated by contour integration using analytic properties of Bessel functions (done in Gottfried's book). We obtain for $r\to\infty$

$$\int_{-\infty}^{+\infty} dq\frac{q^2 j_l(qr)j_l\left(qr'\right)}{k^2-q^2+i\delta} \to \frac{-\pi k e^{ikr}}{kr}\int_0^\infty dr' r'^2 j_l\left(kr'\right)A_l(r',k).$$

So we find as $r \to \infty$,

$$A_l(r,k) \to -\frac{1}{2ikr}\left\{e^{-i\left(kr-\frac{l\pi}{2}\right)} - e^{i\left(kr-\frac{l\pi}{2}\right)}\left[\underbrace{1-2ik\int_0^\infty dr' r'^2 \frac{2m}{\hbar^2}V(r')j_l(kr')A_l(r',k)}_{\text{outgoing}}\right]\right\}.$$

Let

$$\boxed{e^{2i\delta_l(k)} = 1-2ik\int_0^\infty dr' r'^2 j_l\left(kr'\right)\frac{2m}{\hbar^2}V(r')A_l\left(r',k\right),}$$

then

$$A_l(r,k) \to \frac{e^{i\delta_l(k)}}{kr}\sin\left(kr-\frac{l\pi}{2}+\delta_l(k)\right).$$

For large r: $\delta_l(k) = l$th partial wave phase shift. These are the important quantities to find.

3 Scattering amplitude and partial wave scattering amplitude

Write

$$f\left(\mathbf{k}',\mathbf{k}\right) = f(k,\theta) \quad \text{with} \quad \theta = \text{ angle } \mathbf{k}' \text{ makes to } \mathbf{k}.$$

Then

$$\begin{aligned} f(k,\theta) &= (2\pi)^{3/2}\lim_{r\to\infty}\left[\left(\psi_k(r)-\psi_{ok}(r)\right)re^{-ikr}\right] \\ &= \sum_{l=0}^{\infty} i^l(2l+1)P_\ell(\cos\theta)\lim_{r\to\infty}\left[A_l(r,k)-j_l(kr')e^{-ikr}\right] \\ &= \sum_{l=0}^{\infty} il(2l-1)P_l(\cos\theta)\frac{e^{2i\delta_l(k)}-1}{2iki^l} \end{aligned}$$

Hence, we have

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

We often rewrite this in terms of the shifts for each l via defining

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

In this case, we have defined

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

which can be rewritten as

$$f_l(k) = -\int_0^\infty dr r^2 j_l(kr)\frac{2m}{\hbar^2}V(r)A_l(r,k)\boxed{\operatorname{Im} f_l(k) = \frac{1}{k}\sin^2\delta_l(k) = k|f_l(k)|^2}$$

This is like an optical theorem for each partial wave, which yields

$$\boxed{\mathrm{Im}(f_l(k)^{-1}) = -k.}$$

The scattering cross section is given by

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

Plugging in the definitions gives

$$\begin{aligned}\sigma(k) &= \sum_{ll'}(2l+1)(2l'+1)\int d\Omega_k P_l(\cos\theta)P_{l'}(\cos\theta)e^{i(\delta_l-\delta_{l'})}\frac{\sin\delta_l\sin\delta_{l'}}{k^2} \\ &= \sum_l 2(2l+1)\frac{\sin^2\delta_l(k)}{k^2}\cdot 2\pi\end{aligned}$$

So, we have that

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

which is determined entirely by the phase shifts.

The Born approximation for the partial wave replaces $A_l(r,k)$ by $j_l(kr)$, so

$$\begin{aligned}e^{2i\delta_l^B(k)} - 1 &\cong -2ik\int_0^\infty dr\, r^2 j_l^2(kr)\frac{2m}{\hbar^2}V(r) \\ &\cong 2i\delta_l^B(k) \;\text{ since the phase shift is small when V is small}\end{aligned}$$

Hence,

$$\boxed{\delta_d^\beta(h) \cong -k\frac{2m}{\hbar^2}\int_0^\infty dr\, r^2 j_l^2(kr)V(r).}$$

4 Attractive delta-shell potential

Now, let us try an example: Attractive delta shell potential

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

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

So

$$A_l(r,k) - j_l(kr) = \frac{2m}{\hbar^2}\int_0^\infty dr'\, r'^2 V(r') A_l(r',k)(-ik)\begin{cases} j_l(kr)\left(j_l\left(kr'\right) + i\eta_l(kr')\right) \\ \hfill r < r' \\ \left(j_l(kr) + i\eta_l(kr)\right) j_l\left(kr'\right) \\ \hfill r' < r \end{cases}$$

$$= +\,\lambda a^2 A_l(a,k) ik \begin{cases} j_l(kr)\left(j_l(ka) + i\eta_l(ka)\right) & r < a \\ \left(j_l(kr) + i\eta_l(kr)\right) j_l(ka) & r > a \end{cases}$$

$$A_l(a,k) = \frac{j_l(ka)}{1 - ik\lambda a^2 j_l(ka)\left(j_l(ka) + i\eta_l(ka)\right)}$$

$$\text{So } A_l(r,k) = j_l(kr) + \frac{ik\lambda a^2 j_l(ka) \times \begin{cases} j_l(kr)\left(j_l\left(kr'\right) + i\eta_l(kr')\right) \\ \hfill r < a \\ \left(j_l(kr) + i\eta_l(kr)\right) j_l\left(kr'\right) \\ \hfill r > a \end{cases}}{1 - ik\lambda a^2 j_l(ka)(j_l(ka) + i\eta_l(ka))}$$

This means that

$$f_l(k) = -\int_0^\infty dr\, r^2 j_l(kr) \frac{2m}{\hbar^2} V(r) A_l(r,k)$$
$$= \lambda a^2 j_l(ka) A_l(a,k)$$
$$\boxed{f_l(k) = \frac{\lambda a^2 j_l^2(ka)}{1 - ik\lambda a^2 j_l(ka)\left(j_l(ka) + i\eta_l(ka)\right)}}$$

It is common to also note that

$$\tan\delta_l(k) = \frac{\operatorname{Im} f_l(k)}{\operatorname{Re} f_l(k)}, \qquad \text{but } f = \frac{\alpha}{\beta - i\gamma} = \frac{\alpha(\beta + i\gamma)}{\beta^2 + \gamma^2}$$
$$\text{so} \quad \tan\delta = \frac{\gamma}{\beta}$$
$$\boxed{-\tan\delta_l(k) = \frac{k\lambda a^2 j_l^2\,(ka)}{1 + k\lambda a^2 j_l\,(ka)\,\eta_l(ka)}}$$

Let us examine in some limits:

$$\text{high energy} \qquad j_l(ka) \to \frac{1}{ka}\sin\left(ka - \frac{l\pi}{2}\right)$$
$$\eta_l(ka) \to -\frac{1}{ka}\cos\left(ka - \frac{l\pi}{2}\right)$$

$$f_l(k) \to \frac{\frac{\lambda}{k^2}\sin^2(ka - \frac{l\pi}{2})}{1 - i\frac{\lambda}{k}\sin(ka - \frac{l\pi}{2})(\sin(ka - \frac{l\pi}{2}) - i\cos(ka - \frac{l\pi}{2}))}$$
$$= \frac{1}{k}\frac{\lambda\sin^2\left(ka - \frac{l\pi}{2}\right)}{k - i\lambda\sin\left(ka - \frac{l\pi}{2}\right)\left(\sin\left(ka - \frac{l\pi}{2}\right) - i\cos\left(ka \cdot \frac{l\pi}{2}\right)\right)}$$

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

first Born is good

This implies that as $k \to \infty$ $\Rightarrow$ phase shifts are small $\Rightarrow$ first Born is good. So, we have

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

Now for low energy $ka \ll 1$

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

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

$$\begin{aligned}
f_l(h) &\to \frac{\lambda a^2 (ka)^{2l}}{((2l+1)!!)^2}\frac{1}{1 - ik\lambda a^2 \frac{(ka)^l}{(2l-1)!!}\left(\frac{(ka)^l}{(2l+1)!!} - i\frac{(2l-1)!!}{(ka)^{l+1}}\right)} \\
&= \frac{\lambda a^2\left(ka\right)^{2l}}{((2\ell+1)!!)^2}\frac{1}{1 + \frac{k\lambda a^2}{ka}\frac{1}{(2l+1)} - i\lambda a\frac{(ka)^{2l+1}}{[(2l+1)!!]^2}} \\
&= a\frac{\lambda_a\left(ka\right)^{2l}}{[(2l+1)!!]^2}\frac{1}{1 + \frac{\lambda a}{2\lambda+1} - i\lambda a\frac{(ka)^{2l+1}}{[(2l+1)!!]^2}} \\
&= O\left(\left(ka\right)^{2l}\right)
\end{aligned}$$

$$\begin{aligned}
\tan \delta_l(k) &\to \frac{ka\lambda a\left(ka\right)^{2l}}{[(2l+1)!!]^2}\frac{1}{1 + ka\lambda a\frac{(ka)^l}{(2l+1)!!}\left(-\frac{(2l-1)!!}{(ka)^{l+1}}\right)} \\
&\to \frac{\lambda a\left(ka\right)^{2l+1}}{[(2l+1)!!]^2}\frac{1}{1 - \frac{\lambda a}{2l+1}}
\end{aligned}$$

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

which implies that s-wave scattering dominates at low energies.

These two results are useful rules of thumb when thinking about scattering.