Scattering Theory

Historically, data regarding quantum phenomena has been obtained from two main sources--the study of spectroscopic lines, and scattering experiments.

We have already developed theories which account for some aspects of the spectra of hydrogen-like atoms.

Let us now examine the quantum theory of scattering.

The Lipmann-Schwinger equation

Consider time-independent scattering theory, for which the Hamiltonian of the system is written

$$H = H_0 + H_1, \tag{7.1}$$

where H_0 is the Hamiltonian of a free particle of mass m,

$$H_0 = \frac{p^2}{2\,m}, \tag{7.2}$$

and H_1 represents the non-time-varying source of the scattering. Let $|\phi\rangle$ be an energy eigenket of H_0,

$$H_0\,|\phi\rangle = E\,|\phi\rangle, \tag{7.3}$$

whose wave-function $\langle \mathbf{r}'|\phi\rangle$ is $\phi(\mathbf{r}')$. This state is a plane-wave state or, possibly, a spherical-wave state. Schrödinger's equation for the scattering problem is

$$(H_0 + H_1)|\psi\rangle = E\,|\psi\rangle, \tag{7.4}$$

where $|\psi\rangle$ is an energy eigenstate of the total Hamiltonian whose wave-function $\langle \mathbf{r}'|\psi\rangle$ is $\psi(\mathbf{r}')$. In general, both H_0 and $H_0 + H_1$ have continuous energy spectra: *i.e.*, their energy eigenstates are unbound. We require a solution of Eq. (7.4) which satisfies the boundary condition $|\psi\rangle \to |\phi\rangle$ as $H_1 \to 0$. Here, $|\phi\rangle$ is a solution of the free particle Schrödinger equation, (7.3), corresponding to the same energy eigenvalue.

Formally, the desired solution can be written

$$|\psi\rangle = |\phi\rangle + \frac{1}{E - H_0} H_1 |\psi\rangle. \tag{7.5}$$

Note that we can recover Eq. (7.4) by operating on the above equation with $E - H_0$, and making use of Eq. (7.3). Furthermore, the solution satisfies the boundary condition $|\psi\rangle \to |\phi\rangle$ as $H_1 \to 0$. Unfortunately, the operator $(E - H_0)^{-1}$ is *singular*: *i.e.*, it produces infinities when it operates on an eigenstate of H_0 corresponding to the eigenvalue E. We need a prescription for dealing with these infinities, otherwise the above solution is useless. The standard prescription is to make the energy eigenvalue E slightly complex. Thus,

$$|\psi^{\pm}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\,\epsilon} H_1 |\psi^{\pm}\rangle, \tag{7.6}$$

where ϵ is real, positive, and small. Equation (7.6) is called the *Lipmann-Schwinger equation*, and is non-singular as long as $\epsilon > 0$. The physical significance of the $\pm$ signs will become apparent later on.

The Lipmann-Schwinger equation can be converted into an *integral equation* via left multiplication by $\langle \mathbf{r}|$. Thus,

$$\psi^{\pm}(\mathbf{r}) = \phi(\mathbf{r}) + \int \left\langle \mathbf{r} \left| \frac{1}{E - H_0 \pm i\,\epsilon} \right| \mathbf{r}' \right\rangle \langle \mathbf{r}'|H_1|\psi^{\pm}\rangle \, d^3\mathbf{r}'. \tag{7.7}$$

Adopting the Schrödinger representation, we can write the scattering problem (7.4) in the form

$$(\nabla^2 + k^2)\,\psi(\mathbf{r}) = \frac{2\,m}{\hbar^2}\langle \mathbf{r}|H_1|\psi\rangle, \tag{7.8}$$

where

$$E = \frac{\hbar^2 k^2}{2\,m}. \tag{7.9}$$

This equation is called *Helmholtz's equation*, and can be inverted using standard Green's function techniques. Thus,

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + \frac{2\,m}{\hbar^2}\int G(\mathbf{r}, \mathbf{r}')\langle \mathbf{r}'|H_1|\psi\rangle \, d^3\mathbf{r}', \tag{7.10}$$

where

$$(\nabla^2 + k^2)\, G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'). \tag{7.11}$$

Note that the solution (7.10) satisfies the boundary condition $|\psi\rangle \rightarrow |\phi\rangle$ as $H_1 \rightarrow 0$. As is well-known, the Green's function for the Helmholtz problem is given by

$$G(\mathbf{r}, \mathbf{r}') = -\frac{\exp(\pm i\, k\, |\mathbf{r} - \mathbf{r}'|)}{4\pi\, |\mathbf{r} - \mathbf{r}'|}. \tag{7.12}$$

Thus, Eq. (7.10) becomes

$$\psi^{\pm}(\mathbf{r}) = \phi(\mathbf{r}) - \frac{2\, m}{\hbar^2} \int \frac{\exp(\pm i\, k\, |\mathbf{r} - \mathbf{r}'|)}{4\pi\, |\mathbf{r} - \mathbf{r}'|}\, \langle \mathbf{r}' | H_1 | \psi \rangle\, d^3\mathbf{r}'. \tag{7.13}$$

A comparison of Eqs. (7.7) and (7.13) suggests that the kernel to Eq. (7.7) takes the form

$$\left\langle \mathbf{r} \left| \frac{1}{E - H_0 \pm i\, \epsilon} \right| \mathbf{r}' \right\rangle = -\frac{2\, m}{\hbar^2}\, \frac{\exp(\pm i\, k\, |\mathbf{r} - \mathbf{r}'|)}{4\pi\, |\mathbf{r} - \mathbf{r}'|}. \tag{7.14}$$

It is not entirely clear that the $\pm$ signs correspond on both sides of this equation. In fact, they do, as is easily proved by a more rigorous derivation of this result.

$$\psi^{\pm}(\mathbf{r}) = \phi(\mathbf{r}) + \int \left\langle \mathbf{r} \left| \frac{1}{E - H_0 \pm i\, \epsilon} \right| \mathbf{r}' \right\rangle \langle \mathbf{r}' | H_1 | \psi^{\pm} \rangle\, d^3\mathbf{r}'. \tag{7.7}$$

Green's Functions Method

$$L(x)u(x) = f(x)$$

$$u(x) = L^{-1}(x)f(x)$$

$$LL^{-1} = L^{-1}L = 1$$

we define the inverse operator as

$$L^{-1}f = \int dx' G(x;x')f(x')$$

where the kernel *G(x;x')* is the *Green's Function* associated with the differential operator *L*

Note that *G(x;x')* is a two-point function which depends on *x* and *x'*

The Green's function *G(x;x')* then satisfies

$$L(x)G(x;x') = \delta(x-x')$$

The solution can then be written in terms of the Green's function as

$$u(x) = \int dx' G(x;x')f(x')$$

$$\begin{aligned} Lu(x) &= L\int dx' G(x;x')f(x') \\ &= \int dx' LG(x;x')f(x') \\ &= \int dx' \delta(x-x')f(x') \\ &= f(x) \end{aligned}$$

Green's Function for Laplace's Equation

$$L(x)u(x) = f(x) \qquad L(x)G(x;x') = \delta(x-x') \qquad u(x) = \int dx' G(x;x') f(x')$$

$$\int_V \nabla\cdot\hat{A}\, dV = \int_S \hat{A}\cdot d\hat{\sigma}. \qquad A = \phi\nabla\psi - \psi\nabla\phi$$

$$\nabla\cdot\hat{A} = \nabla\cdot(\phi\nabla\psi - \psi\nabla\phi) = (\nabla\phi)\cdot(\nabla\psi) + \phi\nabla^2\psi - (\nabla\phi)\cdot(\nabla\psi) - \psi\nabla^2\phi = \phi\nabla^2\psi - \psi\nabla^2\phi.$$

$$\int_V (\phi\nabla^2\psi - \psi\nabla^2\phi)dV = \int_S (\phi\nabla\psi - \psi\nabla\phi)\cdot d\hat{\sigma}. \qquad LG(x,x') = \nabla^2 G(x,x') = \delta(x-x').$$

$$\nabla^2\Phi(x) = \rho(x) \qquad \Phi(x) \longrightarrow \Phi(x) \qquad \psi \longrightarrow G(x;x') \Rightarrow \qquad \nabla^2\psi = \delta(x-x')$$

$$\int_V \phi(x')\delta(x-x') - G(x,x')\nabla^2\phi(x')\, d^3x' = \int_S [\phi(x')\nabla' G(x,x') - G(x,x')\nabla'\phi(x')]\cdot d\hat{\sigma}'$$

$$\phi(x) = \int_V G(x,x')\rho(x')\, d^3x' + \int_S [\phi(x')\nabla' G(x,x') - G(x,x')\nabla'\phi(x')]\cdot d\hat{\sigma}'.$$

$$\Phi(x) = \int dx' G(x;x')\rho(x') \qquad G(x;x') = \frac{1}{|x-x'|} \qquad \Phi(x) = \int \frac{\rho(x')dx'}{|x-x'|}$$

Green's Function for Helmholtz's Equation

$$\left(\nabla^2 + k^2\right)u = 0$$

$$LG(\mathbf{x};\mathbf{x}') = \nabla^2 G(\mathbf{x};\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$$

$$\delta(\mathbf{x}-\mathbf{x}') = \delta(x-x')\delta(y-y')\delta(z-z')$$

$$u(\mathbf{q}) = \frac{1}{(2\pi)^3}\int_{-\infty}^{+\infty} u(\mathbf{r})e^{-i\mathbf{q}.\mathbf{r}}d\mathbf{r}$$

$$u(\mathbf{r}) = \int_{-\infty}^{+\infty} u(\mathbf{q})e^{i\mathbf{q}.\mathbf{r}}d\mathbf{q}$$

We can prove that:

$$G(\mathbf{x};\mathbf{x}') = \frac{1}{4\pi}\frac{e^{ik.(\mathbf{x}-\mathbf{x}')}}{\left|\mathbf{x}-\mathbf{x}'\right|}$$

$$H = H_0 + V$$

$$\langle \mathbf{x} | \psi^{(\pm)} \rangle = \langle \mathbf{x} | \phi \rangle + \int d^3x' \left\langle \mathbf{x} \left| \frac{1}{E - H_0 \pm i\varepsilon} \right| \mathbf{x}' \right\rangle \langle \mathbf{x}' | V | \psi^{(\pm)} \rangle$$

$$H_0 = \frac{\mathbf{p}^2}{2m}$$

$$\langle \mathbf{x} | \phi \rangle = \frac{e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}}{(2\pi\hbar)^{3/2}}$$

$$H_0 | \phi \rangle = E | \phi \rangle$$

$$\int d^3x \langle \mathbf{p}' | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{p} \rangle = \delta^{(3)}(\mathbf{p} - \mathbf{p}')$$

$$(H_0 + V) | \psi \rangle = E | \psi \rangle$$

$$\langle \mathbf{p} | \psi^{(\pm)} \rangle = \langle \mathbf{p} | \phi \rangle + \frac{1}{E - (p^2/2m) \pm i\varepsilon} \langle \mathbf{p} | V | \psi^{(\pm)} \rangle$$

$$| \psi \rangle = \frac{1}{E - H_0} V | \psi \rangle + | \phi \rangle$$

$$G_\pm(\mathbf{x}, \mathbf{x}') \equiv \frac{\hbar^2}{2m} \left\langle \mathbf{x} \left| \frac{1}{E - H_0 \pm i\varepsilon} \right| \mathbf{x}' \right\rangle$$

$$| \psi^{(\pm)} \rangle = | \phi \rangle + \frac{1}{E - H_0 \pm i\varepsilon} V | \psi^{(\pm)} \rangle$$

$$G_\pm(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{x} - \mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|}$$

$$\frac{\hbar^2}{2m} \left\langle \mathbf{x} \left| \frac{1}{E - H_0 \pm i\varepsilon} \right| \mathbf{x}' \right\rangle = \frac{\hbar^2}{2m} \int d^3p' \int d^3p'' \langle \mathbf{x} | \mathbf{p}' \rangle$$

$$\times \left\langle \mathbf{p}' \left| \frac{1}{E - (\mathbf{p}'^2/2m) \pm i\varepsilon} \right| \mathbf{p}'' \right\rangle \langle \mathbf{p}'' | \mathbf{x}' \rangle$$

$$\left\langle \mathbf{p}' \left| \frac{1}{E - (\mathbf{p}'^2/2m) \pm i\varepsilon} \right| \mathbf{p}'' \right\rangle = \frac{\delta^{(3)}(\mathbf{p}' - \mathbf{p}'')}{E - (\mathbf{p}'^2/2m) \pm i\varepsilon}$$

$$\langle \mathbf{x} | \mathbf{p}' \rangle = \frac{e^{i\mathbf{p}' \cdot \mathbf{x}/\hbar}}{(2\pi\hbar)^{3/2}}, \qquad \langle \mathbf{p}'' | \mathbf{x}' \rangle = \frac{e^{-i\mathbf{p}' \cdot \mathbf{x}'/\hbar}}{(2\pi\hbar)^{3/2}}$$

$$\frac{\hbar^2}{2m} \int \frac{d^3p'}{(2\pi\hbar)^3} \frac{e^{i\mathbf{p}' \cdot (\mathbf{x}-\mathbf{x}')/\hbar}}{[E - (\mathbf{p}'^2/2m) \pm i\varepsilon]}$$

$$\frac{1}{(2\pi)^3} \int_0^\infty q^2\, dq \int_0^{2\pi} d\phi \int_{-1}^{+1} \frac{d(\cos\theta)\, e^{i|\mathbf{q}||\mathbf{x}-\mathbf{x}'|\cos\theta}}{k^2 - q^2 \pm i\varepsilon}$$

$$= \frac{-1}{8\pi^2} \frac{1}{i|\mathbf{x}-\mathbf{x}'|} \int_{-\infty}^{+\infty} \frac{dq\,q\left(e^{iq|\mathbf{x}-\mathbf{x}'|} - e^{-iq|\mathbf{x}-\mathbf{x}'|}\right)}{q^2 - k^2 \mp i\varepsilon}$$

$$= -\frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}$$

$$\langle \mathbf{x}' | V | \psi^{(\pm)} \rangle = \int d^3x'' \langle \mathbf{x}' | V | \mathbf{x}'' \rangle \langle \mathbf{x}'' | \psi^{(\pm)} \rangle$$
$$= V(\mathbf{x}') \langle \mathbf{x}' | \psi^{(\pm)} \rangle.$$

$$\langle \mathbf{x} | \psi^{(\pm)} \rangle = \langle \mathbf{x} | \phi \rangle - \frac{2m}{\hbar^2} \int d^3x' \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} V(\vec{\mathbf{x}}') \langle \mathbf{x}' | \psi^{(\pm)} \rangle$$

$$(\nabla^2 + k^2) G_{\pm}(\mathbf{x}, \mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}')$$

$$\langle \mathbf{x} | \psi^{(\pm)} \rangle = \langle \mathbf{x} | \phi \rangle - \frac{2m}{\hbar^2} \int d^3x' \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \langle \mathbf{x}' | V | \psi^{(\pm)} \rangle$$

$$\langle \mathbf{x}' | V | \mathbf{x}'' \rangle = V(\mathbf{x}') \delta^{(3)}(\mathbf{x}' - \mathbf{x}'')$$

Let us suppose that the scattering Hamiltonian, H_1, is only a function of the position operators. This implies that

$$\langle \mathbf{r}'|H_1|\mathbf{r}\rangle = V(\mathbf{r})\,\delta(\mathbf{r}-\mathbf{r}'). \tag{7.15}$$

We can write

$$\begin{aligned}\langle \mathbf{r}'|H_1|\psi^\pm\rangle &= \int \langle \mathbf{r}'|H_1|\mathbf{r}''\rangle\langle \mathbf{r}''|\psi^\pm\rangle\, d^3\mathbf{r}'' \\ &= V(\mathbf{r}')\,\psi^\pm(\mathbf{r}'). \end{aligned} \tag{7.16}$$

Thus, the integral equation (7.13) simplifies to

$$\psi^\pm(\mathbf{r}) = \phi(\mathbf{r}) - \frac{2\,m}{\hbar^2}\int \frac{\exp(\pm i\,k\,|\mathbf{r}-\mathbf{r}'|)}{4\pi\,|\mathbf{r}-\mathbf{r}'|}\,V(\mathbf{r}')\,\psi^\pm(\mathbf{r}')\, d^3\mathbf{r}'. \tag{7.17}$$

Suppose that the initial state $|\phi\rangle$ is a plane-wave with wave-vector $\mathbf{k}$ (*i.e.*, a stream of particles of definite momentum $\mathbf{p} = \hbar\,\mathbf{k}$). The ket corresponding to this state is denoted $|\mathbf{k}\rangle$. The associated wave-function takes the form

$$\langle \mathbf{r}|\mathbf{k}\rangle = \frac{\exp(\,i\,\mathbf{k}\cdot\mathbf{r})}{(2\pi)^{3/2}}. \tag{7.18}$$

$$\psi^\pm(\mathbf{r}) = \phi(\mathbf{r}) - \frac{2\,m}{\hbar^2}\int \frac{\exp(\pm i\,k\,|\mathbf{r}-\mathbf{r}'|\,)}{4\pi\,|\mathbf{r}-\mathbf{r}'|}\,\langle \mathbf{r}'|H_1|\psi\rangle\, d^3\mathbf{r}'. \tag{7.13}$$

The wave-function is normalized such that

$$\begin{aligned}\langle \mathbf{k}|\mathbf{k}'\rangle &= \int \langle \mathbf{k}|\mathbf{r}\rangle \langle \mathbf{r}|\mathbf{k}'\rangle \, d^3\mathbf{r} \\ &= \int \frac{\exp[-i\,\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')]}{(2\pi)^3}\, d^3\mathbf{r} = \delta(\mathbf{k}-\mathbf{k}'). \end{aligned} \tag{7.19}$$

Suppose that the scattering potential $V(\mathbf{r})$ is only non-zero in some relatively localized region centred on the origin ($\mathbf{r} = 0$). Let us calculate the wave-function $\psi(\mathbf{r})$ a long way from the scattering region. In other words, let us adopt the ordering $r \gg r'$. It is easily demonstrated that

$$|\mathbf{r} - \mathbf{r}'| \simeq r - \hat{\mathbf{r}}\cdot\mathbf{r}' \tag{7.20}$$

to first-order in r'/r, where

$$\hat{\mathbf{r}} = \frac{\mathbf{r}}{r} \tag{7.21}$$

is a unit vector which points from the scattering region to the observation point.

$$|\mathbf{x}| \gg |\mathbf{x}'|, \tag{7.1.23}$$

as depicted in Figure 7.1.

Introducing

$$r = |\mathbf{x}| \qquad r' = |\mathbf{x}'| \tag{7.1.24}$$

and

$$\alpha = \angle(\mathbf{x}, \mathbf{x}'), \tag{7.1.25}$$

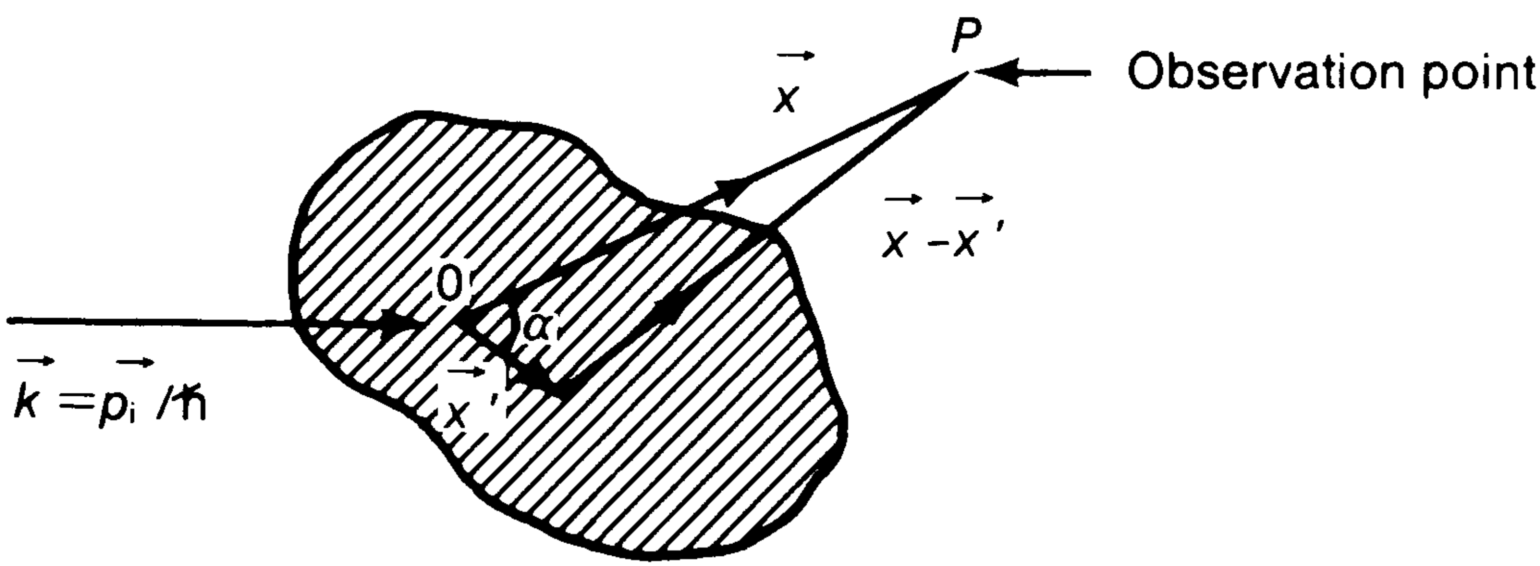


FIGURE 7.1. Finite-range scattering potential. The *observation point P* is where the wave function $\langle \mathbf{x}|\psi^{(\pm)}\rangle$ is to be evaluated, while the contribution to the integral in Equation (7.1.22) is for $|\mathbf{x}'|$ less than the range of the potential, as depicted by the shaded region of the figure.

we have for $r \gg r'$,

$$|\mathbf{x}-\mathbf{x}'| = \sqrt{r^2 - 2rr'\cos\alpha + r'^2}$$

$$= r\left(1 - \frac{2r'}{r}\cos\alpha + \frac{r'^2}{r^2}\right)^{1/2} \tag{7.1.26}$$

$$\simeq r - \hat{\mathbf{r}}\cdot\mathbf{x}'$$

where

$$\hat{\mathbf{r}} \equiv \frac{\mathbf{x}}{|\mathbf{x}|}. \tag{7.1.27}$$

Also define

$$\mathbf{k}' \equiv k\hat{\mathbf{r}}. \tag{7.1.28}$$

The motivation for this definition is that $\mathbf{k}'$ represents the propagation vector for waves reaching observation point $\mathbf{x}$. We then obtain

$$e^{\pm ik|\mathbf{x}-\mathbf{x}'|} \simeq e^{\pm ikr} e^{\mp i\mathbf{k}'\cdot\mathbf{x}'} \tag{7.1.29}$$

for large r. It is legitimate to replace $1/|\mathbf{x}-\mathbf{x}'|$ by just $1/r$. Furthermore, to get rid of the $\hbar$'s in expressions such as $1/(2\pi\hbar)^{3/2}$, it is convenient to use $|\mathbf{k}\rangle$ rather than $|\mathbf{p}_i\rangle$, where

$$\mathbf{k} \equiv \frac{\mathbf{p}_i}{\hbar}. \tag{7.1.30}$$

Let us define

$$\mathbf{k}' = k\,\hat{\mathbf{r}}. \tag{7.22}$$

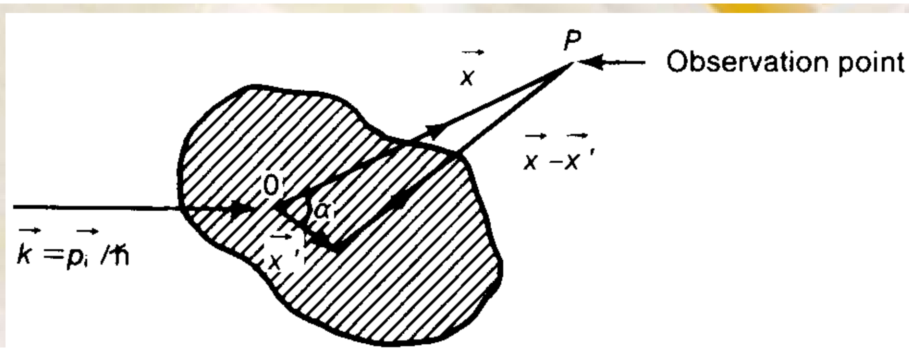
Clearly, $\mathbf{k}'$ is the wave-vector for particles which possess the same energy as the incoming particles (*i.e.*, $k' = k$), but propagate from the scattering region to the observation point. Note that

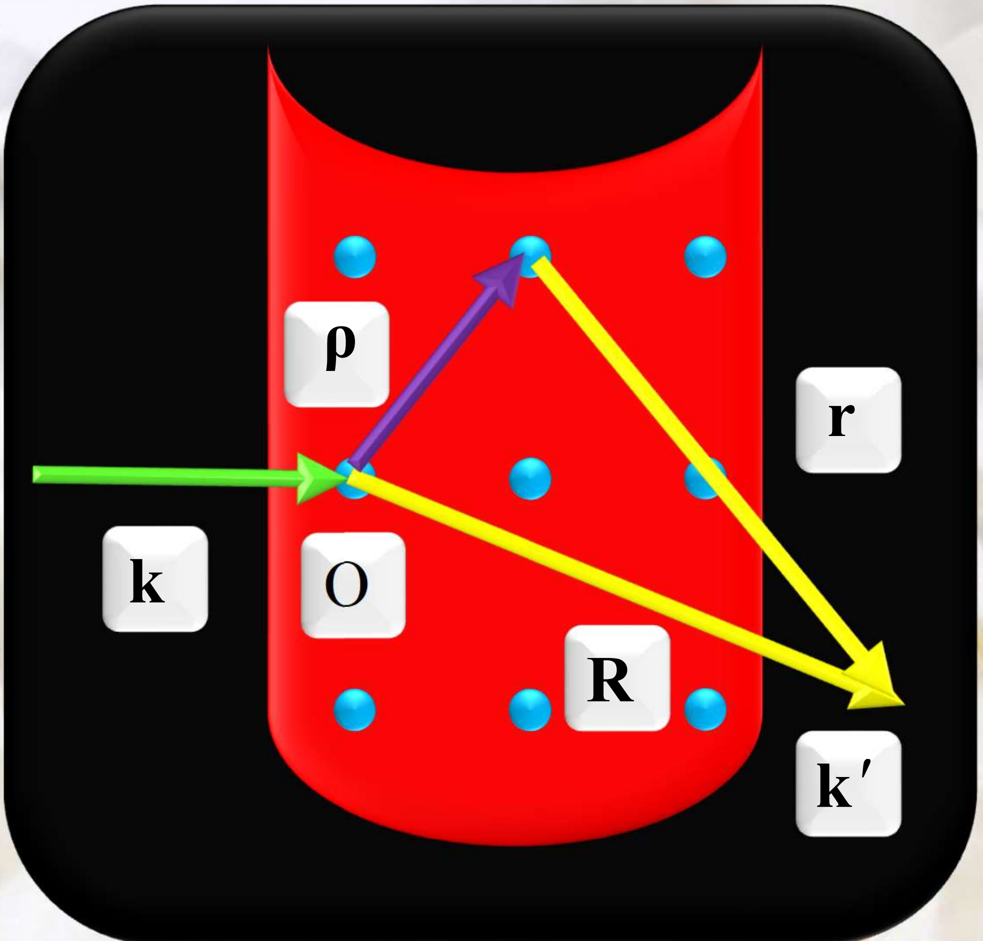
$$\exp(\pm i\,k\,|\mathbf{r} - \mathbf{r}'|\,) \simeq \exp(\pm i\,k\,r)\,\exp(\mp i\,\mathbf{k}'\cdot\mathbf{r}'). \tag{7.23}$$

In the large-r limit, Eq. (7.17) reduces to

$$\psi(\mathbf{r})^{\pm} \simeq \frac{\exp(\,i\,\mathbf{k}\cdot\mathbf{r})}{(2\pi)^{3/2}} - \frac{m}{2\pi\,\hbar^2}\frac{\exp(\pm i\,k\,r)}{r}\int \exp(\mp i\,\mathbf{k}'\cdot\mathbf{r}')\,V(\mathbf{r}')\,\psi^{\pm}(\mathbf{r}')\,d^3\mathbf{r}'. \tag{7.24}$$

The first term on the right-hand side is the incident wave. The second term represents a spherical wave centred on the scattering region. The plus sign (on $\psi^{\pm}$) corresponds to a wave propagating away from the scattering region, whereas the minus sign corresponds to a wave propagating towards the scattering region.





$$E(\boldsymbol{\rho}) = E_0 \exp[i\mathbf{k}.\boldsymbol{\rho}]$$

$$E_{sc} = CE(\boldsymbol{\rho}) \frac{\exp[i\mathbf{k}'.\mathbf{r}]}{r}$$

$$E_{sc} = \frac{CE_0}{r} \exp[i(\mathbf{k}.\boldsymbol{\rho} + kr)]$$

$$\mathbf{r} = \mathbf{R} - \boldsymbol{\rho}$$

$$r^2 = R^2 + \rho^2 - 2\boldsymbol{\rho}.\mathbf{R}$$

$$r^2 = R^2 + \rho^2 - 2\rho R \cos(\hat{\boldsymbol{\rho}}, \hat{\mathbf{R}})$$

$$r = \sqrt{R^2 + \rho^2 - 2\rho R \cos(\hat{\boldsymbol{\rho}}, \hat{\mathbf{R}})}$$

$$\cong R\left(1 - \rho / R \cos(\hat{\boldsymbol{\rho}}, \hat{\mathbf{R}})\right)$$

$$E_{sc} = \frac{CE_0}{r} \exp\left[i\left(\mathbf{k}.\boldsymbol{\rho} + kR - k\rho\cos(\hat{\boldsymbol{\rho}}, \hat{\mathbf{R}})\right)\right]$$

$$E_{sc} = \frac{CE_0}{r} \exp[ikR] \exp\left[i\left(\mathbf{k}.\boldsymbol{\rho} - \mathbf{k}'.\boldsymbol{\rho}\right)\right]$$

$$E_{sc} = CE_0 \frac{\exp[ikR]}{r} \exp\left[i\left(\mathbf{k} - \mathbf{k}'\right).\boldsymbol{\rho} \right]$$

$$E_{sc} \cong CE_0 \frac{\exp[ikR]}{R} \exp\left[i\left(\mathbf{k} - \mathbf{k}'\right).\boldsymbol{\rho} \right]$$

$$E_{sc} \cong CE_0 \frac{\exp[ikR]}{R} \exp\left[-i\Delta\mathbf{k}.\boldsymbol{\rho} \right]$$

$$E_{sc} \propto n(\mathbf{r})$$

$$E_{sc} \cong CE_0 \frac{\exp[ikR]}{R} \underbrace{\int_{\text{all crystal}} n(\boldsymbol{\rho}) \exp\left[-i\Delta\mathbf{k}.\boldsymbol{\rho} \right] d\boldsymbol{\rho}}_{\text{scattering amplitude}}$$

It is obvious that the former represents the physical solution. Thus, the wave-function a long way from the scattering region can be written

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\left[\exp(\,i\,\mathbf{k}\cdot\mathbf{r}) + \frac{\exp(\,i\,k r)}{r} f(\mathbf{k}', \mathbf{k})\right], \tag{7.25}$$

where

$$\begin{aligned} f(\mathbf{k}', \mathbf{k}) &= -\frac{(2\pi)^2\, m}{\hbar^2}\int \frac{\exp(-i\,\mathbf{k}'\cdot\mathbf{r}')}{(2\pi)^{3/2}}\, V(\mathbf{r}')\,\psi(\mathbf{r}')\, d^3\mathbf{r}' \\ &= -\frac{(2\pi)^2\, m}{\hbar^2}\,\langle \mathbf{k}'|H_1|\psi\rangle. \end{aligned} \tag{7.26}$$

Let us define the differential cross-section $d\sigma/d\Omega$ as the number of particles per unit time scattered into an element of solid angle $d\Omega$, divided by the incident flux of particles. Recall, from Sect. 4, that the probability flux (*i.e.*, the particle flux) associated with a wave-function ψ is

$$\mathbf{j} = \frac{\hbar}{m}\mathrm{Im}(\psi^*\,\nabla\psi). \tag{7.27}$$

Thus, the probability flux associated with the incident wave-function,

$$\frac{\exp(\,i\,\mathbf{k}\cdot\mathbf{r})}{(2\pi)^{3/2}}, \tag{7.28}$$

is

$$\mathbf{j}_{inci} = \frac{\hbar}{(2\pi)^3\,m}\,\mathbf{k}. \tag{7.29}$$

Likewise, the probability flux associated with the scattered wave-function,

$$\frac{\exp(\,i\,k\,r)}{(2\pi)^{3/2}}\frac{f(\mathbf{k}',\mathbf{k})}{r}, \tag{7.30}$$

is

$$\mathbf{j}_{scat} = \frac{\hbar}{(2\pi)^3\,m}\frac{|f(\mathbf{k}',\mathbf{k})|^2}{r^2}\,k\,\hat{\mathbf{r}}. \tag{7.31}$$

Now,

(7.32)

Thus, $|f(\mathbf{k}',\mathbf{k})|^2$ gives the differential cross-section for particles with incident momentum $\hbar\,\mathbf{k}$ to be scattered into states whose momentum vectors are directed in a range of solid angles $d\Omega$ about $\hbar\,\mathbf{k}'$. Note that the scattered particles possess the same energy as the incoming particles (*i.e.*, $k' = k$). This is always the case for scattering Hamiltonians of the form shown in Eq. (7.15).

giving

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}',\mathbf{k})|^2. \tag{7.33}$$