Physics 531

Lecture 22: Collisions – Review

Collisions play a central role in atomic-molecular physics. Rutherford's discovery of the nucleus of the atom was made through the scattering of alpha particles. Various astrophysical processes are driven by collisions involving atoms and molecules. In contemporary physics, collisions between ultra-cold atoms are central to the properties of quantum denerate gas such as Bose-Einstein condensates and Fermi-degenerate gases.

Basic Concepts

Collisions can occur between systems where one or more object is an "elementary" particle (e.g. electron, photon) or composite object (e.g. atom or molecule). In the latter case, the internal structure allows for a rich variety of scattering processes. Consider two particles A and B

Possible processes

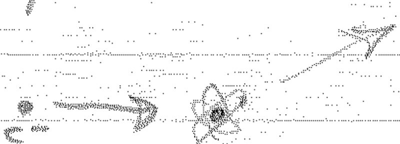
- Elastic collision $A + B \rightarrow A + B$
- Inellastic collision $A + B \rightarrow A + B^*$
- Reaction $A + B \rightarrow C + D$

  or $C_1 + C_2 + \quad + C_n$

A possible mode of fragmentation is known as a <u>channel</u>. In a elastic collision the particles "exit" on the same channel in which they "entered". In an inelastic or reaction collision, the exit channel differs from the entrance. A channel is said to be <u>open</u> if it is energetically allowed, otherwise it is said to be <u>closed</u>. Certain channels open when the incoming particles have sufficient energy. This is known as a <u>threshold</u>.

<u>Example: Electron scattering on hydrogen</u>

Consider electron incident on hydrogen in ground state. Taking the mass of the proton infinite compared to electron, the center of mass is approximated at hydrogen atom



H(1s)

- Elastic: $e^- + H(1s) \rightarrow e^- + H(1s)$

- Inelastic: $e^- + H(1s) \rightarrow e^- + H^*$

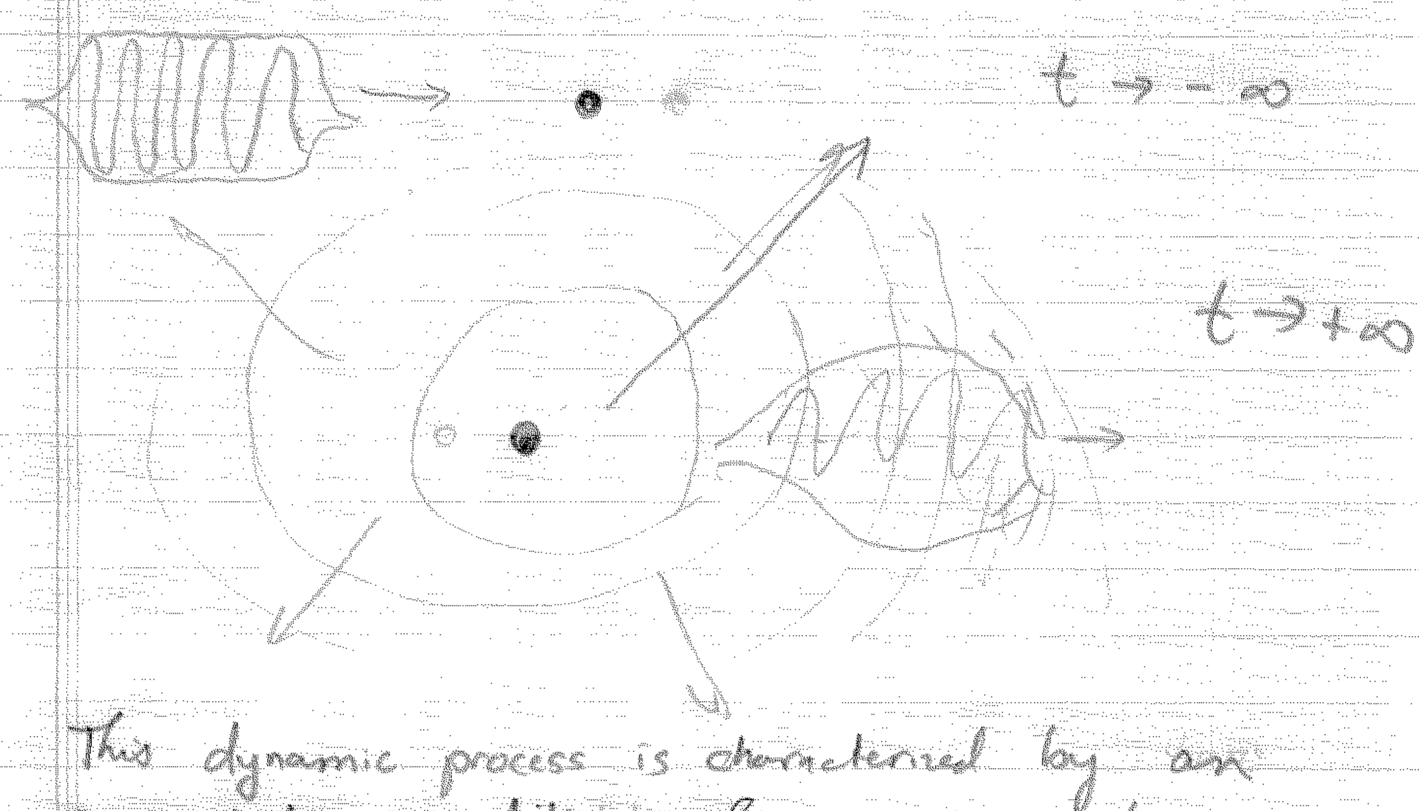
  Thresholds at energies $E_n = 13.6\left(1 - \frac{1}{n^2}\right)$ $n = 2, 3, \ldots \infty$

- Reaction (ionization): $e^- + H(1s) \rightarrow 2e^- + (\text{proton})$

Scattering Eigenstates

Scattering is a dynamic process and thus should be described by a time-dependent equation of motion. Nonetheless, we can characterize the scattering process by considering the stationary states associated with unbound eigenstates of the time-independent Schrödinger eq.

Consider a long-wave packet (quasi-monochromatic) of a scatterer, incident on a fixed target



This dynamic process is characterized by an asymptotic condition of a near-plane wave at $t \to -\infty$.

We define interacting state which asymptotically connects to a free particle "in" state by

$$\lim_{t \to -\infty} \left(\hat{U}(t) |\Psi^{(+)}\rangle - \hat{U}_0(t) |\Psi_{in}\rangle \right) = 0$$

where $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ $\hat{U}_0 = e^{-i\hat{H}_0 t/\hbar}$

or $|\Psi^{(+)}\rangle = \hat{\Omega}_+ |\Psi_{in}\rangle$

where $\hat{\Omega}_+ = \lim_{t \to -\infty} \hat{U}^\dagger(t) \hat{U}_0(t)$ Møller operator

We can define "scattering" stationary states with an asymptotic "in" state as a plane wave formally.

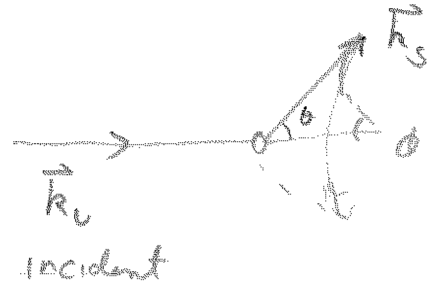
$$|\Psi^{(+)}_{\vec{k}_i}\rangle = \hat{\Omega}_+ |\vec{k}_i\rangle$$

The states $\Psi^{(+)}_{\vec{k}}(\vec{x})$ are the solutions to the T.I.S.E. Ignoring any internal degrees of freedom the wave Eq. is

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) \Psi(\vec{r}) = E \Psi(\vec{r}) = \frac{\hbar^2 k^2}{2m} \Psi(\vec{r})$$

Solution following from a retarded Greens function

$$\Psi^{(+)}_{\vec{k}_i}(\vec{r}) = A \left(e^{i\vec{k}_i \cdot \vec{r}} + f_k(\theta, \phi) \frac{e^{ikr}}{r} \right)$$

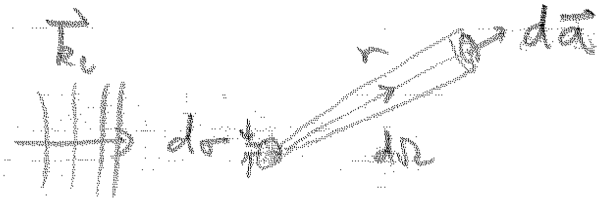
Where 

$f_k(\theta, \phi)$ is known as the scattering amplitude.

Because we have ignored internal degrees of freedom, only elastic scattering is possible.

<u>Scattering Cross - Section</u>

We as bound states are characterized by an energy eigenvalue, scattering states are characterized by a differential cross section



The rate of dectection is proportional to the probability flux through the detector aperature

$$R_{detect} = \left[(\vec{j}_{scat}) \cdot \vec{e}_r \right] r^2 d\Omega \qquad \text{Incident flux} = \vec{j}_{inc} \cdot \vec{e}_z$$

$$\vec{j} = \text{Re}\left[\psi^* \frac{\vec{p}}{m} \psi \right] = \text{Im}\left(\frac{\hbar}{m} \psi^* \vec{\nabla} \psi \right)$$

$$\vec{j}_{inc} = |A|^2 \frac{\hbar \vec{k}_i}{m} \qquad \vec{j}_{scat} \cdot \vec{e}_r = \text{Im}\left(\frac{\hbar}{m} \psi_{sc}^* \frac{\partial}{\partial r} \psi_{sc} \right) = |A|^2 \frac{\hbar k}{m}$$

$|f(\theta, \phi)|^2/$

$\therefore$ $R_{dect} = |A|^2 \frac{\hbar k}{m} \; |f_k(\theta,\phi)|^2 \, d\Omega \equiv |A|^2 \frac{\hbar k \, d\sigma}{m}$

$$\therefore \boxed{\frac{d\sigma}{d\Omega} = |f_k(\theta,\phi)|^2}$$

- S-matrix

An important construct in quantum mechanics is the Scattering operator (or S-matrix). As we have defined an "in" state as the free particle state that connects to the true state at $t \to -\infty$, we can define an "out" state as the free particle state which connects to the true state at $t \to +\infty$.

$$|\Psi_{out}\rangle = \hat{\Omega}_- |\Psi\rangle \qquad \hat{\Omega}_- = \lim_{t \to +\infty} \hat{U}^\dagger(t) \hat{U}_0(t)$$

$$\hat{S} \equiv \hat{\Omega}_-^\dagger \hat{\Omega}_+ \Rightarrow \boxed{|\Psi_{out}\rangle = \hat{S} |\Psi_{in}\rangle}$$

$\hat{S}$ map input asymptote to the out-state

Scattering transition probability amplitude

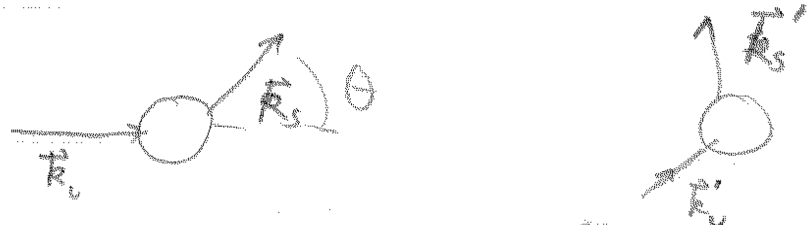
$$\langle \vec{k}_S | \hat{S} | \vec{k}_i \rangle = \delta^{(3)}(\vec{k}_i - \vec{k}_S) - \frac{i\hbar^2}{2m} \delta(E_{k_S} - E_{k_i}) \, f(\vec{k}_S \leftarrow \vec{k}_i)$$

Scattering amplitude $f(\vec{k}_S \leftarrow \vec{k}_i)$ = (constant) $\langle \vec{k}_S | (\hat{S} - 1) | \vec{k}_i \rangle$

Central Potentials and Partial Wave Expansion

If there is a central force between the target and scatterer, the interaction potential is spherically symmetric

$\Rightarrow$ S matrix rotationally invariant



$$f(\vec{k}_s \leftarrow \vec{k}_i) = f(\vec{k}_s' \leftarrow \vec{k}_i')$$

For a fixed $\vec{k}_i$, f has azimuthal symmetry

$$\Rightarrow f(\vec{k}_s \leftarrow \vec{k}_i) = f(E,\theta)$$

Can expand in a complete set of Legendre polynomial

Define "partial wave" scattering amplitude

$$f_\ell(E) = \int d(\cos\theta)\, f(E,\theta)\, P_\ell(\cos\theta)$$

$$\Rightarrow \boxed{f(\vec{k}_s \leftarrow \vec{k}_i) = \sum_{\ell=0}^{\infty} (2\ell+1) f_\ell(E)\, P_\ell(\cos\theta)}$$

We thus seek the partial wave amplitude $f_\ell(E)$

Free partical in spherical Coordinates

$$\hat{H} = \frac{\hat{P}^2}{2m} = \frac{\hat{P}_{rad}^2}{2m} + \frac{\hat{L}^2}{2mr^2}$$

⇒ Can define states a free particle with define angular momentum (rather than definite momentum) these are known as "partial waves"

$$\psi_{k,\ell,m}(\vec{r}) = R_{k\ell}(r)\, Y_{\ell,m}(\theta,\phi)$$

$$R_{k\ell} = A\, j_\ell(kr) + B\, n_\ell(kr)$$

↖spherical Bessel / Neuman function

For free particle including origin only $j_\ell(kr)$ ($n_\ell(kr)$ blow up)

Note: Spherical Hankel $h_\ell^{(\pm)}(kr) = j_\ell(kr) \pm i n_\ell(kr)$

≡ outgoing/incoming spherical waves

$j_0(kr) = \frac{\sin kr}{kr}$, $n_0(kr) = \frac{\cos(kr)}{kr}$, $h_0^{(\pm)}(kr) = \mp i \frac{e^{\pm ikr}}{r}$

Note representations: $\langle \vec{r} | k\ell m \rangle = R_{k\ell}(r)\, Y_{\ell,m}(\theta,\phi)$

momentum space $\langle \vec{p} | k\ell m \rangle = \frac{\hbar}{\sqrt{mk}}\, \delta(E_p - E_k)\, Y^\ell_m(\vec{p}/p)$

S-matrix eigenvalues

Since $\hat{S}$ has only on asymptotic states, for spherical symmetric potentials, the partial waves are eigenvectors of $\hat{S}$

$$\hat{S}\,|k,l,m\rangle = \underbrace{S_l(k)}_{\text{independent of } m}\,|k,l,m\rangle = \underbrace{e^{2i\delta_l(k)}}_{\text{phase, unitary}}|k,l,m\rangle$$

Now, $\langle \vec{k}_s|\hat{S}-1|\vec{k}_i\rangle = \frac{-i\hbar^2}{2\pi m}\,\delta(E_{k_s}-E_{k_i})\,f(\vec{k}_s \leftarrow \vec{k}_i)$

$$= \int_0^\infty dE \sum_{l,m} \langle\vec{k}_s|\underbrace{(\hat{S}-1)|klm\rangle}_{(e^{2i\delta_l(k)}-1)\,|klm\rangle}\langle klm|\vec{k}_i\rangle$$

$$= \frac{\hbar^2}{mk}\,\delta(E_{k_i}-E_{k_s})\sum_l (e^{2i\delta_l(k)}-1)\underbrace{\sum_m Y_{l,m}(\vec{e}_{k_s})\,Y^*_{l,m}(\vec{e}_{k_i})}_{\text{(addition theorem) } = \frac{2l+1}{4\pi}P_l(\cos\theta)}$$

$$\therefore\ f(\vec{k}_s \leftarrow \vec{k}_i) = \sum_l (2l+1)\left(\frac{e^{2i\delta_l(k)}-1}{2ik}\right)P_l(\cos\theta)$$

$$\Rightarrow \boxed{f_l(k) = \frac{e^{2i\delta_l(k)}-1}{2ik} = \frac{e^{i\delta_l(k)}\sin\delta_l(k)}{k}}$$

Given the partial wave decomposition, the total cross-section decomposes into

$$\sigma_{total} = \int d\Omega \frac{d\sigma}{d\Omega} = \int d\Omega \, |f(E,\theta)|^2$$

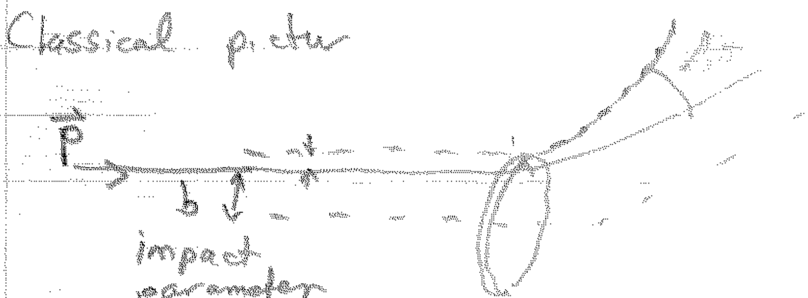
using orthogonality

$$= \sum_{l=0}^{\infty} \underbrace{4\pi (2l+1) \, |f_l(E)|^2}_{\sigma_l}$$

$\Rightarrow$ Partial cross-section $\boxed{\sigma_l = 4\pi (2l+1) \frac{\sin^2 \delta_l(E)}{k^2}}$

<u>Physical interpretation</u>

Classical picture



$L = pb$

$$\Delta\sigma_L = 2\pi b \, \Delta b = \frac{2\pi L \Delta L}{p^2}$$

$L = \hbar l$

$p = \hbar k$

Cross-section in the range $\hbar l \to \hbar (l+1)$

$\Delta L = \hbar$

$$\Rightarrow \Delta\sigma_L^{semi} = \frac{2\pi (\hbar l) \hbar}{\hbar^2 k^2} = \frac{2\pi l}{k^2}$$

from wave interference

$$\Delta\sigma_L^{quant} = \frac{4\pi}{k^2} (2l+1) \xrightarrow[l \to \infty]{} 4\left(\frac{2\pi}{k^2} l\right)$$