12 - Scattering Theory

- Aim of Section:
  - Outline quantum theory of scattering.

Introduction

- Historically, data regarding quantum phenomena was obtained from two main sources.
- Firstly, study of spectroscopic lines, and, secondly, analysis of data from scattering experiments.
- Let us now examine quantum theory of scattering.
- We shall treat scattering as an essentially two-particle effect.
- As is well known, when viewed in center of mass frame, two particles of masses m_1 and m_2, and position vector $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively, interacting via potential $V(\mathbf{x}_1 - \mathbf{x}_2)$, can be treated as a single body of reduced mass $\mu_{12} = m_1\, m_2/(m_1 + m_2)$, and position vector $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$, moving in fixed potential $V(\mathbf{x})$.
- For this reason, we can, without loss of generality, focus our study on quantum theory of particles scattered by fixed potentials.

Fundamental Equations - I

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

$$H = H_0 + H_1,$$

where

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

is Hamiltonian of a free particle of mass m, and H_1 represents non-time-varying source of scattering.

- Let $|\phi\rangle$ be an energy eigenket of H_0,

$$H_0\,|\phi\rangle = E\,|\phi\rangle, \tag{1}$$

whose wavefunction is $\phi(\mathbf{x})$. This wavefunction is assumed to be a plane wave.

Fundamental Equations - II

- Schrödinger's equation for scattering problem is

$$(H_0 + H_1)\,|\psi\rangle = E\,|\psi\rangle, \tag{2}$$

  where $|\psi\rangle$ is an energy eigenstate of total Hamiltonian whose wavefunction is $\psi(\mathbf{x})$.
- In general, both H_0 and $H_0 + H_1$ have continuous energy spectra: that is, their energy eigenstates are unbound.
- We require a solution of (2) that satisfies boundary condition $|\psi\rangle \to |\phi\rangle$ as $H_1 \to 0$.
- Here, $|\phi\rangle$ is a solution of free-particle Schrödinger equation, (1), that corresponds to same energy eigenvalue as $|\psi\rangle$.

Fundamental Equations - III

- Adopting Schrödinger representation, we can write scattering equation, (2), in form

$$(\nabla^2 + k^2)\,\psi(\mathbf{x}) = \frac{2\,m}{\hbar^2}\,\langle\mathbf{x}|H_1|\psi\rangle, \qquad (3)$$

where

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

- Here, $|\mathbf{x}'\rangle$ is a state whose wavefunction is $\delta^3(\mathbf{x}-\mathbf{x}')$. It follows that

$$\mathbf{x}\,|\mathbf{x}'\rangle = \mathbf{x}'\,|\mathbf{x}'\rangle.$$

  In other words, $|\mathbf{x}'\rangle$ is an eigenstate of position operator, $\mathbf{x}$, corresponding to eigenvalue $\mathbf{x}'$.
- Follows that

$$\langle\mathbf{x}|\psi\rangle = \psi(\mathbf{x}).$$

Fundamental Equations - IV

- (3) is known as Helmholtz equation, and can be inverted using standard Green's function techniques. Thus,

$$\psi(\mathbf{x}) = \phi(\mathbf{x}) + \frac{2\,m}{\hbar^2}\int G(\mathbf{x},\mathbf{x}')\,\langle\mathbf{x}'|H_1|\psi\rangle\,d^3\mathbf{x}', \qquad (4)$$

  where

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

  Here, $\delta^3(\mathbf{x})$ is a three-dimensional Dirac delta function.
- Note that solution (4) satisfies previously mentioned constraint $|\psi\rangle \rightarrow |\phi\rangle$ as $H_1 \rightarrow 0$.
- As is well known, Green's function for Helmholtz equation is given by

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

- Thus, (4) becomes

$$\psi^{\pm}(\mathbf{x}) = \phi(\mathbf{x}) - \frac{2\,m}{\hbar^2}\int \frac{\exp(\pm\mathrm{i}\,k\,|\mathbf{x}-\mathbf{x}'|\,)}{4\pi\,|\mathbf{x}-\mathbf{x}'|}\,\langle\mathbf{x}'|H_1|\psi^{\pm}\rangle\,d^3\mathbf{x}'. \qquad (5)$$

Fundamental Equations - V

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

$$\langle \mathbf{x}' | H_1 | \mathbf{x} \rangle = V(\mathbf{x})\, \delta^3(\mathbf{x} - \mathbf{x}'). \tag{6}$$

- We can write

$$\langle \mathbf{x}' | H_1 | \psi^{\pm} \rangle = \int \langle \mathbf{x}' | H_1 | \mathbf{x}'' \rangle \langle \mathbf{x}'' | \psi^{\pm} \rangle \, d^3\mathbf{x}''$$
$$= \int V(\mathbf{x}')\, \delta^3(\mathbf{x}' - \mathbf{x}'')\, \psi(\mathbf{x}'')\, d^3\mathbf{x}'' = V(\mathbf{x}')\, \psi^{\pm}(\mathbf{x}'),$$

where use has been made of standard completeness relation $\int |\mathbf{x}''\rangle\langle \mathbf{x}''|\, d^3\mathbf{x}'' = 1$.

- Thus, integral equation (5) simplifies to give

$$\psi^{\pm}(\mathbf{x}) = \phi(\mathbf{x}) - \frac{2\, m}{\hbar^2} \int \frac{\exp(\pm \mathrm{i}\, k\, |\mathbf{x} - \mathbf{x}'|)}{4\pi\, |\mathbf{x} - \mathbf{x}'|}\, V(\mathbf{x}')\, \psi^{\pm}(\mathbf{x}')\, d^3\mathbf{x}'. \tag{7}$$

Fundamental Equations - VI

- Suppose that initial state, $|\phi\rangle$, possesses a plane-wave wavefunction with wavevector $\mathbf{k}$ (i.e., it corresponds to a stream of particles of definite momentum $\mathbf{p} = \hbar\,\mathbf{k}$).
- Ket corresponding to this state is denoted $|\mathbf{k}\rangle$.
- Thus,

$$\phi(\mathbf{x}) \equiv \langle \mathbf{x}|\mathbf{k}\rangle = \frac{\exp(\,\mathrm{i}\,\mathbf{k}\cdot\mathbf{x})}{(2\pi)^{3/2}}. \tag{8}$$

- Preceding wavefunction is conveniently normalized such that

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \int \langle \mathbf{k}|\mathbf{x}\rangle\langle \mathbf{x}|\mathbf{k}'\rangle\, d^3\mathbf{x} = \int \frac{\exp[-\mathrm{i}\,\mathbf{x}\cdot(\mathbf{k}-\mathbf{k}')]}{(2\pi)^3}\, d^3\mathbf{x}$$

$$= \delta^3(\mathbf{k}-\mathbf{k}').$$

Fundamental Equations - VII

- Suppose that scattering potential, $V(\mathbf{x})$, is non-zero only in some relatively localized region centered on origin ($\mathbf{x} = \mathbf{0}$).
- Let us calculate total wavefunction, $\psi(\mathbf{x})$, far from scattering region. In other words, let us adopt ordering $r \gg r'$, where $r = |\mathbf{x}|$ and $r' = |\mathbf{x}'|$.
- It is easily demonstrated that

$$|\mathbf{x} - \mathbf{x}'| \simeq r - \mathbf{e}_r \cdot \mathbf{x}'$$

to first order in r'/r, where $\mathbf{e}_r = \mathbf{x}/r$ is a unit vector that is directed from scattering region to observation point.
- Let us define

$$\mathbf{k}' = k\,\mathbf{e}_r.$$

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

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

Fundamental Equations - VIII

- In large-r limit, (7) and (8) reduce to

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

- First term on right-hand side of previous equation is incident wave.
- Second term represents a spherical wave centered on scattering region.
- Plus sign (on $\psi^{\pm}$) corresponds to a wave propagating away from scattering region, whereas minus sign corresponds to a wave propagating toward scattering region.
- It is obvious that former sign represents physical solution.

Fundamental Equations - IX

- Thus, wavefunction far from scattering region can be written

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

where

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

Fundamental Equations - X

- Let us define differential scattering cross-section, $d\sigma/d\Omega$, as number of particles per unit time scattered into an element of solid angle $d\Omega$, divided by incident particle flux.
- Probability current (which is proportional to particle flux) associated with a wavefunction ψ is

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

- Thus, particle flux associated with incident wavefunction,

$$\frac{\exp(\,\mathrm{i}\,\mathbf{k}\cdot\mathbf{x})}{(2\pi)^{3/2}},$$

is proportional to

$$\mathbf{j}_{\mathrm{incident}} = \frac{\hbar\,\mathbf{k}}{(2\pi)^3\,m}. \tag{9}$$

Fundamental Equations - XI

- Likewise, particle flux associated with scattered wavefunction,

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

is proportional to

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

- Now, by definition,

$$\frac{d\sigma}{d\Omega}\,d\Omega = \frac{r^2\,d\Omega\,|\mathbf{j}_{\rm scattered}|}{|\mathbf{j}_{\rm incident}|},$$

giving

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}',\mathbf{k})|^2. \tag{10}$$

Fundamental Equations - XII

- Thus, $|f(\mathbf{k}', \mathbf{k})|^2$ is 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 scattered particles possess same energy as incoming particles (i.e., $k' = k$). This is always case for scattering Hamiltonians of form specified in (6).

Born Approximation - I

- (10) is not particularly useful, as it stands, because quantity $f(\mathbf{k}', \mathbf{k})$ depends on unknown ket $|\psi\rangle$.
- Recall that $\psi(\mathbf{x}) \equiv \langle \mathbf{x}|\psi\rangle$ is solution of integral equation

$$\psi(\mathbf{x}) = \phi(\mathbf{x}) - \frac{m}{2\pi\,\hbar^2} \int \frac{\exp(\mathrm{i}\,k\,|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}\,V(\mathbf{x}')\,\psi(\mathbf{x}')\,d^3\mathbf{x}', \tag{11}$$

  where $\phi(\mathbf{x})$ is wavefunction of incident state.
- According to previous equation, total wavefunction is a superposition of incident wavefunction and a great many spherical waves emitted from scattering region.
- Strength of spherical wave emitted at a given point in scattering region is proportional to local value of scattering potential, $V(\mathbf{x})$, as well as local value of wavefunction, $\psi(\mathbf{x})$.

Born Approximation - II

- Suppose, however, that scattering is not particularly intense. In this case, it is reasonable to suppose that total wavefunction, $\psi(\mathbf{x})$, does not differ substantially from incident wavefunction, $\phi(\mathbf{x})$.
- Thus, we can obtain an expression for $\psi(\mathbf{x})$ by making substitution

$$\psi(\mathbf{x}) \rightarrow \phi(\mathbf{x}) = \frac{\exp(\mathrm{i}\,\mathbf{k}\cdot\mathbf{x})}{(2\pi)^{3/2}}$$

  on right-hand side of (11).
- This simplification is known as Born approximation.

Born Approximation - III

- Born approximation yields

$$f(\mathbf{k}', \mathbf{k}) \simeq -\frac{m}{2\pi\,\hbar^2} \int \exp\left[\,\mathrm{i}\,(\mathbf{k} - \mathbf{k}') \cdot \mathbf{x}'\right] V(\mathbf{x}')\, d^3\mathbf{x}'.$$

- Thus, $f(\mathbf{k}', \mathbf{k})$ is proportional to Fourier transform of scattering potential, $V(\mathbf{x})$, with respect to relative wavevector, $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}'$.

Born Approximation - IV

- For a spherically symmetric scattering potential,

$$f(\mathbf{k}',\mathbf{k}) \simeq -\frac{m}{2\pi\,\hbar^2}\int_0^\infty\int_0^\pi\int_0^{2\pi} \mathrm{e}^{\,\mathrm{i}\,q\,r'\cos\theta'}\,V(r')'\,r'^{\,2}\,\sin\theta'\,dr'\,d\theta'\,d\varphi,$$

giving

$$f(\mathbf{k}',\mathbf{k}) \simeq -\frac{2\,m}{\hbar^2\,q}\int_0^\infty r\,V(r)\sin(q\,r)\,dr. \tag{12}$$

- Hence, it is clear that, for special case of a spherically symmetric potential, $f(\mathbf{k}',\mathbf{k})$ depends only on magnitude of relative wavevector, $\mathbf{q} = \mathbf{k} - \mathbf{k}'$, and is independent of its direction.
- Now, it is easily demonstrated that

$$q \equiv |\mathbf{k} - \mathbf{k}'| = 2\,k\,\sin(\theta/2), \tag{13}$$

where θ is angle subtended between vectors $\mathbf{k}$ and $\mathbf{k}'$.
- In other words, θ is angle of scattering.

Born Approximation - V

- Recall that vectors $\mathbf{k}$ and $\mathbf{k}'$ have same length, as a consequence of energy conservation.
- It follows that, according to Born approximation, $f(\mathbf{k}', \mathbf{k}) = f(\theta)$ for a spherically symmetric scattering potential, $V(r)$. Moreover, $f(\theta)$ is real.
- Finally, differential scattering cross-section, $d\sigma/d\Omega = |f(\theta)|^2$, is invariant under transformation $V \to -V$.
- In other words, pattern of scattering is identical for attractive and repulsive scattering potentials of same strength.

Born Approximation - VI

- Consider scattering by a Yukawa potential,

$$V(r) = \frac{V_0 \exp(-\mu\, r)}{\mu\, r}, \tag{14}$$

where V_0 is a constant, and $1/\mu$ measures "range" of potential.

- It follows from (12) that

$$f(\theta) = -\frac{2\, m\, V_0}{\hbar^2\, \mu} \frac{1}{q^2 + \mu^2},$$

because

$$\int_0^\infty \exp(-\mu\, r)\, \sin(q\, r)\, dr = \frac{q}{q^2 + \mu^2}.$$

- Thus, Born approximation yields a differential cross-section for scattering by a Yukawa potential of form

$$\frac{d\sigma}{d\Omega} \simeq \left(\frac{2\, m\, V_0}{\hbar^2\, \mu}\right)^2 \frac{1}{\left[4\, k^2\, \sin^2(\theta/2) + \mu^2\right]^2}.$$

Born Approximation - VII

- Yukawa potential reduces to familiar Coulomb potential in limit $\mu \to 0$, provided that $V_0/\mu \to Z\,Z'\,e^2/4\pi\,\epsilon_0$. Here, $Z\,e$ and $Z'\,e$ are electric charges of two interacting particles.
- In Coulomb limit, previous Born differential cross-section transforms into

$$\frac{d\sigma}{d\Omega} \simeq \left(\frac{2\,m\,Z\,Z'\,e^2}{4\pi\,\epsilon_0\,\hbar^2}\right)^2 \frac{1}{16\,k^4\,\sin^4(\theta/2)}.$$

- Recalling that $\hbar\,k$ is equivalent to $|\mathbf{p}|$, where $\mathbf{p}$ is momentum of incident particles, preceding equation can be rewritten

$$\frac{d\sigma}{d\Omega} \simeq \left(\frac{Z\,Z'\,e^2}{16\pi\,\epsilon_0\,E}\right)^2 \frac{1}{\sin^4(\theta/2)}, \tag{15}$$

  where $E = p^2/(2\,m)$ is kinetic energy of incident particles.
- (15) is identical to well-known Rutherford scattering cross-section formula of classical physics.

Born Approximation - VIII

- Born approximation is valid provided $\psi(\mathbf{x})$ is not significantly different from $\phi(\mathbf{x})$ in scattering region.
- It follows, from (11), that condition that must be satisfied in order that $\psi(\mathbf{x}) \simeq \phi(\mathbf{x})$ in vicinity of $\mathbf{x} = \mathbf{0}$ is

$$\left| \frac{m}{2\pi\,\hbar^2} \int \frac{\exp(\,{\rm i}\,k\,r')}{r'}\,V(\mathbf{x}')\,d^3\mathbf{x}' \right| \ll 1. \tag{16}$$

- Consider special case of Yukawa potential, (14). At low energies (i.e., $k \ll \mu$), we can replace $\exp(\,{\rm i}\,k\,r')$ by unity, giving

$$\frac{2\,m}{\hbar^2}\frac{|V_0|}{\mu^2} \ll 1$$

as condition for validity of Born approximation.
- Now, criterion for Yukawa potential to develop a bound state turns out to be

$$\frac{2\,m}{\hbar^2}\frac{|V_0|}{\mu^2} \geq 2.7, \tag{17}$$

provided V_0 is negative.

Born Approximation - IX

- Thus, if potential is strong enough to form a bound state then Born approximation is likely to break down.
- In high-k limit (i.e., $k \gg \mu$), (16) yields

$$\frac{2\,m}{\hbar^2}\frac{|V_0|}{\mu\,k} \ll 1.$$

- This inequality becomes progressively easier to satisfy as k increases, implying that Born approximation becomes more accurate at high incident particle energies

Born Expansion - I

- As we have seen, quantum scattering theory requires solution of integral equation,

$$\psi(\mathbf{x}) = \phi(\mathbf{x}) - \frac{m}{2\pi\,\hbar^2}\int \frac{\exp(\,\mathrm{i}\,k\,|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}\,V(\mathbf{x}')\,\psi(\mathbf{x}')\,d^3\mathbf{x}',$$

  where $\phi(\mathbf{x}) = \exp(\,\mathrm{i}\,\mathbf{k}\cdot\mathbf{x})/(2\pi)^{3/2}$ is incident wavefunction, and $V(\mathbf{x})$ scattering potential.
- An obvious approach, in weak-scattering limit, is to solve preceding equation via a series of successive approximations. That is,

$$\psi^{(1)}(\mathbf{x}) = \phi(\mathbf{x}) - \frac{m}{2\pi\,\hbar^2}\int \frac{\exp(\,\mathrm{i}\,k\,|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}\,V(\mathbf{x}')\,\phi(\mathbf{x}')\,d^3\mathbf{x}',$$

$$\psi^{(2)}(\mathbf{x}) = \phi(\mathbf{x}) - \frac{m}{2\pi\,\hbar^2}\int \frac{\exp(\,\mathrm{i}\,k\,|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}\,V(\mathbf{x}')\,\psi^{(1)}(\mathbf{x}')\,d^3\mathbf{x}',$$

$$\psi^{(3)}(\mathbf{x}) = \phi(\mathbf{x}) - \frac{m}{2\pi\,\hbar^2}\int \frac{\exp(\,\mathrm{i}\,k\,|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}\,V(\mathbf{x}')\,\psi^{(2)}(\mathbf{x}')\,d^3\mathbf{x}',$$

  and so on.

Born Expansion - II

- Assuming that $V(\mathbf{x})$ is only non-negligible relatively close to origin, and taking limit $|\mathbf{x}| \to \infty$, we find that

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

  where

$$f(\mathbf{k}', \mathbf{k}) = f^{(1)}(\mathbf{k}', \mathbf{k}) + f^{(2)}(\mathbf{k}', \mathbf{k}) + f^{(3)}(\mathbf{k}', \mathbf{k}) + \cdots.$$

- First two terms in previous series, which is generally known as Born expansion, are

$$f^{(1)}(\mathbf{k}', \mathbf{k}) = -\frac{m}{2\pi\,\hbar^2} \int \mathrm{e}^{\,\mathrm{i}\,(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}'}\, V(\mathbf{x}')\, d^3\mathbf{x}', \tag{18}$$

$$f^{(2)}(\mathbf{k}', \mathbf{k}) = \left(\frac{m}{2\pi\,\hbar^2}\right)^2 \iint \mathrm{e}^{\,\mathrm{i}\,(\mathbf{k}\cdot\mathbf{x}''-\mathbf{k}'\cdot\mathbf{x}')}\, \frac{\mathrm{e}^{\,\mathrm{i}\,k\,|\mathbf{x}'-\mathbf{x}''|}}{|\mathbf{x}'-\mathbf{x}''|}\, V(\mathbf{x}')\, V(\mathbf{x}'')\, d^3\mathbf{x}'\, d^3\mathbf{x}''.$$

Born Expansion - III

- Of course, we recognize (18) as Born approximation discussed previously.
- In other words, Born approximation essentially involves truncating Born expansion after its first term.
- Incidentally, it can be proved that Born expansion converges for all k (for a spherically symmetric scattering potential) provided; a) $\int_0^\infty r\,|V(r)|\,dr < \infty$; b) $\int_0^\infty r^2\,|V(r)|\,dr < \infty$; and; c) $-|V(r)|$ is too weak to form a bound state.
- Furthermore, criterion for convergence becomes less stringent at high k.

Partial Waves - I

- We can assume, without loss of generality, that incident wavefunction is characterized by a wavevector, $\mathbf{k}$, that is aligned parallel to z-axis.
- Scattered wavefunction is characterized by a wavevector, $\mathbf{k}'$, that has same magnitude as $\mathbf{k}$, but, in general, points in a different direction.
- Direction of $\mathbf{k}'$ is specified by polar angle θ (i.e., angle subtended between two wavevectors), and an azimuthal angle φ measured about z-axis.
- (12) and (13) strongly suggest that for a spherically symmetric scattering potential [i.e., $V(\mathbf{x}) = V(r)$], scattering amplitude is a function of θ only: that is,

$$f(\theta, \varphi) = f(\theta).$$

- Let us assume that this is case.

Partial Waves - II

- It follows that neither incident wavefunction,

$$\phi(\mathbf{x}) = \frac{\exp(\mathrm{i}\,k\,z)}{(2\pi)^{3/2}} = \frac{\exp(\mathrm{i}\,k\,r\cos\theta)}{(2\pi)^{3/2}}, \tag{19}$$

nor total wavefunction far from scattering region,

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\left[\exp(\mathrm{i}\,k\,r\cos\theta) + \frac{\exp(\mathrm{i}\,k\,r)\,f(\theta)}{r}\right], \tag{20}$$

depend on azimuthal angle, φ.

Partial Waves - III

- Outside range of scattering potential, $\phi(\mathbf{x})$ and $\psi(\mathbf{x})$ both satisfy free-space Schrödinger equation,

$$(\nabla^2 + k^2)\,\psi = 0. \qquad (21)$$

- Consider most general solution to this equation that is independent of azimuthal angle, φ.
- Separation of variables (in spherical coordinates) yields

$$\psi(r,\theta) = \sum_{l=0,\infty} R_l(r)\,P_l(\cos\theta) \qquad (22)$$

- Legendre polynomials, $P_l(\cos\theta)$, are related to associated Legendre functions, $P_l^m(\cos\theta)$, as well as spherical harmonics, $Y_l^m(\theta,\varphi)$, via $P_l(\cos\theta) = P_l^0(\cos\theta)$, and

$$P_l(\cos\theta) = \sqrt{\frac{4\pi}{2\,l+1}}\,Y_l^0(\theta,\varphi),$$

respectively.

Partial Waves - IV

- (21) and (22) can be combined to give

$$r^2 \frac{d^2 R_l}{dr^2} + 2\, r\, \frac{dR_l}{dr} + [k^2\, r^2 - l\,(l+1)]\, R_l = 0.$$

- Two independent solutions to this equation are spherical Bessel function, $j_l(k\, r)$, and Neumann function, $\eta_l(k\, r)$, where

$$j_l(y) = y^l \left(-\frac{1}{y}\frac{d}{dy}\right)^l \frac{\sin y}{y}, \qquad (23)$$

$$\eta_l(y) = -y^l \left(-\frac{1}{y}\frac{d}{dy}\right)^l \frac{\cos y}{y}. \qquad (24)$$

- Note that spherical Bessel functions are well behaved in limit $y \to 0$, whereas Neumann functions become singular.

Partial Waves - V

- Asymptotic behavior of these functions in limit $y \to \infty$ is

$$j_l(y) \to \frac{\sin(y - l\pi/2)}{y}, \tag{25}$$

$$\eta_l(y) \to -\frac{\cos(y - l\pi/2)}{y}. \tag{26}$$

Partial Waves - VI

- We can write

$$\exp(\mathrm{i}\,k\,r\cos\theta) = \sum_{l=0,\infty} a_l\,j_l(k\,r)\,P_l(\cos\theta),$$

  where the a_l are constants.
- Of course, there are no Neumann functions in this expansion because they are not well behaved as $r \rightarrow 0$ (whereas function on left-hand side is clearly finite at $r = 0$).
- As is well known, Legendre polynomials are orthogonal functions,

$$\int_{-1}^{1} P_n(\mu)\,P_m(\mu)\,d\mu = \frac{\delta_{n\,m}}{n+1/2}, \tag{27}$$

  so we can invert preceding expansion to give

$$a_l\,j_l(k\,r) = (l+1/2)\int_{-1}^{1} \exp(\mathrm{i}\,k\,r\,\mu)\,P_l(\mu)\,d\mu.$$

Partial Waves - VII

- Now,
$$j_l(y) = \frac{(-\mathrm{i})^l}{2} \int_{-1}^{1} \exp(\mathrm{i}\, y\, \mu)\, P_l(\mu)\, d\mu,$$
for $l = 0, \infty$.
- Thus, a comparison of previous equations yields
$$a_l = \mathrm{i}^l\,(2\,l + 1),$$
giving
$$\exp(\mathrm{i}\,k\,r\cos\theta) = \sum_{l=0,\infty} \mathrm{i}^l\,(2\,l+1)\,j_l(k\,r)\,P_l(\cos\theta). \qquad (28)$$
- Preceding expression specifies how a plane wave can be decomposed into a series of spherical waves.
- Latter waves are usually referred to as partial waves.

Partial Waves - VIII

- Most general expression for total wavefunction outside scattering region is

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} [A_l\, j_l(k\, r) + B_l\, \eta_l(k\, r)]\, P_l(\cos\theta), \quad (29)$$

  where the A_l and B_l are constants.
- Note that Neumann functions are allowed to appear in this expansion, because its region of validity does not include origin.
- In large-r limit, total wavefunction reduces to

$$\psi(\mathbf{x}) \simeq \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} \left[A_l\, \frac{\sin(k\, r - l\, \pi/2)}{k\, r} - B_l\, \frac{\cos(k\, r - l\, \pi/2)}{k\, r}\right] P_l(\cos\theta),$$

  where use has been made of (25) and (26).

Partial Waves - IX

- Previous expression can also be written

$$\psi(\mathbf{x}) \simeq \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} C_l \, \frac{\sin(k\,r - l\,\pi/2 + \delta_l)}{k\,r} \, P_l(\cos\theta), \quad (30)$$

where

$$A_l = C_l \, \cos\delta_l, \quad (31)$$

$$B_l = -C_l \, \sin\delta_l. \quad (32)$$

Partial Waves - X

- (30) yields

$$\psi(\mathbf{x}) \simeq \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} C_l \left[\frac{e^{\,i\,(k\,r - l\,\pi/2 + \delta_l)} - e^{-i\,(k\,r - l\,\pi/2 + \delta_l)}}{2\,i\,k\,r} \right] P_l(\cos\theta), \tag{33}$$

  which contains both incoming and outgoing spherical waves.
- What is source of incoming waves?
- Obviously, they must form part of large-r asymptotic expansion of incident wavefunction.
- In fact, it is easily seen from (19), (25), and (28) that

$$\phi(\mathbf{x}) \simeq \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} i^l\,(2\,l+1) \left[\frac{e^{\,i\,(k\,r - l\,\pi/2)} - e^{-i\,(k\,r - l\,\pi/2)}}{2\,i\,k\,r} \right] P_l(\cos\theta), \tag{34}$$

  in large-r limit.
- Now, (19) and (20) give

$$(2\pi)^{3/2}\,[\psi(\mathbf{x}) - \phi(\mathbf{x})] = \frac{\exp(\,i\,k\,r)}{r}\,f(\theta). \tag{35}$$

Partial Waves - XI

- Note that right-hand side consists only of an outgoing spherical wave.
- This implies that coefficients of incoming spherical waves in large-r expansions of $\psi(\mathbf{x})$ and $\phi(\mathbf{x})$ must be equal.
- It follows from (33) and (34) that

$$C_l = (2\,l+1)\,\exp[\,\mathrm{i}\,(\delta_l + l\,\pi/2)], \tag{36}$$

which leads to

$$\phi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} \mathrm{i}^l\,(2\,l+1)\,\frac{\sin(k\,r - l\,\pi/2)}{k\,r}\,P_l(\cos\theta), \tag{37}$$

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} \mathrm{i}^l\,(2\,l+1)\,\mathrm{e}^{\,\mathrm{i}\,\delta_l}\,\frac{\sin(k\,r - l\,\pi/2 + \delta_l)}{k\,r}\,P_l(\cos\theta). \tag{38}$$

Partial Waves - XII

- Thus, it is apparent that effect of scattering is to introduce a phase-shift, δ_l, into lth partial wave.
- Finally, (35) yields

$$f(\theta) = \sum_{l=0,\infty} (2\,l+1)\,\frac{\exp(\,\mathrm{i}\,\delta_l)}{k}\,\sin\delta_l\,P_l(\cos\theta). \tag{39}$$

- Clearly, determining scattering amplitude, $f(\theta)$, via a decomposition into partial waves (i.e., spherical waves), is equivalent to determining phase-shifts, δ_l.

Partial Waves - XIII

- It is helpful to write

$$\phi(\mathbf{r}) = \sum_{l=0,\infty} \left[\phi_l^+(r,\theta) + \phi_l^-(r,\theta)\right], \tag{40}$$

$$\psi(\mathbf{r}) = \sum_{l=0,\infty} \left[S_l\,\phi_l^+(r,\theta) + \phi_l^-(r,\theta)\right], \tag{41}$$

where

$$\phi_l^-(r,\theta) = -\frac{(2\,l+1)}{(2\pi)^{3/2}}\,\frac{\mathrm{e}^{-\mathrm{i}\,(k\,r-l\,\pi)}}{2\,\mathrm{i}\,k\,r}\,P_l(\cos\theta) \tag{42}$$

is an ingoing spherical wave, whereas

$$\phi_l^+(r,\theta) = \frac{(2\,l+1)}{(2\pi)^{3/2}}\,\frac{\mathrm{e}^{\,\mathrm{i}\,k\,r}}{2\,\mathrm{i}\,k\,r}\,P_l(\cos\theta) \tag{43}$$

is an outgoing spherical wave.

- Moreover,

$$S_l = \mathrm{e}^{\,\mathrm{i}\,2\,\delta_l}. \tag{44}$$

[See (37) and (38).]

Partial Waves - XIII

- Note that $\phi_l^-(r,\theta)$ and $\phi_l^+(r,\theta)$ are both eigenstates of magnitude of total orbital angular momentum about origin belonging to eigenvalues $\sqrt{l\,(l+1)}\,\hbar$.
- Thus, in preforming a partial wave expansion, we have effectively separated incoming and outgoing particles into streams possessing definite angular momenta about origin.
- Moreover, effect of scattering is to introduce an angular-momentum-dependent phase-shift into outgoing particle streams.

Partial Waves - XIV

- Net outward particle flux through a sphere of radius r, centered on origin, is proportional to

$$\oint r^2 j_r \, d\Omega,$$

where $\mathbf{j} = (\hbar/m)\,\mathrm{Im}(\psi^*\,\nabla\psi)$ is probability current.

- It follows that

$$\oint r^2\, j_r\, d\Omega = \frac{\hbar}{8\pi^2\, k\, m} \sum_{l=0,\infty} (2\,l+1)\,(|S_l|^2 - 1), \qquad (45)$$

where use has been made of (27).

- Of course, net particle flux must be zero, otherwise number of particles would not be conserved.
- Particle conservation is ensured by fact that $|S_l| = 1$ for all l. [See (44).]

Optical Theorem - I

- Differential scattering cross-section, $d\sigma/d\Omega$, is simply modulus squared of scattering amplitude, $f(\theta)$. [See (10).]
- Total scattering cross-section is defined as

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

$$= \frac{1}{k^2}\oint d\varphi \int_{-1}^{1} \sum_{l=0,\infty}\sum_{l'=0,\infty}(2\,l+1)\,(2\,l'+1)\exp[\,{\rm i}\,(\delta_l-\delta_{l'})]$$

$$\times \sin\delta_l\,\sin\delta_{l'}\,P_l(\mu)\,P_{l'}(\mu)\,d\mu, \quad (46)$$

where $\mu = \cos\theta$.

- It follows that

$$\sigma_{\rm total} = \frac{4\pi}{k^2}\sum_{l=0,\infty}(2\,l+1)\,\sin^2\delta_l, \quad (47)$$

where use has been made of (27).

Optical Theorem - II

- A comparison of preceding expression with (39) reveals that

$$\sigma_{\text{total}} = \frac{4\pi}{k}\,\mathrm{Im}\,[f(0)] = \frac{4\pi}{k}\,\mathrm{Im}\,[f(\mathbf{k},\mathbf{k})], \qquad (48)$$

  because $P_l(1) = 1$.
- This result is known as optical theorem, and is a consequence of fact that very existence of scattering requires scattering in forward ($\theta = 0$) direction, in order to interfere with incident wave, and thereby reduce probability current in that direction.

Optical Theorem - III

- It is conventional to write

$$\sigma_{\rm total} = \sum_{l=0,\infty} \sigma_l,$$

where

$$\sigma_l = \frac{4\pi}{k^2}\,(2\,l+1)\,\sin^2\delta_l \tag{49}$$

is termed lth partial scattering cross-section: that is, contribution to total scattering cross-section from lth partial wave.

- Note that (at fixed k) maximum value for lth partial scattering cross-section occurs when associated phase-shift, δ_l, takes value $\pi/2$.

Determination of Phase-Shifts - I

- Let us now consider how partial wave phase-shifts, δ_l, can be evaluated.
- Consider a spherically symmetric potential, $V(r)$, that vanishes for $r > a$, where a is termed range of potential.
- In region $r > a$, wavefunction $\psi(\mathbf{x})$ satisfies free-space Schrödinger equation, (21).
- According to (29), (31), (32), and (36), most general solution of this equation that is consistent with no incoming spherical waves, other than those contained in incident wave, is

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} \mathrm{i}^l\,(2\,l+1)\,A_l(r)\,P_l(\cos\theta), \tag{50}$$

where

$$A_l(r) = \exp(\,\mathrm{i}\,\delta_l)\,\left[\cos\delta_l\,j_l(k\,r) - \sin\delta_l\,\eta_l(k\,r)\right]. \tag{51}$$

Determination of Phase-Shifts - II

- Note that Neumann functions are allowed to appear in previous expression, because its region of validity does not include torigin (where $V \neq 0$).
- Logarithmic derivative of lth radial wavefunction, $A_l(r)$, just outside range of potential is given by

$$\beta_{l+} = k\,a\left[\frac{\cos\delta_l\,j_l'(k\,a) - \sin\delta_l\,\eta_l'(k\,a)}{\cos\delta_l\,j_l(k\,a) - \sin\delta_l\,\eta_l(k\,a)}\right],$$

  where $j_l'(x)$ denotes $dj_l(x)/dx$, et cetera.
- Previous equation can be inverted to give

$$\tan\delta_l = \frac{k\,a\,j_l'(k\,a) - \beta_{l+}\,j_l(k\,a)}{k\,a\,\eta_l'(k\,a) - \beta_{l+}\,\eta_l(k\,a)}. \tag{52}$$

- Thus, problem of determining phase-shift, δ_l, is equivalent to that of determining β_{l+}.

Determination of Phase-Shifts - III

- Most general solution to Schrödinger's equation inside range of potential ($r < a$) that does not depend on azimuthal angle, φ, is

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0,\infty} \mathrm{i}^l \, (2\,l+1)\, A_l(r)\, P_l(\cos\theta), \tag{53}$$

where

$$A_l(r) = \frac{u_l(r)}{r}, \tag{54}$$

and

$$\frac{d^2 u_l}{dr^2} + \left[k^2 - \frac{2\,m}{\hbar^2}\,V - \frac{l\,(l+1)}{r^2}\right] u_l = 0. \tag{55}$$

- Boundary condition

$$u_l(0) = 0 \tag{56}$$

ensures that radial wavefunction is well behaved at origin.

Determination of Phase-Shifts - IV

- We can launch a well-behaved solution of previous equation from $r = 0$, integrate out to $r = a$, and form logarithmic derivative [of $A_l(r)$]

$$\beta_{l-} = \frac{1}{(u_l/r)} \frac{d(u_l/r)}{dr}\bigg|_{r=a}.$$

- Because $\psi(\mathbf{x})$ and its first derivatives are necessarily continuous for physically acceptable wavefunctions, it follows that

$$\beta_{l+} = \beta_{l-}.$$

- Phase-shift, δ_l, is then obtained from (52).

Hard-Sphere Scattering - I

- Let us try out scheme outlined previously using a particularly simple example.
- Consider scattering by a hard sphere, for which potential is infinite for $r < a$, and zero for $r > a$.
- It follows that $\psi(\mathbf{x})$ is zero in region $r < a$, which implies that $u_l = 0$ for all l.
- Thus,

$$\beta_{l-} = \beta_{l+} = \infty$$

  for all l.
- (52) yields

$$\tan\delta_l = \frac{j_l(k\,a)}{\eta_l(k\,a)}. \tag{57}$$

- In fact, this result is most easily obtained from obvious requirement that $A_l(a) = 0$. [See (51).]

Hard-Sphere Scattering - II

- Consider $l = 0$ partial wave, which is usually referred to as S-wave.
- (57) gives

$$\tan\delta_0 = \frac{\sin(k\,a)/k\,a}{-\cos(k\,a)/ka} = -\tan(k\,a),$$

where use has been made of (23) and (24).

- It follows that

$$\delta_0 = -k\,a. \tag{58}$$

- S-wave radial wavefunction is

$$\begin{aligned} A_0(r) &= \exp(-\mathrm{i}\,k\,a)\left[\frac{\cos(k\,a)\,\sin(k\,r) - \sin(k\,a)\,\cos(k\,r)}{k\,r}\right] \\ &= \exp(-\mathrm{i}\,k\,a)\,\frac{\sin[k\,(r-a)]}{k\,r}. \end{aligned} \tag{59}$$

[See (51).]

Hard-Sphere Scattering - III

- Corresponding radial wavefunction for incident wave takes form

$$\tilde{A}_0(r) = \frac{\sin(k\, r)}{k\, r}.$$

[See (37), (38), (50), and (58).]

- It is clear that actual $l = 0$ radial wavefunction is similar to incident $l = 0$ wavefunction, except that it is phase-shifted by $k\, a$.

Hard-Sphere Scattering - IV

- Let us consider low- and high-energy asymptotic limits of $\tan\delta_l$.
- Low energy corresponds to $k\,a \ll 1$.
- In this limit, spherical Bessel functions and Neumann functions reduce to

$$j_l(k\,r) \simeq \frac{(k\,r)^l}{(2\,l+1)!!},$$

$$\eta_l(k\,r) \simeq -\frac{(2\,l-1)!!}{(k\,r)^{l+1}},$$

  where $n!! = n\,(n-2)\,(n-4)\cdots 1$.
- It follows that

$$\tan\delta_l = \frac{-(k\,a)^{2\,l+1}}{(2\,l+1)\,[(2\,l-1)!!]^2}.$$

- It is clear that we can neglect δ_l, with $l > 0$, with respect to δ_0.

Hard-Sphere Scattering - V

- In other words, at low energy, only S-wave scattering (i.e., spherically symmetric scattering) is important.
- It follows from (10), (39), and (58) that

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2(k\,a)}{k^2} \simeq a^2 \tag{60}$$

for $k\,a \ll 1$.

- Note that total cross-section,

$$\sigma_{\rm total} = \oint \frac{d\sigma}{d\Omega}\,d\Omega = 4\pi\,a^2,$$

is four times geometric cross-section, $\pi\,a^2$ (i.e., cross-section for classical particles bouncing off a hard sphere of radius a).

- However, low-energy scattering implies relatively long de Broglie wavelengths, so we would not expect to obtain classical result in this limit.

Hard-Sphere Scattering - VI

- Consider high-energy limit, $k\,a \gg 1$.
- At high energies, by analogy with classical scattering, scattered particles with largest angular momenta about origin have angular momenta $\hbar\,k\,a$ (i.e., product of their incident momenta, $\hbar\,k$, and their maximum possible impact parameters, a).
- Given that particles in lth partial wave have angular momenta $\sqrt{l\,(l+1)}\,\hbar$, we deduce that all partial waves up to $l_{\rm max} \simeq k\,a$ contribute significantly to scattering cross-section.
- It follows from (47) that

$$\sigma_{\rm total} = \frac{4\pi}{k^2} \sum_{l=0,l_{\rm max}} (2\,l+1)\,\sin^2\delta_l. \tag{61}$$

Hard-Sphere Scattering - VII

- Making use of (57), as well as asymptotic expansions (25) and (26), we find that

$$\sin^2\delta_l = \frac{\tan^2\delta_l}{1+\tan^2\delta_l} = \frac{j_l^2(k\,a)}{j_l^2(k\,a)+\eta_l^2(k\,a)} = \sin^2(k\,a - l\,\pi/2).$$

- In particular,

$$\sin^2\delta_l + \sin^2\delta_{l+1} = \sin^2(k\,a - l\,\pi/2) + \cos^2(k\,a - l\,\pi/2) = 1.$$

- Hence, it is a good approximation to write

$$\sigma_{\rm total} \simeq \frac{2\pi}{k^2}\sum_{l=0,l_{\rm max}}(2\,l+1) = \frac{2\pi}{k^2}\,(l_{\rm max}+1)^2 \simeq 2\pi\,a^2.$$

- This is twice classical result, which is somewhat surprising, because we might expect to obtain classical result in short-wavelength limit.

Hard-Sphere Scattering - VIII

- In fact, for hard-sphere scattering, all incident particles with impact parameters less than a are deflected.
- However, in order to produce a shadow behind sphere, there must be scattering in forward direction (recall optical theorem) to produce destructive interference with incident plane wave.
- Effective cross-section associated with this forward scattering is $\pi\, a^2$, which, when combined with cross-section for classical reflection, $\pi\, a^2$, gives actual cross-section of $2\pi\, a^2$.

Low-Energy Scattering - I

- In general, at low energies (i.e., when $1/k$ is much larger than range of potential), partial waves with $l > 0$ make a negligible contribution to scattering cross-section.
- It follows that, with a finite-range potential, only S-wave (i.e., spherically symmetric) scattering is important at such energies.

Low-Energy Scattering - II

- As a specific example, let us consider scattering by a finite potential well, characterized by $V = V_0$ for $r < a$, and $V = 0$ for $r \geq a$
- Here, V_0 is a constant.
- Potential is repulsive for $V_0 > 0$, and attractive for $V_0 < 0$.
- External wavefunction is given by [see (51)]

$$A_0(r) = \exp(\mathrm{i}\,\delta_0)\,\left[j_0(k\,r)\cos\delta_0 - \eta_0(k\,r)\sin\delta_0\right]$$
$$= \frac{\exp(\mathrm{i}\,\delta_0)\,\sin(k\,r+\delta_0)}{k\,r},$$

  where use has been made of (23) and (24).
- Internal wavefunction follows from (55). We obtain

$$A_0(r) = B\,\frac{\sin(k'\,r)}{r}, \tag{62}$$

  where use has been made of boundary condition (56).

Low-Energy Scattering - III

- Here, B is a constant, and

$$E - V_0 = \frac{\hbar^2 k'^2}{2m}. \tag{63}$$

- Note that (62) only applies when $E > V_0$.
- For $E < V_0$, we have

$$A_0(r) = B\,\frac{\sinh(\kappa\,r)}{r},$$

where

$$V_0 - E = \frac{\hbar^2 \kappa^2}{2m}. \tag{64}$$

- Matching $A_0(r)$, and its radial derivative, at $r = a$ yields

$$\tan(k\,a + \delta_0) = \frac{k}{k'}\,\tan(k'\,a) \tag{65}$$

for $E > V_0$, and

$$\tan(k\,a + \delta_0) = \frac{k}{\kappa}\,\tanh(\kappa\,a)$$

for $E < V_0$.

Low-Energy Scattering - IV

- Consider an attractive potential, for which $E > V_0$.
- Suppose that $|V_0| \gg E$ (i.e., depth of potential well is much larger than energy of incident particles), so that $k' \gg k$.
- As can be seen from (65), unless $\tan(k'\,a)$ becomes extremely large, right-hand side of equation is much less than unity, so replacing tangent of a small quantity with quantity itself, we obtain

$$k\,a + \delta_0 \simeq \frac{k}{k'}\,\tan(k'\,a).$$

- This yields

$$\delta_0 \simeq k\,a\left[\frac{\tan(k'\,a)}{k'\,a} - 1\right].$$

- According to (61), total scattering cross-section is given by

$$\sigma_{\rm total} \simeq \frac{4\pi}{k^2}\sin^2\delta_0 = 4\pi\,a^2\left[\frac{\tan(k'\,a)}{k'\,a} - 1\right]^2. \qquad (66)$$

Low-Energy Scattering - V

- Now,

$$k' \, a = \sqrt{k^2 \, a^2 + \frac{2 \, m \, |V_0| \, a^2}{\hbar^2}}, \tag{67}$$

so for sufficiently small values of $k \, a$,

$$k' \, a \simeq \sqrt{\frac{2 \, m \, |V_0| \, a^2}{\hbar^2}}.$$

- It follows that total (S-wave) scattering cross-section is independent of energy of incident particles (provided that this energy is sufficiently small).

Low-Energy Scattering - VI

- Note that there are values of $k' a$ (e.g., $k' a \simeq 4.493$) at which scattering cross-section (66) vanishes, despite very strong attraction of potential.
- In reality, cross-section is not exactly zero, because of contributions from $l > 0$ partial waves. But, at low incident energies, these contributions are small.
- It follows that there are certain values of $|V_0|$, a, and k that give rise to almost perfect transmission of incident wave.
- This is called Ramsauer-Townsend effect, and has been observed experimentally.

Resonant Scattering - I

- There is a significant exception to energy independence of scattering cross-section at low incident energies described previously.
- Suppose that quantity $(2\,m\,|V_0|\,a^2/\hbar^2)^{1/2}$ is slightly less than $\pi/2$.
- As incident energy increases, $k'a$, which is given by (67), can reach value $\pi/2$.
- In this case, $\tan(k'\,a)$ becomes infinite, so we can no longer assume that right-hand side of (65) is small.
- In fact, at value of incident energy at which $k'\,a = \pi/2$, it follows from (65) that $k\,a + \delta_0 = \pi/2$, or $\delta_0 \simeq \pi/2$ (because we are assuming that $k\,a \ll 1$).
- This implies that

$$\sigma_{\rm total} = \frac{4\pi}{k^2}\sin^2\delta_0 = 4\pi\,a^2\left(\frac{1}{k^2\,a^2}\right).$$

Resonant Scattering - II

- Note that total scattering cross-section now depends on energy. Furthermore, magnitude of cross-section is much larger than that given in (66) for $k' a \neq \pi/2$ (because $k a \ll 1$, whereas $k' a \sim 1$).
- Origin of rather strange behavior just described is easily explained.
- Condition

$$\sqrt{\frac{2\, m\, |V_0|\, a^2}{\hbar^2}} = \frac{\pi}{2}$$

  is equivalent to condition that a spherical well of depth $|V_0|$ possesses a bound state at zero energy.
- Thus, for a potential well that satisfies preceding equation, energy of scattering system is essentially same as energy of bound state.

Resonant Scattering - III

- In this situation, an incident particle would like to form a bound state in potential well.
- However, bound state is not stable, because system has a small positive energy.
- Nevertheless, this sort of resonant scattering is best understood as capture of an incident particle to form a metastable bound state, followed by decay of bound state and release of particle.
- Cross-section for resonant scattering is generally far higher than that for non-resonant scattering.

Resonant Scattering - IV

- We have seen that there is a resonant effect when phase-shift of S-wave takes value $\pi/2$.
- There is nothing special about $l = 0$ partial wave, so it is reasonable to assume that there is a similar resonance when phase-shift of lth partial wave is $\pi/2$.
- Suppose that δ_l attains value $\pi/2$ at incident energy E_0, so that

$$\delta_l(E_0) = \frac{\pi}{2}.$$

- Let us expand $\cot\delta_l$ in vicinity of resonant energy:

$$\cot\delta_l(E) = \cot\delta_l(E_0) + \left(\frac{d\cot\delta_l}{dE}\right)_{E=E_0}(E - E_0) + \cdots$$

$$= -\left(\frac{1}{\sin^2\delta_l}\frac{d\delta_l}{dE}\right)_{E=E_0}(E - E_0) + \cdots.$$

Resonant Scattering - V

- Defining

$$\left[\frac{d\delta_l(E)}{dE}\right]_{E=E_0} = \frac{2}{\Gamma},$$

we obtain

$$\cot\delta_l(E) = -\frac{2}{\Gamma}(E - E_0) + \cdots.$$

- Recall, from (49), that contribution of lth partial wave to total scattering cross-section is

$$\sigma_l = \frac{4\pi}{k^2}(2\,l+1)\,\sin^2\delta_l = \frac{4\pi}{k^2}(2\,l+1)\,\frac{1}{1+\cot^2\delta_l}.$$

- Thus,

$$\sigma_l \simeq \frac{4\pi}{k^2}(2\,l+1)\,\frac{\Gamma^2/4}{(E-E_0)^2+\Gamma^2/4}$$

which is known as Breit-Wigner formula.

- Variation of partial cross-section, σ_l, with incident energy has form of a classical resonance curve.

Resonant Scattering - VI

- Quantity Γ is width of resonance (in energy).
- We can interpret Breit-Wigner formula as describing absorption of an incident particle to form a metastable state, of energy E_0, and lifetime $\tau = \hbar/\Gamma$.

Elastic and Inelastic Scattering - I

- From before, for case of a spherically symmetric scattering potential, scattered wave is characterized by

$$f(\theta) = \sum_{l=0,\infty} (2\,l+1)\,f_l\,P_l(\cos\theta), \tag{68}$$

where

$$f_l = \frac{\exp(\mathrm{i}\,\delta_l)}{k}\,\sin\delta_l = \frac{S_l - 1}{2\,\mathrm{i}\,k} \tag{69}$$

is amplitude of lth partial wave, whereas δ_l is associated phase-shift.

- Here,

$$S_l = \mathrm{e}^{\,\mathrm{i}\,2\,\delta_l}.$$

- Moreover, fact that $|S_l| = 1$ ensures that scattering is elastic (i.e., that number of particles is conserved).
- Finally, net elastic scattering cross-section can be written

$$\sigma_{\rm elastic} = \frac{4\pi}{k^2}\sum_{l=0,\infty}(2\,l+1)\,\sin^2\delta_l = 4\pi\sum_{l=0,\infty}(2\,l+1)\,|f_l|^{\,2}. \tag{70}$$

Elastic and Inelastic Scattering - II

- Turns out that many scattering experiments are characterized by absorption of some of incident particles.
- Such absorption may induce a change in quantum state of target, or, perhaps, emergence of another particle.
- Note that scattering that does not conserve particle number is known as inelastic scattering.
- We can take inelastic scattering into account in our analysis by writing

$$S_l = \eta_l \, \mathrm{e}^{\,\mathrm{i}\, 2\,\delta_l}, \tag{71}$$

  where real parameter η_l is such that

$$0 \leq \eta_l \leq 1.$$

- It follows from (69) that

$$f_l = \frac{\eta_l \, \sin(2\,\delta_l)}{2\,k} + \mathrm{i}\left[\frac{1-\eta_l\,\cos(2\,\delta_l)}{2\,k}\right].$$

Elastic and Inelastic Scattering - III

- Hence, according to (70), net elastic scattering cross-section becomes

$$\sigma_{\rm elastic} = 4\pi \sum_{l=0,\infty} (2\,l+1)\,|f_l|^{\,2}$$

$$= \frac{\pi}{k^2} \sum_{l=0,\infty} (2\,l+1)\left[1+\eta_l^{\,2} - 2\,\eta_l\,\cos(2\,\delta_l)\right]. \qquad (72)$$

- Net inelastic scattering (i.e., absorption) cross-section follows from (9) and (45):

$$\sigma_{\rm inelastic} = \frac{\oint r^{\,2}\,(-j_r)\,d\Omega}{|{\bf j}_{\rm incident}|} = \frac{\pi}{k^2} \sum_{l=0,\infty} (2\,l+1)\left(1-|S_l|^{\,2}\right)$$

$$= \frac{\pi}{k^2} \sum_{l=0,\infty} (2\,l+1)\left(1-\eta_l^{\,2}\right). \qquad (73)$$

Elastic and Inelastic Scattering - IV

- Thus, total cross-section is

$$\sigma_{\rm total} = \sigma_{\rm elastic} + \sigma_{\rm inelastic}$$
$$= \frac{2\pi}{k^2} \sum_{l=0,\infty} (2\,l+1)\,[1-\eta_l\,\cos(2\,\delta_l)].$$

- Note, from (68), (69), and (71) that

$${\rm Im}[f(0)] = \frac{1}{2\,k} \sum_{l=0,\infty} (2\,l+1)\,[1-\eta_l\,\cos(2\,\delta_l)].$$

- In other words,

$$\sigma_{\rm total} = \frac{4\pi}{k}\,{\rm Im}[f(0)].$$

- Hence, we deduce that optical theorem still applies in presence of inelastic scattering.

Elastic and Inelastic Scattering - V

- If $\eta_l = 1$ then there is no absorption, and lth partial wave is scattered in a completely elastic manner.
- On other hand, if $\eta_l = 0$ then there is total absorption of lth partial wave.
- However, such absorption is necessarily accompanied by some degree of elastic scattering.
- In order to illustrate this important point, let us investigate special case of scattering by a black sphere.
- Such a sphere has a well-defined edge of radius a, and is completely absorbing.
- Consider short-wavelength scattering characterized by $k\,a \gg 1$.
- In this case, we expect all partial waves with $l \leq l_{\rm max}$, where $l_{\rm max} \simeq k\,a$, to be completely absorbed (because, by analogy with classical physics, impact parameters of associated particles are less than a), and all other partial waves to suffer neither absorption nor scattering.

Elastic and Inelastic Scattering - VI

- In other words, $\eta_l = 0$ for $0 \leq l_{\max}$, and $\eta_l = 1$, $\delta_l = 0$ for $l > l_{\max}$.
- It follows from (72) and (73) that

$$\sigma_{\text{elastic}} = \frac{\pi}{k^2} \sum_{l=0,l_{\max}} (2\,l+1) = \frac{\pi}{k^{\,2}}\,(1+l_{\max})^{\,2} \simeq \pi\,a^2,$$

and

$$\sigma_{\text{inelastic}} = \frac{\pi}{k^2} \sum_{l=0,l_{\max}} (2\,l+1) = \frac{\pi}{k^{\,2}}\,(1+l_{\max})^{\,2} \simeq \pi\,a^2.$$

- Thus, total scattering cross-section is

$$\sigma_{\text{total}} = \sigma_{\text{elastic}} + \sigma_{\text{inelastic}} = 2\pi\,a^2.$$

- This result seems a little strange, at first, because, by analogy with classical physics, we would not expect total cross-section to exceed cross-section presented by sphere.
- Nor would we expect a totally absorbing sphere to give rise to any elastic scattering.

Elastic and Inelastic Scattering - V

- In fact, this reasoning is incorrect. Absorbing sphere removes flux proportional to $\pi\, a^2$ from incident wave, which leads to formation of a shadow behind sphere.
- However, a long way from sphere, shadow gets filled in.
- In other words, shadow is not visible infinitely far downstream of sphere.
- Only way in which this can occur is via diffraction of some of incident wave around edges of sphere.
- Actually, amount of incident wave that must be diffracted is same amount as was removed from wave by absorption. Thus, scattered flux is also proportional to $\pi\, a^2$.

Elastic and Inelastic Scattering - VI

- Consider low-energy scattering by a hard-sphere potential.
- This process is dominated by S-wave (i.e., $l = 0$) scattering.
- Moreover, phase-shift of S-wave takes form

$$\delta_0 = -k\,a,$$

where k is wavenumber of incident particles, and a is radius of sphere.

- Note that low-energy limit corresponds to $k\,a \ll 1$.
- It follows that

$$S_0 = \mathrm{e}^{\,\mathrm{i}\,2\,\delta_0} \simeq 1 - 2\,\mathrm{i}\,k\,a.$$

- We can generalize previous analysis to take absorption into account by writing

$$S_0 \simeq 1 - 2\,\mathrm{i}\,k\,\alpha,$$

where α is complex, $k\,|\alpha| \ll 1$, and $\mathrm{Im}(\alpha) < 0$.

Elastic and Inelastic Scattering - VII

- According to (72) and (73),

$$\sigma_{\rm elastic} \simeq \frac{\pi}{k^2}\left|S_0 - 1\right|^2 \simeq 4\pi\,|\alpha|^2, \tag{74}$$

$$\sigma_{\rm inelastic} \simeq \frac{\pi}{k^2}\left(1 - |S_0|^2\right) \simeq \frac{4\pi\,{\rm Im}(-\alpha)}{k}. \tag{75}$$

- We conclude that low-energy elastic scattering cross-section is again independent of incident particle velocity (which is proportional to k), whereas inelastic cross-section is inversely proportional to particle velocity.
- Consequently, as incident particle velocity decreases, inelastic scattering becomes more and more important in comparison with elastic scattering.

Scattering of Identical Particles - I

- Consider two identical particles that scatter off one another.
- In center of mass frame, there is no way of distinguishing a deflection of a particle through an angle θ, and a deflection through an angle $\pi - \theta$, because momentum conservation demands that if one of particles is scattered in direction characterized by angle θ then other is scattered in direction characterized by $\pi - \theta$.
- Here, for sake of simplicity, we are assuming that scattering potential is spherically symmetric, which implies that motion of two particles is confined to a fixed plane passing through origin.

Scattering of Identical Particles - II

- In classical mechanics, differential cross-section for scattering is affected by identity of particles because number of particles counted by a detector located at angular position θ is sum of counts due to two particles, which implies that

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

[See (10).]

Scattering of Identical Particles - III

- In quantum mechanics, overall wavefunction must be either symmetric or antisymmetric under interchange of identical particles, depending on whether particles in question are bosons or fermions, respectively.
- If spatial wavefunction is symmetric then (20) is replaced by

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\left(\mathrm{e}^{\,\mathrm{i}\,k\,r\cos\theta} + \mathrm{e}^{-\mathrm{i}\,k\,r\cos\theta} + \frac{\mathrm{e}^{\,\mathrm{i}\,k\,r}}{r}\left[f(\theta)+f(\pi-\theta)\right]\right),$$

and associated differential scattering cross-section becomes

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

[See (10).]

Scattering of Identical Particles - IV

- On other hand, if spatial wavefunction is antisymmetric then (20) is replaced by

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\left(\mathrm{e}^{\,\mathrm{i}\,k\,r\cos\theta} - \mathrm{e}^{-\mathrm{i}\,k\,r\cos\theta} + \frac{\mathrm{e}^{\,\mathrm{i}\,k\,r}}{r}\left[f(\theta) - f(\pi-\theta)\right]\right),$$

and associated differential scattering cross-section is written

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

Scattering of Identical Particles - V

- For case of two identical spin-zero (i.e., boson) particles (e.g., α-particles), spatial wavefunction is symmetric with respect to particle interchange, which implies that

$$\frac{d\sigma}{d\Omega} = |f(\theta) + f(\pi - \theta)|^2$$
$$= |f(\theta)|^2 + |f(\pi - \theta)|^2 + [f^*(\theta)\, f(\pi - \theta) + f(\theta)\, f^*(\pi - \theta)].$$

- Previous result differs from classical one because of interference term (i.e., final term on right-hand side), which leads to an enhancement of differential scattering cross-section at $\theta = \pi/2$.
- In fact,

$$\left(\frac{d\sigma}{d\Omega}\right)_{\theta=\pi/2} = 4\,[f(\pi/2)]^{\,2},$$

whereas

$$\left(\frac{d\sigma_{\rm classical}}{d\Omega}\right)_{\theta=\pi/2} = 2\,[f(\pi/2)]^{\,2}.$$

Scattering of Identical Particles - VI

- For case of two identical spin-$1/2$ (i.e., fermion) particles (e.g., electrons or protons), overall wavefunction is antisymmetric under particle interchange.
- If two particles are in spin singlet state then spatial wavefunction is symmetric (because spin wavefunction is antisymmetric), and

$$\frac{d\sigma_{\rm singlet}}{d\Omega} = |f(\theta)+f(\pi-\theta)|^2$$
$$= |f(\theta)|^2 + |f(\pi-\theta)|^2 + [f^\ast(\theta)\,f(\pi-\theta) + f(\theta)\,f^\ast(\pi-\theta)].$$

- On other hand, if two particles are in spin triplet state then spatial wavefunction is antisymmetric (because spin wavefunction is symmetric), which leads to

$$\frac{d\sigma_{\rm triplet}}{d\Omega} = |f(\theta)-f(\pi-\theta)|^2$$
$$= |f(\theta)|^2 + |f(\pi-\theta)|^2 - [f^\ast(\theta)\,f(\pi-\theta) + f(\theta)\,f^\ast(\pi-\theta)].$$

Scattering of Identical Particles - VII

- In former case, interference term leads to an enhancement (with respect to the classical case) of differential scattering cross-section at $\theta = \pi/2$: that is,

$$\left(\frac{d\sigma_{\rm singlet}}{d\Omega}\right)_{\theta=\pi/2} = 4\,[f(\pi/2)]^{\,2}.$$

- In latter case, interference term leads to complete suppression of scattering in direction $\theta = \pi/2$: that is,

$$\left(\frac{d\sigma_{\rm triplet}}{d\Omega}\right)_{\theta=\pi/2} = 0.$$

Scattering of Identical Particles - VIII

- Consider mutual scattering of two unpolarized beams of spin-$1/2$ particles.
- All spin states are equally likely, so probability of finding a given pair of particles (one from each beam) in triplet state is three times that of finding it in singlet state, which implies that

$$\left(\frac{d\sigma_{\rm unpolarized}}{d\Omega}\right) = \frac{1}{4}\left(\frac{d\sigma_{\rm singlet}}{d\Omega}\right) + \frac{3}{4}\left(\frac{d\sigma_{\rm triplet}}{d\Omega}\right)$$
$$= |f(\theta)|^2 + |f(\pi-\theta)|^2$$
$$- \frac{1}{2}\left[f^*(\theta)\, f(\pi-\theta) + f(\theta)\, f^*(\pi-\theta)\right].$$

- In this case, interference term leads to incomplete suppression (with respect to classical case) of differential scattering cross-section at $\theta = \pi/2$: that is,

$$\left(\frac{d\sigma_{\rm unpolarized}}{d\Omega}\right)_{\theta=\pi/2} = [f(\pi/2)]^2.$$