Phys 506 lecture 22: 3D scattering and the generalized optical theorem

1 Scattering in three dimensions

In 3D, the Lipmann-Schwinger equation still holds

$$|\psi_k\rangle = |\psi_{0,k}\rangle + G_{0,+}(E)\hat{V}\,|\psi_k\rangle$$

with $E = \frac{\hbar^2 k^2}{2m}$ and

$$\hat{G}_{0,+}(E) = \frac{1}{E_0 - \hat{H}_0 + i\delta}.$$

If we evaluate in the coordinate representation, we have

$$\left\langle \mathbf{r} \middle| \hat{G}_{0,+}(E) \middle| \mathbf{r}' \right\rangle = -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}.$$

This derivation required contour integration and was skipped, although the derivation is fairly straightforward to complete. So,

$$\psi_k(\mathbf{r}) = \psi_{0,k}(\mathbf{r}) - \frac{1}{4\pi}\int d^3r'\,\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\frac{2m}{\hbar^2}V(\mathbf{r}')\psi_k(\mathbf{r}')$$

for three-dimensional scattering.

2 Scattering amplitude

Now focus on the behavior for large r. If $V(r')$ is nonzero only for small $|\mathbf{r}'|$ and decays fast for large $|\mathbf{r}'|$, we can expand

$$\begin{aligned}
|\mathbf{r}-\mathbf{r}'| \approx r\left|\frac{\mathbf{r}'}{r} - \frac{\mathbf{r}'}{r}\right| &= r\sqrt{1 - \frac{2\mathbf{r}\cdot\mathbf{r}'}{r^2} + \frac{r'^2}{r^2}} \\
&= r\left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2} - \frac{1}{2}\frac{(\mathbf{r}\cdot\mathbf{r}')^2}{r^4} + \frac{1}{2}\frac{r'^2}{r^2} + \cdots\right) \\
&\approx r - \mathbf{e}_r\cdot\mathbf{r}',
\end{aligned}$$

to lowest order. So,

$$\begin{aligned}
\frac{1}{|\mathbf{r}-\mathbf{r}'|} &\approx \frac{1}{r}\frac{1}{(1 - \mathbf{e}_r\cdot\mathbf{e}_{r'}\frac{r'}{r})} \\
&\approx \frac{1}{r}\left(1 + \mathbf{e}_r\cdot\mathbf{e}_{r'}\frac{r'}{r}\right) \\
&= \frac{1}{r} + \frac{\mathbf{e}_r\cdot\mathbf{e}_{r'}r'}{r^2}
\end{aligned}$$

and

$$k|\mathbf{r}-\mathbf{r}'| \approx kr\left(1-\mathbf{e}_r\cdot\mathbf{e}_{r'}\frac{r'}{r}+\cdots\right).$$

Define $\mathbf{k}'=\mathbf{e}_r k$ so that $|\mathbf{k}'|=|\mathbf{k}|=k$. Then,

$$k|\mathbf{r}-\mathbf{r}'| = kr-\mathbf{k}'\cdot\mathbf{r}'+\cdots$$

and

$$\psi_{\mathbf{k}}(\mathbf{r})=\psi_{0,k}(r)-\frac{1}{4\pi}\int d^3r'\frac{e^{ikr-i\mathbf{k}'\cdot\mathbf{r}'}}{r}\left(1+\mathbf{e}_r\cdot\mathbf{e}_{r'}\frac{r'}{r}\right)\frac{2m}{\hbar^2}V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}).$$

But $\psi_{0,k}(r)=\frac{1}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{r}}$, so

$$\psi_{\mathbf{k}}(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}\left(e^{i\mathbf{k}\cdot\mathbf{r}}+\frac{e^{ikr}}{r}f(\mathbf{k}',\mathbf{k})\right)+O\left(\frac{r'}{r}\right),$$

where $f(\mathbf{k}',\mathbf{k})$ is called the *scattering amplitude* and is defined by

$$f(\mathbf{k}',\mathbf{k})=-\frac{4\pi^2 m}{\hbar^2}\left\langle\psi_{0,\mathbf{k}'}\middle|\hat{V}\middle|\psi_k\right\rangle,$$

which has units of length. It can be thought of as the amplitude of an outgoing spherical wave in the direction $\mathbf{k}'$. Then, $|f(\mathbf{k}',\mathbf{k})|^2$ is the probability to observe some particle with momentum $\hbar\mathbf{k}'$ after scattering (where $\hbar\mathbf{k}$ was the incident momentum).

3 The differential cross section

The differential cross section is defined via

$$\frac{d\sigma}{d\Omega_{\mathbf{k}'}}=\frac{\text{prob/time/solid angle of scattering in }\mathbf{k}'\text{ direction}}{\text{prob/time/area of incident flux of particles}}$$

where σ is the cross section defined through

$$\sigma=\int d\Omega\,\frac{d\sigma}{d\Omega},$$

which has units of area. The cross section is a function of the incident momentum $\hbar\mathbf{k}$ or incident energy E, but does not depend on the frame of reference. Gottfried tells us how to find

$$\frac{d\sigma}{d\Omega_{\mathbf{k}'}}=|f(\mathbf{k}',\mathbf{k})|^2.$$

4 Transition matrix and the generalized optical theorem

These results are often summarized in terms of the *transition matrix* (or T-matrix).

$$|\psi_k\rangle=|\psi_{0,k}\rangle+\hat{G}_{0,+}(E)\hat{V}\,|\psi_k\rangle$$

$$\Longrightarrow\ |\psi_k\rangle=(1-\hat{G}_{0,+}(E)\hat{V})^{-1}\,|\psi_{0,k}\rangle=\hat{\Omega}_+(E)\,|\psi_{0,k}\rangle$$

where $\hat{\Omega}_+(E)$ is called the Möller wave matrix. Then,

$$f(\mathbf{k},\mathbf{k}') = -\frac{4\pi^2 m}{\hbar^2}\left\langle \psi_{0,\mathbf{k}'}\middle|\hat{V}\middle|\psi_k\right\rangle = -\frac{4\pi^2 m}{\hbar^2}\left\langle \psi_{0,\mathbf{k}'}\middle|\hat{V}\hat{\Omega}_+(E)\middle|\psi_{0,\mathbf{k}'}\right\rangle.$$

Then, define the T-matrix with the following:

$$\hat{T}(E) = \hat{V}\hat{\Omega}_+(E)$$

so that

$$f(\mathbf{k},\mathbf{k}') = -\frac{4\pi^2 m}{\hbar^2}T_{\mathbf{k},\mathbf{k}'}(E).$$

$\hat{T}(E)$ also satisfies the operator equations:

$$\hat{T} = \hat{V}\left[1-\hat{G}_{0,+}\hat{V}\right]^{-1}$$

$$\implies \hat{T} - \hat{T}\hat{G}_{0,+}\hat{V} = \hat{V}$$

or

$$\boxed{\hat{T} = \hat{V} + \hat{T}\hat{G}_{0,+}\hat{V}.}$$

Also,

$$\begin{aligned}\hat{T} &= \hat{V} + \hat{V}\hat{G}_{0,+}\hat{V} + \hat{V}\hat{G}_{0,+}\hat{V}\hat{G}_{0,+}\hat{V} + \cdots \\ &= \left[1-\hat{V}\hat{G}_{0,+}\right]^{-1}.\end{aligned}$$

Therefore,

$$\hat{T} = \hat{V} + \hat{V}\hat{G}_{0,+}\hat{T}$$

Since $\hat{G}_{0,\pm} = \frac{1}{E-\hat{H}_0\pm i\delta}$, we have $\hat{G}^\dagger_{0,+}(E) = \hat{G}_{0-}(E)$. Then, taking Hermitian conjugates yields

$$\hat{T}^\dagger = \hat{V} + \hat{T}^\dagger\hat{G}_{0-}\hat{V} = \hat{V} + \hat{V}\hat{G}_{0-}\hat{T}^\dagger.$$

Recall Dirac's identity:

$$\frac{1}{x\pm i\delta} = \frac{P}{x} \mp i\pi\delta(x),$$

where P denotes a principal value. So,

$$\begin{aligned}\hat{T} - \hat{T}^\dagger &= \hat{V} + \hat{V}\hat{G}_{0,+}\hat{T} - \hat{V} - \hat{T}^\dagger\hat{G}_{0,-}\hat{V} \\ &= \hat{T}\hat{G}_{0,+}\hat{T} - \hat{T}^\dagger\hat{G}_{0,-}\hat{V}\hat{G}_{0,+}\hat{T} - \hat{T}^\dagger\hat{G}_{0,-}\hat{T} + \hat{T}^\dagger\hat{G}_{0,-}\hat{V}\hat{G}_{0,+}\hat{T} \\ &= \hat{T}^\dagger(\hat{G}_{0,+} - \hat{G}_{0,-})\hat{T}.\end{aligned}$$

But,

$$\hat{G}_{0,+} - \hat{G}_{0,-} = -2\pi i\delta(E-\hat{H}_0)$$

$$\implies \boxed{\hat{T} - \hat{T}^\dagger = -2\pi i\hat{T}^\dagger\delta(E-\hat{H}_0)\hat{T}}$$

This is known as the *generalized optical theorem*. Then, let's take matrix elements and introduce complete sets of states on both sides of the delta function. This gives us

$$T_{\mathbf{k},\mathbf{k}'}(E) - T^*_{\mathbf{k},\mathbf{k}'}(E) = -2\pi i\int d^3k''\int d^3k'''\, T^*_{\mathbf{k}'',\mathbf{k}'}(E)\left\langle \mathbf{k}''\middle|\delta(E-\hat{H}_0)\middle|\mathbf{k}'''\right\rangle T_{\mathbf{k}''',\mathbf{k}}(E)$$

But

$$\left\langle \mathbf{k}'' \middle| \delta(E - \hat{H}_0) \middle| \mathbf{k}''' \right\rangle = \delta\left(E - \frac{\hbar^2 \mathbf{k}''}{2m}\right) \langle \mathbf{k}'' | \mathbf{k}''' \rangle = \delta\left(E - \frac{\hbar^2 \mathbf{k}''^2}{2m}\right) \delta^3(\mathbf{k}'' - \mathbf{k}'''),$$

so the integral can be done over $\mathbf{k}'''$. Furthermore,

$$\begin{aligned} \int d^3k'' \delta\left(E - \frac{\hbar^2 \mathbf{k}''^2}{2m}\right) &= \int_0^\infty dk''\, k''^2 \int d\Omega_{\mathbf{k}''} \delta\left(E - \frac{\hbar^2 \mathbf{k}''^2}{2m}\right) \\ &= \frac{mk}{\hbar^2} \int d\Omega_{\mathbf{k}''}. \end{aligned}$$

So,

$$T_{\mathbf{k},\mathbf{k}'}(E) - T^*_{\mathbf{k},\mathbf{k}'}(E) = -\frac{i\pi mk}{\hbar^2} \int d\Omega_{\mathbf{k}''} T^*_{\mathbf{k}'',\mathbf{k}'}(E) T_{\mathbf{k}''',\mathbf{k}}(E).$$

Multiply across by $-\frac{4\pi^2 m}{\hbar^2}$ to get

$$\boxed{f(\mathbf{k}', \mathbf{k}) - f^*(\mathbf{k}', \mathbf{k}) = \frac{ik}{2\pi} \int d\Omega_{\mathbf{k}''} f(\mathbf{k}'', \mathbf{k}) f^*(\mathbf{k}'', \mathbf{k}'),}$$

which is the generalized optical theorem for scattering amplitudes. For forward scattering, $\mathbf{k} = \mathbf{k}'$ and $\theta = 0$.

$$\begin{aligned} \mathrm{Im} f(\mathbf{k}', \mathbf{k}) &= \frac{k}{2\pi} \int d\Omega_{\mathbf{k}''} |f(\mathbf{k}'', \mathbf{k})|^2 \\ &= \frac{k}{2\pi} \int d\Omega_{\mathbf{k}''} \frac{d\sigma(k)}{d\Omega_{\mathbf{k}''}} = \frac{k}{2\pi} \sigma(k) \end{aligned}$$

So,

$$\boxed{\sigma(k) = \frac{4\pi}{k} \mathrm{Im} f(\mathbf{k}', \mathbf{k}).}$$

5 Born series

The scattering amplitude satisfies

$$f(\mathbf{k}', \mathbf{k}) = -\frac{4\pi^2 m}{\hbar^2} \left\langle \psi_{0,\mathbf{k}'} \middle| \left(1 - \hat{V} \hat{G}_{0,+}(E)\right)^{-1} \hat{V} \middle| \psi_{0,\mathbf{k}'} \right\rangle = \sum_{n=1}^{\infty} f_n(\mathbf{k}', \mathbf{k}),$$

where n counts powers of $\hat{V}$. Define the Nth Born approximation by truncating the sum at N.

$$f^{(N)}(\mathbf{k}', \mathbf{k}) = \sum_{n=1}^{N} f_n(\mathbf{k}', \mathbf{k}).$$

Therefore,

$$\begin{aligned} f^{(1)}(\mathbf{k}', \mathbf{k}) &= -\frac{4\pi^2 m}{\hbar^2} \left\langle \psi_{0,\mathbf{k}'} \middle| \hat{V} \middle| \psi_{0,\mathbf{k}} \right\rangle \\ &= -\frac{m}{2\pi\hbar^2} \int d^3r\, e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} V(\mathbf{r}) \\ &= \tilde{V}(\mathbf{k}' - \mathbf{k}), \end{aligned}$$

which is simply the Fourier transform of $V(\mathbf{r})$. Also note that $\left\langle \psi_{0,\mathbf{k}'} \middle| \hat{V} \middle| \psi_{0,\mathbf{k}} \right\rangle = \frac{1}{(2\pi)^3} \tilde{V}(\mathbf{k}' - \mathbf{k})$, so

$$f^{(2)}(\mathbf{k}', \mathbf{k}) = -\frac{m}{2\pi\hbar^2} \left(\tilde{V}(\mathbf{k}' - \mathbf{k}) + (2\pi)^3 \int d^3k'' \left\langle \psi_{0,\mathbf{k}'} \middle| \hat{V} \middle| \psi_{0,\mathbf{k}''} \right\rangle \left\langle \psi_{0,\mathbf{k}''} \middle| \hat{G}_{0,+}(E) \hat{V} \middle| \psi_{0,\mathbf{k}} \right\rangle \right).$$

But

$$\left\langle \psi_{0,\mathbf{k}''} \right| \hat{G}_{0,+}(E) = \frac{1}{E - \frac{\hbar^2 k''^2}{2m} + i\delta} \left\langle \psi_{0,\mathbf{k}''} \right|,$$

so

$$f^{(2)}(\mathbf{k}', \mathbf{k}) = -\frac{m}{2\pi\hbar^2} \left(\tilde{V}(\mathbf{k}' - \mathbf{k}) + \int \frac{d^3k''}{(2\pi)^3} \frac{\tilde{V}(\mathbf{k}' - \mathbf{k}'')\tilde{V}(\mathbf{k}'' - \mathbf{k})}{E - \frac{\hbar^2 k''^2}{2m} + i\delta} \right)$$

and so on.