Lecture 20

Scattering theory

Scattering theory

Scattering theory is important as it underpins one of the most ubiquitous tools in physics.

- Almost everything we know about nuclear and atomic physics has been discovered by scattering experiments,

  e.g. Rutherford's discovery of the nucleus, the discovery of sub-atomic particles (such as quarks), etc.

- In low energy physics, scattering phenomena provide the standard tool to explore solid state systems,

  e.g. neutron, electron, x-ray scattering, etc.

- As a general topic, it therefore remains central to any advanced course on quantum mechanics.

- In these two lectures, we will focus on the general methodology leaving applications to subsequent courses.

Scattering theory: outline

- Notations and definitions; lessons from classical scattering
- Low energy scattering: method of partial waves
- High energy scattering: Born perturbation series expansion
- Scattering by identical particles
- Bragg scattering.

Scattering phenomena: background

- In an idealized scattering experiment, a sharp beam of particles (A) of definite momentum **k** are scattered from a localized target (B).
- As a result of collision, several outcomes are possible:

$$
\mathrm{A}+\mathrm{B} \longrightarrow \left\{ \begin{array}{ll} \mathrm{A}+\mathrm{B} & \text{elastic} \\ \left.\begin{array}{l} \mathrm{A}+\mathrm{B}^* \\ \mathrm{A}+\mathrm{B}+\mathrm{C} \end{array}\right\} & \text{inelastic} \\ \mathrm{C} & \text{absorption} \end{array} \right.
$$

- In high energy and nuclear physics, we are usually interested in deep inelastic processes.
- To keep our discussion simple, we will focus on **elastic processes** in which both the energy and particle number are conserved – although many of the concepts that we will develop are general.

Scattering phenomena: differential cross section

Both classical and quantum mechanical scattering phenomena are characterized by the scattering cross section, σ.

- Consider a collision experiment in which a detector measures the number of particles per unit time, $N\, d\Omega$, scattered into an element of solid angle $d\Omega$ in direction (θ, ϕ).
- This number is proportional to the incident flux of particles, j_{I} defined as the number of particles per unit time crossing a unit area normal to direction of incidence.
- Collisions are characterised by the **differential cross section** defined as the ratio of the number of particles scattered into direction (θ, ϕ) per unit time per unit solid angle, divided by incident flux,

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{N}{j_{\mathrm{I}}}}$$

Scattering phenomena: cross section

- From the differential, we can obtain the **total cross section** by integrating over all solid angles

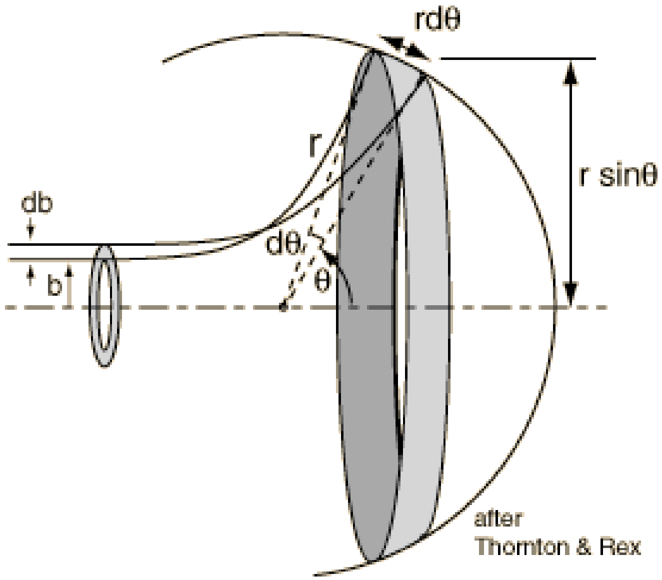
$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, \sin\theta \frac{d\sigma}{d\Omega}$$

- The cross section, which typically depends sensitively on energy of incoming particles, has dimensions of area and can be separated into $\sigma_{\mathrm{elastic}}$, $\sigma_{\mathrm{inelastic}}$, σ_{abs}, and σ_{total}.
- In the following, we will focus on elastic scattering where internal energies remain constant and no further particles are created or annihilated,

  e.g. low energy scattering of neutrons from protons.
- However, before turning to quantum scattering, let us consider classical scattering theory.

Scattering phenomena: classical theory

- In classical mechanics, for a central potential, $V(r)$, the angle of scattering is determined by **impact parameter** $b(\theta)$.
- The number of particles scattered per unit time between θ and $\theta + d\theta$ is equal to the number incident particles per unit time between b and $b + db$.
- Therefore, for incident flux $j_{\rm I}$, the number of particles scattered into the solid angle $d\Omega = 2\,\pi \sin\theta\, d\theta$ per unit time is given by

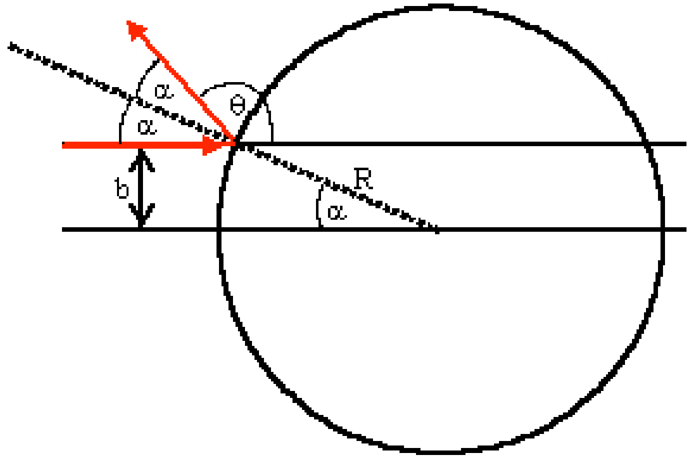


$$N\, d\Omega = 2\,\pi \sin\theta\, d\theta\, N = 2\pi b\, db\, j_{\rm I}$$

$$\boxed{\text{i.e.} \quad \frac{d\sigma(\theta)}{d\Omega} = \frac{N}{j_{\rm I}} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|}$$

Scattering phenomena: classical theory

$$\boxed{\frac{d\sigma(\theta)}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|}$$



- For elastic scattering from a hard (impenetrable) sphere,

$$b(\theta) = R\sin\alpha = R\sin\left(\frac{\pi-\theta}{2}\right) = -R\cos(\theta/2)$$

- As a result, we find that $\left|\frac{db}{d\theta}\right| = \frac{R}{2}\sin(\theta/2)$ and

$$\boxed{\frac{d\sigma(\theta)}{d\Omega} = \frac{R^2}{4}}$$

- As expected, total scattering cross section is just $\int d\Omega \frac{d\sigma}{d\Omega} = \pi R^2$, the projected area of the sphere.

Scattering phenomena: classical theory

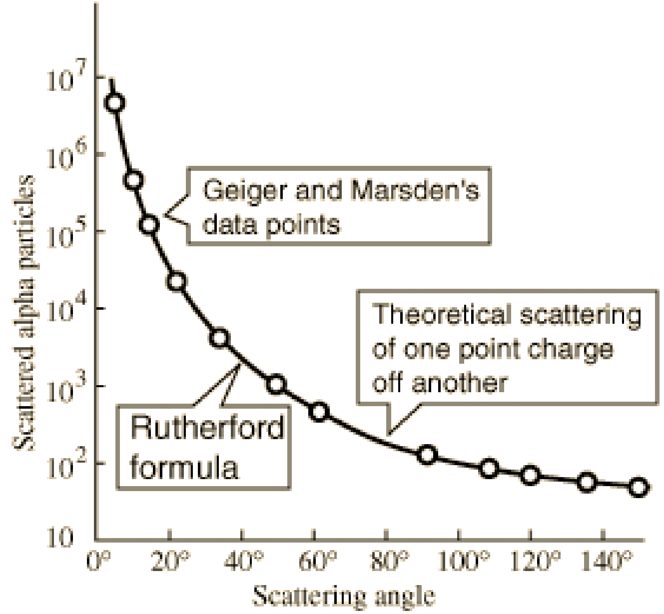
- For **classical Coulomb scattering**,

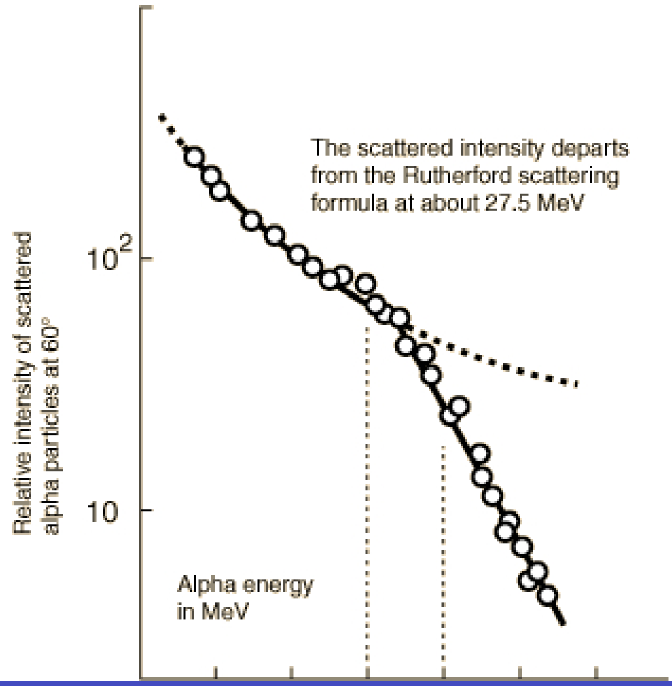
$$V(r) = \frac{\kappa}{r}$$

particle follows hyperbolic trajectory.

- In this case, a straightforward calculation obtains the **Rutherford formula:**

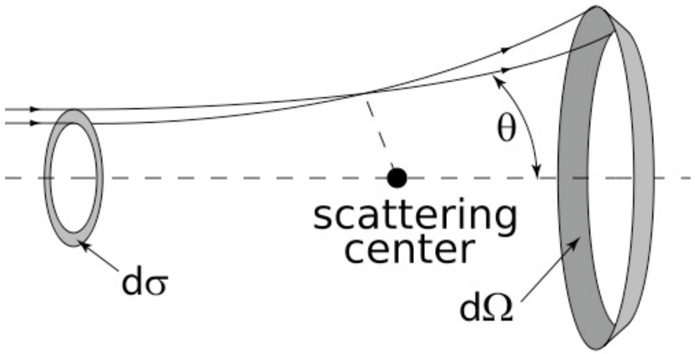
$$\boxed{\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{\kappa^2}{16E^2}\frac{1}{\sin^4\theta/2}}$$





Quantum scattering: basics and notation

- Simplest scattering experiment: plane wave impinging on localized potential, $V(\mathbf{r})$, e.g. electron striking atom, or α particle a nucleus.
- Basic set-up: flux of particles, all at the same energy, scattered from target and collected by detectors which measure angles of deflection.



- In principle, if all incoming particles represented by wavepackets, the task is to solve time-dependent Schrödinger equation,

$$\boxed{i\hbar\partial_t\Psi(\mathbf{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right]\Psi(\mathbf{r},t)}$$

and find probability amplitudes for outgoing waves.

Quantum scattering: basics and notation

- However, if beam is "switched on" for times long as compared with "encounter-time", steady-state conditions apply.
- If wavepacket has well-defined energy (and hence momentum), may consider it a plane wave: $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-iEt/\hbar}$.
- Therefore, seek solutions of time-*independent* Schrödinger equation,

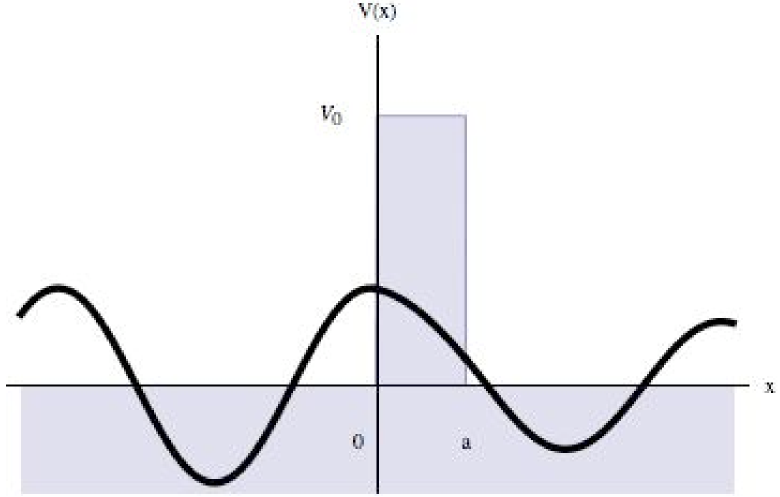
$$\boxed{E\psi(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r})}$$

  subject to boundary conditions that incoming component of wavefunction is a plane wave, $e^{i\mathbf{k}\cdot\mathbf{r}}$ (cf. 1d scattering problems).
- $E = (\hbar\mathbf{k})^2/2m$ is energy of incoming particles while flux given by,

$$\mathbf{j} = -i\frac{\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) = \frac{\hbar\mathbf{k}}{m}$$

Lessons from revision of one-dimension

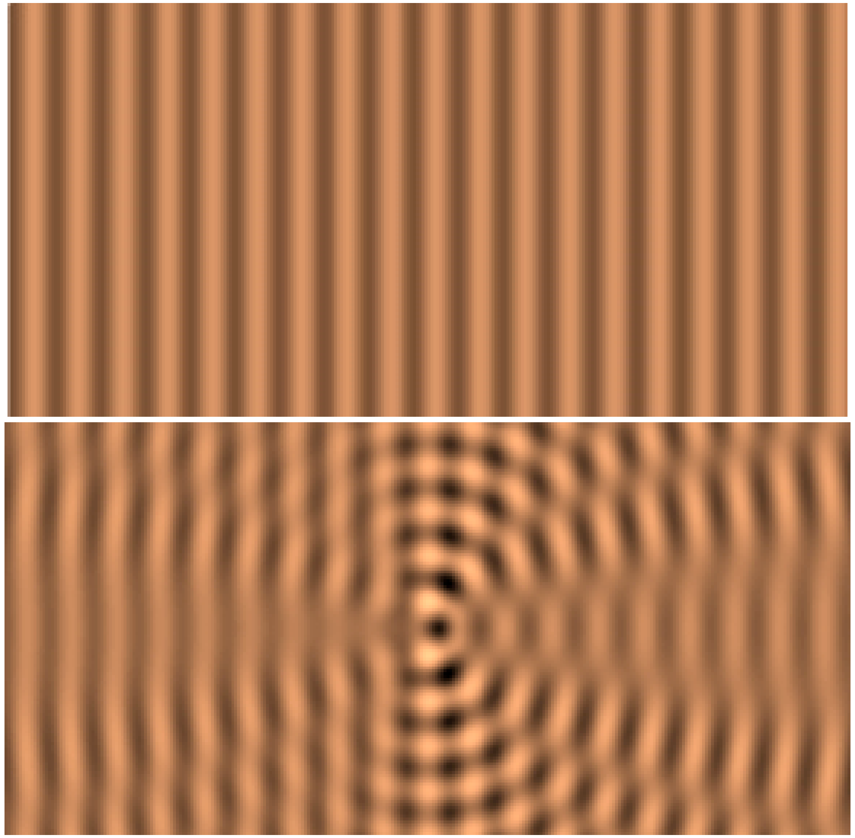
- In one-dimension, interaction of plane wave, e^{ikx}, with localized target results in degree of reflection and transmission.

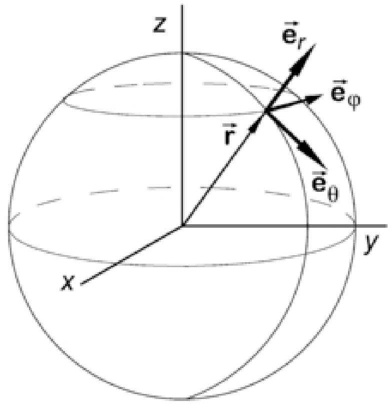


- Both components of outgoing scattered wave are plane waves with wavevector $\pm k$ (energy conservation).
- Influence of potential encoded in **complex amplitude** of reflected and transmitted wave – fixed by time-independent Schrödinger equation subject to boundary conditions (flux conservation).

Scattering in more than one dimension

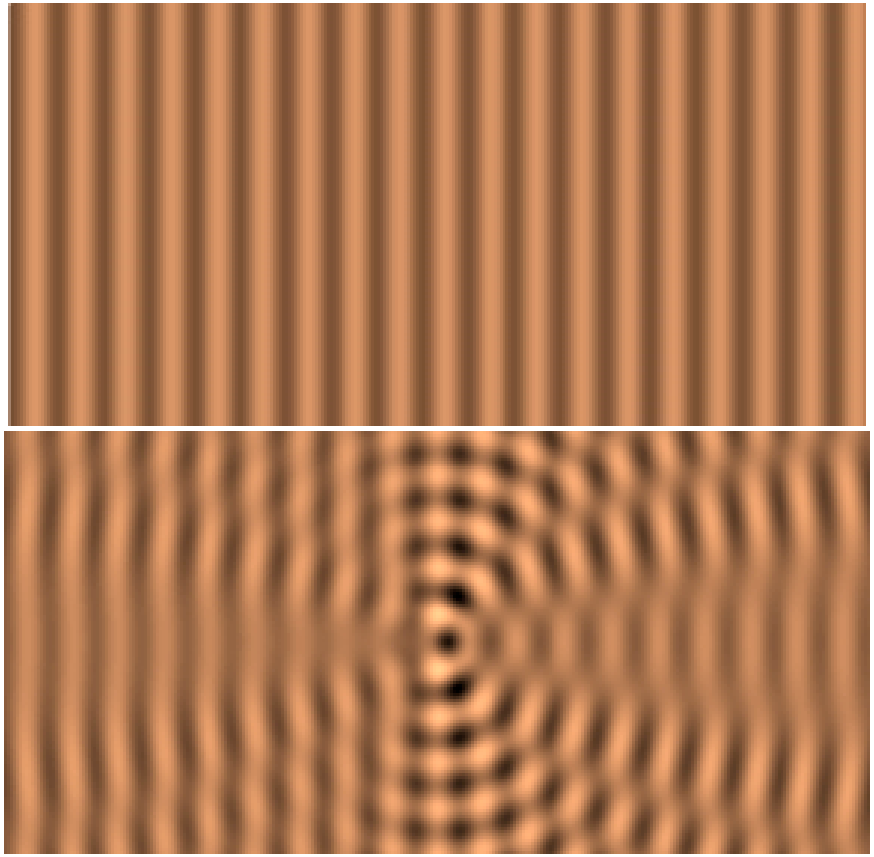
- In higher dimension, phenomenology is similar – consider plane wave incident on localized target:





- Outside localized target region, wavefunction involves superposition of incident plane wave and scattered (spherical wave)

Scattering phenomena: partial waves



- If we define z-axis by $\mathbf{k}$ vector, plane wave can be decomposed into superposition of incoming and outgoing spherical wave:
- If $V(r)$ isotropic, short-ranged (faster than $1/r$), and **elastic** (particle/energy conserving), scattering wavefunction given by,

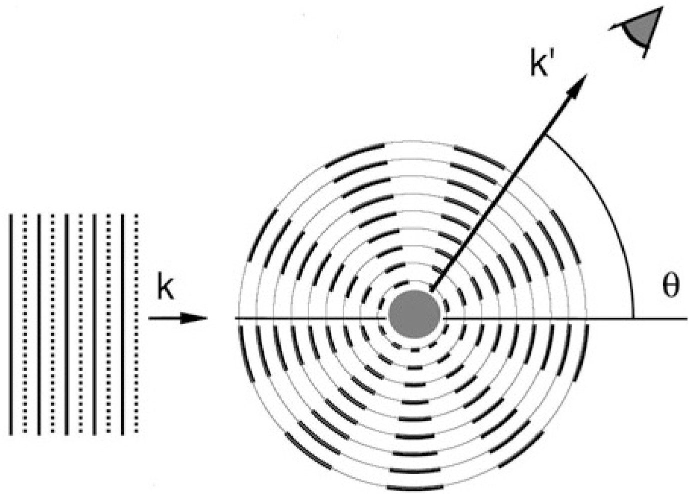
$$i \quad \infty \qquad \left[e^{-i(kr-\ell\pi/2)} \qquad e^{i(kr-\ell\pi/2)} \right]$$

Scattering phenomena: partial waves

$$\boxed{\psi(\mathbf{r}) \simeq \frac{i}{2k}\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\left[\frac{e^{-i(kr-\ell\pi/2)}}{r} - S_\ell(k)\frac{e^{i(kr-\ell\pi/2)}}{r}\right]P_\ell(\cos\theta)}$$

- If we set, $\psi(\mathbf{r}) \simeq e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}$

$$\boxed{f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\theta)}$$

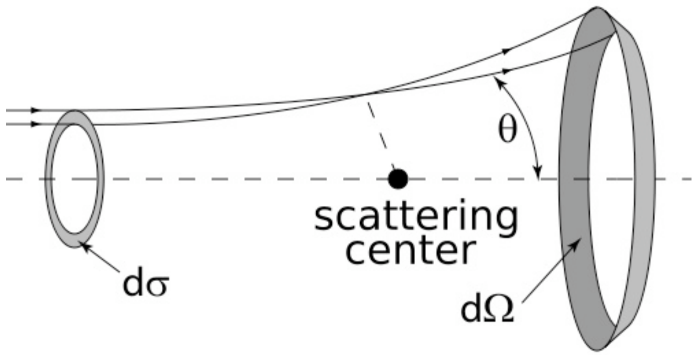


where $f_\ell(k) = \frac{S_\ell(k)-1}{2ik}$ define **partial wave scattering amplitudes**.

- i.e. $f_\ell(k)$ are defined by phase shifts, $\delta_\ell(k)$, where $S_\ell(k) = e^{2i\delta_\ell(k)}$.
  But how are phase shifts related to cross section?

Scattering phenomena: scattering cross section

$$\boxed{\psi(\mathbf{r}) \simeq e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}}$$



- Particle flux associated with $\psi(\mathbf{r})$ obtained from current operator,

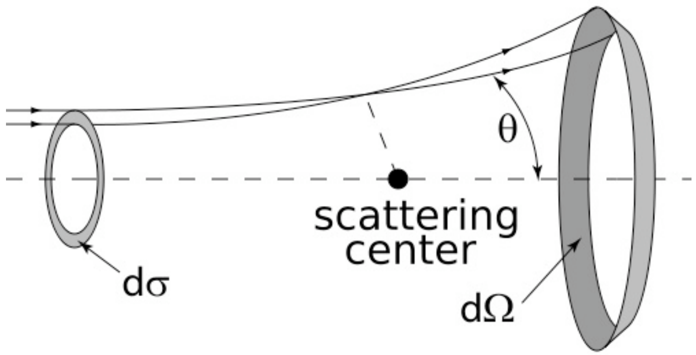
$$\mathbf{j} = -i\frac{\hbar}{m}(\psi^*\nabla\psi + \psi\nabla\psi^*) = -i\frac{\hbar}{m}\mathrm{Re}[\psi^*\nabla\psi]$$
$$= -i\frac{\hbar}{m}\mathrm{Re}\left\{\left[e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}\right]^*\nabla\left[e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}\right]\right\}$$

- Neglecting rapidly fluctuation contributions (which average to zero)

$$\mathbf{j} = \frac{\hbar\mathbf{k}}{m} + \frac{\hbar k}{m}\hat{\mathbf{e}}_r\frac{|f(\theta)|^2}{r^2} + O(1/r^3)$$

Scattering phenomena: scattering cross section

$$\mathbf{j} = \frac{\hbar\mathbf{k}}{m} + \frac{\hbar k}{m}\hat{\mathbf{e}}_r \frac{|f(\theta)|^2}{r^2} + O(1/r^3)$$



- (Away from direction of incident beam, $\hat{\mathbf{e}}_k$) the flux of particles crossing area, $dA = r^2 d\Omega$, that subtends solid angle $d\Omega$ at the origin (i.e. the target) given by

$$N d\Omega = \mathbf{j}\cdot\hat{\mathbf{e}}_r dA = \frac{\hbar k}{m}\frac{|f(\theta)|^2}{r^2} r^2 d\Omega + O(1/r)$$

- By equating this flux with the incoming flux $j_{\mathrm{I}} \times d\sigma$, where $j_{\mathrm{I}} = \frac{\hbar k}{m}$, we obtain the **differential cross section**,

$$\boxed{d\sigma = \frac{N d\Omega}{j_{\mathrm{I}}} = \frac{\mathbf{j}\cdot\hat{\mathbf{e}}_r\, dA}{j_{\mathrm{I}}} = |f(\theta)|^2\, d\Omega, \qquad \text{i.e. } \frac{d\sigma}{d\Omega} = |f(\theta)|^2}$$

Scattering phenomena: partial waves

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta)|^2, \qquad f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\theta)}$$

- From the expression for $\frac{d\sigma}{d\Omega}$, we obtain the total scattering cross-section:

$$\sigma_{\rm tot} = \int d\sigma = \int |f(\theta)|^2 d\Omega$$

- With orthogonality relation, $\displaystyle\int d\Omega\, P_\ell(\cos\theta)P_{\ell'}(\cos\theta) = \frac{4\pi}{2\ell+1}\delta_{\ell\ell'}$,

$$\sigma_{\rm tot} = \sum_{\ell,\ell'}(2\ell+1)(2\ell'+1)f_\ell^*(k)f_{\ell'}(k)\underbrace{\int d\Omega P_\ell(\cos\theta)P_{\ell'}(\cos\theta)}_{4\pi\delta_{\ell\ell'}/(2\ell+1)}$$

$$= 4\pi\sum_\ell(2\ell+1)|f_\ell(k)|^2$$

Scattering phenomena: partial waves

$$\sigma_{\rm tot} = 4\pi \sum_\ell (2\ell+1)|f_\ell(k)|^2, \qquad f(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1) f_\ell(k) P_\ell(\cos\theta)$$

- Making use of the relation $f_\ell(k) = \frac{1}{2ik}(e^{2i\delta_\ell(k)} - 1) = \frac{e^{i\delta_\ell(k)}}{k} \sin\delta_\ell$,

$$\boxed{\sigma_{\rm tot} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2\delta_\ell(k)}$$

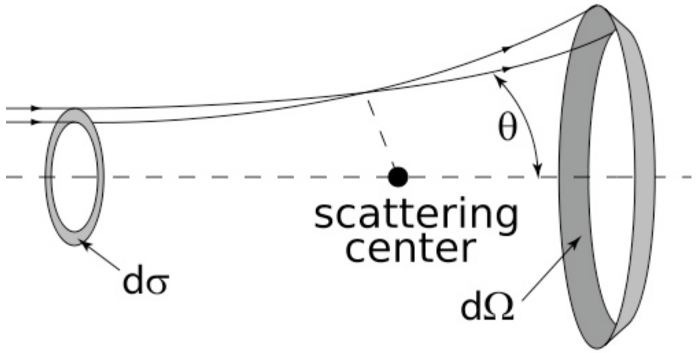
- Since $P_\ell(1) = 1$, $f(0) = \sum_\ell (2\ell+1) f_\ell(k) = \sum_\ell (2\ell+1) \frac{e^{i\delta_\ell(k)}}{k} \sin\delta_\ell$,

$$\boxed{\mathrm{Im}\, f(0) = \frac{k}{4\pi} \sigma_{\rm tot}}$$

One may show that this “sum rule”, known as **optical theorem**, encapsulates particle conservation.

Method of partial waves: summary

$$\boxed{\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}}$$



- The quantum scattering of particles from a localized target is fully characterised by the differential cross section,

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

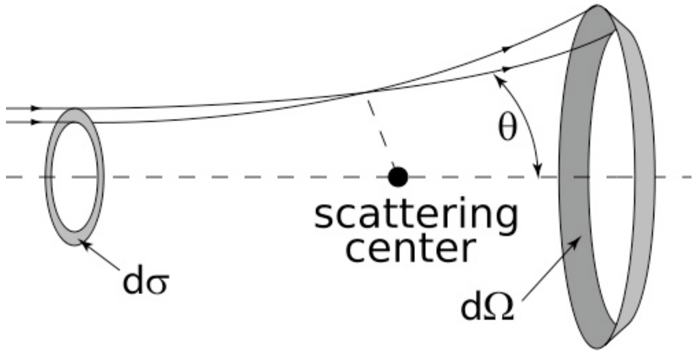
- The scattering amplitude, $f(\theta)$, which depends on the energy $E = E_k$, can be separated into a set of partial wave amplitudes,

$$f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\theta)$$

where partial amplitudes, $f_\ell(k) = \frac{e^{i\delta_\ell}}{k}\sin\delta_\ell$ defined by scattering phase shifts $\delta_\ell(k)$. **But how are phase shifts determined?**

Method of partial waves

- For scattering from a central potential, the scattering amplitude, f, must be symmetrical about axis of incidence.



- In this case, both scattering wavefunction, $\psi(\mathbf{r})$, and scattering amplitudes, $f(\theta)$, can be expanded in Legendre polynomials,

$$\psi(\mathbf{r}) = \sum_{\ell=0}^{\infty} R_\ell(r) P_\ell(\cos\theta)$$

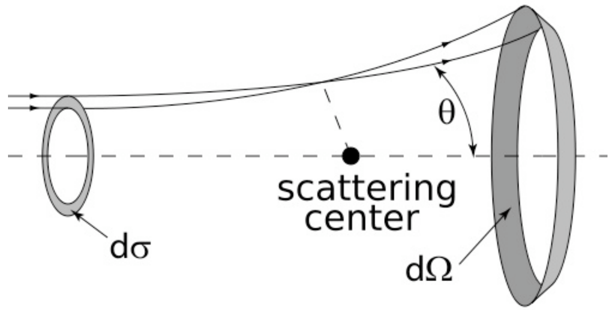
  cf. wavefunction for hydrogen-like atoms with $m = 0$.

- Each term in expansion known as **partial wave**, and is simultaneous eigenfunction of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ having eigenvalue $\hbar^2\ell(\ell+1)$ and 0, with $\ell = 0, 1, 2, \cdots$ referred to as $s, p, d, \cdots$ waves.

- From the asymtotic form of $\psi(\mathbf{r})$ we can determine the phase shifts $\delta_\ell(k)$ and in turn the partial amplitudes $f_\ell(k)$.

Method of partial waves

$$\psi(\mathbf{r}) = \sum_{\ell=0}^{\infty} R_\ell(r) P_\ell(\cos\theta)$$



- Starting with Schrödinger equation for scattering wavefunction,

$$\left[\frac{\hat{\mathbf{p}}^2}{2m} + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \qquad E = \frac{\hbar^2 k^2}{2m}$$

separability of $\psi(\mathbf{r})$ leads to radial equation,

$$\left[-\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{2}{r}\partial_r - \frac{\ell(\ell+1)}{r^2}\right) + V(r)\right] R_\ell(r) = \frac{\hbar^2 k^2}{2m} R_\ell(r)$$

- Rearranging equation, we obtain the radial equation,

$$\boxed{\left[\partial_r^2 + \frac{2}{r}\partial_r - \frac{\ell(\ell+1)}{r^2} - U(r) + k^2\right] R_\ell(r) = 0}$$

where $U(r) = 2mV(r)/\hbar^2$ represents effective potential.

Method of partial waves

$$\boxed{\left[\partial_r^2 + \frac{2}{r}\partial_r - \frac{\ell(\ell+1)}{r^2} - U(r) + k^2\right] R_\ell(r) = 0}$$

- Providing potential sufficiently short-ranged, scattering wavefunction involves superposition of incoming and outgoing spherical waves,

$$R_\ell(r) \simeq \frac{i}{2k}\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\left(\frac{e^{-i(kr-\ell\pi/2)}}{r} - e^{2i\delta_\ell(k)}\frac{e^{i(kr-\ell\pi/2)}}{r}\right)$$

$$R_0(r) \simeq \frac{1}{kr}e^{i\delta_0(k)}\sin(kr+\delta_0(k))$$

- However, at low energy, $kR \ll 1$, where R is typical range of potential, s-wave channel ($\ell = 0$) dominates.
- Here, with $u(r) = rR_0(r)$, radial equation becomes,

$$\boxed{\left[\partial_r^2 - U(r) + k^2\right] u(r) = 0}$$

with boundary condition $u(0) = 0$ and, as expected, outside radius

Method of partial waves

$$\boxed{\left[\partial_r^2 - U(r) + k^2\right] u(r) = 0}$$

- Alongside phase shift, δ_0 it is convenient to introduce **scattering length**, a_0, defined by condition that $u(a_0) = 0$ for $kR \ll 1$, i.e.

$$\begin{aligned} u(a_0) &= \sin(ka_0 + \delta_0) = \sin(ka_0)\cos\delta_0 + \cos(ka_0)\sin\delta_0 \\ &= \sin\delta_0\left[\cot\delta_0 \sin(ka_0) + \cos(kr)\right] \simeq \sin\delta_0\left[ka_0\cot\delta_0 + 1\right] \end{aligned}$$

leads to scattering length $a_0 = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0(k)$.

- From this result, we find the scattering cross section

$$\boxed{\sigma_{\rm tot} = \frac{4\pi}{k^2}\sin^2\delta_0(k) \overset{k\to 0}{\simeq} \frac{4\pi}{k^2}\frac{(ka_0)^2}{1+(ka_0)^2} \simeq 4\pi a_0^2}$$

i.e. a_0 characterizes effective size of target.

Example I: Scattering by hard-sphere

$$\boxed{\left[\partial_r^2 - U(r) + k^2\right] u(r) = 0, \qquad a_0 = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0}$$

- Consider hard sphere potential,

$$U(r) = \begin{cases} \infty & r < R \\ 0 & r > R \end{cases}$$

- With the boundary condition $u(R) = 0$, suitable for an impenetrable sphere, the scattering wavefunction given by

$$u(r) = A\sin(kr + \delta_0), \qquad \delta_0 = -kR$$

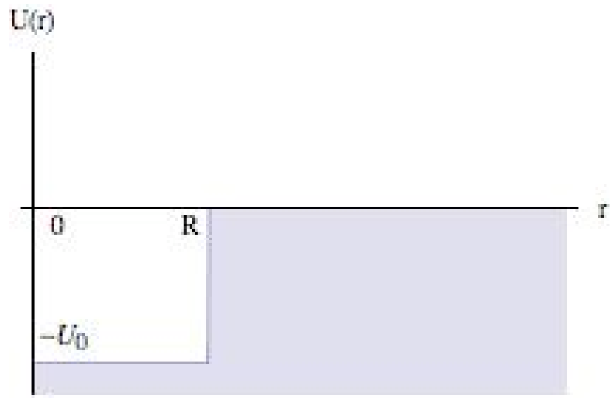
- i.e. scattering length $a_0 \simeq R$, $f_0(k) = \frac{e^{ikR}}{k}\sin(kR)$, and the total scattering cross section is given by,

$$\sigma_{\rm tot} \simeq 4\pi\frac{\sin^2(kR)}{k^2} \simeq 4\pi R^2$$

Factor of 4 enhancement over classical value, πR^2, due to diffraction processes at sharp potential.

Example II: Scattering by attractive square well

$$\left[\partial_r^2 - U(r) + k^2\right] u(r) = 0$$



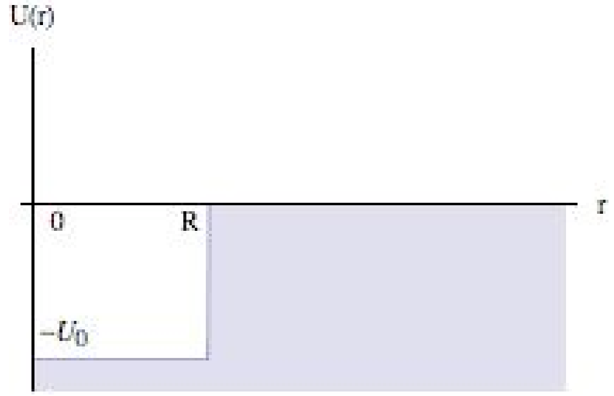
- As a proxy for scattering from a binding potential, let us consider quantum particles incident upon an attractive square well potential, $U(r) = -U_0\theta(R-r)$, where $U_0 > 0$.
- Once again, focussing on low energies, $kR \ll 1$, this translates to the radial potential,

$$\left[\partial_r^2 + U_0\theta(R-r) + k^2\right] u(r) = 0$$

with the boundary condition $u(0) = 0$.

Example II: Scattering by attractive square well

$$\boxed{\left[\partial_r^2 + U_0\theta(R-r) + k^2\right] u(r) = 0}$$



- From this radial equation, we obtain the solution,

$$u(r) = \begin{cases} C\sin(Kr) & r < R \\ \sin(kr + \delta_0) & r > R \end{cases}$$

  where $K^2 = k^2 + U_0 > k^2$ and δ_0 denotes scattering phase shift.

- From continuity of wavefunction and derivative at $r = R$,

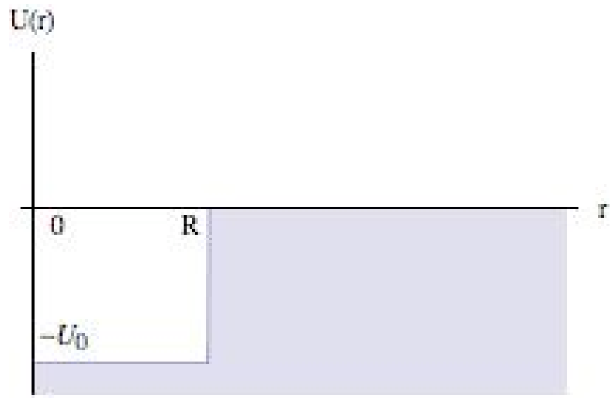
$$C\sin(KR) = \sin(kR + \delta_0), \qquad CK\cos(KR) = k\cos(kR + \delta_0)$$

  we obtain the self-consistency condition for $\delta_0 = \delta_0(k)$,

$$\boxed{K\cot(KR) = k\cot(kR + \delta_0)}$$

Example II: Scattering by attractive square well

$$\boxed{K\cot(KR) = k\cot(kR + \delta_0)}$$



- From this result, we obtain

$$\tan\delta_0(k) = \frac{k\tan(KR) - K\tan(kR)}{K + k\tan(kR)\tan(KR)}, \qquad K^2 = k^2 + U_0$$

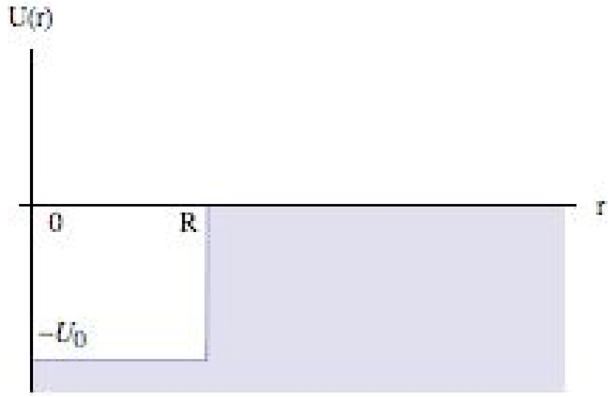
- With $kR \ll 1$, $K \simeq U_0^{1/2}(1 + O(k^2/U_0))$, find scattering length,

$$\boxed{a_0 = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0 \simeq -R\left(\frac{\tan(KR)}{KR} - 1\right)}$$

which, for $KR < \pi/2$ leads to a negative scattering length.

Example II: Scattering by attractive square well

$$\boxed{a_0 = -\lim_{k\to 0}\frac{1}{k}\tan\delta_0 \simeq -R\left(\frac{\tan(KR)}{KR}-1\right)}$$



- So, at low energies, the scattering from an attractive square potential leads to the $\ell = 0$ phase shift,

$$\boxed{\delta_0 \simeq -ka_0 \simeq kR\left(\frac{\tan(KR)}{KR}-1\right)}$$

- and total scattering cross-section,

$$\sigma_{\rm tot} \simeq \frac{4\pi}{k^2}\sin^2\delta_0(k) \simeq 4\pi R^2\left(\frac{\tan(KR)}{KR}-1\right)^2, \qquad K \simeq U_0^{1/2}$$

- **But what happens when $KR \simeq \pi/2$?**

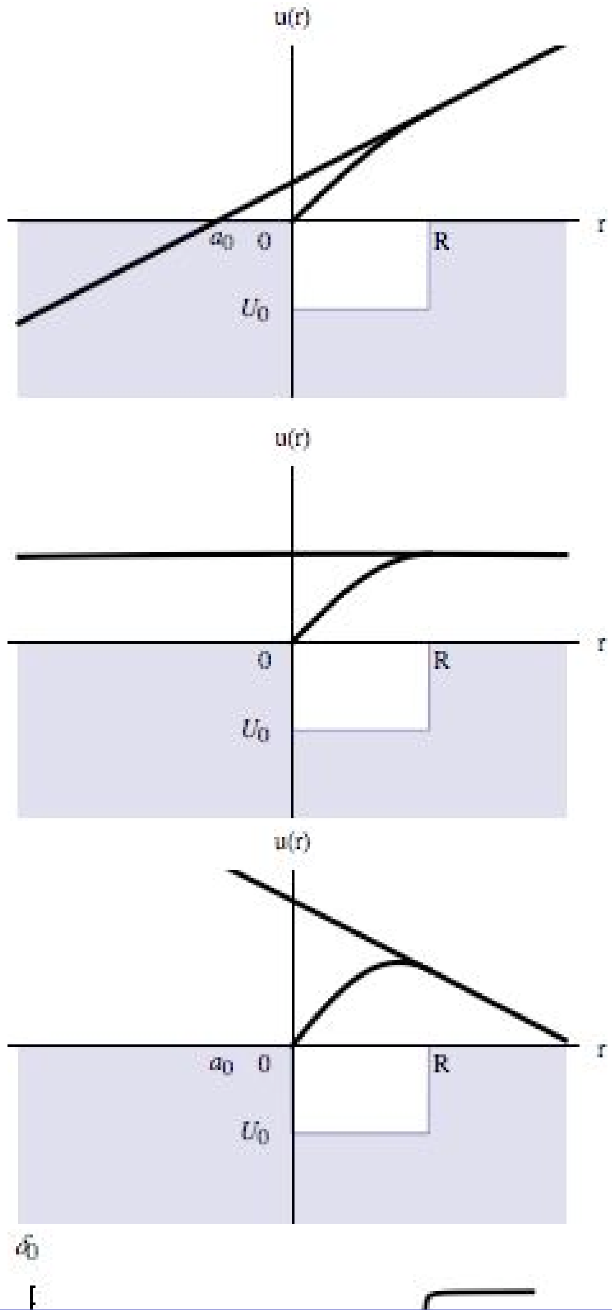
Example II: Scattering by attractive square well

$$\boxed{a_0 \simeq -R\left(\frac{\tan(KR)}{KR} - 1\right), \qquad K \simeq U_0^{1/2}}$$

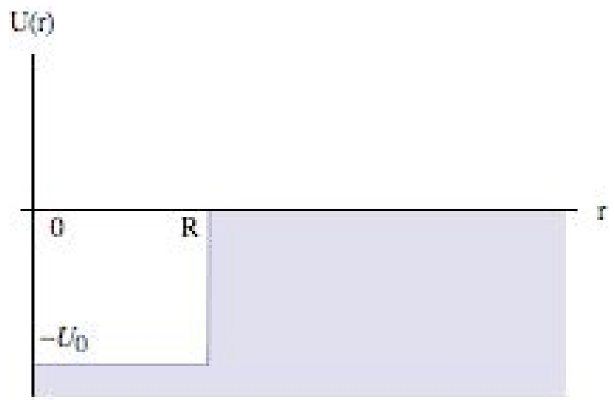
- If $KR \ll 1$, $a_0 < 0$ and wavefunction drawn towards target – hallmark of attractive potential.

- As $KR \to \pi/2$, both scattering length a_0 and cross section $\sigma_{\rm tot} \simeq 4\pi a_0^2$ diverge.

- As KR increased, a_0 turns positive, wavefunction pushed away from target (cf. repulsive potential) until $KR = \pi$ when $\sigma_{\rm tot} = 0$ and process repeats.



Example II: Scattering by attractive square well



- In fact, when $KR = \pi/2$, the attractive square well just meets the criterion to host a single s-wave bound state.
- At this value, there is a **zero energy resonance** leading to the divergence of the scattering length, and with it, the cross section – the influence of the target becomes effectively infinite in range.
- When $KR = 3\pi/2$, the potential becomes capable of hosting a second bound state, and there is another resonance, and so on.
- When $KR = n\pi$, the scattering cross section vanishes identically and the target becomes invisible – the **Ramsauer-Townsend effect**.

Resonances

- More generally, the ℓ-th partial cross-section

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\frac{1}{1+\cot^2\delta_\ell(k)}, \qquad \sigma_{\text{tot}} = \sum_\ell \sigma_\ell$$

  takes maximum value if there is an energy at which $\cot\delta_\ell$ vanishes.

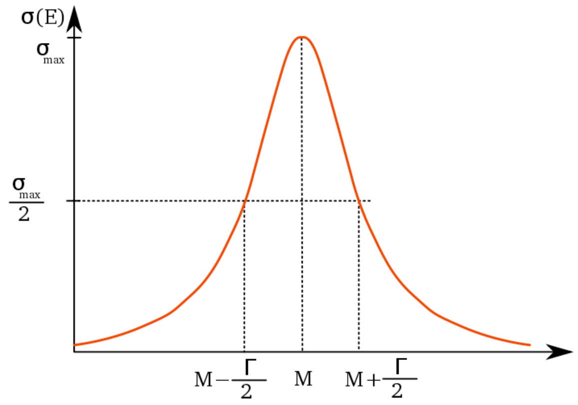
- If this occurs as a result of $\delta_\ell(k)$ increasing rapidly through odd multiple of $\pi/2$, cross-section exhibits a narrow peak as a function of energy – a **resonance**.

- Near the resonance,

$$\cot\delta_\ell(k) = \frac{E_{\mathrm{R}} - E}{\Gamma(E)/2}$$

  where E_{R} is resonance energy.

Resonances



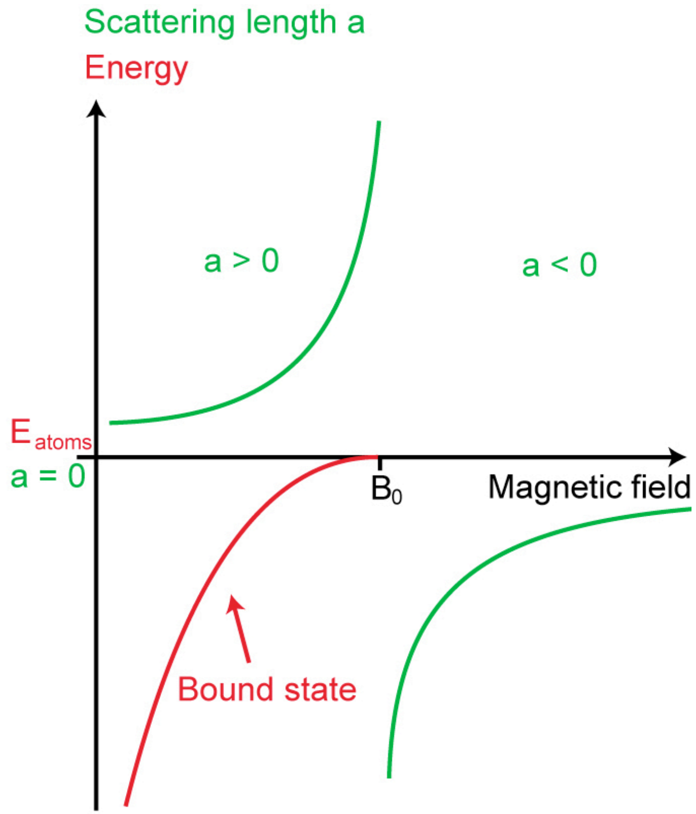
- If $\Gamma(E)$ varies slowly in energy, partial cross-section in vicinity of resonance given by **Breit-Wigner formula**,

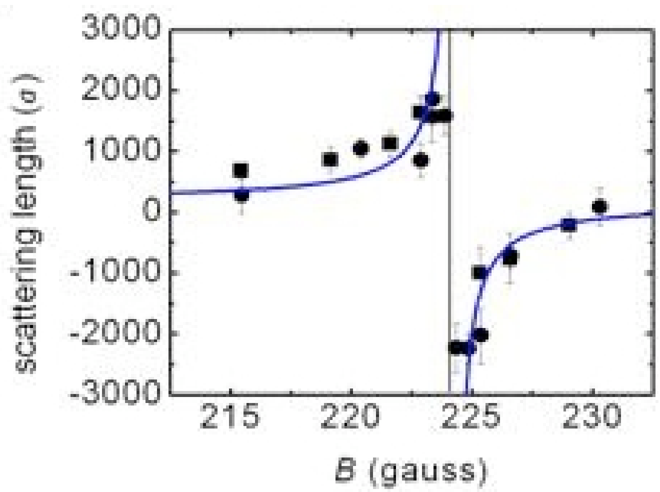
$$\boxed{\sigma_\ell(E) = \frac{4\pi}{k^2}(2\ell+1)\frac{\Gamma^2(E_\mathrm{R})/4}{(E-E_\mathrm{R})^2+\Gamma^2(E_\mathrm{R})/4}}$$

- Physically, at $E = E_\mathrm{R}$, the amplitude of the wavefunction within the potential region is high and the probability of finding the scattered particle inside the well is correspondingly high.
- The parameter $\Gamma = \hbar/\tau$ represents typical lifetime, τ, of metastable bound state formed by particle in potential.

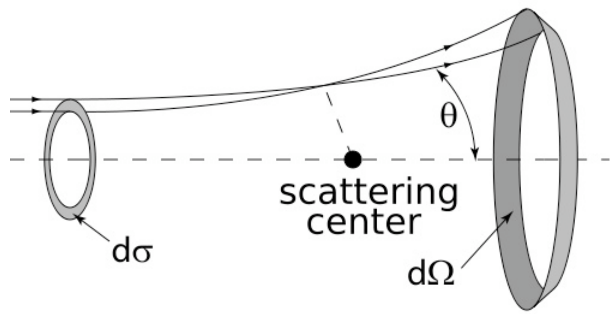
Application: Feshbach resonance phenomena

- Ultracold atomic gases provide arena in which resonant scattering phenomena exploited – far from resonance, neutral alkali atoms interact through short-ranged van der Waals interaction.
- However, effective strength of interaction can be tuned by allowing particles to form virtual bound state – a resonance.
- By adjusting separation between entrance channel states and bound state through external magnetic field, system can be tuned through resonance.
- This allows effective interaction to be tuned from repulsive to attractive simply by changing external field.





Scattering theory: summary



- The quantum scattering of particles from a localized target is fully characterised by differential cross section,

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta)|^2}$$

where $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta, \phi)\frac{e^{ikr}}{r}$ denotes scattering wavefunction.

- The scattering amplitude, $f(\theta)$, which depends on the energy $E = E_k$, can be separated into a set of partial wave amplitudes,

$$f(\theta) = \sum_{\ell=0}^{\infty}(2\ell + 1)f_\ell(k)P_\ell(\cos\theta)$$

where $f_\ell(k) = \frac{e^{i\delta_\ell}}{k}\sin\delta_\ell$ defined by scattering phase shifts $\delta_\ell(k)$.

Scattering theory: summary

- The partial amplitudes/phase shifts fully characterise scattering,

$$\boxed{\sigma_{\mathrm{tot}} = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell(k)}$$

- The individual scattering phase shifts can then be obtained from the solutions to the radial scattering equation,

$$\boxed{\left[\partial_r^2 + \frac{2}{r}\partial_r - \frac{\ell(\ell+1)}{r^2} - U(r) + k^2\right] R_\ell(r) = 0}$$

- Although this methodology is "straightforward", when the energy of incident particles is high (or the potential weak), many partial waves contribute.
- In this case, it is convenient to switch to a different formalism, the Born approximation.

Lecture 21

Scattering theory: Born perturbation series expansion

Recap

- Previously, we have seen that the properties of a scattering system,

$$\left[\frac{\hat{\mathbf{p}}^2}{2m} + V(r)\right]\psi(\mathbf{r}) = \frac{\hbar^2 k^2}{2m}\psi(\mathbf{r})$$

  are encoded in the scattering amplitude, $f(\theta, \phi)$, where

$$\boxed{\psi(\mathbf{r}) \simeq e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta, \phi)\frac{e^{ikr}}{r}}$$

- For an isotropic scattering potential $V(r)$, the scattering amplitudes, $f(\theta)$, can be obtained as an expansion in harmonics, $P_\ell(\cos\theta)$.
- At low energies, $k \longrightarrow 0$, this **partial wave expansion** is dominated by small ℓ.
- At higher energies, when many partial waves contribute, expansion is inconvenient – helpful to develop a different methodology, the **Born series expansion**

Lippmann-Schwinger equation

- Returning to Schrödinger equation for scattering wavefunction,

$$\left(\nabla^2 + k^2\right) \psi(\mathbf{r}) = U(\mathbf{r})\psi(\mathbf{r})$$

with $V(\mathbf{r}) = \frac{\hbar^2 U(\mathbf{r})}{2m}$, general solution can be written as

$$\boxed{\psi(\mathbf{r}) = \phi(\mathbf{r}) + \int G_0(\mathbf{r}, \mathbf{r}')U(\mathbf{r}')\psi(\mathbf{r}')d^3r'}$$

where $\left(\nabla^2 + k^2\right) \phi(\mathbf{r}) = 0$ and $\left(\nabla^2 + k^2\right) G_0(\mathbf{r}, \mathbf{r}') = \delta^d(\mathbf{r} - \mathbf{r}')$.

- Formally, these equations have the solution

$$\boxed{\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}, \qquad G_0(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}}$$

Lippmann-Schwinger equation

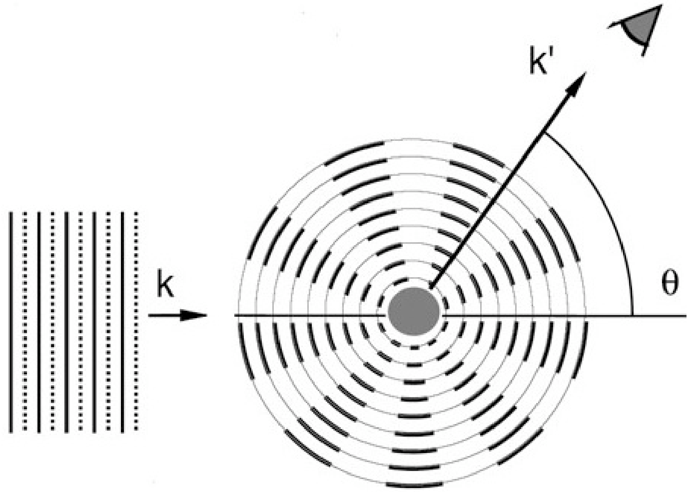
- Together, leads to **Lippmann-Schwinger equation:**

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int d^3r'\, \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')}$$

- In far-field, $|\mathbf{r}-\mathbf{r}'| \simeq r - \hat{\mathbf{e}}_r \cdot \mathbf{r}' + \cdots$,

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \simeq \frac{e^{ikr}}{r} e^{-i\mathbf{k}'\cdot\mathbf{r}'}$$

where $\mathbf{k}' \equiv k\hat{\mathbf{e}}_r$.



- i.e. $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}$ where, with $\phi_{\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}}$,

$$\boxed{f(\theta,\phi) \simeq -\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\cdot\mathbf{r}'} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}') \equiv -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U|\psi_{\mathbf{k}}\rangle}$$

Lippmann-Schwinger equation

$$\boxed{f(\theta,\phi) = -\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\cdot\mathbf{r}'}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}') \equiv -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U|\psi_{\mathbf{k}}\rangle}$$

- The corresponding differential cross-section:

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 = \frac{m^2}{(2\pi)^2\hbar^4}|T_{\mathbf{k},\mathbf{k}'}|^2}$$

where, in terms of the original scattering potential, $V(\mathbf{r}) = \frac{\hbar^2 U(\mathbf{r})}{2m}$,

$$\boxed{T_{\mathbf{k},\mathbf{k}'} = \langle\phi_{\mathbf{k}'}|V|\psi_{\mathbf{k}}\rangle}$$

denotes the transition matrix element.

Born approximation

$$\boxed{\psi(\mathbf{r}) = \phi(\mathbf{r}) + \int G_0(\mathbf{r}, \mathbf{r}')U(\mathbf{r}')\psi(\mathbf{r}')d^3r' \qquad (*)}$$

- At zeroth order in $V(\mathbf{r})$, scattering wavefunction translates to unperturbed incident plane wave, $\psi_{\mathbf{k}}^{(0)}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$.
- In this approximation, (*) leads to expansion first order in U,

$$\psi_{\mathbf{k}}^{(1)}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int d^3r' \, G_0(\mathbf{r}, \mathbf{r}')U(\mathbf{r}')\psi_{\mathbf{k}}^{(0)}(\mathbf{r}')$$

- and then to second order in U,

$$\psi_{\mathbf{k}}^{(2)}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int d^3r' \, G_0(\mathbf{r}, \mathbf{r}')U(\mathbf{r}')\psi_{\mathbf{k}}^{(1)}(\mathbf{r}')$$

  and so on.
- i.e. expressed in coordinate-independent basis,

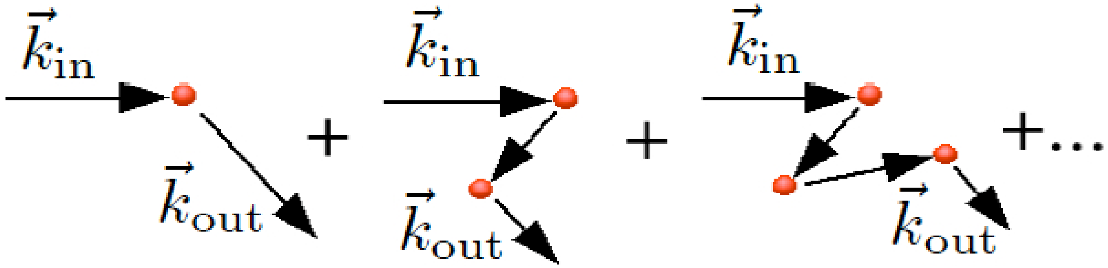
$$\boxed{|\psi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}}\rangle + \hat{G}_0\hat{U}|\phi_{\mathbf{k}}\rangle + \hat{G}_0\hat{U}\hat{G}_0\hat{U}|\phi_{\mathbf{k}}\rangle + \cdots = \sum_{n=0}^{\infty}(\hat{G}_0\hat{U})^n|\phi_{\mathbf{k}}\rangle}$$

Born approximation

$$|\psi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}}\rangle + \hat{G}_0\hat{U}|\phi_{\mathbf{k}}\rangle + \hat{G}_0\hat{U}\hat{G}_0\hat{U}|\phi_{\mathbf{k}}\rangle + \cdots = \sum_{n=0}^{\infty}(\hat{G}_0\hat{U})^n|\phi_{\mathbf{k}}\rangle$$

- Then, making use of the identity $f(\theta,\phi) = -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U|\psi_{\mathbf{k}}\rangle$, scattering amplitude expressed as **Born series** expansion

$$f = -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U + UG_0U + UG_0UG_0U + \cdots|\phi_{\mathbf{k}}\rangle$$



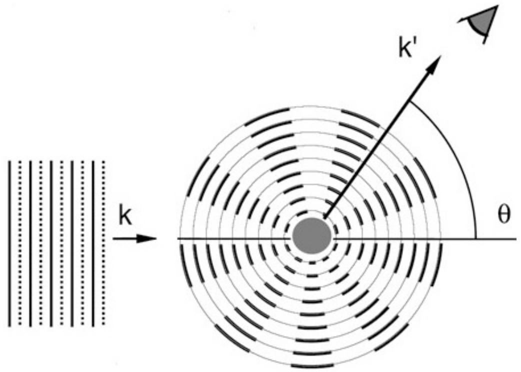
- Physically, incoming particle undergoes a sequence of multiple scattering events from the potential.

Born approximation

$$\boxed{f = -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U + UG_0U + UG_0UG_0U + \cdots|\phi_{\mathbf{k}}\rangle}$$

- Leading term in Born series known as **first Born approximation**,

$$\boxed{f_{\mathrm{Born}} = -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U|\phi_{\mathbf{k}}\rangle}$$



- Setting $\boldsymbol{\Delta} = \mathbf{k} - \mathbf{k}'$, where $\hbar\boldsymbol{\Delta}$ denotes momentum transfer, Born scattering amplitude for a central potential

$$f_{\mathrm{Born}}(\Delta) = -\frac{1}{4\pi}\int d^3r\, e^{i\boldsymbol{\Delta}\cdot\mathbf{r}}U(\mathbf{r}) = -\int_0^\infty r dr\,\frac{\sin(\Delta r)}{\Delta}U(r)$$

where, noting that $|\mathbf{k}'| = |\mathbf{k}|$, $\Delta = 2k\sin(\theta/2)$.

Example: Coulomb scattering

- Due to long range nature of the Coulomb scattering potential, the boundary condition on the scattering wavefunction does not apply.
- We can, however, address the problem by working with the screened (Yukawa) potential, $U(r) = U_0 \frac{e^{-r/\alpha}}{r}$, and taking $\alpha \to \infty$. For this potential, one may show that (exercise)

$$f_{\rm Born} = -U_0 \int_0^\infty dr \, \frac{\sin(\Delta r)}{\Delta} e^{-r/\alpha} = -\frac{U_0}{\alpha^{-2} + \Delta^2}$$

Therefore, for $\alpha \to \infty$, we obtain

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{U_0^2}{16 k^4 \sin^4 \theta/2}}$$

which is just the **Rutherford formula**.

From Born approximation to Fermi's Golden rule

- Previously, in the leading approximation, we found that the transition rate between states and i and f induced by harmonic perturbation $Ve^{i\omega t}$ is given by Fermi's Golden rule,

$$\boxed{\Gamma_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar}|\langle \mathrm{f}|V|\mathrm{i}\rangle|^2\delta(\hbar\omega - (E_{\mathrm{f}} - E_{\mathrm{i}}))}$$

- In a three-dimensional scattering problem, we should consider the initial state as a plane wave state of wavevector $\mathbf{k}$ and the final state as the continuum of states with wavevectors $\mathbf{k}'$ with $\omega = 0$.

- In this case, the total transition (or scattering) rate into a fixed solid angle, $d\Omega$, in direction (θ, ϕ) given by

$$\Gamma_{\mathbf{k}\to\mathbf{k}'} = \sum_{\mathbf{k}'\in d\Omega} \frac{2\pi}{\hbar}|\langle \mathbf{k}'|V|\mathbf{k}\rangle|^2\delta(E_{\mathbf{k}} - E_{\mathbf{k}'}) = \frac{2\pi}{\hbar}|\langle \mathbf{k}'|V|\mathbf{k}\rangle|^2 g(E_k)$$

where $g(E_k) = \sum_{k'}\delta(E_k - E_{k'}) = \frac{dn}{dE}$ is density of states at energy $E_k = \frac{\hbar^2 k^2}{2m}$.

From Born approximation to Fermi's Golden rule

$$\boxed{\Gamma_{\mathbf{k}\to\mathbf{k}'} = \frac{2\pi}{\hbar}|\langle\mathbf{k}'|V|\mathbf{k}\rangle|^2 g(E_k)}$$

- With

$$g(E_k) = \frac{dn}{dk}\frac{dk}{dE} = \frac{k^2 d\Omega}{(2\pi/L)^3}\frac{1}{\hbar^2 k/m}$$

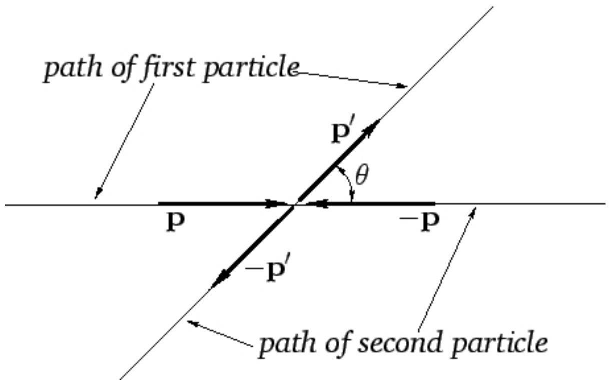
and incident flux $j_{\mathrm{I}} = \hbar k/m$, the differential cross section,

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{1}{L^3}\frac{\Gamma_{\mathbf{k}\to\mathbf{k}'}}{j_{\mathrm{I}}} = \frac{1}{(4\pi)^2}|\langle\mathbf{k}'|\frac{2mV}{\hbar^2}|\mathbf{k}\rangle|^2}$$

- **At first order, Born approximation and Golden rule coincide.**

Scattering by identical particles

- So far, we have assumed that incident particles and target are distinguishable. When scattering involves identical particles, we have to consider quantum statistics:



- Consider scattering of two identical particles. In centre of mass frame, if an outgoing particle is detected at angle θ to incoming, it could have been (a) deflected through θ, or (b) through $\pi - \theta$.
- Classically, we could tell whether (a) or (b) by monitoring particles during collision – however, in quantum scattering, we cannot track.

Scattering by identical particles

- Therefore, in centre of mass frame, we must write scattering wavefunction in appropriately symmetrized/antisymmetrized form – for bosons,

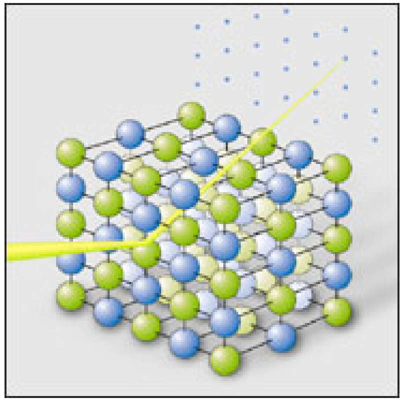
$$\psi(\mathbf{r}) = e^{ikz} + e^{-ikz} + (f(\theta) + f(\pi - \theta))\frac{e^{ikr}}{r}$$

- The differential cross section is then given by

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2}$$

as opposed to $|f(\theta)|^2 + |f(\pi - \theta)|^2$ as it would be for distinguishable particles.

Scattering by an atomic lattice



- As a final application of Born approximation, consider scattering from crystal lattice: At low energy, scattering amplitude of particles is again independent of angle (s-wave).

  - In this case, the solution of the Schrödinger equation by a single atom i located at a point $\mathbf{R}_i$ has the asymptotic form,

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_i)} + f\frac{e^{ik|\mathbf{r}-\mathbf{R}_i|}}{|\mathbf{r}-\mathbf{R}_i|}$$

  - Since $k|\mathbf{r}-\mathbf{R}_i| \simeq kr - \mathbf{k}'\cdot\mathbf{R}_i$, with $\mathbf{k}' = k\hat{\mathbf{e}}_r$ we have

$$\boxed{\psi(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{R}_i}\left[e^{i\mathbf{k}\cdot\mathbf{r}} + fe^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_i}\frac{e^{ikr}}{r}\right]}$$

  - From this result, we infer effective scattering amplitude,

$$f(\theta) = f\exp\left[-i\mathbf{\Delta}\cdot\mathbf{R}_i\right], \qquad \mathbf{\Delta} = \mathbf{k}' - \mathbf{k}$$

Scattering by an atomic lattice

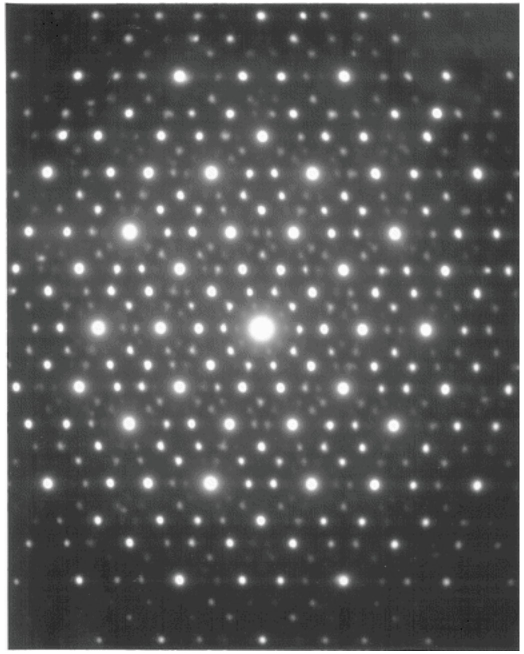
- If we consider scattering from a crystal lattice, we must sum over all atoms leading to the total differential scattering cross-section,

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \left| f \sum_{\mathbf{R}_i} \exp\left[-i\boldsymbol{\Delta} \cdot \mathbf{R}_i\right] \right|^2$$

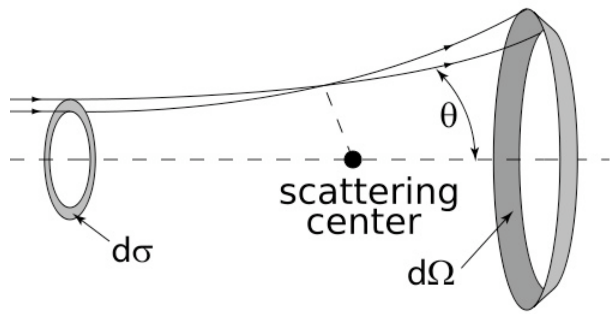
- For periodic cubic crystal of dimension L^d, sum translates to **Bragg condition**,

$$\frac{d\sigma}{d\Omega} = |f|^2 \frac{(2\pi)^3}{L^3} \delta^{(3)}(\mathbf{k}' - \mathbf{k} - 2\pi\mathbf{n}/L)$$

where integers $\mathbf{n}$ known as **Miller indices of Bragg planes**.



Scattering theory: summary



- The quantum scattering of particles from a localized target is fully characterised by differential cross section,

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta)|^2}$$

where $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}$ denotes scattering wavefunction.

- The scattering amplitude, $f(\theta)$, which depends on the energy $E = E_k$, can be separated into a set of partial wave amplitudes,

$$f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\cos\theta)$$

where $f_\ell(k) = \frac{e^{i\delta_\ell}}{k}\sin\delta_\ell$ defined by scattering phase shifts $\delta_\ell(k)$.

Scattering theory: summary

- The partial amplitudes/phase shifts fully characterise scattering,

$$\boxed{\sigma_{\rm tot} = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(k)}$$

- The individual scattering phase shifts can then be obtained from the solutions to the radial scattering equation,

$$\boxed{\left[\partial_r^2 + \frac{2}{r}\partial_r - \frac{\ell(\ell+1)}{r^2} - U(r) + k^2\right] R_\ell(r) = 0}$$

- Although this methodology is "straightforward", when the energy of incident particles is high (or the potential weak), many partial waves contribute.
- In this case, it is convenient to switch to a different formalism, the Born approximation.

Scattering theory: summary

- Formally, the solution of the scattering wavefunction can be presented as the integral (Lippmann-Schwinger) equation,

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int d^3r' \, \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')}$$

- This expression allows the scattering amplitude to be developed as a power series in the interaction, $U(\mathbf{r})$.
- In the leading approximation, this leads to the Born approximation for the scattering amplitude,

$$f_{\mathrm{Born}}(\boldsymbol{\Delta}) = -\frac{1}{4\pi}\int d^3r e^{i\boldsymbol{\Delta}\cdot\mathbf{r}} U(\mathbf{r})$$

where $\boldsymbol{\Delta} = \mathbf{k} - \mathbf{k}'$ and $\Delta = 2k\sin(\theta/2)$.