Theory of Scattering

A parallel beam of particles of given momentum is directed towards a target which deflects or scatters the particles in various direction. The scattered particles diverge. Eventually at large distance from the target, their motion is directed radically outward. For convenience, we choose a coordinate system with the origin at the position of the target or scattering centre, and Z- axis in the direction of incident beam. The direction of any scattered particle is indicated by polar angles (θ,ϕ) with the Z axis taken as polar axis

θ is the angle of scattering, ie angle between the scattered and incident directions. These two directions together define the plane of scattering. The azimuthal angle ϕ specifies the orientation of this plane with respect to some reference plane containing Z axis.

For more details see
https://www.physics.harvard.edu/uploads/files/thesesPDF/lupusax.pdf

Scattering crossection

Consider a scattering experiment in which a steady incident beam is maintained for an indefinitely long time. Incident flux is defined as the number of particles crossing unit area taken normal to the beam direction per unit time and is denoted by 'F'. In this experiment 'F' is independent of time.

These beam strikes the target and a steady stream of scattered particles followed. Let 'ΔN' be the number of particles scattered into a small solid angle $\Delta\Omega$ about the direction (θ,ϕ) in time Δt.

$\therefore \Delta N$ is proportional to $\Delta\Omega\ \Delta t$ and to incident flux F

$$\Delta N \;\alpha\; \Delta\Omega\ \Delta t\ F$$

Or $$\Delta N = \frac{d\sigma}{d\Omega}(\theta,\phi)\ \Delta\Omega\ \Delta t\ F \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (1)$$

The proportionality constant $\frac{d\sigma}{d\Omega}$, which depends on θ and ϕ is called the differential scattering crossection. It depends only the parameters of incident particles and nature of the target. The total scattering crossection σ is obtained from it by integration over all directions.

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \frac{d\sigma}{d\Omega} \sin\theta\, d\theta\, d\phi \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

In most of the cases, we consider $\frac{d\sigma}{d\Omega}$ is independent of ϕ, then (2) becomes

$$\sigma = \int_0^{\pi} \frac{d\sigma}{d\Omega}\, 2\pi \sin\theta\, d\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

σ has the dimension of area.

For more details watch https://www.youtube.com/watch?v=twdF0EIbFds

Scattering amplitude

→Wave mechanical picture of scattering

When particles involved in the scattering process are quantum mechanical objects, we must describe then by a wave function. The phenomenon of scattering is manifested as a distortion in the stationary wave pattern, caused by the presence of scattering centre. At large distance from the scattering centre r →∞, the form of the wave function u(x) must consist of a part u_{inc} corresponding to the parallel beam of incident particles and u_{sc} representing the scattered particles moving radially outward from the centre

$$u(x) \underset{r \to \infty}{\longrightarrow} u_{inc} + u_{sc} \quad \ldots\ldots\ldots\ldots\ldots (4)$$

The beam of incident particles with momentum ħk can be represented by the plane wave

$$u_{inc} = e^{ikz}$$

Where k is the propagation constant.

Let $|u_{in\,c}|^2$ be the number of incident particles per unit volume. Then the incident flux F is

$$F_{in} = |u\ in\ c|^2\ V = \frac{\hbar k}{m} \qquad \ldots\ldots\ldots\ldots\ldots (5)$$

(since $|uin\ c|^2 = 1$, normalized wave fun)

Assume that the scattering is elastic, then the scattered particles will have the same momentum as the incident ones. And since the scatterd wave move radically they must be spherical.

$$u_{sc} \ \alpha \ \frac{e^{ikr}}{r}$$

$$\text{Or} \quad u_{sc} = f(\theta,\phi)\,\frac{e^{ikr}}{r} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Where the proportionality factor is f(θ,ϕ) which is direction dependent and is called scattering amplitude.

Flux of scattered particles.

$$F_{sc} = |u_{sc}|^2 V = |u_{sc}| \frac{\hbar K}{m}$$

Then number of particles scattered

$$\Delta N = \text{flux} * \text{area} * \text{time}$$

$$= |u_{sc}|^2 \frac{\hbar K}{m} \Delta S \, \Delta t$$

$$= |f(\theta,\phi)|^2 \frac{e^{ikr} \bar{e}^{ikr}}{r^2} \frac{\hbar K}{m} r^2 \Delta\Omega \, \Delta t \text{ .... (7)}$$

$$\Delta N = |f(\theta,\phi)|^2 \frac{\hbar K}{m} \Delta\Omega \, \Delta t \text{ ....(8)}$$

But we know that

$$\Delta N = \frac{d\sigma}{d\Omega} \Delta\Omega \, \Delta t \; F$$

Equating (4) and (5) and substituting the value of F from (2) we get

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = |f(\theta,\phi)|^2 \text{ .... (9)}$$

By this relation, f (θ,ϕ)is called scattering amplitude .

Now at r → α , the wave function

$$u(x) \rightarrow e^{iKz} + f(\theta,\phi) \frac{e^{ikr}}{r} \text{ ....(10)}$$

We assume that a steady (time independent) incident beam is maintained. Then the wave function will be stationary and it will obey time independent Schrödinger equation

$$[\frac{-\hbar^2}{2m}\nabla^2 + V]\,\psi\,(r) = E\,\psi\,(r) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

Here $\psi = u(x)$

$$\therefore\ [\frac{-\hbar^2}{2m}\nabla^2 + V]\,u(x) = E\,u(x)$$

It is possible to get a formal solution for the scattering amplitude by transferring (7) to an integral equation. To accomplish this we make use of greens function method.

Expression for scattering amplitude using Greens function

For full detailed theory of Green's function read

http://www.math.caltech.edu/~dinakar/08-Ma1cAnalytical-Notes-chap.6.pdf

From (7)

We have

$$\frac{\hbar^2}{2m}\nabla^2\psi(r) + V\,\psi\,(r) = \frac{\hbar^2 K^2}{2m}\psi(r)$$

$$\text{Or}\quad \frac{\hbar^2}{2m}(k^2+\nabla^2)\,\psi(r) = V\,\psi\,(r)$$

$$(\nabla^2 + k^2)\,\varphi\,(r) = \frac{2m}{\hbar^2} V\,\varphi\,(v) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (12)$$

Put $\frac{2m\,v}{\hbar^2}$ = u (r)

∴ (8) becomes

$$(\nabla^2 + k^2)\, \varphi(r) = U(r)\, \varphi(r) \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \;(13)$$

At large distance,

$$\psi(r) = \psi\, inc + \psi\, sc$$

$$= e^{ikr} + f(\theta,\phi)\, \frac{e^{ikr)}}{r}$$

$$= u(x)$$

∴ (9) Become

$$(\nabla^2 + k^2)\, e^{ikr} + (\nabla^2 + k^2)\, \psi s = u(r)\; \psi(r) \text{ -------------- } (14)$$

But for r→∞

$$(\nabla^2 + k^2)\, e^{ikr} = 0$$

∴ (10) reduces to

$$(\nabla^2 + k^2)\, \psi s = u(r)\; \psi(r) = -\rho(r) \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (15)$$

Eqn (11) is an in homogeneous equation and the inhomogeneous term depends on ψ(r). Its solution is obtained by greens function method.

Let Ω (x,∇) be any liner differential operator, then any function

G (x,x′)such that

$$\Omega\,(X,\nabla)\,G\,(x,x') = \delta\,(x-x') \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ (16)$$

is said to be a greens function for the operator Ω.

here we can written as

$$(\Delta^2 + k^2)\,G\,(r-r') = \delta(r-r')$$

and the general solution of any in homogeneous equation

$$\Omega\,(r,\Delta)\,u(r) = F\,(r) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(17)$$

is of the from u (r) = $\int G\,(r,r')\ \mathrm{f}\,(r')\,d\tau'$

hence ψ(s) can be written

$$\psi(s) = \int G\,(r,r')\,\rho\,(r')\,d\tau'$$

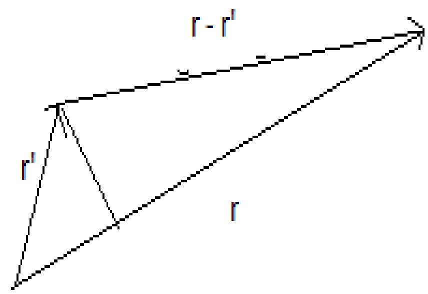
using greens fun technique and contour integration, we get

$$G(r,r') = \frac{-\exp(ik|r-r'|)}{4\pi|r-r'|}$$

$$\therefore \psi(s) = -\frac{1}{4\pi} = \int \frac{-\exp(ik|r-r'|)}{|r-r'|}\,\rho\,(r')\,d\tau' \text{-------------------- } (18)$$

Where $\rho\,(r') = u(r')\,\psi(r')$

Where r is the position of the scattered particle after being scattered is the region r' ≡0. The scattered wave ψs at point ‘r’ has the form of the superposition of spherical waves originating from all points r' with amplitudes u(r') ψ(r'). The following figure illustrates the vectors r and r'.



$$|r - r'| = r - \hat{n}.r'$$

$$k|r - r'| = kr - k'.r'$$

Since r is very large, replacing lr-r'l in the denominator of equation (18) by r, the wave function ψ(r) can be written as

$$\psi(r) \rightarrow \exp(ik.r) - \frac{1}{4\pi}\int \frac{\exp i\,(kr - k'.r')}{r} u(r')\,\psi(r')d\tau' \text{ ----------- (19)}$$

Eq (15) is the integral equation for the wave function. Now comparing Eq (19) and (i), we get

$$f(\theta,\phi) = -\frac{1}{4\pi}\int \exp(-ik'r')u(r')\psi(r')d\tau') \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (20)$$

from which differential scattering cross section $\frac{d\sigma}{d\Omega}$ can be calculated

Now to find f(θ,ϕ), we must know ψ(r'). ψ(r') is evaluated using an iterative procedure developed by Born know as the Born approximation.

The Born approximation

In the first Born approximation ψ(r') is the integral (16) is replaced by the incoming plane wave exp (ik.r'). This leads to an improved value for the wave function ψ(r) which is used in the integral in the second Born approximation. This iterative procedure continues till both the input and output Ψ s are almost equal. As higher order approximations are complicated, we only consider the first born approximation.

Replacing Ψ (r') in the integral in Eq (16) by exp (ik.r') we get

$$f(\theta)= -\frac{1}{4\pi}\int \exp[i(k-k^1).r\,')\ u(r')d\tau\,' \quad \text{------------------------- (21)}$$

where k and k' are wave vectors in the incident and scattered directions respectively. The quality (k-k') ħ=qħ is the momentum transfer from the incident particle to scatter particle. The change in momentum qħ due to collision is given by

$$q\hbar = (k-k')\,\hbar$$

$$|q| = 2\,|k|\sin\frac{\theta}{2}$$

replacing (k-k') in Eq (21) we get,

$$f(\theta) = -\frac{1}{4\pi}\int \exp(iq.r\,')\ ')\ u(r')d\tau\,' \quad \text{----------------- (22)}$$

The angular integration is carried out by taking the direction of q as the polar axis.

From figure we have q = 2k $\sin\frac{\theta}{2}$. The scattering amplitude in the Born approximation, considered as a function of q is the Fourier transform of the potential.In the most important special case when V is spherically symmetric, we can reduce (18) to an integral of r alone, by going over to spherical polar coordinaties with the direction of q chosen as the polar axis.

So $f(\theta) = -\frac{1}{4\pi}\int_0^\infty \int_0^\pi \int_0^{2\pi} \exp(iq\, r' \cos\theta')\, V(r')\, r'^2 \sin\theta' dr' d\theta' d\phi'$-----(23)

Solving above integral and substituting

$$u(r') = \frac{2m}{\hbar^2} V(r'), \text{ we get}$$

$$f(\theta) = -\frac{2\mu}{\hbar^2}\int_0^\infty \frac{\sin(qr')}{qr'}\, V(r')\, r'^2 dr' \quad \text{-----------------------(24)}$$

An important feature Born approximation formula Eq (20) is that f depends on the momentum transfer only, and not on the initial momentum and the angle of scattering separately. And the amplitude for a momentum transfer to is the value of the Fourier transform of the potential function V(r) at this particular q.

Validity of Born approximation

In Born approximation $\Psi(r')$ m Eq (16) was replaced by exp (ikr') which is valid only if the scattered wave Ψs is small compared to the plane wave. The scattered wave Ψs is likely to be maximum in the interaction region, where $r \equiv 0$ with r = 0 in Eq (18) the condition reduces to

$$\left|\frac{1}{4\pi}\right| \frac{\exp(-ikr')}{r'} u(r') \exp(ik.r')\, d\tau' \big| \ll 1 \qquad \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ (25)$$

Where $k.r' = kr' \cos\theta$ and $d\tau' = r'^2 \sin\theta' dr' d\theta' d\phi'$

Carrying out angular integration Eq (21) reduces to

$$\left| \int_0^\infty \frac{\exp(ikr')}{r'} u(r') \frac{\sin(kr')}{kr'} \; r'^2 dr' \right| << 1$$

$$\frac{2\mu}{k\hbar^2} \left| \int_0^\infty \exp(ikr') \sin(kr') V(r') dr' \right| << 1$$

If the energy is sufficiently high, sin (kr') will be a rapidly varying function and the value of the integral in Eq (22) will be very small. A weak potential also make the integral small. Hence Born approximation is valid for weak potentials at high energies.

Scattering by a screened coulomb potential

As an example of Born approximation, we shall consider the scattering of a apotential having charge Z'e by an atomic potential of charge Ze. The interaction between the two is usually screened by the atomic electrons surrounding the nucleus. The potential representing the interaction can be written as

$$V(r) = -\frac{zz'e^2}{r} e^{-\alpha r} \qquad \text{..................(26)}$$

Where α is the parameter which determines the screening by atomic electrons. With this value of V(r), the scattering amplitude f(θ) $in\ Eq$ (20) becomes

$$f(\theta) = \frac{2\mu zz'e^2}{\hbar^2 q} \int_0^\infty \sin(qr') \exp(-\alpha r')\, dr'$$

$$= \frac{2\mu zz'e^2}{\hbar^2 q} \frac{q}{q^2+\alpha^2}$$

$$= \frac{2\mu zz'e^2}{\hbar^2 (q^2+\alpha^2)} \qquad \text{..................(27)}$$

$$\therefore \; \sigma(\theta) = |f(\theta)|^2 = \left[\frac{2\mu zz'e^2}{\hbar^2 q}\right]^2 \frac{1}{(\alpha^2+q^2)^2} \qquad \text{..................(28)}$$

If the momentum transfer q$\gg \alpha$

$$q^2 + \alpha^2 \cong q^2 = 4k^2 \sin^2\frac{\theta}{2} \qquad \text{………………..(29)}$$

And $$\sigma(\theta) = \frac{\mu^2 z^2 z'^2 e^4}{4\hbar^4 k^4 \sin^4(\frac{\theta}{2})} \qquad \text{………………(30)}$$

This is Rutherford's scattering formula for scattering by a coulomb potential$-\frac{zz'e^2}{r}$.

Partial wave analysis

While the Born approximation is basically, a truncation of a perturbation expansion of u(x), the method of partial waves is based upon an expansion of u(x) in terms of angular momentum eigen functions. It is applicable if the potential is spherically symmetric. Partial wave analysis is a low energy approximation which complements the Born approximation.

A plane wave e^{ikz} can be expanded as a linear combination of spherical waves as

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(\text{kr}) P_l(\cos\theta) \qquad \text{……………(31)}$$

j_l(kr) is the spherical Bessel function of order l and P_l are the Legendre polynomials. Each term on the right hand side represents a spherical wave. The plane wave is thus equivalent to the superposition of an infinite number of spherical waves and the individual waves are called partial waves. The waves with l=0,1,2… are called s- wave, the p-wave, d-wave and so on. Asymptotically

$$j_l(\text{kr}) \rightarrow \frac{1}{kr}\sin(\text{kr} - \frac{l\pi}{2})$$

$$e^{ikz} = \sum_{l=0}^{\infty} \frac{i^l(2l+1)}{2ik} P_l(\cos\theta)\frac{1}{r}\left[exp\left(ikr - \ i\frac{l\pi}{2}\right) - exp\left(-ikr + i\frac{l\pi}{2}\right)\right] \text{.......(32)}$$

This form shows that each partial wave can be represented as the sum of an incoming and outgoing spherical wave. In scattering problems the first few spherical waves are the most important ones. The s- partial wave will be independent of the angle θ and hence spherically symmetric about the origin. Result of extremely low energy scattering can be explained satisfactorily with S-wave alone. If the energy is slightly higher, we need p-wave also to explain the observed value.

Scattering by a Central Potential: Partial wave analysis

The schrödinger equation that describes the scattering is given by

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V(r) = E\psi \qquad \text{..........................(33)}$$

$\mu = \frac{mM}{m+M}$, where m is the mass of the incident particles and M is the mass of the target. Since he potential has spherical symmetry we can separate the schrödinger equation in to radial and angular part and obtain solution as

$$\Psi(r,\theta) = R_l(r)P_l\,(\cos\theta) \qquad \text{..........................(34)}$$

Where R_l(r) satisfies the radial equation:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \left[\frac{2\mu E}{\hbar^2} - \frac{2\mu V}{\hbar^2} - \frac{l(l+1)}{r^2}\right]R_l = 0 \text{..........................(35)}$$

Outside the range of potential ($r>r_0$), this equation reduces to the free particle equation:

$$\frac{d^2R_l}{dr^2}+\frac{2}{r}\frac{dR_l}{dr}+\left[k^2-\frac{l(l+1)}{r^2}\right]R_l=0 \qquad \text{...............................(36)}$$

Where $k^2=\frac{2\mu E}{\hbar^2}$

Differential equation (31) has two independent solutions $j_l(kr)$ and $n_l(kr)$, where $j_l(kr)$ is the spherical Bessel function and $n_l(kr)$, is the spherical Neumann function. The general solution is

$$R_l(kr)=A^{'}j_l(kr)-B^{'}n_l(kr)$$

Where $A^{'}$ and $B^{'}$ are constants. Though the function is not finite at r=0 it is retained as we are interested only in the asymptotic solution. Asymptotically we have

$$R_l(kr)=_{r\to\infty}\frac{A^{'}}{kr}\sin(kr-\frac{l\pi}{2})+\frac{B^{'}}{kr}\cos(kr-\frac{l\pi}{2}) \qquad \text{............................(32)}$$

When V(r) ≠ 0, we have the asymptotic solution of Eq. (30) as

$$R_l(kr)=\frac{A_l}{kr}\sin(kr-\frac{l\pi}{2}+\delta_l),\quad l=0,1,2\ldots \qquad \text{................................(37)}$$

Where A_l is a constant and δ_l's are called phase shifts. The phase shift measures the amount by which the phase of the radial function for angular momentum quantum number l differs from the corresponding one for V = 0 case. The most general asymptotic solution is then

$$\Psi(r,\theta) = \sum_{l=0}^{\infty} \frac{A_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) P_l(\cos\theta) \quad \ldots\ldots(38)$$

Where A_l is the asymptotic amplitude. Thus the effect of the scattering potential is to shift the phase of the outgoing waves relative to that of the incoming waves.

After some manipulations of the above equations we can calculate the scattering amplitude as

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \exp(i\delta_l)\, P_l\cos(\theta) \sin\delta_l \quad \text{-------------} \quad (39)$$

The partial wave analysis gives $f(\theta)$ as a sum of contributions from all partial waves.

The Scattering cross section

The differential scattering cross section

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{k^2} \left|\sum_{l=0}^{\infty} (2l+1) \exp(i\delta_l)\, P_l\cos(\theta) \sin\delta_l\right|^2 \quad \ldots\ldots(40)$$

The total cross-section σ *is*

$$\sigma = \int_0^{\pi} \sigma(\theta)\, d\Omega = \int_0^{\pi} \sigma(\theta)\, (2\pi \sin\theta) d\theta = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\delta_l \quad (41)$$

In deriving Eq. (41) orthogonal property of Legendre polynomial is used. The differential and total cross-sections are thus given in terms of the phase shits δ_l of the partial waves.

For s-wave scattering the differential scattering cross-section $\sigma_0(\theta)$ and the total cross-section σ_0 are given by

$$\sigma_0(\theta) = \frac{sin^2(\theta)}{k^2} \text{ and} \sigma_0 = \frac{4\pi}{k^2} sin^2(\delta_0) \qquad \text{.....................(42)}$$

Both cross-sections do not depend on the angle θ. Often s- wave contribution is the most dominant part in most of the experiments. From Eq. (40) it is clear that $\sigma(\theta)$ contains terms representing interference between different partial waves whereas the total cross-section σ in Eq.(41) does not contain such terms.

Optical Theorem

For the case $\theta = 0$, we get from Eq.(35)

$$\text{f}(0) = \frac{1}{k} \sum_{l=0}^{\infty}(2l + 1) \exp(\text{i}\delta_l) \sin\delta_l \qquad \text{................(43)}$$

The imaginary part of this scattering amplitude is given by

$$\text{Im f}(0)= \frac{1}{k} \sum_{l=0}^{\infty}(2l + 1) \exp(\text{i}\delta_l) \, sin^2(\delta_l) \qquad \text{...............(44)}$$

Comparing these two equations we get

$$\sigma = \frac{4\pi}{k} \text{Im } f(0) \qquad \text{……………………..…(45)}$$

This relation is known as Optical theorem in analogy with the relation in optics between the absorption coefficient and the imaginary part of the complex index of refraction.

Scattering length

Evaluation of scattering cross-section needs knowledge of phase shiftsδ_l, l=0,1,2………. In most of the cases the s- wave (l=0) contribution is the predominant one. A simple case occurs if the energy E or kr_0, where r_0 is the range of potential, is very low so that only s-state is involved in the scattering. In such a case we have from Eq.(39)

$$f_0(\theta) = \frac{1}{k} \exp(i\delta_0) \sin\delta_0 \qquad \text{…………………..(46)}$$

The limiting value of energy foe which Eq.(38) is valid is called "zero energy" and that of –f(θ) as E →0 is called "scattering length". Denoted by a.

$$a = \lim_{E\to 0}[-f(\theta)] = -\frac{1}{k} \exp(i\delta_0) \sin\delta_0 \qquad \text{……………………...(47)}$$

It follows from Eqs. (38) and (44) that the zero energy cross-section

$$\sigma_0 = 4\pi a^2 \qquad \text{…………………….(48)}$$

If V(r) is weak, δ_0 will be very small which makes exp($i\delta_0$)$\cong$ 1 and sin$\delta_0 \cong \delta_0$. Consequently from Eq. (44) we get

$$a = \lim_{E\to 0}\left(-\frac{\delta_0}{k}\right) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(49)$$

Or we can say that in the zero energy limit, δ_0 = - ka.

The concept of scattering length is extensively used in the investigation relating to the scattering of thermal neutrons.

Reference

A Text Book of Quantum Mechanics by P M Mathews and K Venkitesan

For a full course watch http://ocw.mit.edu/8-04S16