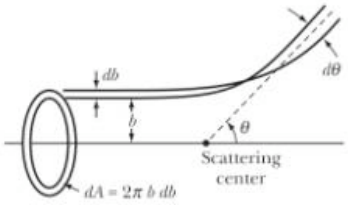
Chapter 14

Scattering theory

Almost everything we know about nuclei and elementary particles has been discovered in scattering experiments, from Rutherford's surprise at finding that atoms have their mass and positive charge concentrated in almost point-like nuclei, to the more recent discoveries, on a far smaller length scale, that protons and neutrons are themselves made up of apparently point-like quarks. More generally, the methods that we have to probe the properties of condensed matter systems rely fundamentally on the notion of scattering. In this section, we will provide a brief introduction to the concepts and methodology of scattering theory.

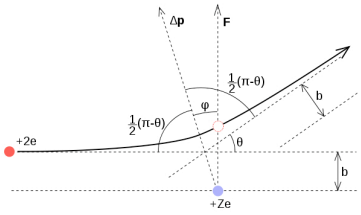
As preparation for the quantum mechanical scattering problem, let us first consider the classical problem. This will allow us to develop (hopefully a revision!) some elementary concepts of scattering theory, and to introduce some notation. In a classical scattering experiment, one considers particles of energy $E = \frac{1}{2}mv_0^2$ (mass m and asymptotic speed v_0), incident upon a target with a central potential $V(r)$. For a repulsive potential, particles are scattered through an angle θ (see figure). The **scattering cross-section**, σ, can be inferred from the number of particles dn scattered into some element of solid angle, $d\Omega$, at angle $(\theta,\ \phi)$, i.e. for an incident flux j_i (number of particles per unit time per unit area), $dn = j_\mathrm{i}\sigma\, d\Omega$. The total cross-section is then obtained as $\sigma_T = \int d\Omega\, \sigma(\theta,\phi) = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi\, \sigma(\theta,\phi)$. The angle of deflection of the beam depends on the impact parameter, b (see figure right). We therefore have that $dn = j_\mathrm{i} b db\, d\phi = j_i \sigma \sin\theta d\theta d\phi$ and



$$\boxed{\sigma(\theta,\phi) = \frac{b}{\sin\theta}\frac{db}{d\theta}\,.}$$

▷ Example: Let us consider then the case of **classical Coulomb scattering** from a repulsive potential $V(r) = \frac{\kappa}{r}$ where $\kappa > 0$. From classical physics, we know that the particle will follow a hyperbolic trajectory with

$$r = \frac{L^2}{m\kappa(e\cos\varphi - 1)}\,,$$



where $\mathbf{r} = (r,\varphi)$ parameterises the relative coordinates of the particle and target,[1] and $e = (1 + \frac{2EL^2}{\kappa^2 m})^{1/2} > 1$ denotes the eccentricity. Since the potential is central, the angular momentum L is conserved and can be fixed asymptotically by the condition $L = mv_0 b$.

To obtain the scattering angle, θ, we can use the relation above to find the limiting angle, $\cos\varphi_0 = 1/e$, where $\varphi_0 = (\pi - \theta)/2$. We therefore have $\tan(\theta/2) = \cot\varphi_0 =$

[1] Note that the angle φ is distinct form the azimuthal angle ϕ associated with the axis of scattering.

$1/\sqrt{e^2-1} = (\frac{m\kappa^2}{2EL^2})^{1/2} = \frac{\kappa}{2Eb}$. Then, from this relation, we obtain the cross-section

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

known as the **Rutherford formula**.

14.1 Basics

Let us now turn to the quantum mechanical problem of a beam of particles incident upon a target. The potential of the target, $V(r)$, might represent that experienced by a fast electron striking an atom, or an α particle colliding with a nucleus. As in the classical problem, the basic scenario involves directing a stream or flux of particles, all at the same energy, at a target and detect how many particles are deflected into a battery of detectors which measure angles of deflection. In principle, if we assume that all the in-going particles are represented by wavepackets of the same shape and size, our challenge is to solve the full time-dependent Schrödinger equation for such a wavepacket,

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

and find the probability amplitudes for out-going waves in different directions at some later time after scattering has taken place. However, if the incident beam of particles is switched on for times very long as compared with the time a particle would take to cross the interaction region, steady-state conditions apply. Moreover, if we assume that the wavepacket has a well-defined energy (and hence momentum), so it is many wavelengths long, and we may consider it a plane wave. Setting $\Psi(\mathbf{r},t) = \psi(\mathbf{r})e^{-iEt/\hbar}$, we may therefore look for solutions $\psi(\mathbf{r})$ of the time-*independent* Schrödinger equation,

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

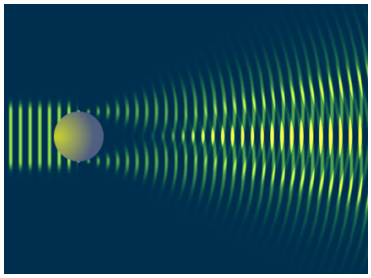
subject to the boundary condition that the incoming component of the wavefunction is a plane wave, $e^{i\mathbf{k}\cdot\mathbf{x}}$. Here $E = \mathbf{p}^2/2m = \hbar^2\mathbf{k}^2/2m$ denotes the energy of the incoming particles while their flux is given by

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

In the one-dimensional geometry, the impact of a plane wave with the localized target resulted in a portion of the wave being reflected and a portion transmitted through the potential region. From energy conservation, we may deduce that both components of the outgoing scattered wave are plane waves with wavevector $\pm k$, while the influence of the potential are encoded in the amplitude of the reflected and transmitted beams, and a potential phase shift. Both amplitudes and phase shifts are then determined by solving the time-independent Schrödinger equation subject to the boundary conditions which ensure energy and flux conservation. In the three-dimensional system, the phenomenology is similar: In this case, the wavefunction well outside the localized target region will involve a superposition of the incident plane wave and the scattered (spherical wave),[2]

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

[2]Here, by localized, we mean a potential which is sufficiently short-ranged. At this stage, it is not altogether clear what constraint this implies. But it will turn out that it excludes the Coulomb potential!



where the function $f(\theta, \phi)$ records the relative amplitude and phase of the scattered components along the direction (θ, ϕ) relative to the incident beam.

To place these ideas on a more formal footing, consider the following: If we define the direction of the incoming wave $\mathbf{k}$ to lie along the z-axis, a plane wave can be recast in the form of an incoming and an outgoing spherical wave,

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

where $P_\ell(\cos\theta) = (\frac{4\pi}{2\ell+1})^{1/2} Y_{\ell 0}(\theta)$ denote the Legendre polynomials. If we assume that the potential perturbation, $V(r)$ depends only on the radial coordinate (i.e. that it is spherically symmetric) and that the number of particles are conserved by the potential (the flux of incoming particles is matched by the flux of outgoing),[3] when the potential is sufficient short-ranged (decreasing faster than $1/r$), the scattering wavefunction takes the *asymptotic* form

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

subject to the constraint $|S_\ell(k)| = 1$ following from the conservation of particle flux (i.e. $S_\ell(k) = e^{2i\delta_\ell(k)}$). Physically, the incoming component of the spherical wave is undisturbed by the potential while the separate components of the outgoing spherical wave are subject to a set of phase shifts, $\delta_\ell(k)$. Recast in the form of a perturbation, the asymptotic form of the wavefunction can be straightforwardly rewritten as

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

where the second component of the wavefunction denotes the change in the outgoing spherical wave due to the potential, and

$$\boxed{f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1) f_{\ell}(k) P_{\ell}(\cos\theta)\,,} \tag{14.1}$$

with the coefficents $f_\ell(k) = \frac{1}{2ik}(S_\ell(k) - 1)$ defining the **partial wave scattering amplitudes**.

The corresponding asymptotic flux is then given by

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

In general, an expansion then leads to a formidible collection of contributing terms. However, for most of these contributions, there remains an exponential factor, $e^{\pm ikr(1-\cos\theta)}$ where θ denotes the angle between $\mathbf{k}$ and $\mathbf{r}$. For $r \to \infty$, the small angular integration implied by any physical measurement leads to a fast oscillation of this factor. As a result, such terms are strongly suppressed and can be neglected. Retaining only those terms where the phase cancellation is complete, one obtains,

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

[3]Note that this assumption is not innocent. In a typical high energy physics experiment, the collision energies are high enough to lead to particle production.

The first term represents the incident flux, while the remainder describes the radial flux of scattered particles. In particular, the number of particles crossing the area that subtends a solid angle $d\Omega$ at the origin (the target) is given by

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

Dropping terms of order $1/r$, negligible in the asymptotic limit, one thus obtains the **differential cross-section**, the ratio of the scattered flux to the incident flux, $d\sigma = \frac{m}{\hbar k}\mathbf{j}\cdot\hat{\mathbf{e}}_r dA = |f(\theta)|^2\, d\Omega$, i.e.

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

The total cross-section is then given by $\sigma_{\rm tot} = \int d\sigma = \int |f(\theta)|^2 d\Omega$. Then, making use of the identity $\int d\Omega P_\ell(\cos\theta)P_{\ell'}(\cos\theta) = \frac{4\pi}{2\ell+1}\delta_{\ell\ell'}$, and Eq. (14.1) one obtains (exercise)

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

In particular, noting that $P_\ell(1) = 1$, from Eq. (14.1) it follows that $\mathrm{Im}\, f(0) = \frac{k}{4\pi}\sigma_{\rm tot}$, a relation known as the **optical theorem**.

14.2 Method of partial waves

Having established the basic concepts for the scattering problem, we turn now to consider operationally how the scattering characteristics can be computed. Here, for simplicity, we will focus on the properties of a centrally symmetric potential, $V(r)$, where the scattering wavefunction, $\psi(\mathbf{r})$ (and indeed that scattering amplitudes, $f(\theta)$) must be symmetrical about the axis of incidence, and hence independent of the azimuthal angle, ϕ. In this case, the wavefunction can be expanded in a series of Legendre polynomials,

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

Each term in the series is known as a **partial wave**, and is a simultaneous eigenfunction of the angular momentum operators $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ having eigenvalue $\hbar^2\ell(\ell+1)$ and 0 respectively. Following standard spectroscopic notation, $\ell = 0, 1, 2, \cdots$ are referred to as $s, p, d, \cdots$ waves. The **partial wave amplitudes**, f_ℓ are determined by the radial functions, $R_\ell(r)$, defined by

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

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

▷ Example: To develop the partial wave scattering method, we will consider the problem of quantum **scattering from an attractive square well potential**, $U(r) = -U_0\theta(R-r)$. In this case, the radial wave equation takes the form

$$\left[\partial_r^2 + \frac{2}{r}\partial_r - \frac{\ell(\ell+1)}{r^2} + U_0\theta(R-r) + k^2\right]R_\ell(r) = 0\,.$$

At high energies, many channels contribute to the total scattering amplitude. However, at low energies, the scattering is dominated by the s-wave ($\ell = 0$) channel. In this case, setting $u(r) = rR_0(r)$, the radial equation takes the simple form, $(\partial_r^2 + U_0\theta(R-r) + k^2)u(r) = 0$, with the boundary condition that $u(0) = 0$. We therefore obtain the solution

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

where $K^2 = k^2 + U_0 > k^2$. The continuity condition of the wavefunction and its derivative at $r = R$ translates to the relation $K\cot(KR) = k\cot(kR + \delta_0)$. From this expression, we obtain the $\ell = 0$ phase shift, $\delta_0 = \tan^{-1}(\frac{k}{K}\tan(KR)) - kR$,[4] i.e.

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

Then, unless $\tan(KR) = \infty$ (see below), an expansion at low energy (small k) obtains $\delta_0 \simeq kR(\frac{\tan(KR)}{KR} - 1)$, and the $\ell = 0$ partial cross-section,

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0(k) = \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0(k)} \simeq \frac{4\pi}{k^2}\delta_0^2 = 4\pi R^2\left(\frac{\tan(KR)}{KR} - 1\right)^2.$$

From this result, we find that when $\frac{\tan(KR)}{KR} = 1$, the scattering cross-section vanishes.

An expansion in small k obtains

$$\boxed{k\cot\delta_0 = -\frac{1}{a_0} + \frac{1}{2}r_0k^2 + \cdots,}$$

where $a_0 = (1 - \frac{\tan\gamma}{\gamma})R$, with $\gamma = U_0^{1/2}R$, defines the **scattering length**, and r_0 is the effective range of the interaction. At low energies, $k \to 0$, the scattering cross-section, $\sigma_0 = 4\pi a_0^2$ is fixed by the scattering length alone. If $\gamma \ll 1$, a_0 is negative. As γ is increased, when $\gamma = \pi/2$, both a_0 and σ_0 diverge – there is said to be a zero energy resonance. This condition corresponds to a potential well that is just able to support an s-wave bound state. If γ is further increased, a_0 turns positive – as it would be for an effective repulsive interaction until $\gamma = \pi$ when $\sigma_0 = 0$ and the process repeats with the appearance of a second bound state at $\gamma = 3\pi/2$, and so on.

More generally, the ℓ-th partial cross-section

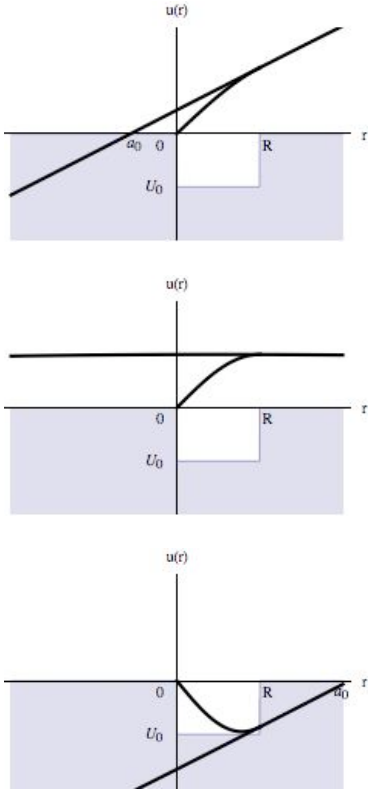
$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\frac{1}{1+\cot^2\delta_\ell(k)},$$

takes its maximum value is there is an energy at which $\cot\delta_\ell$ vanishes. If this occurs as a result of $\delta_\ell(k)$ increasing rapidly through an odd multiple of $\pi/2$, the cross-section exhibits a narrow peak as a function of energy and there is said to be a **resonance**. Near the resonance,

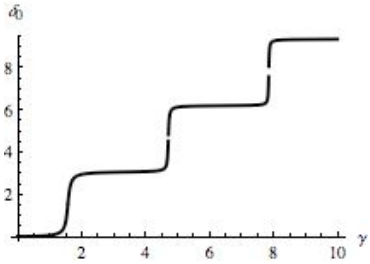
$$\cot\delta_\ell(k) = \frac{E_R - E}{\Gamma(E)/2},$$

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

$$\boxed{\sigma_\ell(E) = \frac{4\pi}{k^2}(2\ell+1)\frac{\Gamma^2(E_R)/4}{(E-E_R)^2 + \Gamma^2(E_R)/4}.} \qquad (14.2)$$



Scattering wavefunction, $u(r)$, for three-dimensional square well potential for $kR = 0.1$ and $\gamma = 1$ (top), $\pi/2$ (middle) and 2 (bottom). Note that the scattering length, a_0 changes from negative to positive as system passes through bound state.



Scattering phase shift for $kR = 0.1$ as a function of γ.

[4] More generally, choosing the solution to be finite at the origin, we find that

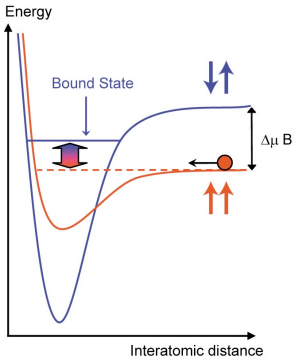
$$R_\ell(r) = N_\ell(K)j_\ell(Kr), \qquad r < R,$$

where $N_\ell(K)$ is a normalization constant. In the exterior region, the general solution can be written as $R_\ell(r) = B_\ell(k)[j_\ell(kr) - \tan\delta_\ell(k)\eta_\ell(kr)]$. Continuity of R_ℓ and the derivative $\partial_r R_\ell$ at the boundary, $r = R$, lead to the following expression for the phase shifts

$$\tan\delta_\ell(k) = \frac{kj'_\ell(kR)j_\ell(KR) - Kj_\ell(kR)j'_\ell(KR)}{k\eta'_\ell(kR)j_\ell(KR) - K\eta_\ell(kR)j'_\ell(KR)}.$$

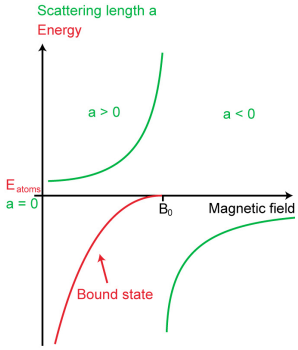
Here $j'_\ell(x) = \partial_x j_\ell(x)$ and similarly η'_ℓ.

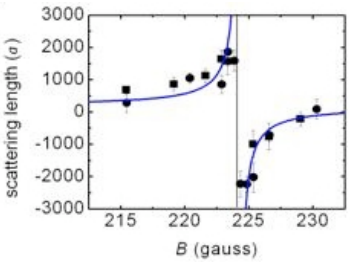
▷ EXERCISE. For a hard-core interaction, $U(r) = U_0\theta(R-r)$, with $U_0 \to \infty$, show that at low energy $\delta_0 = -kR$. As $k \to 0$, show that the differential cross-section is isotropic and given by $\frac{d\sigma}{d\Omega} = R^2$ and $\sigma_{\rm tot} \overset{k\to 0}{\to} 4\pi R^2$.



▷ INFO. Ultracold atomic gases provide a topical arena in which resonant scattering phenomena are exploited. In particular, experimentalists make use of **Feshbach resonance** phenomena to tune the effective interaction between atoms. This tunability arises from the coupling of free unbound atoms to a molecular state in which the atoms are tightly bound. The closer this molecular level lies with respect to the energy of two free atoms, the stronger the interaction between them. In the example on the left, the two free atoms are both "spin up", whereas the molecular state is a "singlet", in which the atoms have opposite spin, adding up to zero total magnetic moment. Thus, a magnetic field shifts the energies of two free atoms relative to the molecular state and thereby controls the interatomic interaction strength.

The interaction between two atoms can be described by the scattering length, shown right as a function of magnetic field close to a Feshbach resonance. On the side where the scattering length is positive, the molecular energy level is lower in energy than the energy of two unbound atoms. The molecular state is thus "real" and stable, and atoms tend to form molecules. If those atoms are fermions, the resulting molecule is a boson. A gas of these molecules can thus undergo Bose-Einstein condensation (BEC). This side of the resonance is therefore called "BEC-side". On the side of the resonance where the scattering length is negative, isolated molecules are unstable. Nevertheless, when surrounded by the medium of others, two fermions can still form a loosely bound pair, whose size can become comparable to or even larger than the average distance between particles. A Bose-Einstein condensate of these fragile pairs is called a "BCS-state", after Bardeen, Cooper and Schrieffer. This is what occurs in superconductors, in which current flows without resistance thanks to a condensate of electron pairs ("Cooper pairs").





14.3 The Born approximation

The partial wave expansion is tailored to the consideration of low-energy scattering processes. At higher energies, when many partial waves contribute, the expansion is not very convenient and it is helpful to develop a different methodology. By developing a general expansion of the scattering wavefunction, $\psi_{\mathbf{k}}(\mathbf{r})$, in terms of the Green function of the scattering potential one may show that,

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int d^3r'\,\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,.} \tag{14.3}$$

Here the subscript $\mathbf{k}$ reminds us that the solution is for a particular incoming plane wave. This integral representation of the scattering wavefunction, known as the Lippmann-Schwinger equation, provides a more useful basis to address situations where the energy of the incoming particles is large and the scattering potential is weak. The elements of the derivation of this equation are summarised in the info box below:

▷ INFO. **Lippmann-Schwinger equation:** For the time-independent Schrödinger

equation $(\nabla^2 + k^2)\psi(\mathbf{r}) = U(\mathbf{r})\psi(\mathbf{r})$, the general solution can be written formally as

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

where $\phi(\mathbf{r})$ is a solution of the homogeneous (free particle) Schrödinger equation, $(\nabla^2 + k^2)\phi(\mathbf{r}) = 0$, and $G_0(\mathbf{r},\mathbf{r}')$ is a Green function of the Laplace operator, $(\nabla^2 + k^2)G_0(\mathbf{r},\mathbf{r}') = \delta^3(\mathbf{r}-\mathbf{r}')$. From the asymptotic behaviour of the boundary condition, it is evident that $\phi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$. In the Fourier basis, the Green function is diagonal and given by $G_0(\mathbf{k},\mathbf{k}') = (2\pi)^3\delta^3(\mathbf{k}-\mathbf{k}')\frac{1}{k^2}$. Transformed back into real space, we have

$$G_0(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\,.$$

Substituted back into the expression for the scattering wavefunction, we obtain the Lippmann-Schwinger equation (14.3).

In the far-field region, $|\mathbf{r}-\mathbf{r}'| \simeq r - \hat{\mathbf{r}}\cdot\mathbf{r}' + \cdots$, i.e.

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

where the vector $\mathbf{k}' = k\hat{\mathbf{e}}_r$ is oriented along the direction of the scattered particle. We therefore find that the scattering wavefunction $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}$ can be expressed in integral form, with the scattering amplitude given by

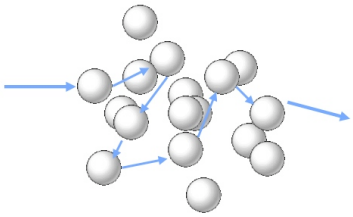
$$\boxed{f(\theta,\phi) = -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U|\psi_{\mathbf{k}}\rangle \equiv -\frac{1}{4\pi}\int d^3r'\, e^{-i\mathbf{k}'\cdot\mathbf{r}}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')\,.} \qquad (14.4)$$

The corresponding differential cross-section can then be expressed as

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

where, cast in terms of the original scattering potential, $V(\mathbf{r}) = \hbar^2U(\mathbf{r})/2m$, $T_{\mathbf{k},\mathbf{k}'} = \langle\phi_{\mathbf{k}'}|V|\psi_{\mathbf{k}}\rangle$ denotes the transition matrix element.

Eq. (14.3) provides a natural means to expand the scattering wavefunction in powers of the interaction potential. At zeroth order in V, the scattering wavefunction is specified by the unperturbed incident plane wave, $\phi^{(0)}_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r})$. Using this approximation, Eq. (14.3) leads to the first order correction,



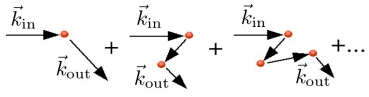
$$\psi^{(1)}_{\mathbf{k}}(\mathbf{r}) = \phi_{\mathbf{k}}(\mathbf{r}) + \int d^3r'\, G_0(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi^{(0)}_{\mathbf{k}}(\mathbf{r}')\,.$$

From this equation, we can use (14.3) to obtain the next term in the series,

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

and so on, i.e.

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



Physically, an incoming particle undergoes a sequence of multiple scattering events from the potential (see schematic on the right). This series expansion is

known as the **Born series**, and the leading term in known as the **first Born approximation** to the scattering amplitude,

$$\boxed{f_{\text{Born}} = -\frac{1}{4\pi}\langle\phi_{\mathbf{k}'}|U|\phi_{\mathbf{k}}\rangle\,.} \tag{14.5}$$

Setting $\boldsymbol{\Delta} = \mathbf{k} - \mathbf{k}'$, where $\hbar\boldsymbol{\Delta}$ denotes the momentum transfer, the Born scattering amplitude for a central potential is given by (exercise)

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

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

Coulomb scattering: Due to the 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) $f_{\text{Born}} = -U_0/(\alpha^{-2} + \Delta^2)$. Therefore, for $\alpha \to \infty$, we obtain

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

which is just the Rutherford formula.

▷ INFO. Previously, we have used time-dependent perturbation theory to develop an expression for the transition rate between states. In the leading order of perturbation theory, we found that the transition rate between states and i and f induced by a potential V is given by Fermi's Golden rule,

$$\Gamma_{\text{i}\to\text{f}} = \frac{2\pi}{\hbar}|\langle\text{f}|V|\text{i}\rangle|^2\delta(E - (E_{\text{f}} - E_{\text{i}}))\,.$$

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 $\mathbf{k}'$. In this case, the total transition (or scattering) rate into a fixed solid angle, $d\Omega$, is given by

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

where $g(E) = \frac{dn}{dE}$ denotes the density of states and both states $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ have energy $E = \hbar^2k^2/2m = \hbar^2k'^2/2m$ – they are said to be "on-shell". As a result, we obtain the density of states $g(E) = \frac{dn}{dk}\frac{dk}{dE} = \frac{k^2d\Omega}{(2\pi/L)^3}\frac{m}{\hbar^2k}$ while the incident flux per unit volume is given by $\hbar k/mL^3$. As a result, we obtain the scattering cross-section, $\frac{d\sigma}{d\Omega} = \frac{\Gamma_{\mathbf{k}\to\mathbf{k}'}}{\hbar k/mL^3}$

$$\frac{d\sigma}{d\Omega} = \frac{1}{(4\pi)^2}|\langle\mathbf{k}'|\frac{2mV}{\hbar^2}|\mathbf{k}\rangle|^2\,.$$

We can therefore recognize that **Fermi's Golden rule is equivalent to the first order Born approximation.**

14.4 INFO: Scattering of identical particles

Until now, we have assumed that the particles involved in the scattering process, the incoming particle and the target, are distinguishable. However, very often we are interested in the scattering of identical quantum particles. In such cases, we

have to consider the influence of quantum statistics on the scattering process. As a preliminary exercise, consider the classical picture of scattering between two identical positively charged particles, e.g. α-particles viewed in the center of mass frame. If an outgoing α particle is detected at an angle θ to the path of the ingoing α-particle, it could be (a) deflected through an angle θ, or (b) deflected through $\pi - \theta$. Classically, we could tell which one it was by watching the collision as it happened, and keeping track. However, in a quantum mechanical scattering process, we cannot keep track of the particles unless we bombard them with photons having wavelength substantially less than the distance of closest approach. This is just like detecting an electron at a particular place when there are two electrons in a one dimensional box: the probability *amplitude* for finding an α particle coming out at angle θ to the ingoing direction of one of them is the sum of the amplitudes (not the sum of the probabilities!) for scattering through θ and $\pi - \theta$.

Writing the asymptotic scattering wavefunction in the standard form for scattering from a fixed target, $\psi(\mathbf{r}) \approx e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$, the two-particle wavefunction in the center of mass frame, in terms of the relative coordinate, is given by symmetrizing:

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

How does the particle symmetry affect the actual scattering rate at an angle θ? If the particles were distinguishable, the differential cross section would be $(\frac{d\sigma}{d\Omega})_{\text{dist.}} = |f(\theta)|^2 + |f(\pi - \theta)|^2$, but quantum mechanically we must compute,

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{indist.}} = |f(\theta) + f(\pi - \theta)|^2\,.$$

This makes a big difference! For example, for scattering through 90^o, where $f(\theta) = f(\pi - \theta)$, the quantum mechanical scattering rate is *twice* the classical (distinguishable) prediction.

Furthermore, if we make the standard expansion of the scattering amplitude $f(\theta)$ in terms of partial waves, $f(\theta) = \sum_{\ell=0}^{\infty}(2\ell + 1)a_\ell P_\ell(\cos\theta)$, then

$$f(\theta) + f(\pi - \theta) = \sum_{l=0}^{\infty}(2\ell + 1)a_\ell\,(P_\ell(\cos\theta) + P_\ell(\cos(\pi - \theta)))\,.$$

Since $P_\ell(-x) = (-1)^\ell P_\ell(x)$, the scattering only takes place in even partial wave states. This is the same thing as saying that the overall wavefunction of two identical bosons is symmetric. So, if they are in an eigenstate of total angular momentum, from $P_\ell(-x) = (-1)^\ell P_\ell(x)$ it has to be a state of even ℓ.

For fermions in an antisymmetric spin state, such as proton-proton scattering with the two proton spins forming a singlet, the spatial wavefunction is symmetric, and the argument is the same as for the boson case above. For *parallel* spin protons, however, the spatial wavefunction has to be *antisymmetric*, and the scattering amplitude will then be $f(\theta) - f(\pi - \theta)$. In this case there is zero scattering at 90^o! Note that for (non-relativistic) equal mass particles, the scattering angle in the center of mass frame is twice the scattering angle in the fixed target (lab) frame.

14.5 Scattering by an atomic lattice

Finally, to close this section, let us say a few words about scattering phenomena in solid state systems. If we ignore spin degrees of freedom, so that we do not have to worry whether an electron does or does not flip its spin during the scattering process, then at low energies, the scattering amplitude of particles from a crystal $f(\theta)$ becomes 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,

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

Now, since

$$k|\mathbf{r}-\mathbf{R}_i| = k\left(\mathbf{r}^2 - 2\mathbf{r}\cdot\mathbf{R}_i + \mathbf{R}_i^2\right)^{1/2} \simeq kr\left(1 - \frac{2\mathbf{r}\cdot\mathbf{R}_i}{r^2}\right)^{1/2} \simeq kr - k\hat{\mathbf{e}}_r\cdot\mathbf{R}_i\,,$$

and $k\hat{\mathbf{e}}_r = \mathbf{k}'$, we have

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

As a result, we can deduce the effective scattering amplitude,

$$f(\theta) = fe^{-i\boldsymbol{\Delta}\cdot\mathbf{R}_i}, \qquad \boldsymbol{\Delta} = \mathbf{k}'-\mathbf{k}\,.$$

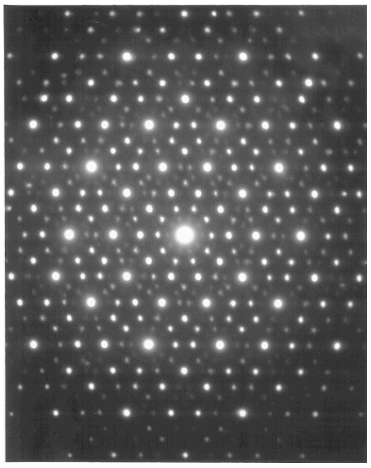
If we consider scattering from a crystal lattice, we must sum over all atoms. In this case, the total differential scattering cross-section is given by

$$\frac{d\sigma}{d\Omega} = \left|f\sum_{\mathbf{R}_i} e^{-i\boldsymbol{\Delta}\cdot\mathbf{R}_i}\right|^2.$$

In the case of a periodic crystal, the sum over atoms translates to the **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 L represents the size of the (cubic) lattice, and $\mathbf{n}$ denote a vector of integers – the **Miller indices of the Bragg planes**. We therefore expect that the differential cross-section is very small expect when $\mathbf{k}'-\mathbf{k} = 2\pi\mathbf{n}/L$. These relations can be generalised straightforwardly to address more complicated crystal structures.



X-ray diffraction pattern of a quasi-crystal.