Advanced Quantum Mechanics

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Scattering Theory

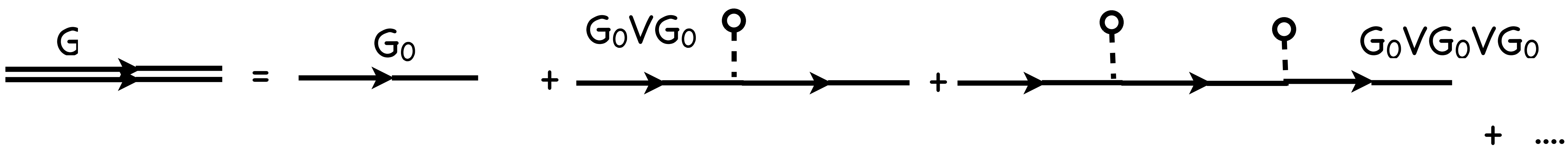
Ref : Sakurai, Modern Quantum Mechanics
Taylor, Quantum Theory of Non-Relativistic Collisions
Landau and Lifshitz, Quantum Mechanics

Recap of Last Class

Basic Set up of Scattering ⟶ cross-section

Time Evolution in presence of potential

$$G^R = G_0^R + G_0^R V G_0^R + G_0^R V G_0^R V G_0^R + \ldots = G_0^R + G_0^R V G^R \qquad (G^R)^{-1} = (G_0^R)^{-1} - V$$



S Matrix

$$S_{\alpha\beta} = \langle \phi_\alpha | \psi_\beta^{(+)}(t \to \infty) \rangle = Lt_{t\to\infty, t'\to -\infty} i G^R(\alpha, t; \beta, t')$$

Elastic Scattering and S(E)

$$S_{\vec{k},\vec{k}'}(E) = \delta_{\vec{k}',\vec{k}} \delta(E - k^2/2m) + i Lt_{t\to\infty, t'\to -\infty} \sum_{k_1} \int \frac{d\omega}{2\pi} G_0^R(k,\omega) V_{kk1} G^R(k_1, k', \omega) e^{i(E-\omega)(t-t')}$$

Incident wave

Involves G rather than G0

Scattered to different out states

Scattering (S) and Transition (T) Matrices

$$S_{\vec{k},\vec{k'}}(E) = \delta_{\vec{k'},\vec{k}}\delta(E-k^2/2m)+iLt_{t\to\infty,t'\to-\infty}\sum_{k_1}\int\frac{d\omega}{2\pi}G_0^R(k,\omega)V_{kk1}G^R(k_1,k',\omega)e^{i(E-\omega)(t-t')}$$

Incident wave

Involves G rather than G_0

Scattered to different out states

Let us define the Transition (T) matrix such that : $(VG^R)_{\alpha\beta}=(TG_0^R)_{\alpha\beta}$

$$iLt_{t\to\infty,t'\to-\infty}e^{iE(t-t')}\int dt_1\int dt_2 G_0^R(k',t,t_1)T_{k'k}(t_1,t_2)G_0^R(k,t_2,t')$$

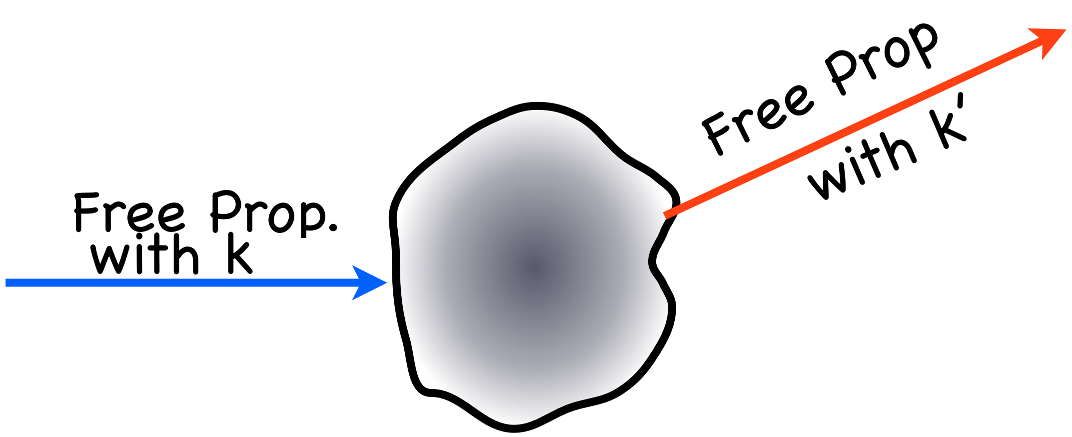
$$= -iLt_{t\to\infty,t'\to-\infty}e^{i(E-(k')^2/2m)t}e^{-i(E-k^2/2m)t'}\int\frac{d\omega}{2\pi}\int dt_1\int dt_2 T_{k'k}(\omega)e^{-i(\omega-(k')^2/2m)t_1}e^{i(\omega-k^2/2m)t_2}$$

$$= -2\pi i\delta(E-(k')^2/2m)\delta(E-k^2/2m)T_{k'k}(E)$$

$T_{kk'}(E)$ incorporates all the effects of scattering in the interction region

$$S_{\vec{k}\vec{k'}}(E) = \delta(E-(k')^2/2m)\delta(E-k^2/2m)[\delta_{\vec{k}\vec{k'}}-2\pi i T_{k'k}(E)]$$

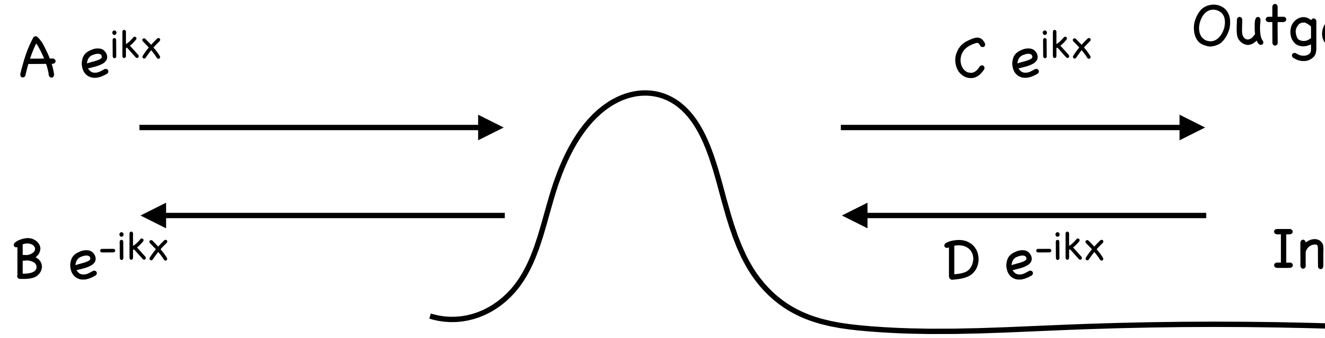
Relation between S and T matrix



The scattered state (1D)

Incident particles with mom k

Outgoing particles with mom k



Incident particles with mom -k

Outgoing particles with mom -k

$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}$$

S Matrix

$$\begin{pmatrix} C \\ B \end{pmatrix} = (1 - 2\pi i T) \begin{pmatrix} A \\ D \end{pmatrix}$$

T Matrix

Nice Properties: Unitarity,
Symmetry

$$S = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix}$$

$|t|^2$ is transmission coeff for left incidence

$|r|^2$ is reflection coeff for left incidence

$|t'|^2$ is transmission coeff for right incidence

$|r'|^2$ is reflection coeff for right incidence

Easily related to reflection and transmission co-effs

Note: Scattering states have particular boundary cond. The eigenstate with hard walls at $x = \pm L$ is different from scattering soln. since it follows different boundary cond.

The scattered state (1D)

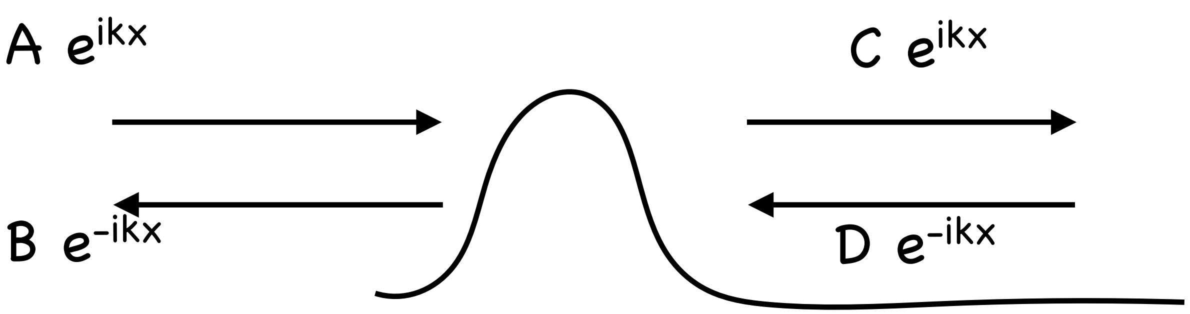
$$S = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix}$$

Unitarity of S

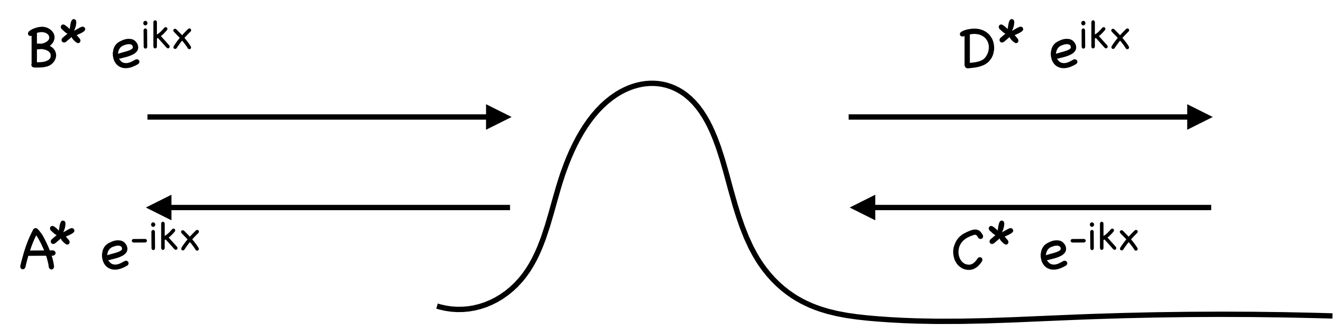
$|r|^2+|t|^2 = |r'|^2+|t'|^2 = 1$

$tr'^* + rt'^* = 0$

Time Reversal Invariance



If this is a solution



So is this

$S^*S = 1$ $\qquad r = r'$

Reflection (Parity) Invariance $\qquad r=r'$, $t = t'$

The scattered state (1D)

$$\begin{pmatrix} C \\ D \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix}$$ Transfer Matrix

Easy to calculate

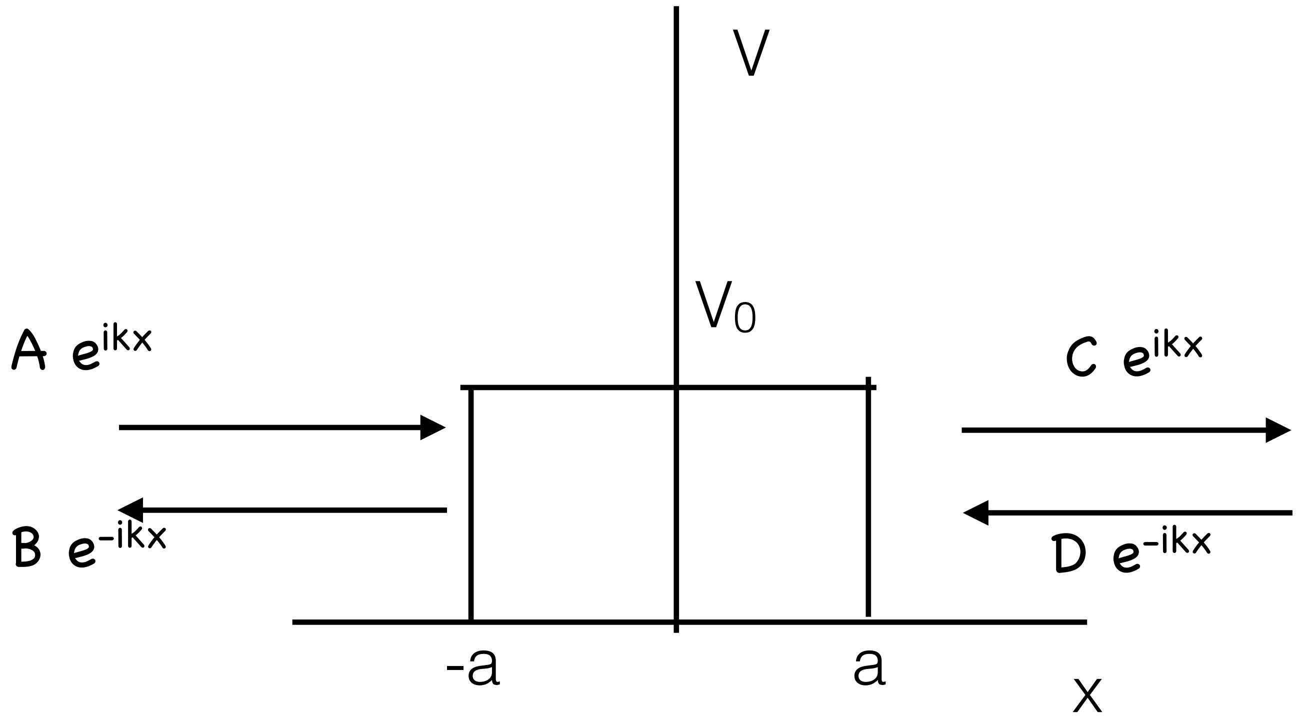
$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}$$ S Matrix

$$M = \frac{1}{S_{22}} \begin{pmatrix} Det(S) & S_{12} \\ -S_{21} & 1 \end{pmatrix} \qquad S = \frac{1}{M_{22}} \begin{pmatrix} Det(M) & M_{12} \\ -M_{21} & 1 \end{pmatrix}$$

Calculation for a repulsive square well

Parity + TR invariance ⟶ $S_{11} = S_{22}$

Follow any Std. QM Book
(Schiff, Merzbacher etc.)



$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (\cos 2k'a) + \frac{\epsilon}{2} \sin 2k'a)\, e^{2ika} & \frac{\eta}{2} \sin 2k'a \\ -\frac{\eta}{2} \sin 2k'a & (\cos 2k'a) - \frac{\epsilon}{2} \sin 2k'a)\, e^{-2ika} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

$k' = [2m(E-V_0)]^{1/2}$ $\quad k = [2mE]^{1/2}$ $\quad \varepsilon = i\,(k^2+k'^2)/2kk'$ $\quad \eta = -i\,(k^2 - k'^2)/2kk'$

The scattered state (3D)

Assume: incident particles have momentum k along z direction
i.e. energy of particles is $E=k^2/2m$

By definition of the propagator $$\psi(\vec{r}) = i\int d^3\vec{r'} G^R(\vec{r},\vec{r'},E)\phi(r')$$ φ is the incident state.

Now, the S matrix connects the incoming and the outgoing states

$|\psi_{out}\rangle = S|\phi_{in}\rangle$ Using $S(E) = I + iG_0^R(E)VG^R(E) = I + iG_0^R(E)TG_0^R(E)$

$$\psi(\vec{r}) = \phi(\vec{r}) + i\int d^3\vec{r}_1 \int d^3\vec{r}_2 \int d^3\vec{r'} G_0^R(\vec{r},\vec{r}_1,E)T(\vec{r_1},\vec{r}_2,E)G_0^R(\vec{r}_2,\vec{r'},E)\phi(\vec{r'})$$

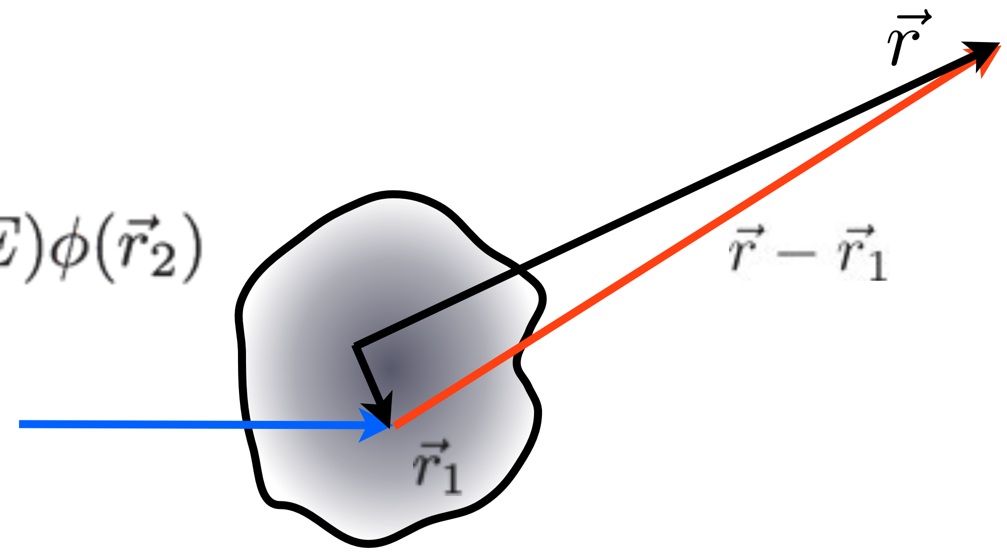
$$= \phi(\vec{r}) + \int d^3\vec{r}_1 \int d^3\vec{r}_2 G_0^R(\vec{r},\vec{r}_1,E)T(\vec{r_1},\vec{r}_2,E)\phi(\vec{r}_2)$$

Now in 3D $$G_0^R(\vec{r},\vec{r'},E) = -\frac{m e^{i\sqrt{2mE}|\vec{r}-\vec{r'}|}}{2\pi|\vec{r}-\vec{r'}|}$$

magnitude of momentum
$$k = \sqrt{2mE}$$

$$\psi(\vec{r}) = \phi(\vec{r}) - \frac{m}{2\pi}\int d^3\vec{r}_1 \int d^3\vec{r}_2 \frac{e^{ik|\vec{r}-\vec{r}_1|}}{|\vec{r}-\vec{r}_1|}T(\vec{r_1},\vec{r}_2,E)\phi(\vec{r}_2)$$

The scattered state (3D)



$$\psi(\vec{r}) = \phi(\vec{r}) - \frac{m}{2\pi}\int d^3\vec{r}_1 \int d^3\vec{r}_2 \frac{e^{ik|\vec{r}-\vec{r}_1|}}{|\vec{r}-\vec{r}_1|} T(\vec{r}_1,\vec{r}_2,E)\phi(\vec{r}_2)$$

For geometry of scattering

$$|\vec{r}| \gg |\vec{r}_1|$$

$$|\vec{r}-\vec{r}_1| = r[1 - 2\hat{r}\cdot\vec{r}_1/r + r_1^2/r^2]^{\frac{1}{2}} \simeq r - \hat{r}\cdot\vec{r}_1$$

For elastic scattering

$$\vec{k} = k\hat{z} \quad \vec{k'} = k\hat{r}$$

So $\quad e^{ik|\vec{r}-\vec{r}_1|} = e^{ikr}e^{-i\vec{k'}\cdot\vec{r}_1}$

and $\quad \dfrac{1}{|\vec{r}-\vec{r}_1|} \simeq \dfrac{1}{r}$

Now, incident state $\quad \phi(\vec{r}) = \dfrac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}$

So, far from the interaction region

$$\psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r}\left(-\frac{m}{2\pi}\right)\int d^3\vec{r}_1 \int d^3\vec{r}_2 e^{-i\vec{k'}\cdot\vec{r}_1} e^{i\vec{k}\cdot\vec{r}_2} T(\vec{r}_1,\vec{r}_2,E)\right]$$

$$\psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r}\left(-4\pi^2 m\right) T(\vec{k'},\vec{k},E)\right]$$

T Matrix and cross section (3D)

Incident wave

Outgoing spherical wavefront

$$\psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r}\left(-4\pi^2 m\right) T(\vec{k'},\vec{k},E)\right]$$

Scattering amplitude

$$\psi(r) = \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r} f(\vec{k},\vec{k'})\right]$$

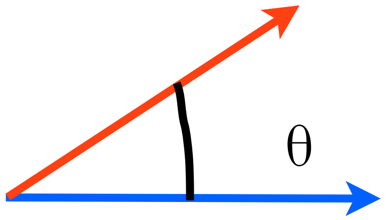
$$f(\vec{k},\vec{k'}) = -4\pi^2 m T(\vec{k'},\vec{k},E)$$

Differential Cross Section

$$\frac{d\sigma}{d\Omega} = |f(\vec{k},\vec{k'})|^2 = |f(E,\vec{k}\cdot\vec{k'})|^2$$

S Matrix ⟶ T Matrix ⟶ Cross Section (Measureable Quantity)

Unitarity of S and Optical Theorem



Statement of Optical Theorem $\mathrm{Im}[f(\theta=0)] = \frac{p\sigma_{tot}}{4\pi}$

Imaginary part of fwd scattering amplitude, which measures how many particles are lost in this dirn., is equal to total number of scattered particles. This is just a restatement of probability conservation.

Unitarity of S $SS^\dagger = [1 - 2\pi i T][1 + 2\pi i T^\dagger] = 1$

$$1 - 2\pi i (T - T^\dagger) + 4\pi^2 T T^\dagger = 1 \qquad\qquad TT^\dagger = -\frac{1}{2\pi i}(T - T^\dagger)$$

Take expectation in p states

$$\int (p')^2 dp' \delta[E - (p')^2/2m] \int d\Omega' T_{\vec{p}\vec{p}'} T^\dagger_{\vec{p}'\vec{p}} = -\frac{1}{2\pi i}(T_{\vec{p}\vec{p}} - T^\dagger_{\vec{p}\vec{p}})$$

$$mp \int d\Omega' |T_{\vec{p}\vec{p}'}|^2 = -\frac{1}{\pi} Im[T_{\vec{p}\vec{p}}]$$

Use $T_{\vec{p}\vec{p}'} = \frac{-1}{4\pi^2 m} f_{\vec{p}\vec{p}'}$ $\qquad Im[f_{\vec{p}\vec{p}}] = \frac{p}{4\pi}\int d\Omega' |f_{\vec{p}\vec{p}'}|^2 = \frac{p}{4\pi}\int d\Omega' |\frac{d\sigma}{d\Omega'} = \frac{p}{4\pi}\sigma_{tot}$

Note: Prob Conservation ⟶ σ_{tot} should include both elastic and inelastic cross section

Singular Potentials and T matrix

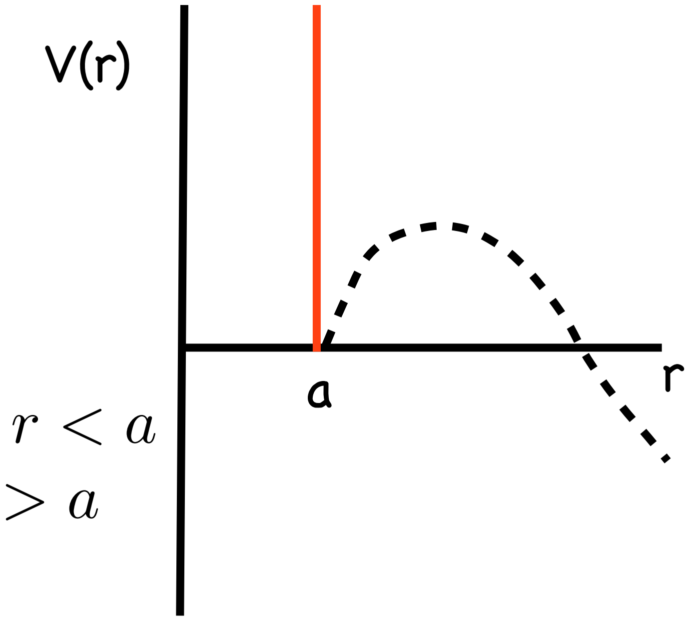
The defining Equation: $VG = TG_0$

The FT of V does not exist, impossible to work with

$$V_{kk'} = \langle k'|V|k\rangle = \langle k'|V|\phi_k\rangle$$

Hard Sphere Model:

$$\begin{aligned} V(r) &= \infty \qquad 0 < r < a \\ &= 0 \qquad r > a \end{aligned}$$



$$T_{kk'} = \langle k'|V|\psi_k^{(+)}\rangle$$ Actual Solution in presence of potential

The wfn in presence of the potential vanishes at r=a and is finite for r>a.

So $T_{kk'}$ is well defined

The system responds to the presence of the infinite potential by avoiding the region where the potential is infinite.

The T matrix incorporates this information and is non-singular.

Born Approximation

Start with the T matrix:

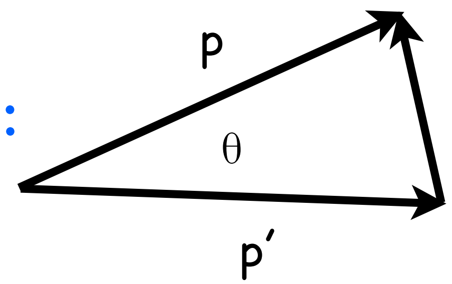
$$T = V + VG_0V + VG_0VG_0V + ...$$

Born. Approx/ 1st Born Approx. (V)

2nd Born Approx. ($V + VG_0V$)

3rd Born Approx. ($V + VG_0V + VG_0VG_0V$)

Scattering Amplitude:



$$q = |\vec{p'} - \vec{p}| = 2p \sin\frac{\theta}{2}$$

- Scattering Ampl. depends only on q
- Scattering Amplitude is real
- dσ/dΩ indep. of sign of V

$$f(\vec{p}, \vec{p'}) = f(\theta) = -4\pi^2 m T_{\vec{p'},\vec{p}} = -4\pi^2 m V_{\vec{p'},\vec{p}} \quad = \frac{2m}{q}\int_0^\infty dr r V(r) \sin qr$$

Validity: $|VG_0V| << |V|$

- Weak potentials
- High Energy of Incident particles

(Time spent in interaction region is small, single scattering dominates)

Violation of Unitarity: $f_{pp'}$ is real: what happens to optical theorem ?

LHS ~ V^2

$$mp\int d\Omega' |T_{\vec{p}\vec{p'}}|^2 = -\frac{1}{\pi} Im[T_{\vec{p}\vec{p}}]$$

Need 2nd Born Approx on RHS to restore optical theorem

Partial Wave Analysis

Rotationally Invariant Potentials: Want to expand in angular momentum states

Simultaneous eigenkets of H_0, L^2 and L_z $\quad |E,l,m\rangle$ with $\quad \langle E',l',m'|E,l,m\rangle = \delta(E-E')\delta_{ll'}\delta_{mm'}$

Use Wigner Eckart Theorem: $\quad \langle E,l',m'|T|E,l,m\rangle = T_l \delta_{ll'}\delta_{mm'}$

Decouples in different l channels, independent of m

Scattering Amplitude:

$$f(\vec{p},\vec{p'}) = -4\pi^2 m \langle \vec{p'}|T|\vec{p}\rangle = -4\pi^2 m \int dE \sum_{lm} \langle \vec{p'}|E,l,m\rangle T_l \langle E,l,m|\vec{p}\rangle$$

Using

$$\langle E,l,m|\vec{p}\rangle = \frac{1}{\sqrt{mp}} Y_l^{m*}(\hat{p})\delta(E-p^2/2m)$$

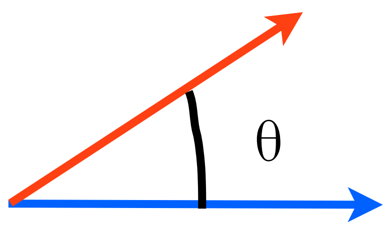
$$f(\vec{p},\vec{p'}) = -\frac{4\pi^2}{p}\sum_{lm} T_l(E) \;\; Y_l^m(\hat{p'})Y_l^{m*}(\hat{p})$$

The initial dirn. can be taken along z axis (θ=0, φ=0) and the final dirn. along (θ, φ=0)

$$f(\vec{p},\vec{p'}) = -\frac{4\pi^2}{p}\sum_{lm} T_l(E) \;\; Y_l^m(\hat{p'})Y_l^{m*}(\hat{p})$$

$$Y_l^m(\theta,0) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)\delta_{m0}$$

$$f(\vec{p},\vec{p'}) = -\frac{\pi}{p}\sum_{l=0}^{\infty}(2l+1)T_l(E)P_l(\cos\theta)$$



Partial Wave Analysis

Define Partial Scattering Amplitude $f_l(p) \equiv -\frac{\pi T_l(E = p^2/2m)}{p}$

$$f(\vec{p}, \vec{p'}) = \sum_{l=0}^{\infty} (2l+1) f_l(p) P_l(\cos\theta)$$

Scattered Wavefunction: $\psi^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \left[e^{i\vec{p}\cdot\vec{r}} + \frac{e^{ipr}}{r} f(\vec{p'}, \vec{p}) \right]$

$$e^{i\vec{p}\cdot\vec{r}} = e^{ipr\cos\theta} = \sum_l i^l (2l+1) j_l(pr) P_l(\cos\theta)$$

Spherical Bessel Functions, consist of both outgoing and incoming waves. Solution of Radial Schrodinger Eqn. for free particles in 3D

$$pr \gg 1 \qquad j_l(pr) \to \frac{e^{i(pr - l\pi/2)} - e^{-i(pr - l\pi/2)}}{2ipr}$$

$$\psi^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \left[\sum_l (2l+1) P_l(\cos\theta) \left(\frac{e^{ipr} - e^{-i(pr - l\pi)}}{2ipr} + f_l(p) \frac{e^{ipr}}{r} \right) \right]$$

$$= \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) \frac{P_l(\cos\theta)}{2ip} \left([1 + 2ipf_l(p)] \frac{e^{ipr}}{r} - \frac{e^{-i(pr - l\pi)}}{r} \right)$$

Scatterer changes co-efficient of outgoing wave. Incoming wave is unaffected

Partial Wave Analysis: S and T Matrices

S matrix is the overlap of the incoming free-particle state and the outgoing scattered state

$$\psi^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) \frac{P_l(\cos\theta)}{2ip} \left([1 + 2ipf_l(p)] \frac{e^{ipr}}{r} - \frac{e^{-i(pr - l\pi)}}{r} \right) \qquad S_l(p) = 1 + 2ipf_l(p)$$

- Probability conservation ---> Incoming flux = Outgoing flux
- Spherical Symmetry ---> L conservation ---> For every l channel, flux in = flux out

Unitarity of S_l : $|S_l(p)| = 1 \Rightarrow S_l(p) = e^{2i\delta_l(p)}$ phase shift in l channel

The phase shifts encode all the information about the scattering potential.

Partial Scattering Amplitude:

$$f_l(p) = \frac{S_l(p) - 1}{2ip} = \frac{e^{2i\delta_l(p)} - 1}{2ip} = \frac{e^{i\delta_l(p)} \sin\delta_l(p)}{p} = \frac{1}{p\cot\delta_l(p) - ip}$$

T Matrix:

$$T_l(p) = -\frac{e^{i\delta_l(p)} \sin\delta_l(p)}{\pi} = \frac{1}{\pi} \frac{1}{\cot\delta_l(p) - i}$$

Scattering Amplitude:

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

Interference of different l channels

Partial Wave Analysis: Cross Section

Total Cross Section:

$$\sigma = \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)|f(\theta)|^2$$

$$= \frac{2\pi}{p^2} \sum_{ll'} (2l+1)(2l'+1) \sin\delta_l(p) \sin\delta_{l'}(p) e^{i[\delta_l(p)-\delta_{l'}(p)]} \int_{-1}^{1} d(\cos\theta) P_l(\cos\theta) P_{l'}(\cos\theta)$$

$$= \frac{4\pi}{p^2} \sum_l (2l+1) \sin^2\delta_l(p)$$

Interference washed out
in angular integration

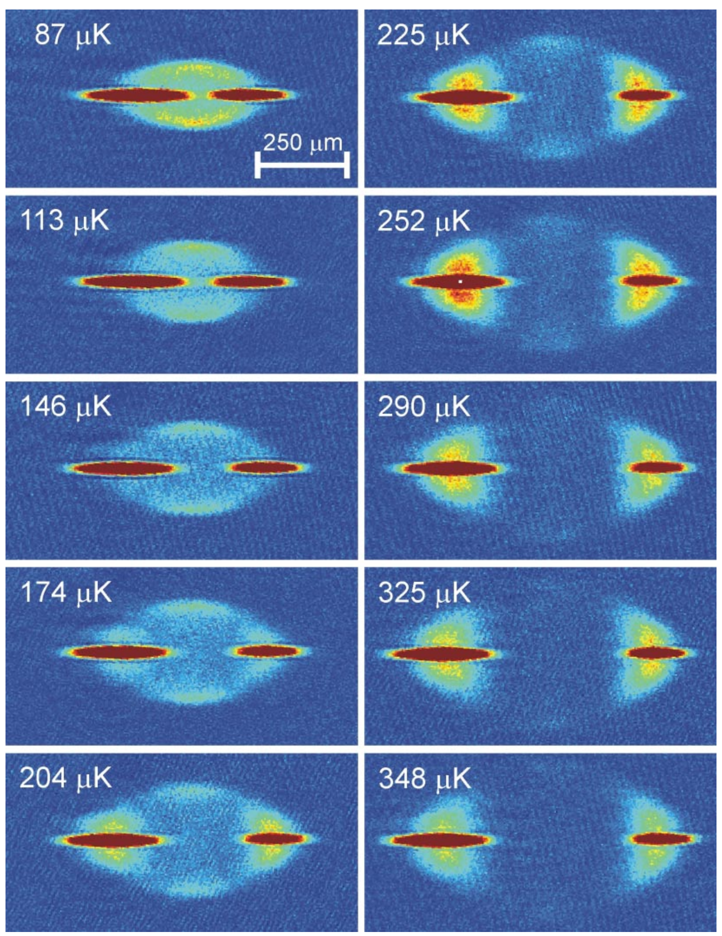
Quick Check of Optical Theorem:

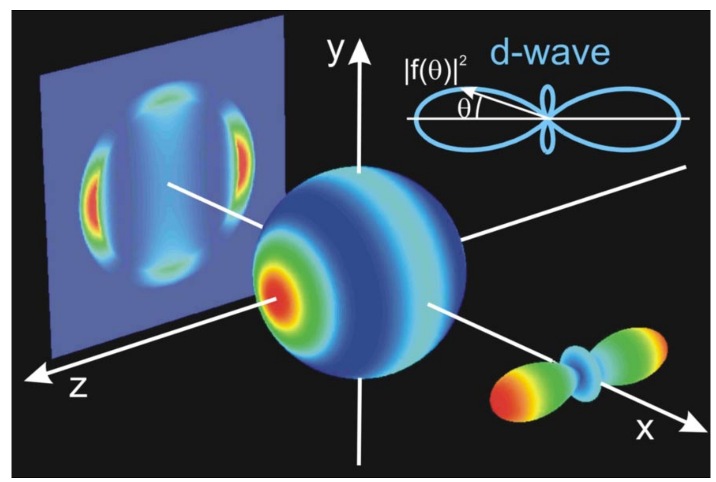
$$\mathrm{Im}[f(\theta=0)] = \sum_l \frac{(2l+1)\mathrm{Im}[e^{i\delta_l(p)}]\sin\delta_l(p)}{p} P_l(\cos\theta=1) \quad = \frac{p}{4\pi}\sigma$$

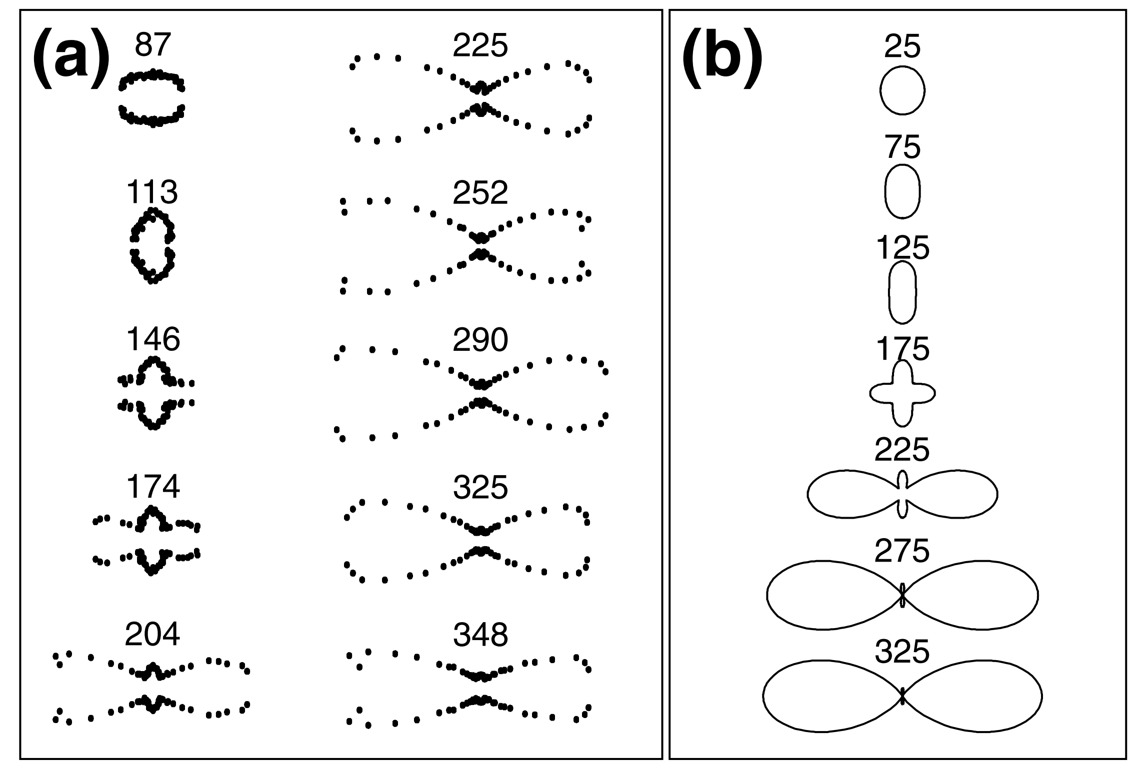
Partial Wave Analysis: Cross Section

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \sum_{ll'} \frac{(2l+1)(2l'+1)}{p^2} P_l(\cos\theta) P_{l'}(\cos\theta) \sin\delta_l(p) \sin\delta_{l'}(p) e^{i[\delta_l(p) - \delta_{l'}(p)]}$$

Note that different l channels contribute additively to scattering amplitude. The differential cross-section includes interference between different channels.







Interference of s and d partial scattering amplitudes in a collision of 2 Rb_{87} atom clouds. Scattered atoms are in the halos. [From : N. Thomas et. al, PRL **93**, 173201 (2004)]