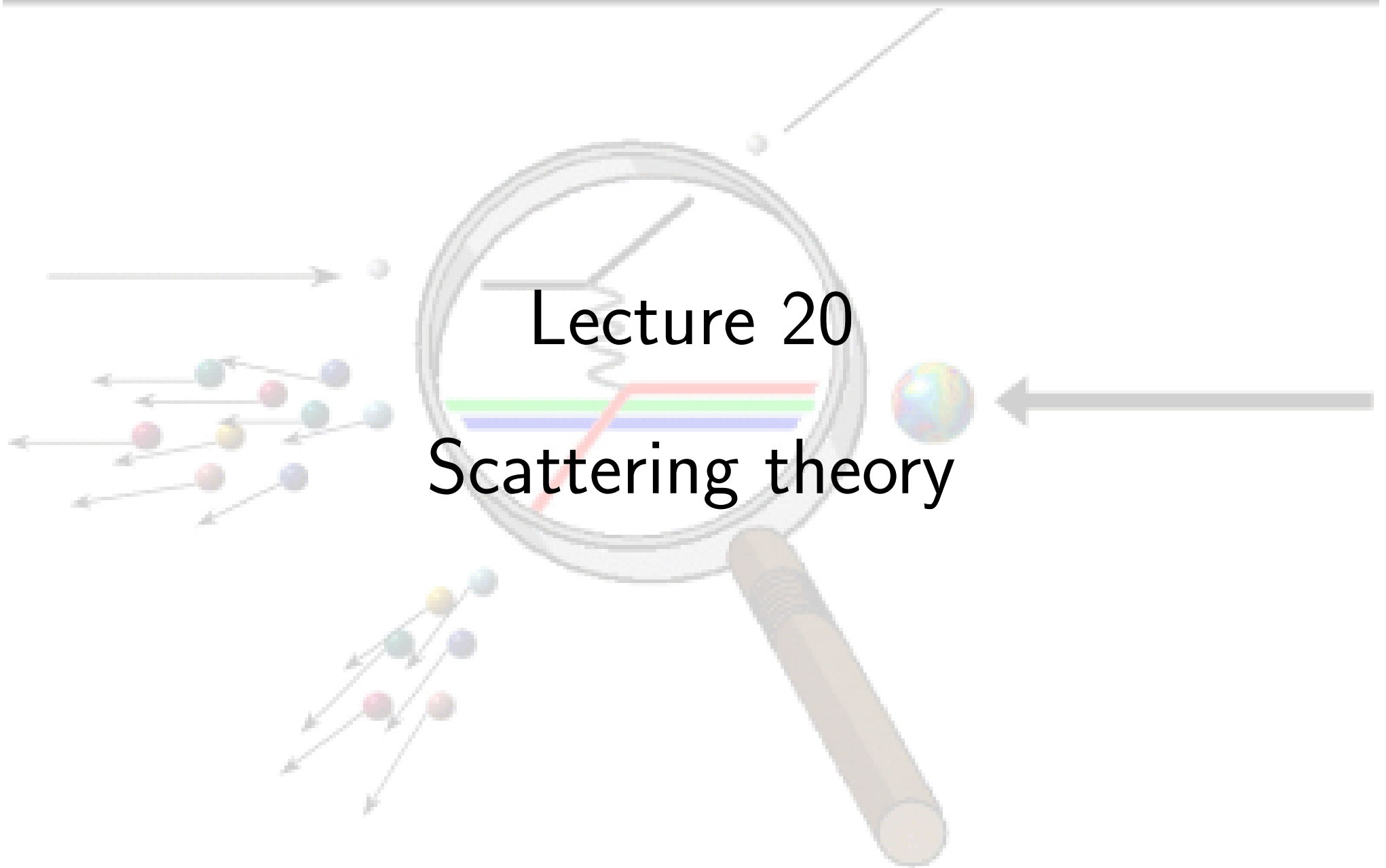


Lecture 20

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 \mathbf{k} are scattered from a localized target (B).
- As a result of collision, several outcomes are possible:

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

- 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,

$$\frac{d\sigma}{d\Omega} = \frac{N}{j_I}$$

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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 σ_{elastic} , $\sigma_{\text{inelastic}}$, 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.

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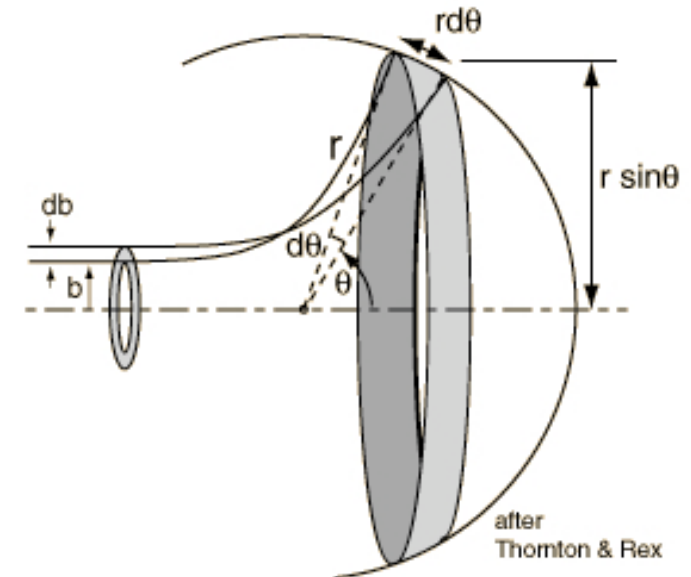
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Scattering phenomena: classical theory

- 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_I , the number of particles scattered into the solid angle $d\Omega = 2\pi \sin\theta d\theta$ per unit time is given by

$$N d\Omega = 2\pi \sin\theta d\theta N = 2\pi b db j_I$$

$$\text{i.e. } \frac{d\sigma(\theta)}{d\Omega} \equiv \frac{N}{j_I} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$$

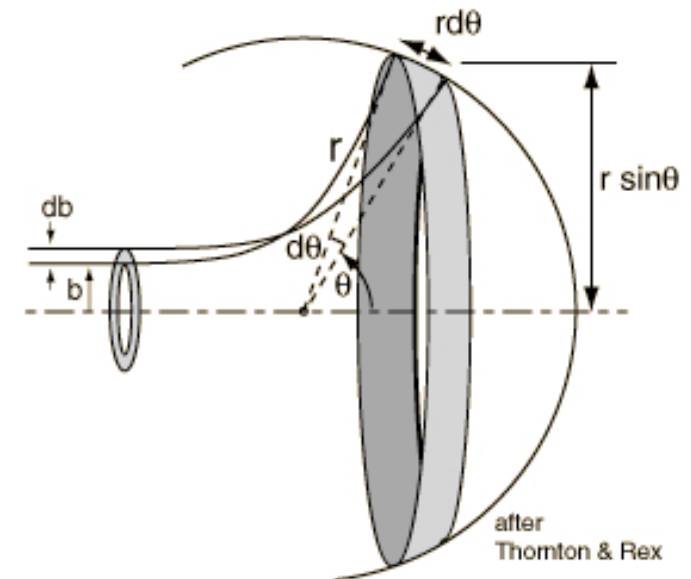


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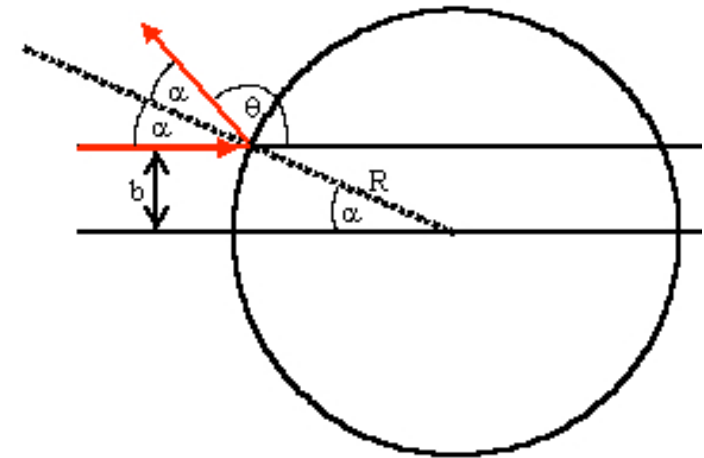
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Scattering phenomena: classical theory

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



- 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

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

- 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**,

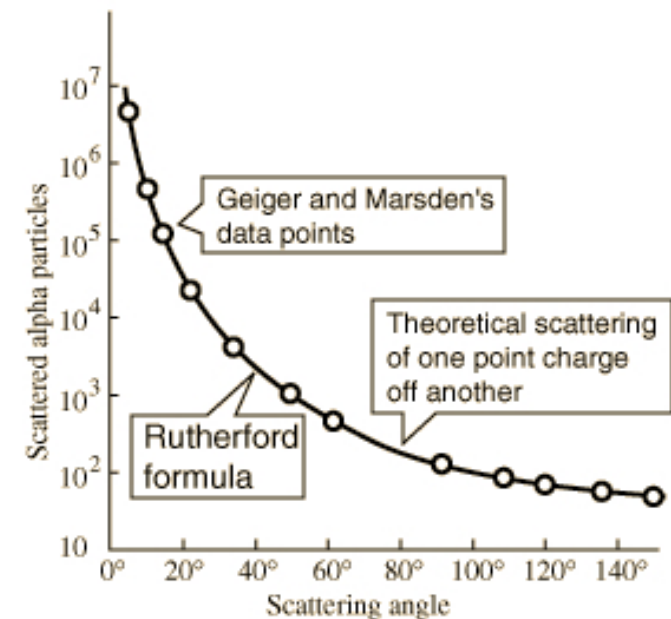
$$V(r) = \frac{\kappa}{r}$$

particle follows hyperbolic trajectory.

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

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

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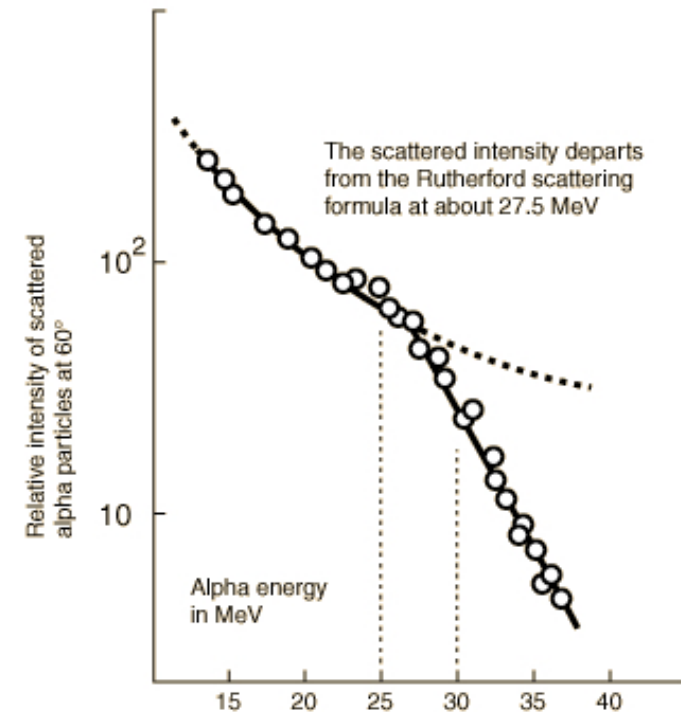
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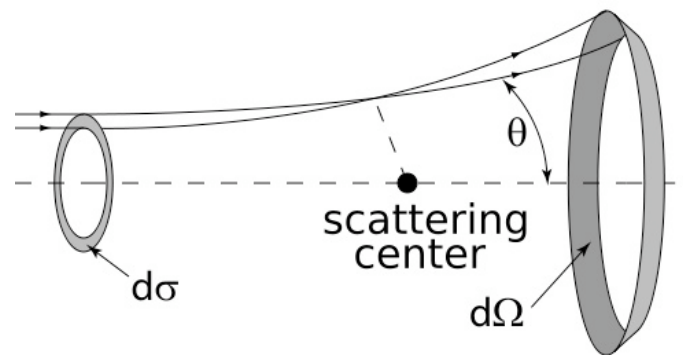
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Quantum scattering: basics and notation

- 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.



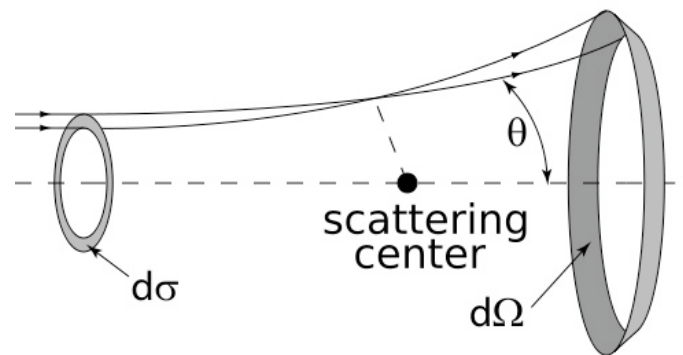
- In principle, if all incoming particles represented by wavepackets, the task is to solve time-dependent Schrödinger equation,

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

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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,

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

subject to boundary conditions that incoming component of wavefunction is a plane wave, $e^{i\mathbf{k}\cdot\mathbf{r}}$ (cf. 1d scattering problems).

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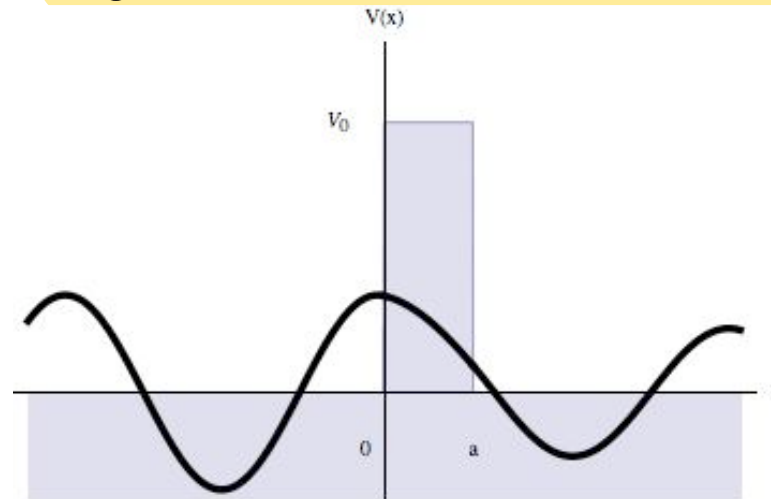
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Lessons from revision of one-dimension

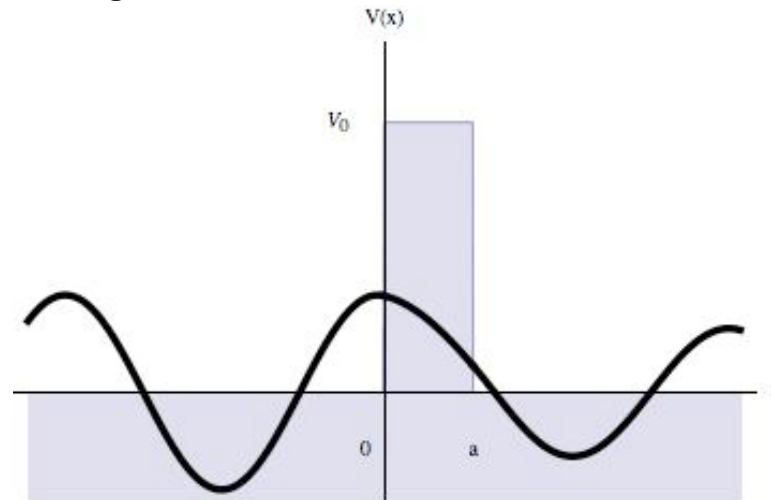
- In one-dimension, interaction of plane wave, e^{ikx} , with localized target results in degree of reflection and transmission.



- Both components of outgoing scattered wave are plane waves with wavevector $\pm k$ (energy conservation).
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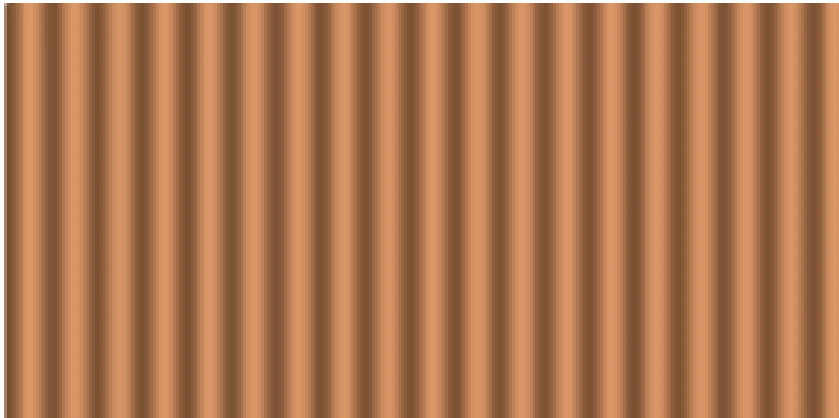
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Scattering in more than one dimension

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



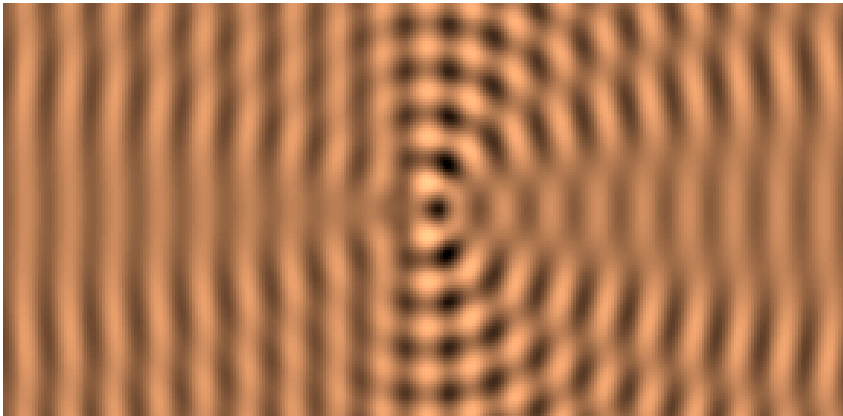
- Outside localized target region, wavefunction involves superposition of incident plane wave and scattered (spherical wave)

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- **Scattering amplitude** $f(\theta, \phi)$ records complex amplitude of component along direction (θ, ϕ) relative to incident beam.

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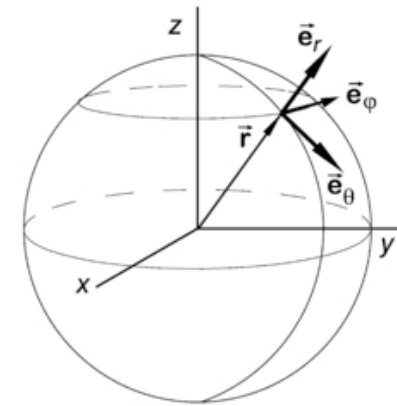
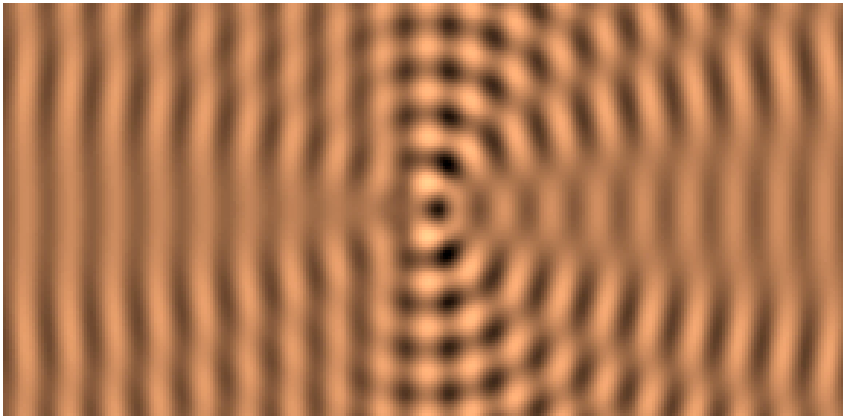
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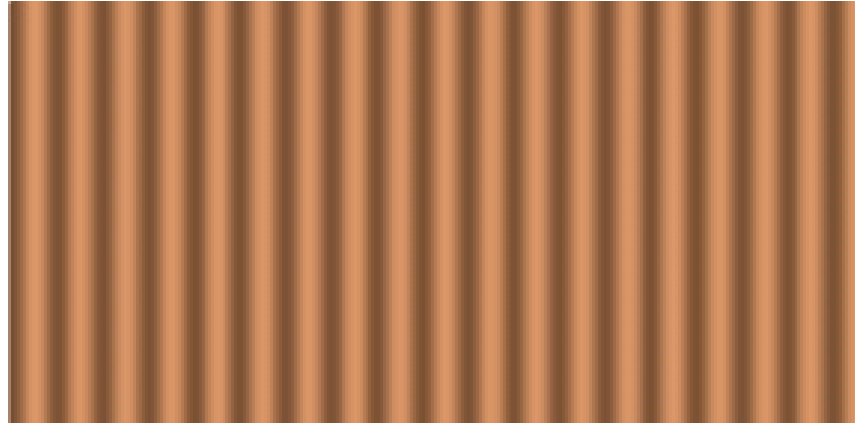


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Scattering phenomena: partial waves

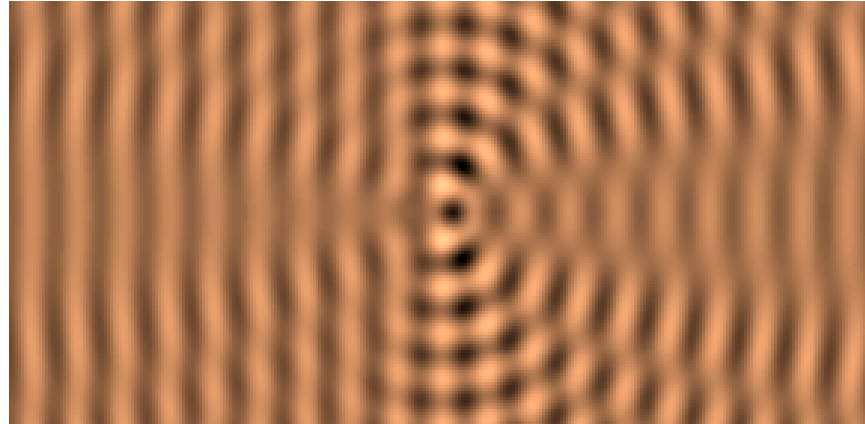


- If we define z-axis by \mathbf{k} vector, plane wave can be decomposed into superposition of incoming and outgoing spherical wave:
- If $V(r)$ isotropic, short-ranged (faster than $1/r$), and **elastic** (particle/energy conserving), scattering wavefunction given by,

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

where $P_{\ell}(\cos \theta) = \left(\frac{4\pi}{2\ell+1}\right)^{1/2} Y_{\ell 0}(\theta)$.

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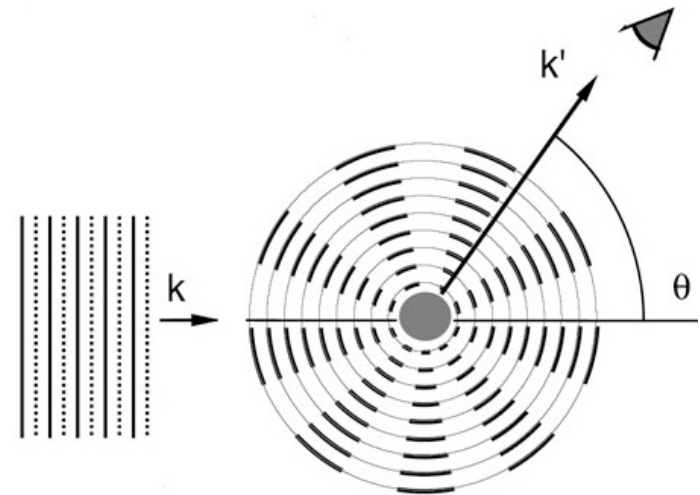
where $|S_{\ell}(k)| = 1$ (i.e. $S_{\ell}(k) = e^{2i\delta_{\ell}(k)}$ with $\delta_{\ell}(k)$ are phase shifts).

Scattering phenomena: partial waves

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

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



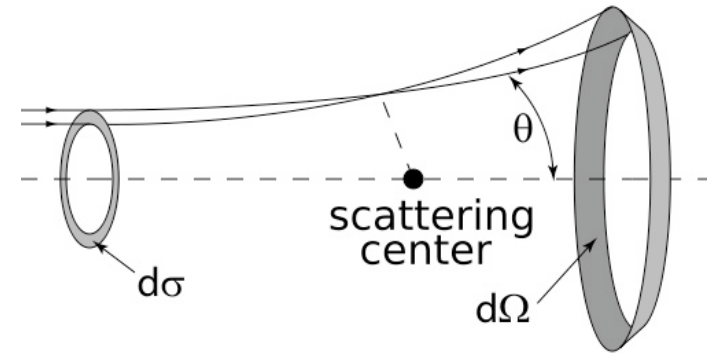
where $f_{\ell}(k) = \frac{S_{\ell}(k) - 1}{2ik}$ define **partial wave scattering amplitudes**.

- 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

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



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

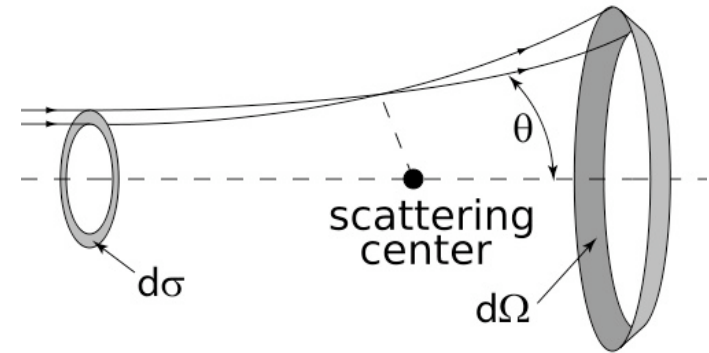
$$\begin{aligned} \mathbf{j} &= -i \frac{\hbar}{m} (\psi^* \nabla \psi + \psi \nabla \psi^*) = -i \frac{\hbar}{m} \text{Re}[\psi^* \nabla \psi] \\ &= -i \frac{\hbar}{m} \text{Re} \left\{ \left[e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta) \frac{e^{ikr}}{r} \right]^* \nabla \left[e^{i\mathbf{k}\cdot\mathbf{r}}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

- Neglecting rapidly fluctuation contributions (which average to zero)

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

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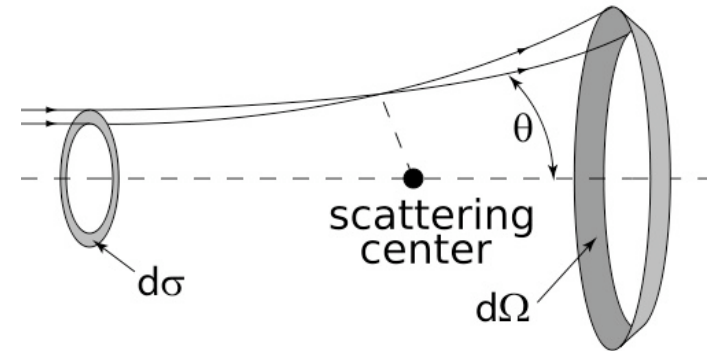
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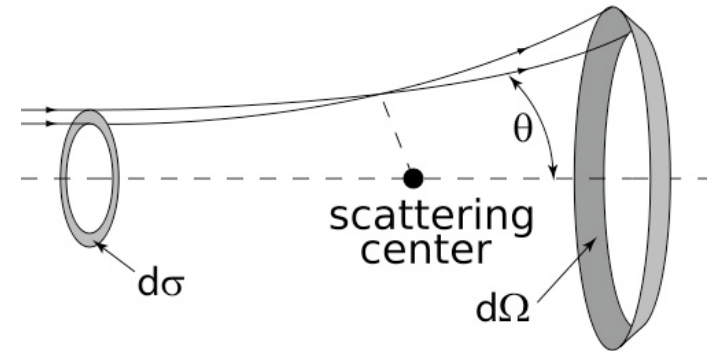
$$Nd\Omega = \mathbf{j} \cdot \hat{\mathbf{e}}_r dA = \frac{\hbar k}{m} \frac{|f(\theta)|^2}{r^2} r^2 d\Omega + O(1/r)$$

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$$d\sigma = \frac{Nd\Omega}{j_I} = \frac{\mathbf{j} \cdot \hat{\mathbf{e}}_r dA}{j_I} = |f(\theta)|^2 d\Omega, \quad \text{i.e. } \frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

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Scattering phenomena: partial waves

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

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

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

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

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

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

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

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

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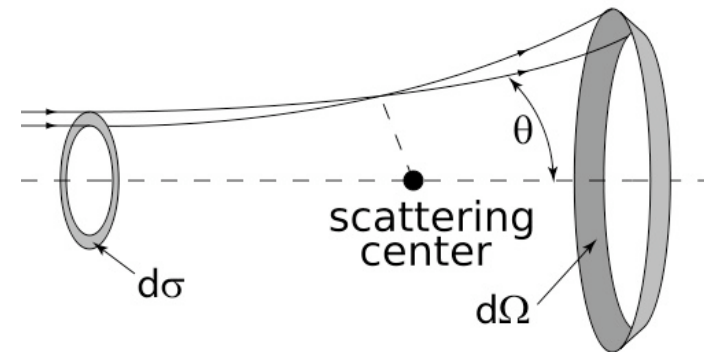
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Method of partial waves: summary

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



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

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

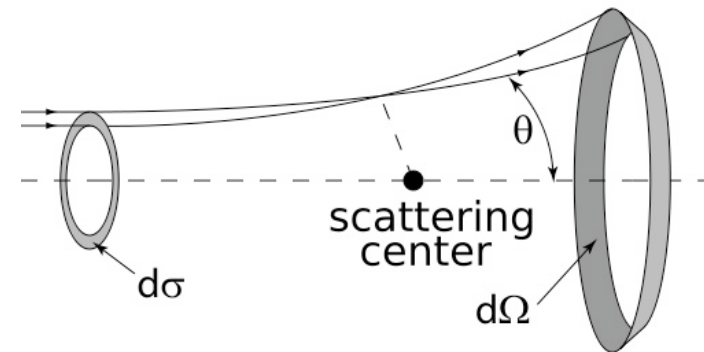
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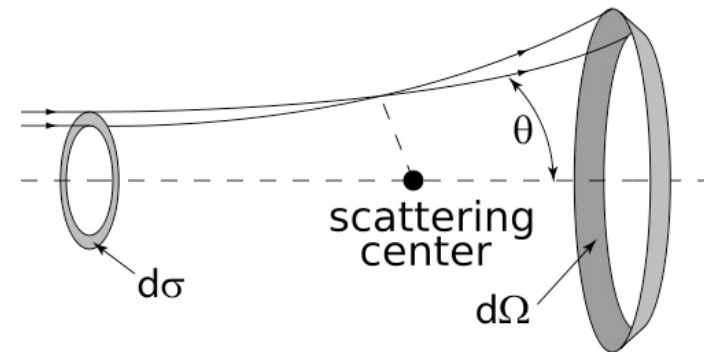
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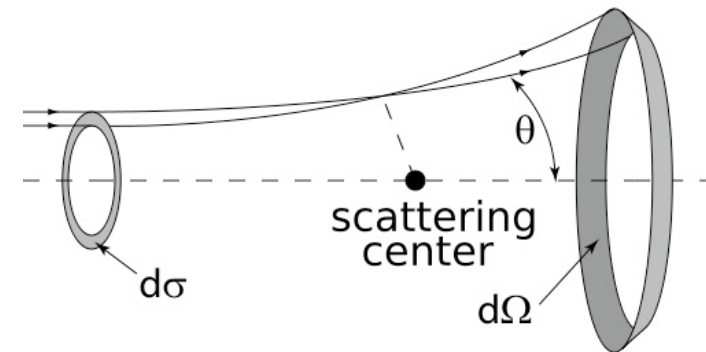
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Method of partial waves

- 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,

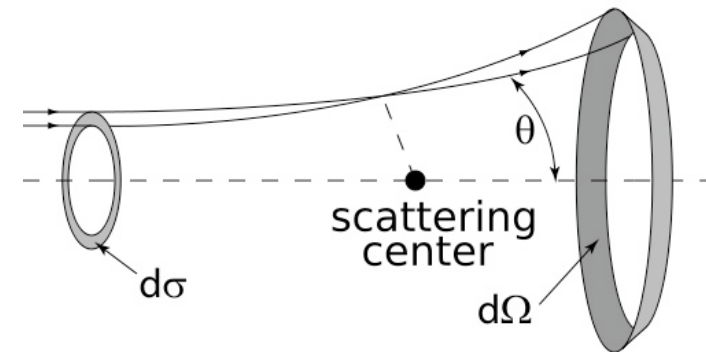
$$\psi(\mathbf{r}) = \sum_{\ell=0}^{\infty} R_{\ell}(r) P_{\ell}(\cos \theta)$$

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 $\ell = 0, 1, 2, \dots$ referred to as s, p, d, \dots waves.
- From the asymptotic form of $\psi(\mathbf{r})$ we can determine the phase shifts $\delta_{\ell}(k)$ and in turn the partial amplitudes $f_{\ell}(k)$.

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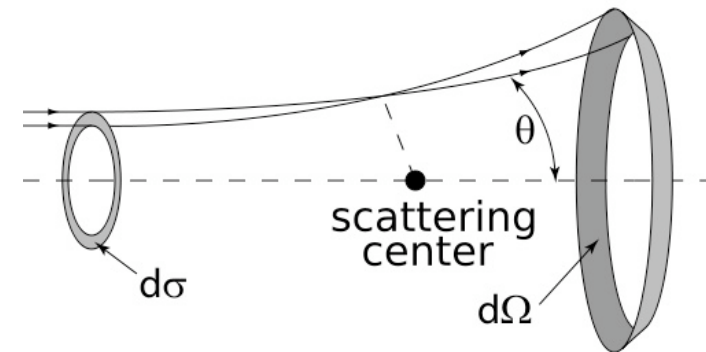
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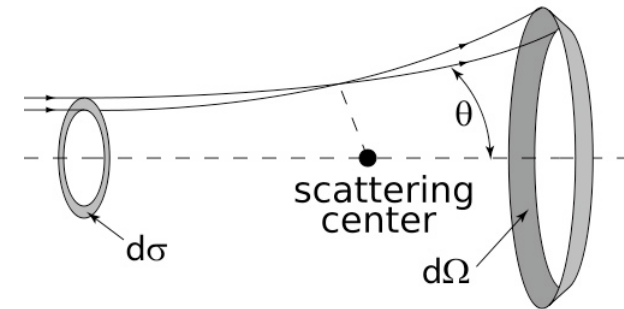
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$$\psi(\mathbf{r}) = \sum_{\ell=0}^{\infty} R_{\ell}(r) P_{\ell}(\cos \theta)$$



- Starting with Schrödinger equation for scattering wavefunction,

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

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

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

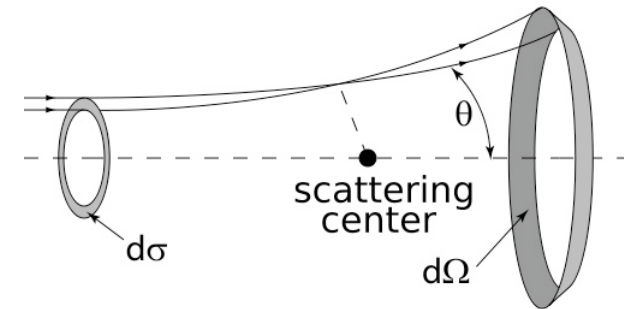
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- Providing potential sufficiently short-ranged, scattering wavefunction involves superposition of incoming and outgoing spherical waves,

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

- 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,

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

with boundary condition $u(0) = 0$ and, as expected, outside radius of potential, R , $u(r) \stackrel{r \gg R}{\simeq} A \sin(kr + \delta_0)$.

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- 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.

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

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

- From this result, we find the scattering cross section

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sin^2 \delta_0(k) \stackrel{k \rightarrow 0}{\simeq} \frac{4\pi}{k^2} \frac{(ka_0)^2}{1 + (ka_0)^2} \simeq 4\pi a_0^2$$

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Example I: Scattering by hard-sphere

$$[\partial_r^2 - U(r) + k^2] u(r) = 0, \quad a_0 = -\lim_{k \rightarrow 0} \frac{1}{k} \tan \delta_0$$

- 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

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

- 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,

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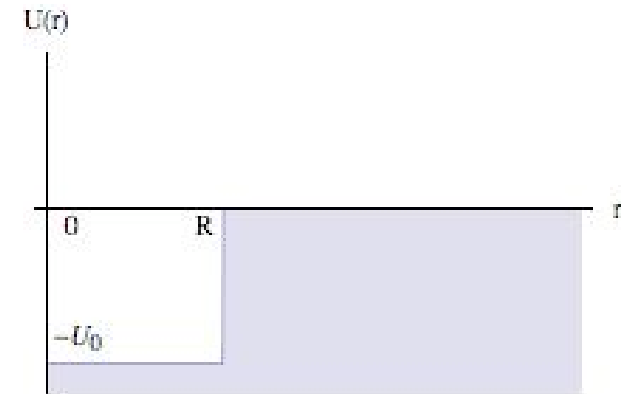
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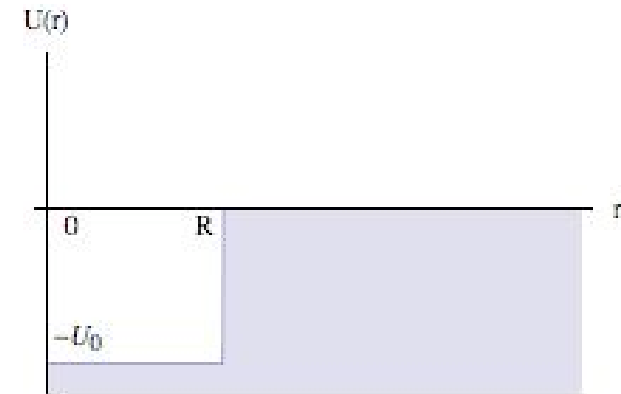
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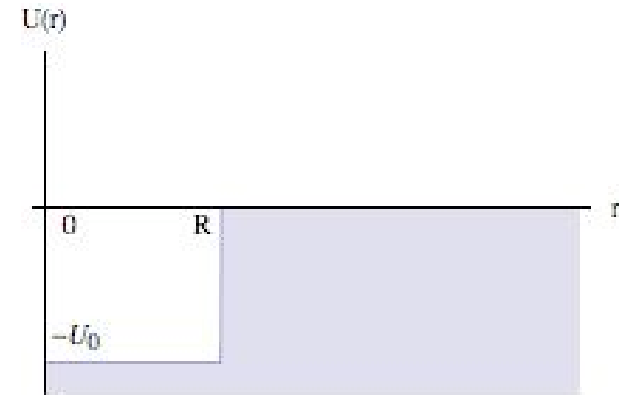
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$$u(r) = \begin{cases} C \sin(Kr) & r < R \\ \sin(kr + \delta_0) & r > R \end{cases}$$

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

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

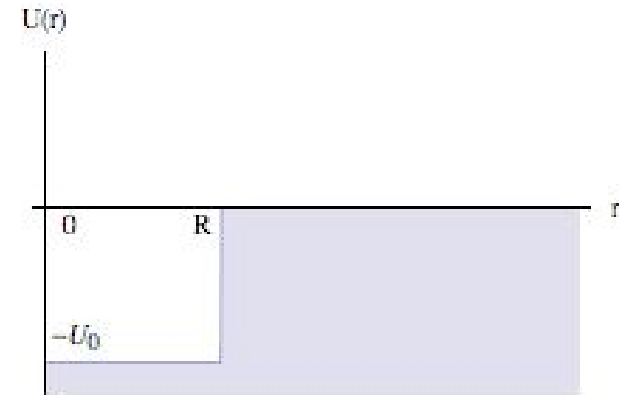
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we obtain the self-consistency condition for $\delta_0 = \delta_0(k)$,

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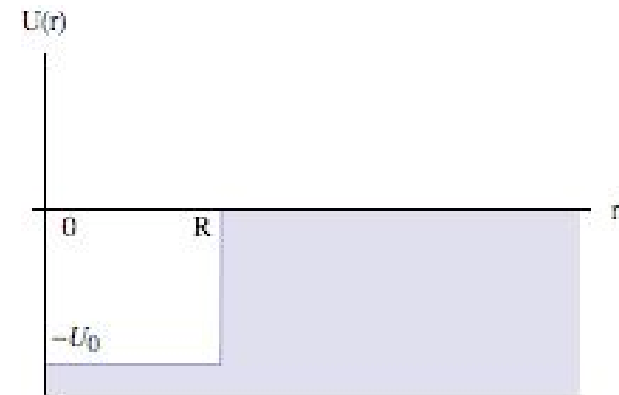
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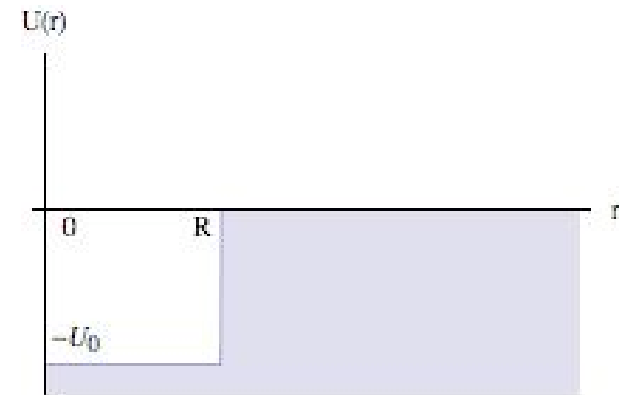
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$$a_0 = -\lim_{k \rightarrow 0} \frac{1}{k} \tan \delta_0 \simeq -R \left(\frac{\tan(KR)}{KR} - 1 \right)$$

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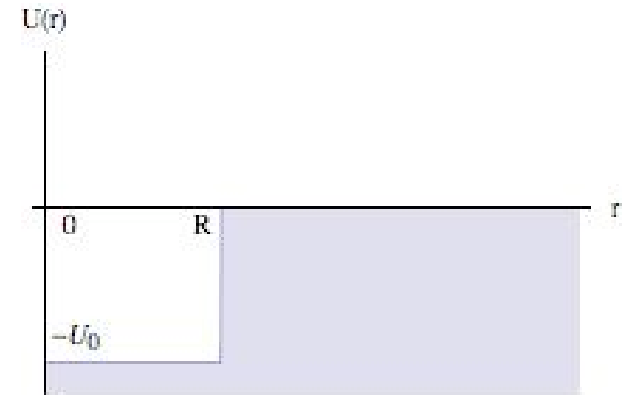
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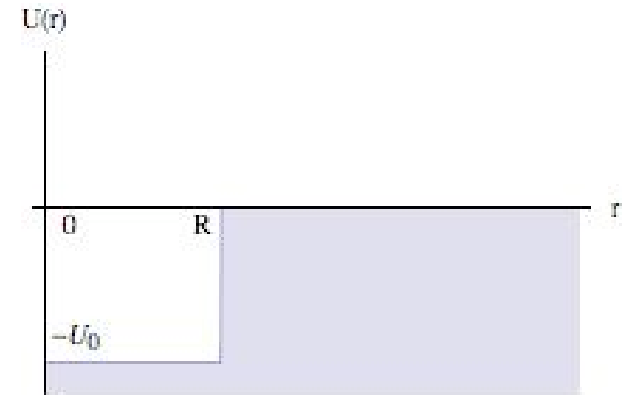
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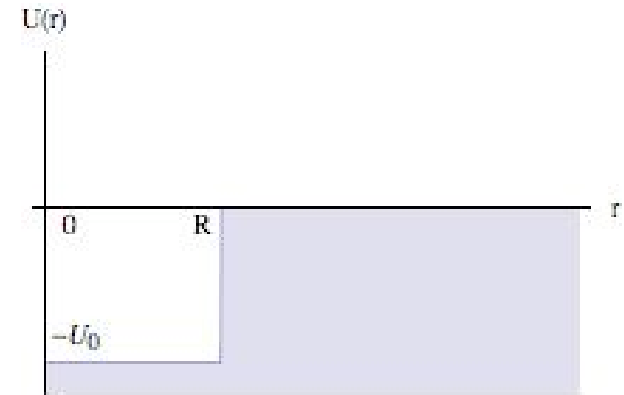
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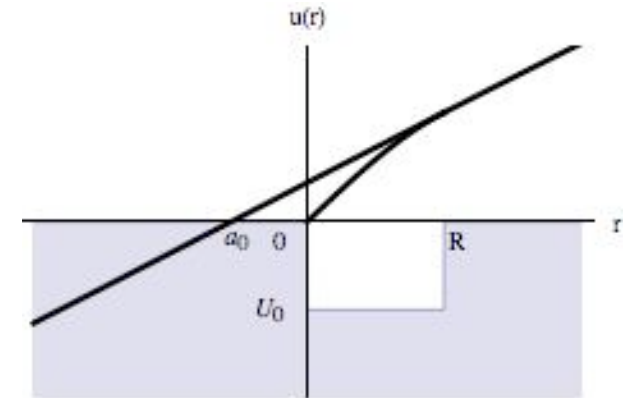
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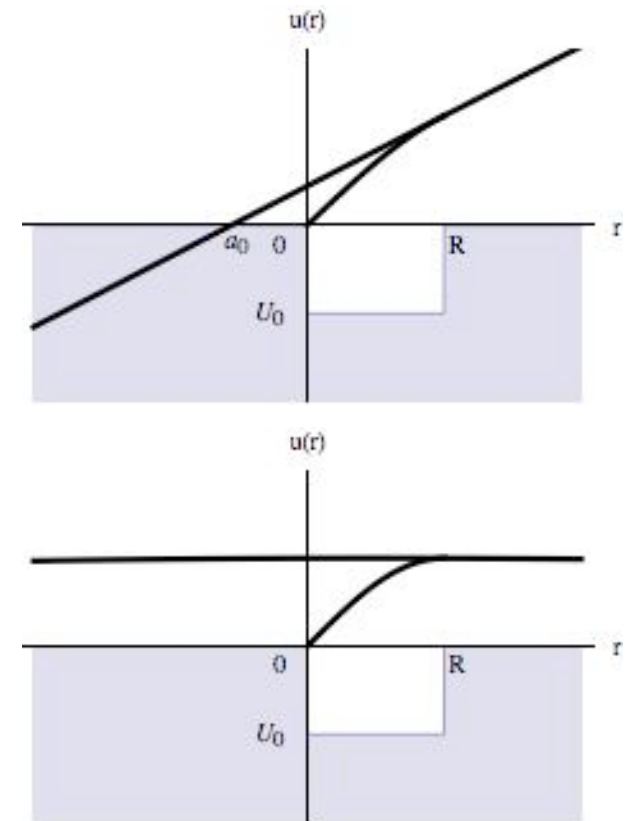
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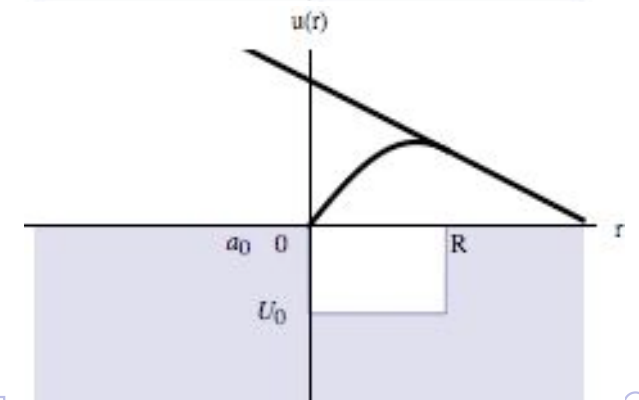
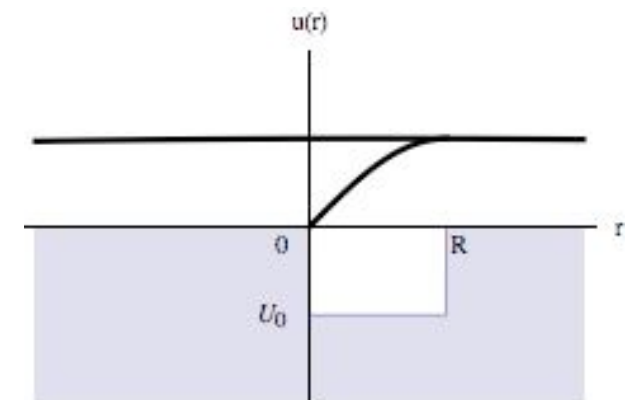
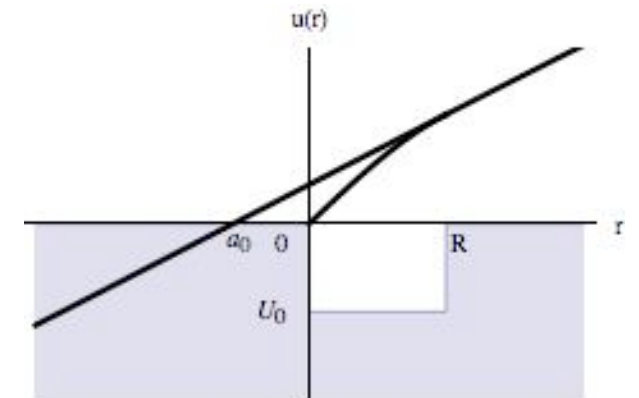
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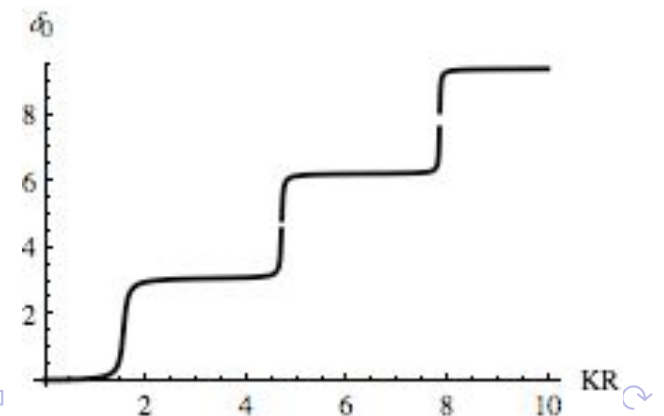
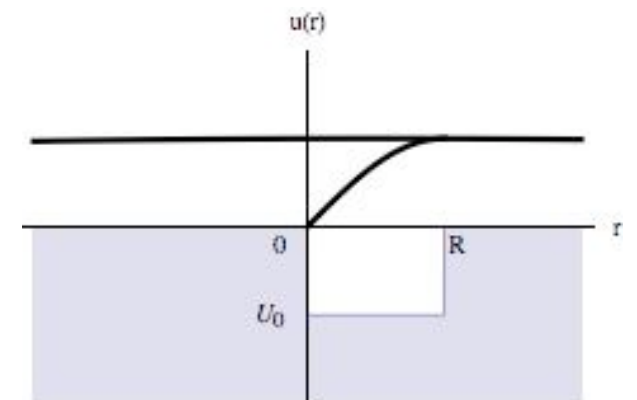
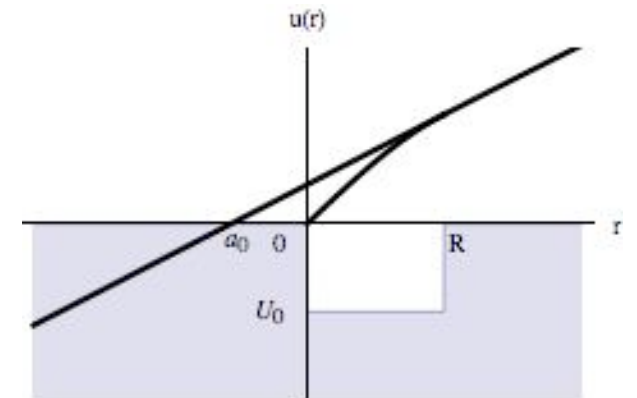


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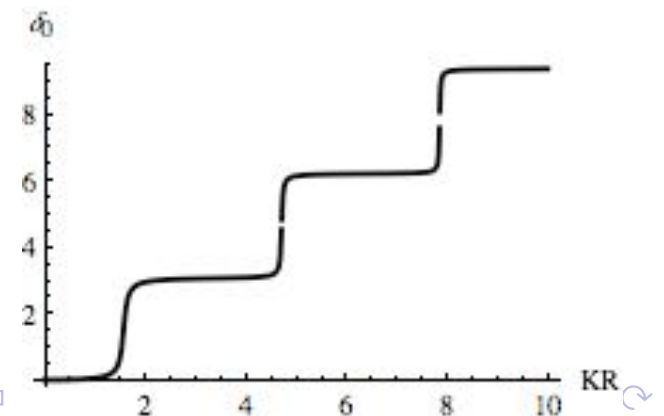
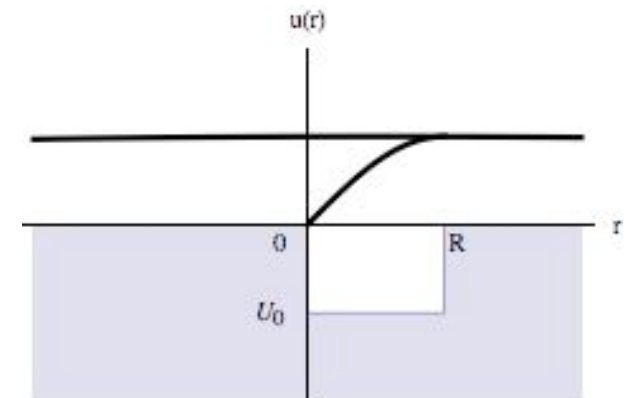
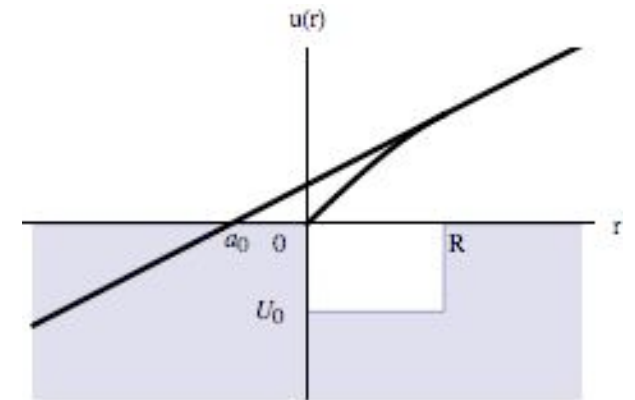
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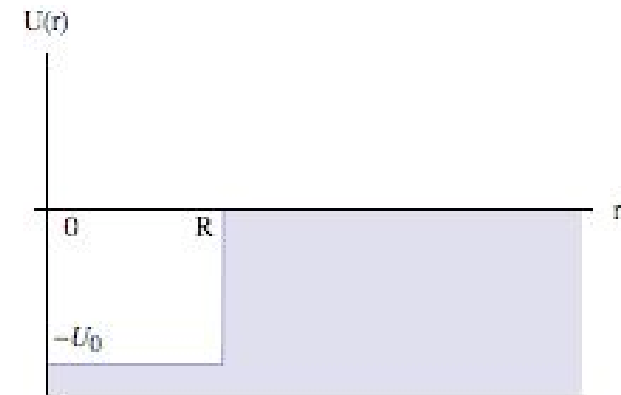
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Example II: Scattering by attractive square well



- 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

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

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,

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

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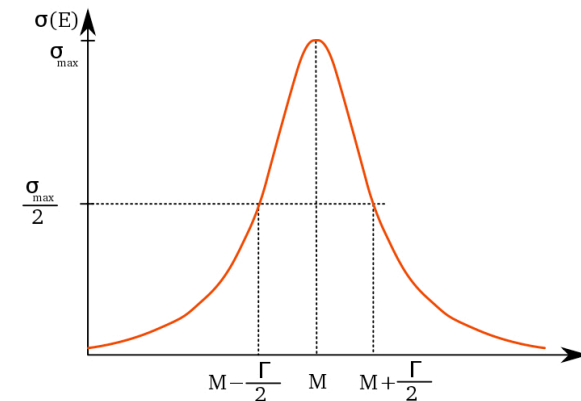
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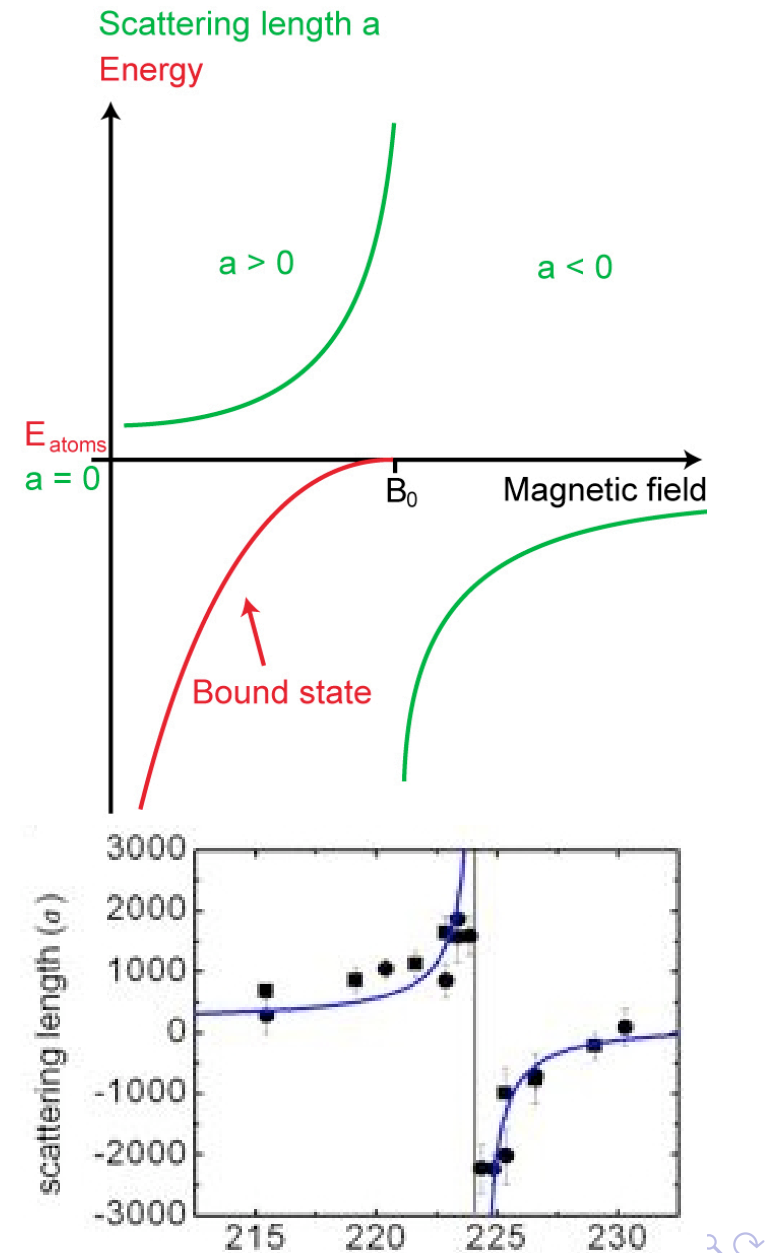
- If $\Gamma(E)$ varies slowly in energy, partial cross-section in vicinity of resonance given by **Breit-Wigner formula**,

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

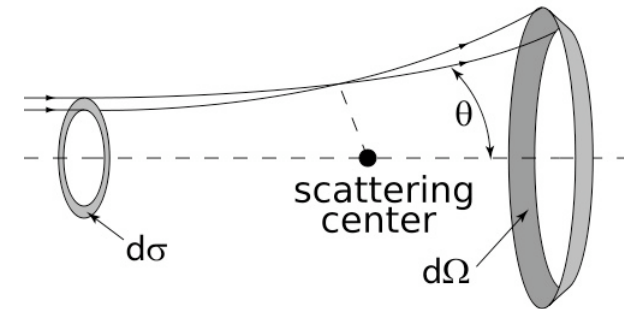
- Physically, at $E = E_R$, the amplitude of the wavefunction within the potential region is high and the probability of finding the scattered particle inside the well is correspondingly high.
- The parameter $\Gamma = \hbar/\tau$ represents typical lifetime, τ , of metastable bound state formed by particle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

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

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,

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

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

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

- 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

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

- 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, $k \rightarrow 0$, 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**

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Lippmann-Schwinger equation

- Returning to Schrödinger equation for scattering wavefunction,

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

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

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

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

- Formally, these equations have the solution

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

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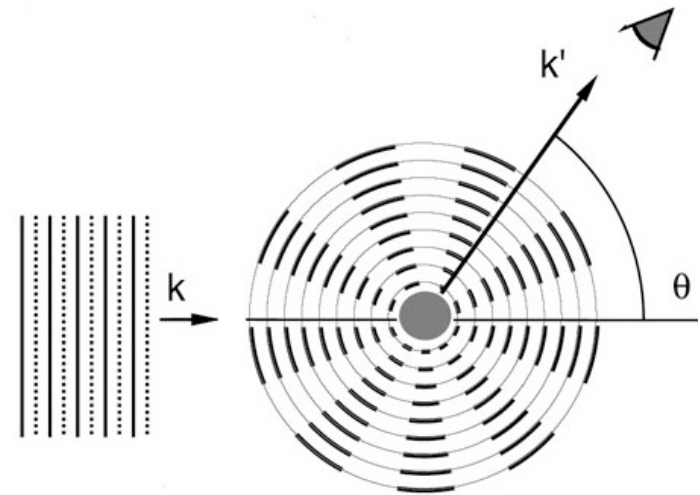
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- In far-field, $|\mathbf{r} - \mathbf{r}'| \simeq r - \hat{\mathbf{e}}_r \cdot \mathbf{r}' + \dots$,

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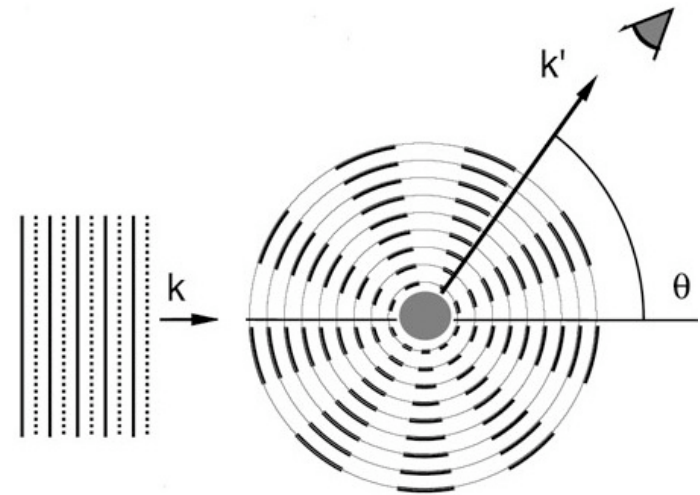
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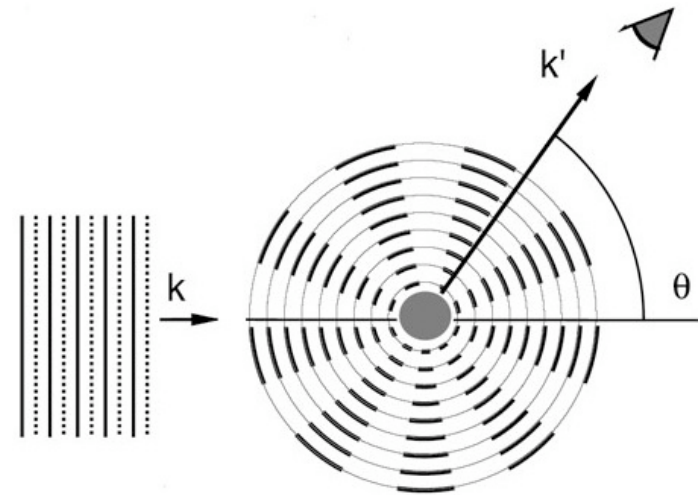
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- The corresponding differential cross-section:

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

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

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

denotes the transition matrix element.

Born approximation

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

- 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 ,

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- and then to second order in U ,

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- i.e. expressed in coordinate-independent basis,

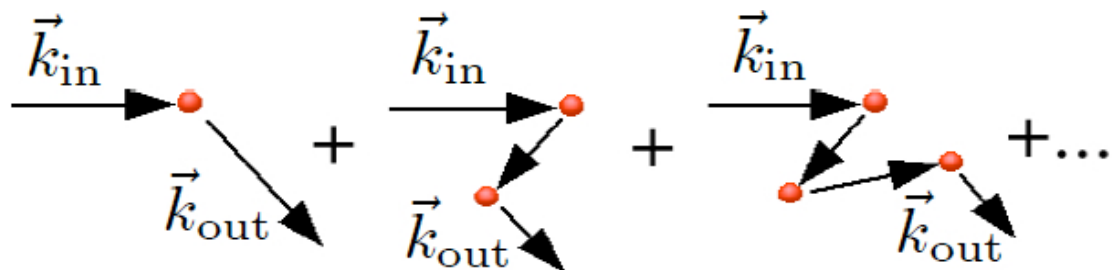
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- Then, making use of the identity $f(\theta, \phi) = -\frac{1}{4\pi} \langle \phi_{\mathbf{k}'} | U | \psi_{\mathbf{k}} \rangle$, scattering amplitude expressed as **Born series** expansion

$$f = -\frac{1}{4\pi} \langle \phi_{\mathbf{k}'} | U + U G_0 U + U G_0 U G_0 U + \cdots | \phi_{\mathbf{k}} \rangle$$



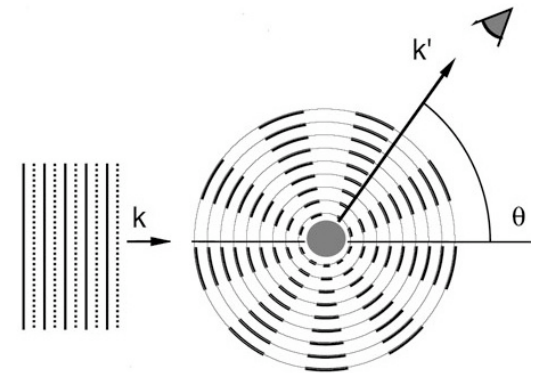
- Physically, incoming particle undergoes a sequence of multiple scattering events from the potential.

Born approximation

$$f = -\frac{1}{4\pi} \langle \phi_{\mathbf{k}'} | U + UG_0 U + UG_0 UG_0 U + \cdots | \phi_{\mathbf{k}} \rangle$$

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

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



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

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

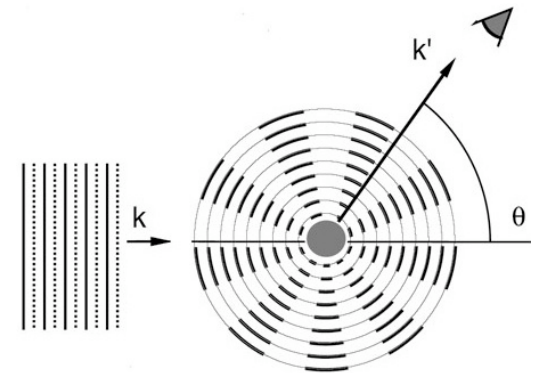
where, noting that $|\mathbf{k}'| = |\mathbf{k}|$, $\Delta = 2k \sin(\theta/2)$.

Born approximation

$$f = -\frac{1}{4\pi} \langle \phi_{\mathbf{k}'} | U + UG_0 U + UG_0 UG_0 U + \cdots | \phi_{\mathbf{k}} \rangle$$

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

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



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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 $\alpha \rightarrow \infty$. For this potential, one may show that (exercise)

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

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

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

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 i and f induced by harmonic perturbation $V e^{i\omega t}$ is given by Fermi's Golden rule,

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} |\langle f | V | i \rangle|^2 \delta(\hbar\omega - (E_f - E_i))$$

- 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

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

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

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From Born approximation to Fermi's Golden rule

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

- With

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

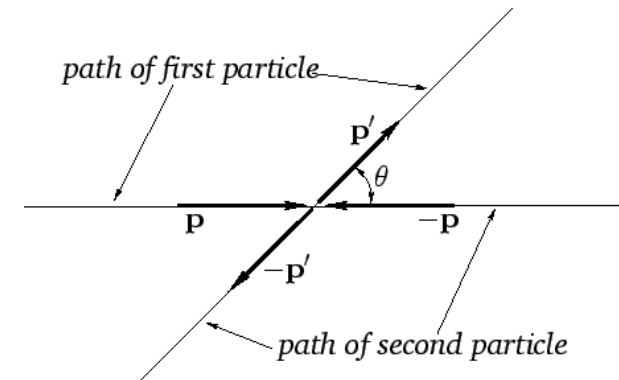
and incident flux $j_I = \hbar k/m$, the differential cross section,

$$\frac{d\sigma}{d\Omega} = \frac{1}{L^3} \frac{\Gamma_{\mathbf{k} \rightarrow \mathbf{k}'}}{j_I} = \frac{1}{(4\pi)^2} |\langle \mathbf{k}' | \frac{2mV}{\hbar^2} | \mathbf{k} \rangle|^2$$

- 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,

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

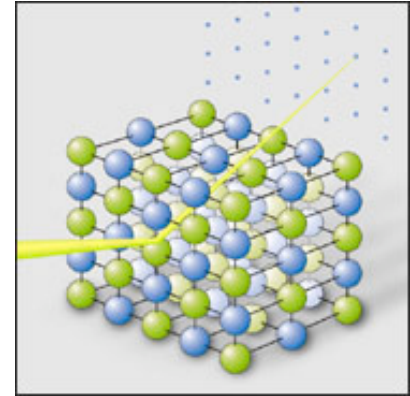
- The differential cross section is then given by

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

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

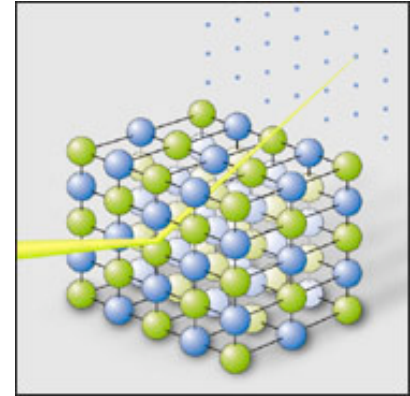
$$\psi(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{R}_i} \left[e^{i\mathbf{k}\cdot\mathbf{r}} + f e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_i} \frac{e^{ikr}}{r} \right]$$

- From this result, we infer effective scattering amplitude,

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

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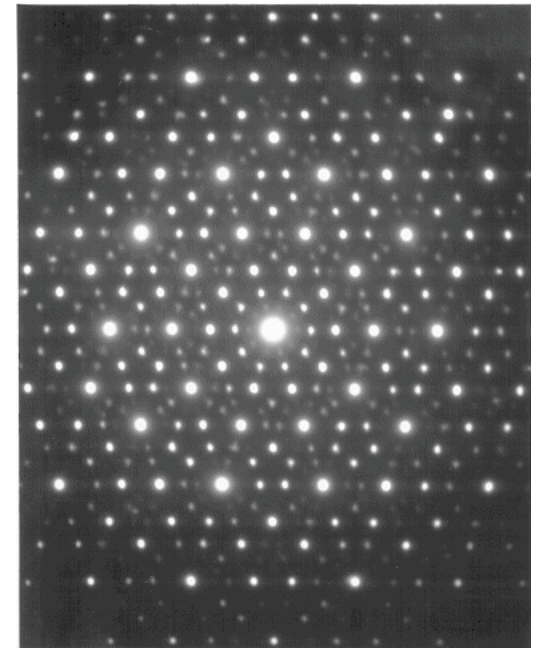
- If we consider scattering from a crystal lattice, we must sum over all atoms leading to the total differential scattering cross-section,

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

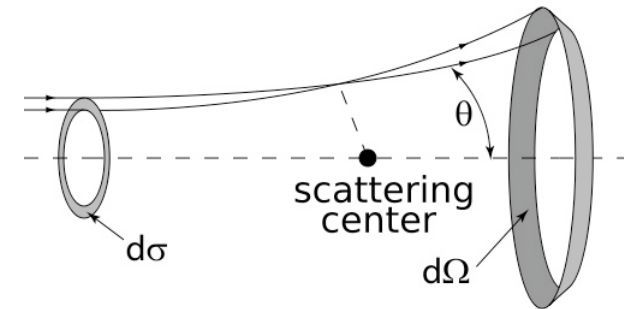
- For periodic cubic crystal of dimension L^d , sum translates to **Bragg condition**,

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

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,

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

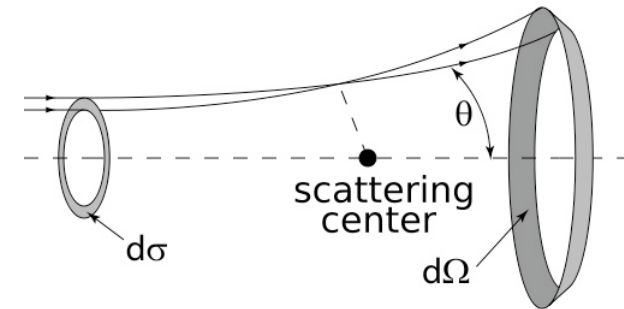
where $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta, \phi) \frac{e^{ikr}}{r}$ denotes scattering wavefunction.

- 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 $\delta_{\ell}(k)$.

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Scattering theory: summary

- The partial amplitudes/phase shifts fully characterise scattering,

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

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

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

- 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,

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

- 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,

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

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