Advanced Quantum Mechanics

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Scattering Theory

Ref : Sakurai, Modern Quantum Mechanics
Taylor, Quantum Theory of Non-Relativistic Collisions
Landau and Lifshitz, Quantum Mechanics

Universality of low energy scattering

We have seen that the low energy scattering from a potential can be characterized by a few parameters

E.g. s-wave scattering can be parametrized by a_s, r_0, etc.

Clearly this cannot depend on all the details of the shape of the potential

For square well $\beta_0 = qa\cot(qa) - 1$

Scattering Length $a_s = \frac{a\beta_0}{1+\beta_0}$

$\frac{q^2}{2m} = E - V_0$

So we can have many different potentials at the microscopic level, whose low energy scattering (say a_s, r_0) are same.

E.g. can choose different V_0 and a for a square well so that qa is fixed. Low energy scattering is same for both. We can even get away with a simpler potential (say delta fn) provided we manage to get the correct scattering length

This is your first glimpse into the general phenomenon of universality:

Many systems which look different on a microscopic scale (i.e. different V) can show same phenomena at low energy. This is at the heart of theoretical endeavours to calculate properties of complicated systems.

delta fn potential and cutoff dependence

Consider s-wave scattering due to a delta function potential $V(r) = g\delta(r)$

$V_{\vec{k}\vec{k'}} = g$

$$T = V + VG_0T$$

$$T = (1 - VG_0)^{-1}V$$

$$= g(1 - gG_0)^{-1}$$

$$Lim_{k\to 0}T(|k| = |k'| = (2mE)^{1/2}) = \frac{4\pi a_s}{m}$$

$$\frac{-m}{4\pi a_s} = \frac{1}{g} + \sum_{k'} G_0(k', E \to 0)$$

$$= \frac{1}{g} - \sum_{k'} \frac{1}{2k'^2/2m}$$

divergent integral, diverges as Λ in 3D

ultraviolet divergence comes from choosing wrong short distance behaviour

You pay a price for simplifying your life too much — a_s is always 0 !!

Two ways out of the conundrum:

A) Work with more realistic potential (say square well)

The range of the potential a, provides a natural cutoff $\Lambda \sim a^{-1}$ and answers are finite. Universality at low energies guarantees that details of V does not matter.

delta fn potential and cutoff dependence

Consider s-wave scattering due to a delta function potential $V(r) = g\delta(r)$

$$V_{\vec{k}\vec{k'}} = g \qquad \frac{-m}{4\pi a_s} = \frac{1}{g} + \sum_{k'} G_0(k', E \to 0) \quad = \frac{1}{g} - \sum_{k'} \frac{1}{2k'^2/2m}$$

ultraviolet divergence comes from choosing wrong short distance behaviour

Two ways out of the conundrum:

B) The potential is a tool to get to the scattering length/cross-section, which is the measureable quantity.

Put an explicit cutoff $$-\frac{m}{4\pi a_s} = \frac{1}{g} - \frac{m}{2\pi^2}\int_0^\Lambda dk' = \frac{1}{g} - \frac{m\Lambda}{2\pi^2}$$

Continue to work with the delta fn (it simplifies your life), but make sure that a_s is finite. Given a scattering length, you can now choose different cutoffs but g will be different for different cutoffs.

$$-\frac{m}{4\pi a_s} = \frac{1}{g(\Lambda)} - \frac{m\Lambda}{2\pi^2}$$

Running coupling g (Λ), ensures physical observables are cutoff independent and finite.

Basic Idea of Renormalization Group procedures

Lets you work with a simplified description for low energy phenomena

T Matrix and Effective Interaction

The other way of doing RG

Let us start with integral eqn form of T = V + VG_0T

$$T(k,k',E) = V(k,k') + \sum_{|k''|} \frac{V(k,k'')T(k'',k',E)}{(E - k''^2/2m + i0^+)}$$

Momentum sum runs all the way

Let us define a new quantity U given by

$$U(k,k',E) = V(k,k') + \sum_{|k''|>\Lambda} \frac{V(k,k'')U(k'',k',E)}{(E - k''^2/2m + i0^+)}$$

Momentum sum runs only over high k" > Λ

We will show that

$$T(k,k',E) = U(k,k',E) + \sum_{|k''|\leq\Lambda} \frac{U(k,k'',E)T(k'',k',E)}{(E - k''^2/2m + i0^+)}$$

Momentum sum runs only over low k" < Λ

U can be thought of as an effective interaction obtained by integrating out high k" modes.

This shows that starting from a microscopic scale, there is a definite procedure to obtain an effective interaction.

One can reproduce the T matrix (at low energies) using this (E dependent) effective interaction and corresponding cutoff

T Matrix and Effective Interaction

$$T(k,k',E) = V(k,k') + \sum_{|k''|} \frac{V(k,k'')T(k'',k',E)}{(E - k''^2/2m + i0^+)} \qquad U(k,k',E) = V(k,k') + \sum_{|k''|>\Lambda} \frac{V(k,k'')U(k'',k',E)}{(E - k''^2/2m + i0^+)}$$

$$T(k,k',E) = U(k,k',E) + \sum_{|k''|\leq\Lambda} \frac{U(k,k'',E)T(k'',k',E)}{(E - k''^2/2m + i0^+)}$$

Let P be the projection operator which projects onto momenta k" < Λ
and Q be the projection operator which projects onto momenta k" > Λ

P+Q=1

Define $G_1 = P\,G_0\,P$ Define $G_2 = Q\,G_0\,Q$ $G_0 = G_1 + G_2$

We have $T = V + VG_0T$ $U = V + VG_2U$ Want to show $T = U + UG_1T$

$U = (1 - VG_2)^{-1}V$

$$(1 - UG_1)^{-1}U = (1 - UG_1)^{-1}(1 - VG_2)^{-1}V$$

$$= [1 - VG_2 - UG_1 + VG_2UG_1]^{-1}V$$

$$= [1 - VG_0 + (V + VG_2U - U)]^{-1}V$$

$$= [1 - VG_0]^{-1}V = T$$

Hence $T = U + UG_1T$

Bound States as Poles of S/T Matrix

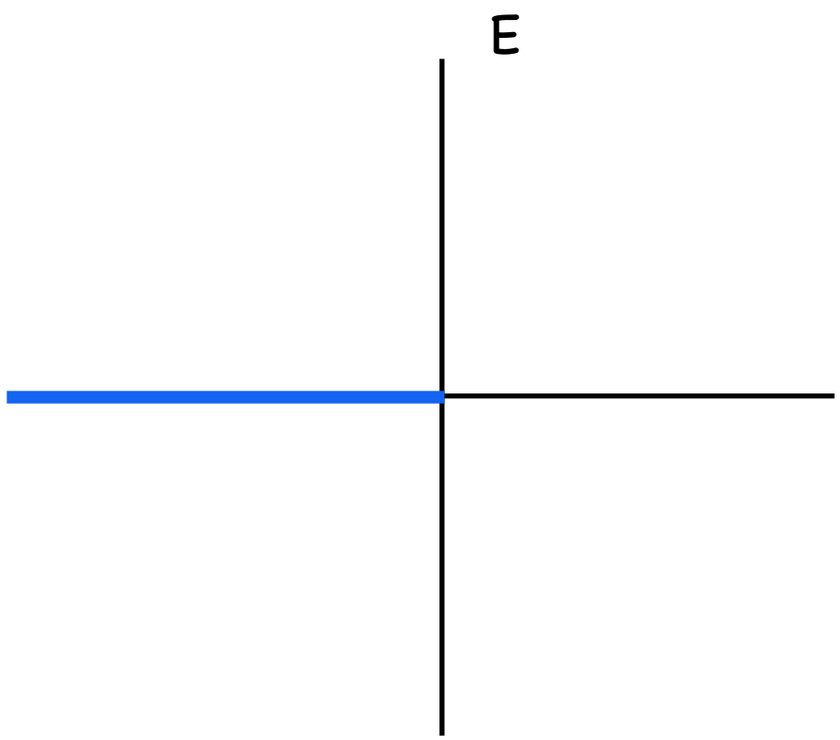
Scattering Solutions far from origin (s-wave) $R(r) \sim S_0(p)\frac{e^{ipr}}{r} - \frac{e^{-ipr}}{r}$

Typical bound state solutions $R(r) \sim \frac{e^{-\kappa r}}{r}$

Suggests that if we analytically continue to complex momenta, S/T matrix can have info about bound states as well.

Convention to work in complex Energy plane

$$u(r) = rR(r) \sim A(E)e^{-\sqrt{-2mE}r} + B(E)e^{\sqrt{-2mE}r}$$

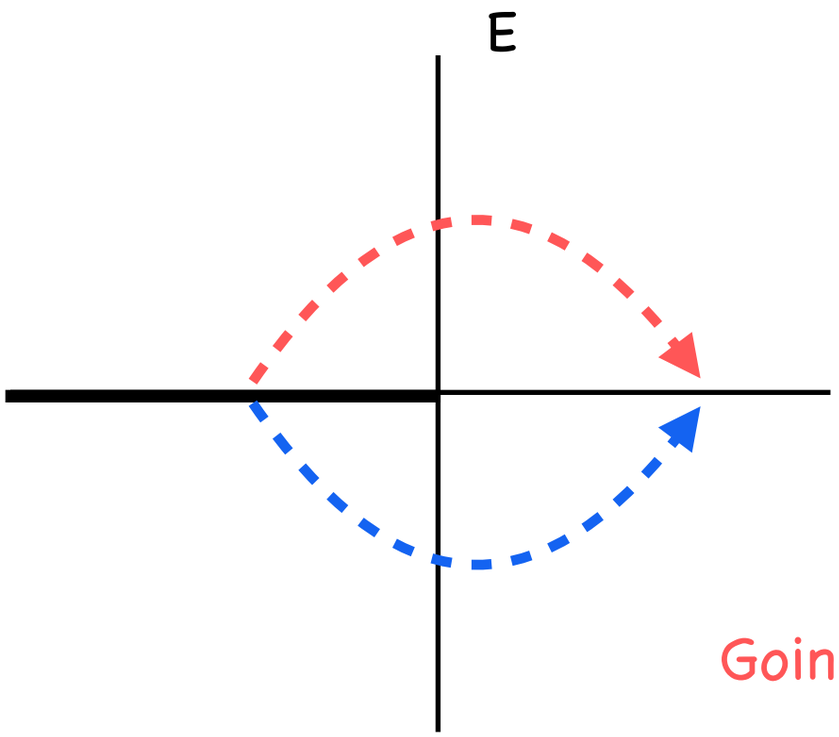


√-E is real and >0, when E is real and < 0

A(E) and B(E) are real on negative real E axis
u(r) is real

A(E*) = A*(E) and B(E*) = B*(E)

Bound States as Poles of S/T Matrix



$$u(r) = rR(r) \sim A(E)e^{-\sqrt{-2mE}r} + B(E)e^{\sqrt{-2mE}r}$$

A(E) and B(E) are real on negative real E axis
u(r) is real

$A(E^*) = A^*(E)$ and $B(E^*) = B^*(E)$

Going from right to left half through upper half plane

$$u(r) \sim A(E)e^{ikr} + B(E)e^{-ikr}$$

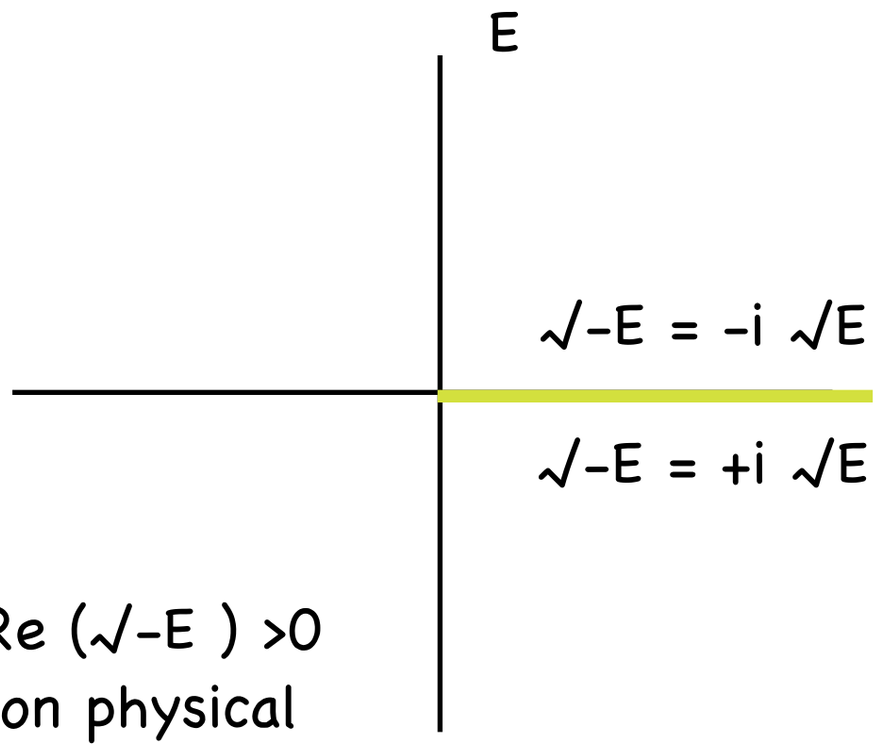
Going from right to left half through lower half plane

$$u(r) \sim A^*(E)e^{-ikr} + B^*(E)e^{ikr}$$

Single valuedness of u for E > 0 ⟶ $A(E) = B^*(E)$

Note that due to presence of √-E in u(r), A(E) and B(E) are not single valued fn.s of E

Bound States as Poles of S/T Matrix



Note that due to presence of √-E in u(r), A(E) and B(E) are not single valued fn.s of E

Branch cut along +ve real axis, makes √-E single valued on the physical Riemann sheet

A(E) and B(E) are single valued

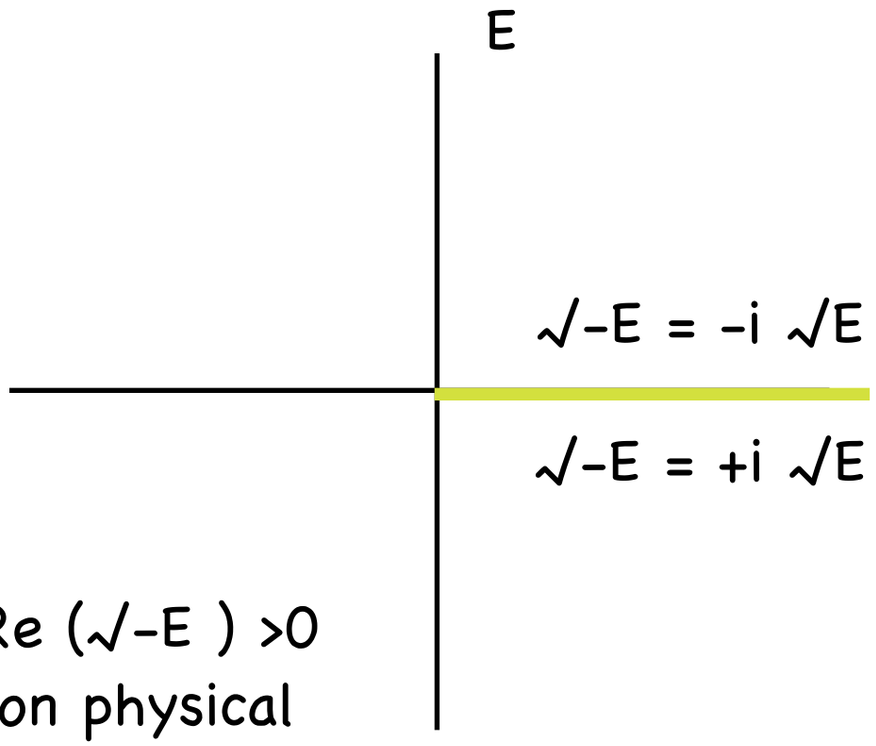
$$u(r) = rR(r) \sim A(E)e^{-\sqrt{-2mE}r} + B(E)e^{\sqrt{-2mE}r}$$

Everywhere on the physical Riemann sheet, first term decays and second term grows.

So, bound states ⟶ B(E) ⟶0 at bound state energy

Real eigenvalues of Schrodinger Eqn ⟶ this must happen on negative real axis. Discrete bound states ⟶ discrete zeroes of B(E)

Bound States as Poles of S/T Matrix



$$u(r) = rR(r) \sim A(E)e^{-\sqrt{-2mE}r} + B(E)e^{\sqrt{-2mE}r}$$

Comparing with

$$u(r) \sim [e^{i(kr+\delta_0)} - e^{-i(kr+\delta_0)}]$$

$$e^{2i\delta_0} = -\frac{A(E)}{B(E)}$$

$$f_0 = \frac{1}{2ik}(e^{2i\delta_0} - 1) = \frac{1}{2\sqrt{-2mE}}\left(\frac{A(E)}{B(E)} + 1\right)$$

Bound States correspond to poles of T/S matrix at negative real E

Also note that when B ⟶0, as diverges with one sign and comes back with another sign.

Bound States as Poles of S/T Matrix

Unitarity of S matrix $S_0 = e^{2i\delta_0}$

Now, by definition of scattering length, as p --> 0 $p \cot \delta_0 \to -1/a \neq 0$

$\delta_0 \to n\pi \qquad S_0 \to 1$

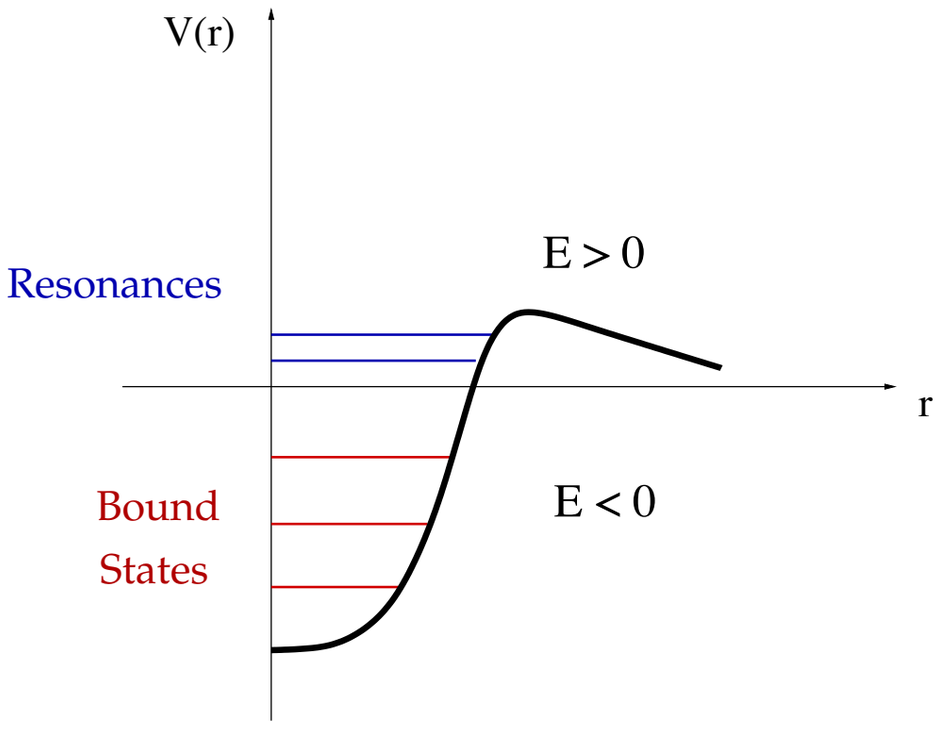
$$S_0 = \frac{g(p) + \alpha p - i\kappa}{p - i\kappa} \qquad g(p) \sim p^2$$

$$f_0(p) = \frac{S_0(p) - 1}{2ip} = \frac{\alpha - 1}{2} \frac{1}{\kappa - ip} + \mathcal{O}(p)$$

by unitarity $\alpha = -1$

Comparing, $\kappa = \frac{1}{a_s}$ Binding Energy : $E_b = \frac{1}{2ma_s^2}$

Resonant Scattering



What happens in other channels?
What happens as we increase energy?

The potential seen by the particles in non s-wave channels consists of two parts, the component of the actual potential in this channel and a centrifugal term $l(l+1)/r^2$.

Depending on the actual potential, this potential can have a maxima at a positive energy. The potential well can then trap quasi-bound states which do not decay at extremely large distances, but behaves like them for large enough distances.

Since we have already seen that dramatic things happen when incident energy coincides with bound state energy, (scattering length and scattering cross section diverges) we may expect something dramatic to happen here as well.

The scattering cross section shows a marked increase (although it does not diverge) for positive incident energies of the particles, when they match the energy of these quasi-bound states. This phenomenon is often called resonant scattering.

Resonant Scattering

To analyze this we go back to our original formula for determining phase-shifts

$$\tan\delta_l(p) = \frac{pRj_l'(pR) - \beta_l(p,R)j_l(pR)}{pRn_l'(pR) - \beta_l(p,R)n_l(pR)}$$

where we have made it explicit that the log-derivative
β_l depends on p and the range R

For low energy $\quad j_l(pR) \sim \frac{(pR)^l}{(2l+1)!!} \quad n_l(pR) \sim \frac{-(2l-1)!!}{(pR)^{l+1}}$

$$\tan\delta_l(p) = \frac{(pR)^{2l+1}}{(2l+1)!!(2l-1)!!}\frac{l-\beta_l(p,R)}{l+1+\beta_l(p,R)}$$

Scattering Amplitude: $\quad f_l(p) = \frac{1}{p\cot\delta_l(p) - ip}$

We have seen in the case of bound states that scattering cross section diverges when the phase shift is either π/2 or 3π/2. At this point, cot(δ_l) is 0. Expanding around this point,

$$\cot\delta_l(E = p^2/2m) = -c(E - E_R) + \mathcal{O}(E - E_R)^2$$

$$\frac{2}{\Gamma} = c = \left.\frac{d(\cot\delta_l)}{dE}\right|_{E=E_R}$$

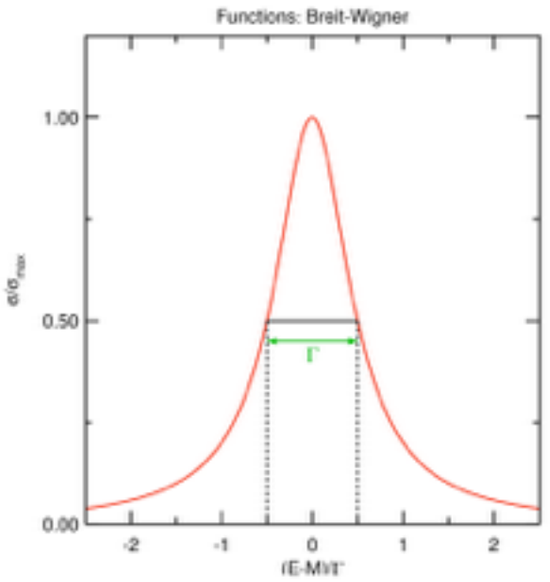
$$f_l(E) = \frac{-1}{p}\frac{1}{c(E-E_R)+i} = -\frac{1}{p}\frac{\Gamma/2}{(E-E_R)+i\Gamma/2}$$

Resonant Scattering

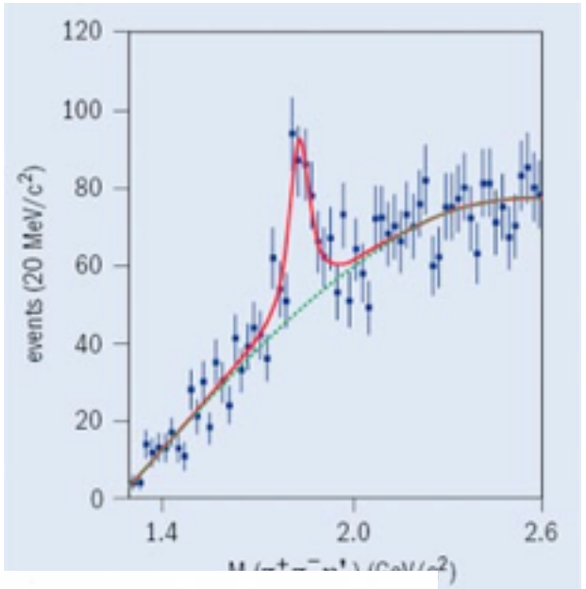
If the dominant contribution to the total scattering cross-section comes from a single resonance,

$$\sigma_l(E) = \frac{4\pi}{p^2}\frac{(2l+1)(\Gamma/2)^2}{(E-E_R)^2+(\Gamma/2)^2}$$

Breit Wigner formula



The Breit Wigner form is the dominant term very close to the resonance. In reality, the Breit Wigner form is superposed on a smooth profile:

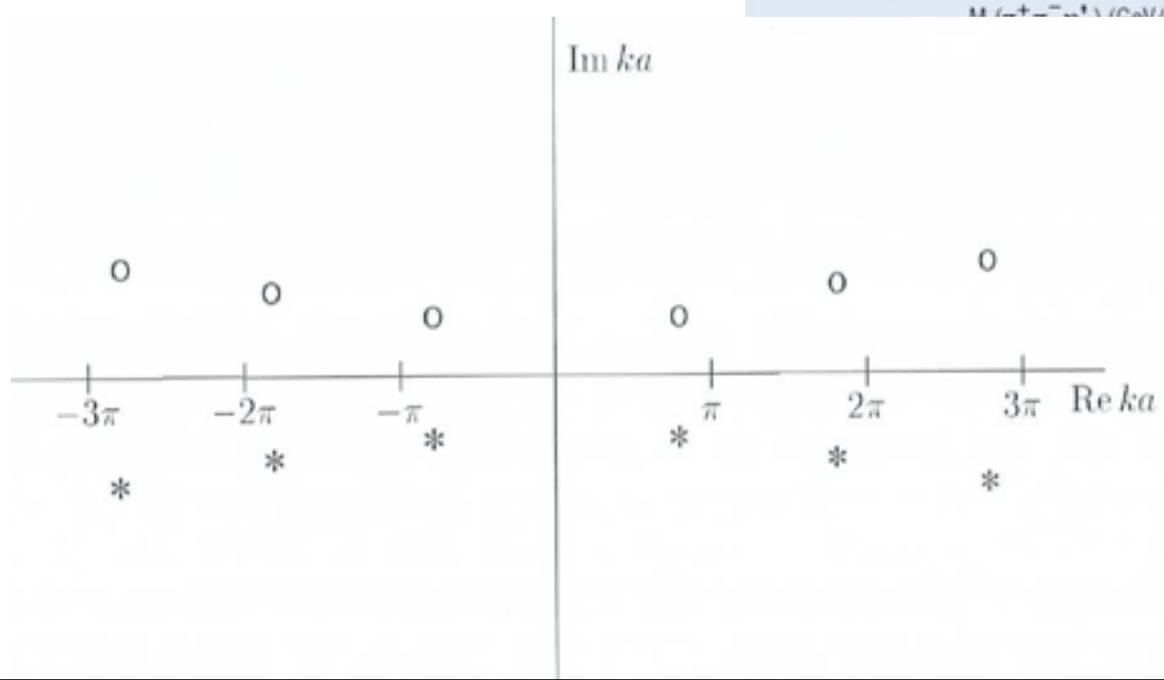


Structure of the S-Matrix for resonance

Poles in lower half-plane.(Contrast with actual bound states)

Symmetrically placed zeroes in the upper half-plane

$$S \sim \frac{p-p_n-i\kappa_n}{p-p_n+i\kappa_n}$$



Scattering from Extended Objects : Form Factors

- Scattering problem defined in terms of interaction potential between incident particle and target

- Realistic situation contains scattering off extended objects; e.g. if the interaction is with electrons of atoms in a target, the electronic charge density is spread over a region determined by the wfns.

$$V(\vec{r}) = \int d\vec{r'} \rho(\vec{r'}) V(\vec{r} - \vec{r'})$$

- In general, the distrn. extends over a lengthscale corresponding to atomic (or nuclear) radii, while the interaction kernel can spread the actual range of the potential further.

- Scattering in the Born Approximation ---> Scattering amplitude is linear in the potential.

- Scattering amplitude is sum of scattering amplitudes, each coming from a point in the charge distrn.

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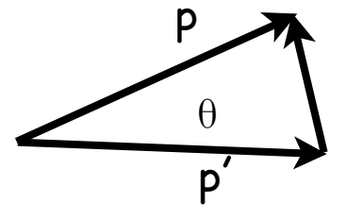
Scattering Amplitude:



$$q = |\vec{p'} - \vec{p}| = 2p\sin\frac{\theta}{2}$$

$$f(\vec{p},\vec{p'}) = f(\theta) = -4\pi^2 m T_{\vec{p'},\vec{p}} = -4\pi^2 m V_{\vec{p'},\vec{p}}$$

$$= -4\pi^2 m \int d\vec{r} V(\vec{r}) e^{i\vec{q}\cdot\vec{r}} = -4\pi^2 m \int d\vec{r} \int d\vec{r'}\rho(\vec{r'}) e^{i\vec{q}\cdot\vec{r'}} V(\vec{r}-\vec{r'}) e^{i\vec{q}\cdot(\vec{r}-\vec{r'})}$$

$$= F(\vec{q})V(\vec{q})$$

$$\frac{d\sigma}{d\Omega} = |F(\vec{q})|^2 |V(\vec{q})|^2$$

Form Factor has info about the distribution → $F(\vec{q}) = \int d\vec{r'}\rho(\vec{r'})e^{i\vec{q}\cdot\vec{r'}}$

Thus, if the interactions are well known, scattering can provide info about distributions in an atom

Scattering from Periodic Structures : Structure Factor

Consider now the problem of scattering off a periodic structure like a lattice. For a concrete example, you can think of neutrons scattering off a lattice (interacting with spins) or light scattering off materials (interacting with charge) etc.

$$V(\vec{r}) = \sum_{j=1}^{N} \rho(\vec{r_j}) V(\vec{r} - \vec{r_j}) = \int d\vec{r'} V(\vec{r} - \vec{r'}) \sum_{j=1}^{N} \rho(\vec{r'}) \delta(\vec{r'} - \vec{r_j})$$

Here r_j is the location of the j^{th} site.

Scattering Amplitude in Born Approximation:

$$f(q) = V(q) \sum_{j=1}^{N} e^{i\vec{q}\cdot\vec{r'}} \rho(\vec{r'}) \delta(\vec{r'} - \vec{r_j})$$

Scattering Cross-Section in Born Approximation:

$$\frac{d\sigma}{d\Omega} = |V(q)|^2 \sum_{jk} \rho(\vec{r_j}) \rho(\vec{r_k}) e^{i\vec{q}\cdot(\vec{r_j} - \vec{r_k})} = |V(q)|^2 S(q)$$

Structure Factor

$$S(q) = \sum_{jk} \rho(\vec{r_j}) \rho(\vec{r_k}) e^{i\vec{q}\cdot(\vec{r_j} - \vec{r_k})}$$

Note that we have treated the potential as if there is just a point particle at lattice sites. In general, there will be extended atomic orbitals at each site. We can also have a unit cell of the lattice made of more than one atom arranged in some way. Thus V(q) may itself be due to extended objects and can be further broken up into a form factor and the potential.

Structure Factor is the Fourier Transform of pair Correlation function