Advanced Quantum Mechanics

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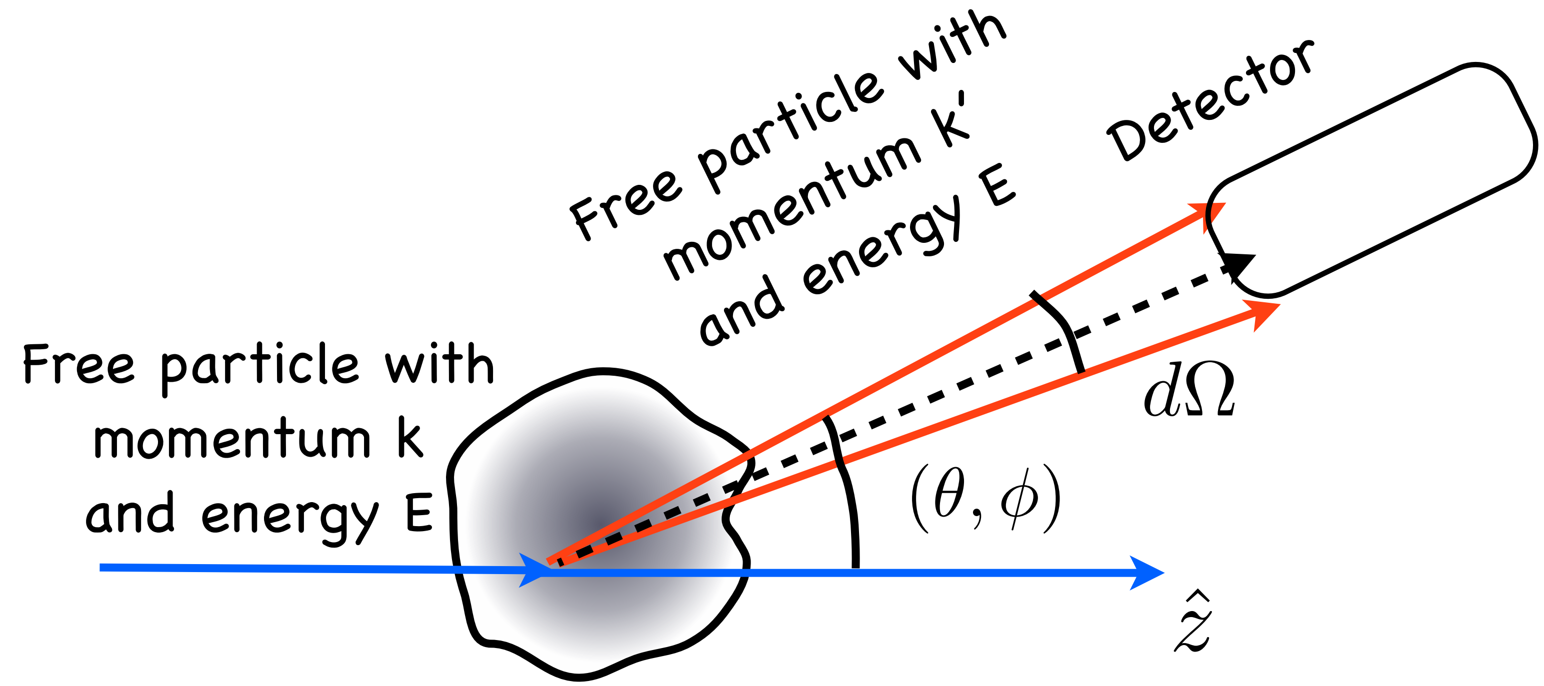
Scattering Theory

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

Recap of Previous Classes

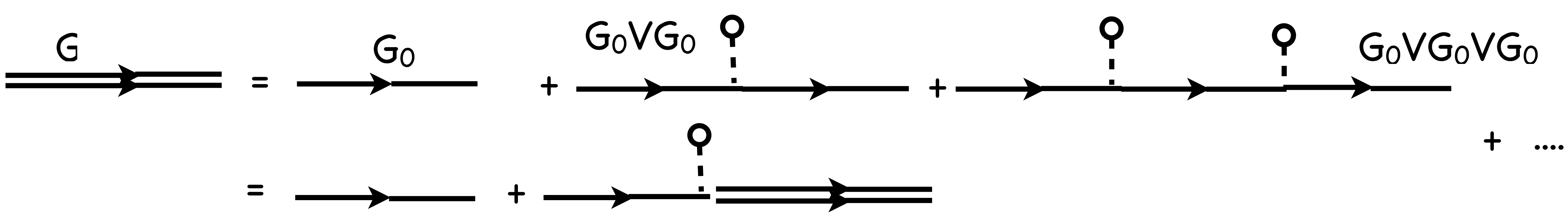


S Matrix and decomposition of scattered state in free particle basis

$$S_{\alpha\beta} = \langle \phi_\alpha | \psi_\beta^{(+)}(t \to \infty) \rangle = Lt_{t\to\infty, t'\to-\infty} iG^R(\alpha, t; \beta, t')$$

Propagator in presence of scatterer

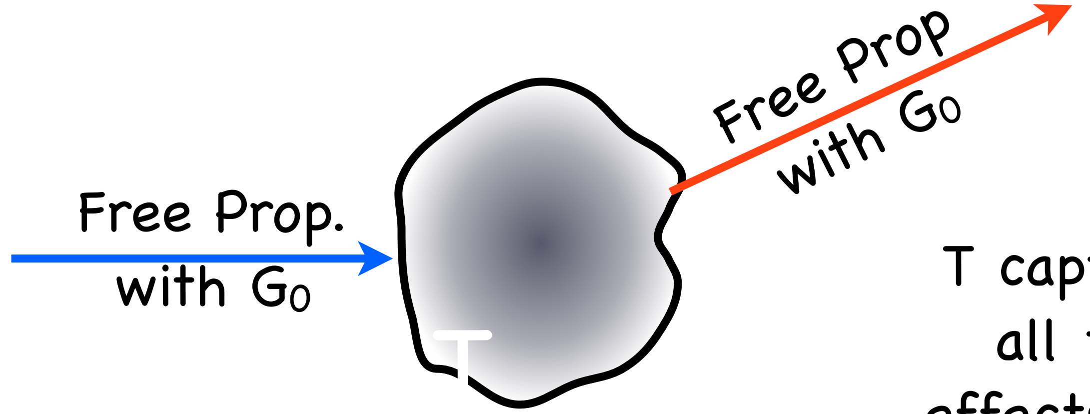
$$G^R = G_0^R + G_0^R V G_0^R + G_0^R V G_0^R V G_0^R + \ldots = G_0^R + G_0^R V G^R$$



Probability conservation ----> Unitarity of S

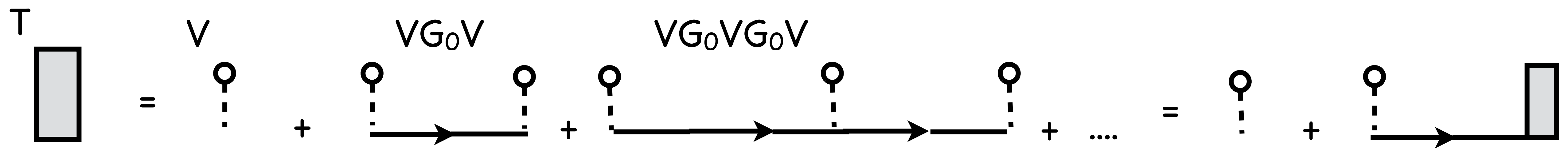
Recap of Previous Classes

$$G^R = G_0^R + G_0^R V G^R = G_0^R + G_0^R T G_0^R$$



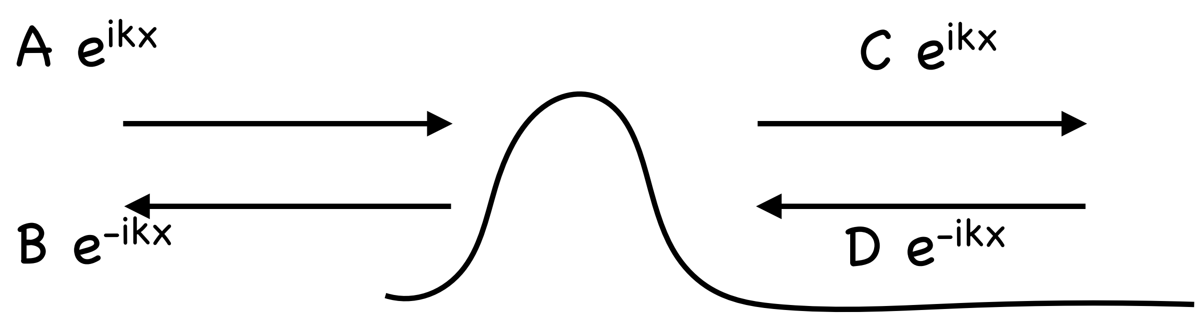
T captures all the effects of V incl. multiple scatterings

$$T = V[1 - G_0 V]^{-1} = V + V G_0 V + V G_0 V G_0 V + \ldots = V + V G_0 T$$



1D Scattered State

$$S = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix}$$



3D Scattered State

$$\psi^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \left[e^{i\vec{p}\cdot\vec{r}} + \frac{e^{ipr}}{r} f(\vec{p'}, \vec{p}) \right]$$

$$f(\vec{k}, \vec{k'}) = -4\pi^2 m T(\vec{k'}, \vec{k}, E)$$

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}, \vec{k'})|^2 = |f(E, \vec{k}\cdot\vec{k'})|^2$$

Recap of Previous Classes

Born Approximation

$$T = V + VG_0V + VG_0VG_0V + \ldots.$$

- V: Born. Approx/ 1st Born Approx.
- $V + VG_0V$: 2nd Born Approx. $q = |\vec{p'} - \vec{p}| = 2p\sin\frac{\theta}{2}$
- $V + VG_0V + VG_0VG_0V$: 3rd Born Approx.

Validity:

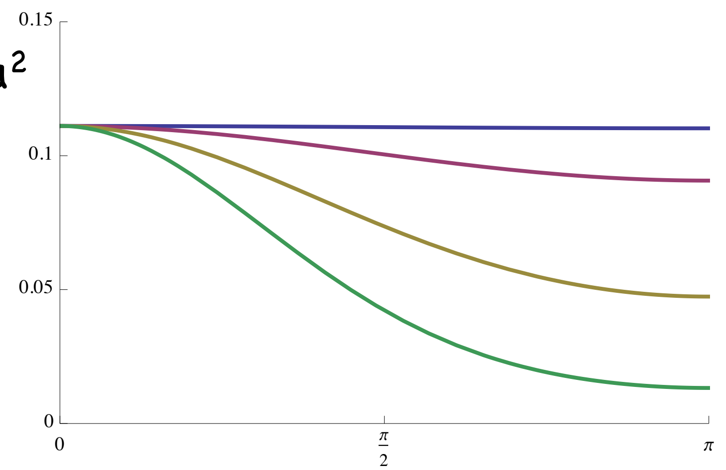
- Weak potentials
- High Energy of Incident particles

A) Square Well

$$V(r) = V_0 \quad 0 < r < a$$
$$= 0 \quad r > a$$

$$f(\theta) = \frac{2mV_0}{q^2}\left[\frac{\sin(qa)}{q} - a\cos(qa)\right]$$

$|f(\theta)|^2\ /a^2$



qa=0.1, 0.5,1.0, 1.5

$2mV_0a^2=1$

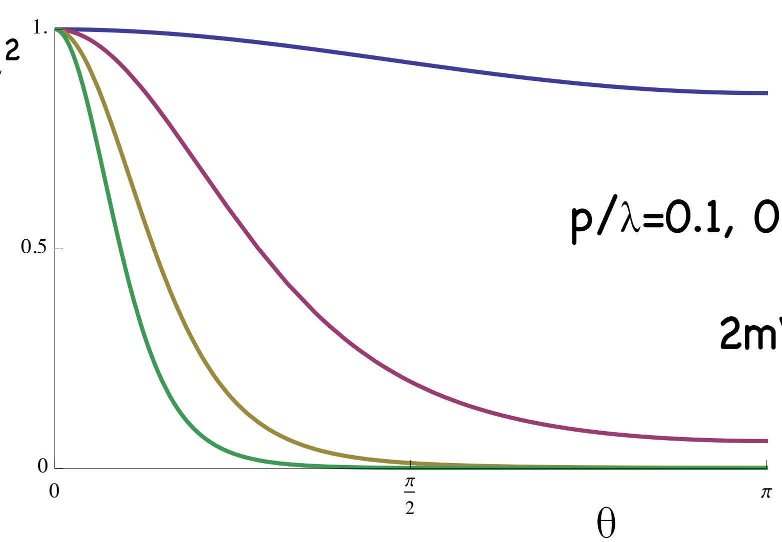
Differential Scattering Cross Section goes down monotonically

B) Yukawa Potential

$$V(r) = \frac{V_0 e^{-\lambda r}}{\lambda r}$$

$$f(\theta) = -\frac{2mV_0}{\lambda}\frac{1}{q^2+\lambda^2}$$

$|f(\theta)|^2\,\lambda^2$



p/λ=0.1, 0.5,1.0, 1.5

$2mV_0/\lambda^2=1$

As λ ---> 0, with V_0/λ fixed, the Yukawa potential goes over to the Coulomb potential.

In this limit, recover the Rutherford cross-section.

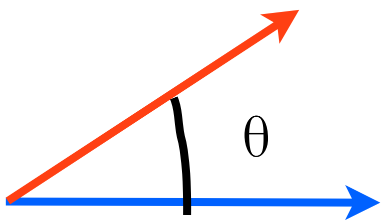
$$\frac{d\sigma}{d\Omega} = \frac{(2m)^2(ZZ'e^2)^2}{16p^4\sin^4(\theta/2)}$$

Recap of Previous Classes

Expansion in Partial waves

$$f(\vec{p},\vec{p'}) = -\frac{4\pi^2}{p}\sum_{lm} T_l(E)\ \ Y_l^m(\hat{p'})Y_l^{m*}(\hat{p})$$

$$f(\vec{p},\vec{p'}) = \sum_{l=0}^{\infty}(2l+1)f_l(p)P_l(\cos\theta)$$



Scattered Wavefunction:

$$\psi^{(+)}(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\sum_l (2l+1)\frac{P_l(\cos\theta)}{2ip}\left([1+2ipf_l(p)]\frac{e^{ipr}}{r} - \frac{e^{-i(pr-l\pi)}}{r}\right)$$

outgoing spherical wave   incoming spherical wave

Conservation of Angular Momentum ⟶ Unitarity of S_l

S Matrix : $S_l(p) = 1 + 2ipf_l(p)$ $|S_l(p)| = 1 \Rightarrow S_l(p) = e^{2i\delta_l(p)}$

phase shift in l channel

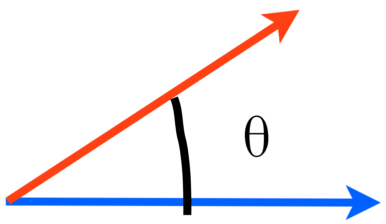
T Matrix: $$T_l(p) = -\frac{e^{i\delta_l(p)}\sin\delta_l(p)}{\pi} = \frac{1}{\pi}\frac{1}{\cot\delta_l(p) - i}$$

Recap of Previous Classes

Expansion in Partial waves

$$f(\vec{p},\vec{p'}) = -\frac{4\pi^2}{p}\sum_{lm} T_l(E)\;\; Y_l^m(\hat{p'})Y_l^{m*}(\hat{p})$$

$$f(\vec{p},\vec{p'}) = \sum_{l=0}^{\infty}(2l+1)f_l(p)P_l(\cos\theta)$$



Scattering Amplitude:

$$f(\theta) = \sum_l (2l+1)P_l(\cos\theta)\frac{e^{i\delta_l(p)}\sin\delta_l(p)}{p}$$

Differential Cross Section:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \sum_{ll'}\frac{(2l+1)(2l'+1)}{p^2}P_l(\cos\theta)P_{l'}(\cos\theta)\sin\delta_l(p)\sin\delta_{l'}(p)e^{i[\delta_l(p)-\delta_{l'}(p)]}$$

interference of different l channels

Total Cross Section:

$$\sigma = \frac{4\pi}{p^2}\sum_l (2l+1)\sin^2\delta_l(p)$$

interference washed out

Low Energy Scattering and few Partial Waves

Use the expansion of a plane wave into spherical waves in 3D

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y_l^{m*}(\hat{k}) Y_l^m(\hat{r})$$

$$V_{\vec{k}\vec{k}'} = \langle \vec{k}' | V | \vec{k} \rangle \quad = \frac{1}{8\pi^3} \int dr r^2 V(r) \int d\Omega_r e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}$$

$$= \frac{2}{\pi} \sum_{ll'} \sum_{mm'} i^{l'-l} \int dr r^2 V(r) j_{l'}(k'r) j_l(kr) Y_{l'}^{m'*}(\hat{k}') Y_l^m(\hat{k}) \int d\Omega_r Y_{l'}^{m'}(\hat{r}) Y_l^{m*}(\hat{r})$$

$$= \frac{2}{\pi} \sum_{lm} \int dr r^2 V(r) j_l(k'r) j_l(kr) Y_l^{m*}(\hat{k}') Y_l^m(\hat{k})$$

Use orthonormality of Y_l^m

Use the fact that k is along z and $Y_l^m(\theta, 0) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \delta_{m0}$

$$= \frac{1}{2\pi^2} \sum_l (2l+1) P_l^m(\cos\theta) \left[\int dr r^2 V(r) j_l(k'r) j_l(kr) \right]$$

Use $j_l(x) \sim x^l$ for x << 1 to show $V_{\vec{k}\vec{k}'} \sim k^l (k')^l$ for small k, k′

How small should k be?

Range of r integral is R_0, the range of potential. So, $kR_0 \ll 1$ for this to be valid

Low Energy Scattering and few Partial Waves

Let us use the self-consistent eqn. for T matrix

$$T_{\vec{k}\vec{k}'}(E) = V_{\vec{k}\vec{k}'} + \int \frac{d^3\vec{q}}{(2\pi)^3} V_{\vec{k}\vec{q}} G_0(\vec{q}, E) T_{\vec{q}\vec{k}'}(E)$$

Note that we want k, k' to be small, but q sum is unrestricted

However, we have $V_{\vec{k}\vec{q}} \sim k^l F(q)$ and $V_{\vec{q}\vec{k}'} \sim (k')^l K(q)$

So, $T_{\vec{k}\vec{k}'}(E) \sim k^l (k')^l$

Expand the series to show that each term has the form $V_{kq} \ldots\ldots V_{pk'}$

Now use the fact that for elastic scattering k=k' and $T_l(E)/k \sim T_{kk'}(E)$

For low $E \ll 1/(2m R_0^2)$

$$T_l(E = k^2/2m = k'^2/2m) \sim k^{2l+1}$$

$$f_l(E = k^2/2m = k'^2/2m) \sim k^{2l}$$

$$\tan\delta_l(E = k^2/2m = k'^2/2m) \sim k^{2l+1}$$

Low E scattering is dominated by a few partial waves

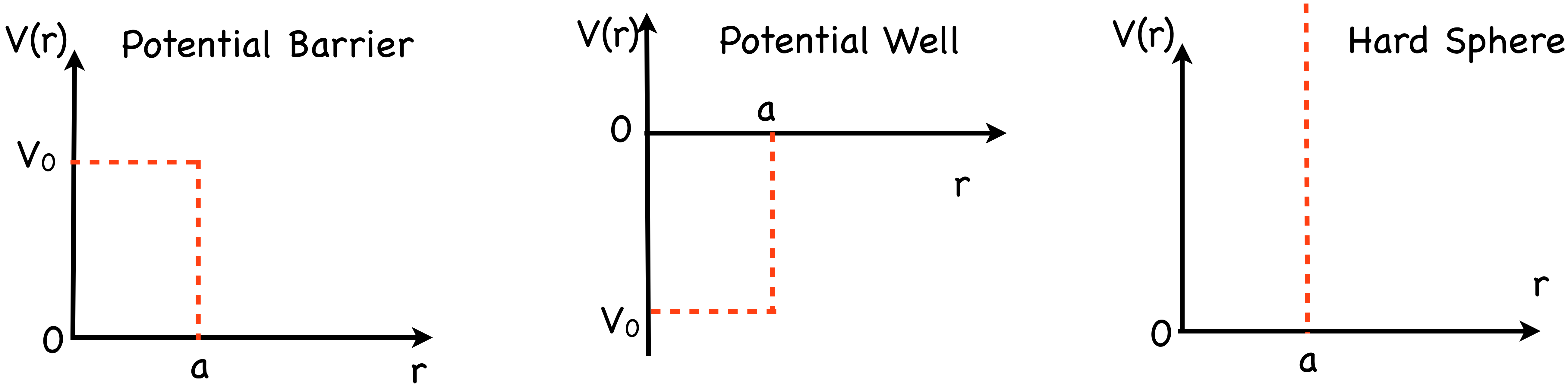
OK to consider only l=0 channel for E —> 0, s-wave scattering

Calculating Phase Shifts in simple potentials

The straight forward approach (works only in few selective cases) is to solve the Schrodinger equation with the potential, and obtain the phase shift from the asymptotic form of the wave-function far from the origin by comparing it with

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) \frac{P_l(\cos\theta)}{2ip} \left(e^{2i\delta_l(p)} \frac{e^{ipr}}{r} - \frac{e^{-i(pr-l\pi)}}{r} \right)$$

Spherically Symmetric Square Potential Well/Barrier:



$$V(r) = V_0 \quad 0 < r < a$$
$$= 0 \quad r > a$$

- Scattering states behave like free particle far from the potential region.
- Since they have KE, we are looking for states with E>0
- The potential well can sustain bound states, but we are not interested in them (for now).

Spherically Symmetric Potential Well/Barrier:

Use spherical co-ord angular part given by $Y^0{}_l$

$$\psi^{(+)}(r,\theta) = \sum_l i^l(2l+1)R_l(r)P_l(\cos\theta) = \sum_l i^l(2l+1)\frac{1}{r}u_l(r)P_l(\cos\theta)$$

Radial Equation: $$-\frac{d^2u_l(r)}{dr^2} + \left[2mV(r) - p^2 + \frac{l(l+1)}{r^2}\right]u_l(r) = 0$$

$$V(r) = V_0 \quad 0 < r < a$$
$$= 0 \quad r > a$$

$r > a$ Free particle solutions far from origin

$$R_l(r) = c_1 j_l(pr) + c_2 n_l(pr) = c^{(1)}h_l^{(1)}(pr) + c^{(2)}h_l^{(2)}(pr)$$

Spherical Bessel Functions Spherical Hankel Functions

$$h_l^{(1(2))}(pr) = j_l(pr) \pm i n_l(pr)$$

$$pr \gg 1$$

$$h_l^{(1(2))}(pr) \sim \pm\frac{e^{\pm i(pr - l\pi/2)}}{ipr}$$

Comparing with

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}}\sum_l(2l+1)\frac{P_l(\cos\theta)}{2ip}\left(e^{2i\delta_l(p)}\frac{e^{ipr}}{r} - \frac{e^{-i(pr-l\pi)}}{r}\right)$$

$$c_l^{(1)} = \frac{1}{2}e^{2i\delta_l(p)} \quad c_l^{(2)} = \frac{1}{2} \qquad R_l(r) = e^{i\delta_l}[\cos\delta_l j_l(pr) - \sin\delta_l n_l(pr)]$$

Spherically Symmetric Potential Well/Barrier:

$$R_l(r) = c_1 j_l(pr) + c_2 n_l(pr) = c^{(1)} h_l^{(1)}(pr) + c^{(2)} h_l^{(2)}(pr)$$

Spherical Bessel Functions Spherical Hankel Functions

Comparing with

$$\psi^{(+)}(r) = \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) \frac{P_l(\cos\theta)}{2ip} \left(e^{2i\delta_l(p)} \frac{e^{ipr}}{r} - \frac{e^{-i(pr - l\pi)}}{r} \right)$$

$$c_l^{(1)} = \frac{1}{2} e^{2i\delta_l(p)} \quad c_l^{(2)} = \frac{1}{2} \qquad R_l(r) = e^{i\delta_l}[\cos\delta_l j_l(pr) - \sin\delta_l n_l(pr)]$$

$c^{(1)}$ and $c^{(2)}$ are obtained from the continuity of the logarithmic derivative at r=a.

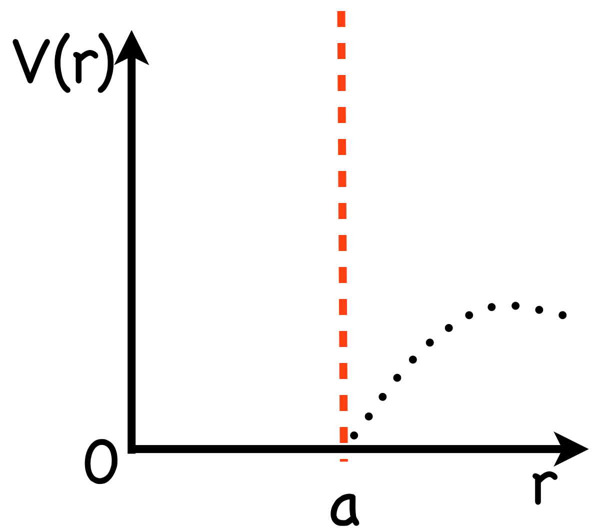
$$\beta_l = \left[\frac{r}{R_l}\frac{dR_l}{dr}\right]\Bigg|_{r=a} \qquad \tan\delta_l(p) = \frac{paj_l'(pa) - \beta_l j_l(pa)}{pan_l'(pa) - \beta_l n_l(pa)}$$

Note that till now we have not used the specific square-wave form of the potential. This result is valid for any potential that vanishes at a finite range

Spherically Symmetric Potential Well/Barrier:

To find the parameter β_l, we need the solution inside the potential region

A) Hard Sphere Potential



Boundary Condition : wfn. vanishes at r=a

$$\beta_l = \left[\frac{r}{R_l} \frac{dR_l}{dr} \right] \Bigg|_{r=a} \qquad \beta_l \to \infty$$

$$\tan \delta_l(p) = \frac{pa j_l'(pa) - \beta_l j_l(pa)}{pa n_l'(pa) - \beta_l n_l(pa)}$$

$$\tan \delta_l(p) = \frac{j_l(pa)}{n_l(pa)}$$

$$j_0(x) = \frac{\sin x}{x} \qquad n_0(x) = -\frac{\cos x}{x}$$

s-wave phase shift $\delta_0(p) = -pa$

$$\frac{d\sigma}{d\Omega}_0 = \frac{\sin^2 \delta_0}{k^2} \simeq a^2 \quad for \quad ka \ll 1$$

Negative phase shift for repulsive potential

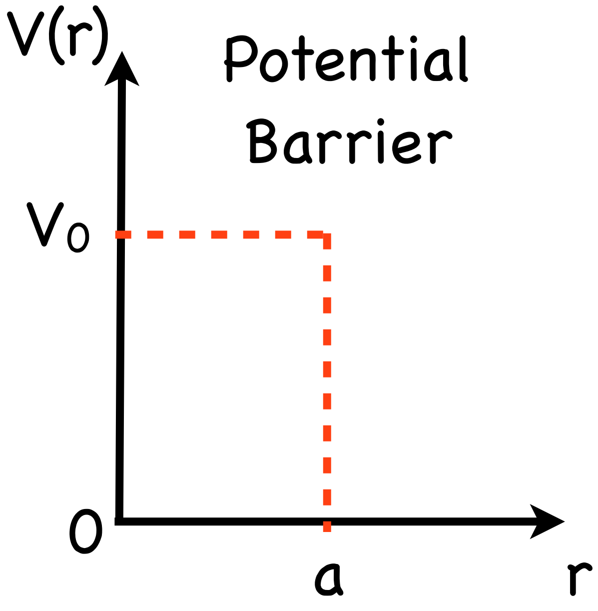
Generically true for finite potential barrier as well.

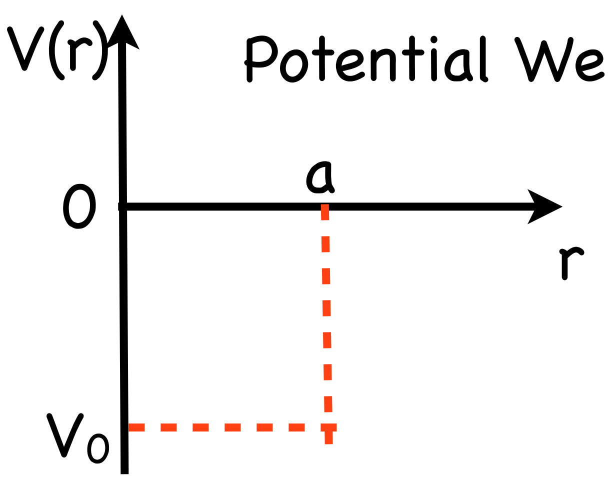
Indicates that the wave-fn is pushed out

Spherically Symmetric Potential Well/Barrier:

To find the parameter β_l, we need the solution inside the potential region

B) Potential Well/ Barrier





Inside Soln.: regular at r=0 $\quad j_l(qr) \quad \frac{q^2}{2m} = E - V_0$

$$\beta_l = \left[\frac{r}{R_l}\frac{dR_l}{dr}\right]\Big|_{r=a} \qquad \beta_l = \frac{qa j_l'(qa)}{j_l(qa)} \qquad \tan\delta_l(p) = \frac{p j_l'(pa) - q j_l'(qa) j_l(pa)/j_l(qa)}{p n_l'(pa) - q j_l'(qa) n_l(pa)/j_l(qa)}$$

$$\delta_l(p) \sim p^{2l+1}$$

Square Potential Well: s-wave Scattering

Consider the l=0 channel in the low energy limit $\tan\delta_l(p) \sim -pa_s$ s-wave scattering length

For square well $\beta_l = \frac{qaj_l'(qa)}{j_l(qa)}$ Using $j_0(x) = \frac{\sin x}{x}$ $\beta_0 = qa\cot(qa) - 1$

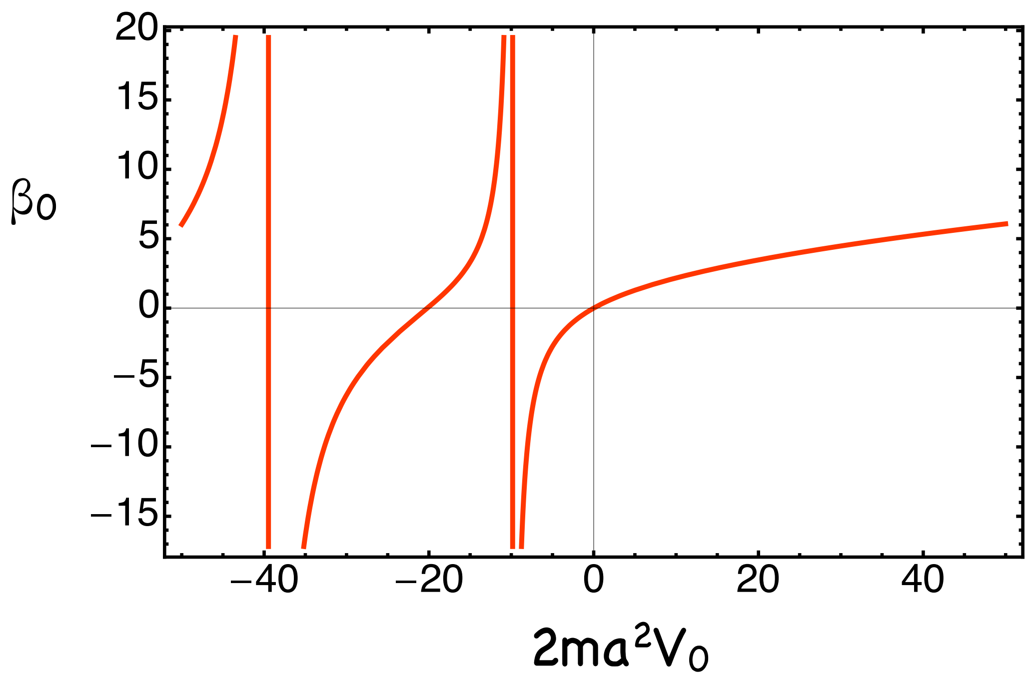
Scattering Length $a_s = \frac{a\beta_0}{1+\beta_0}$

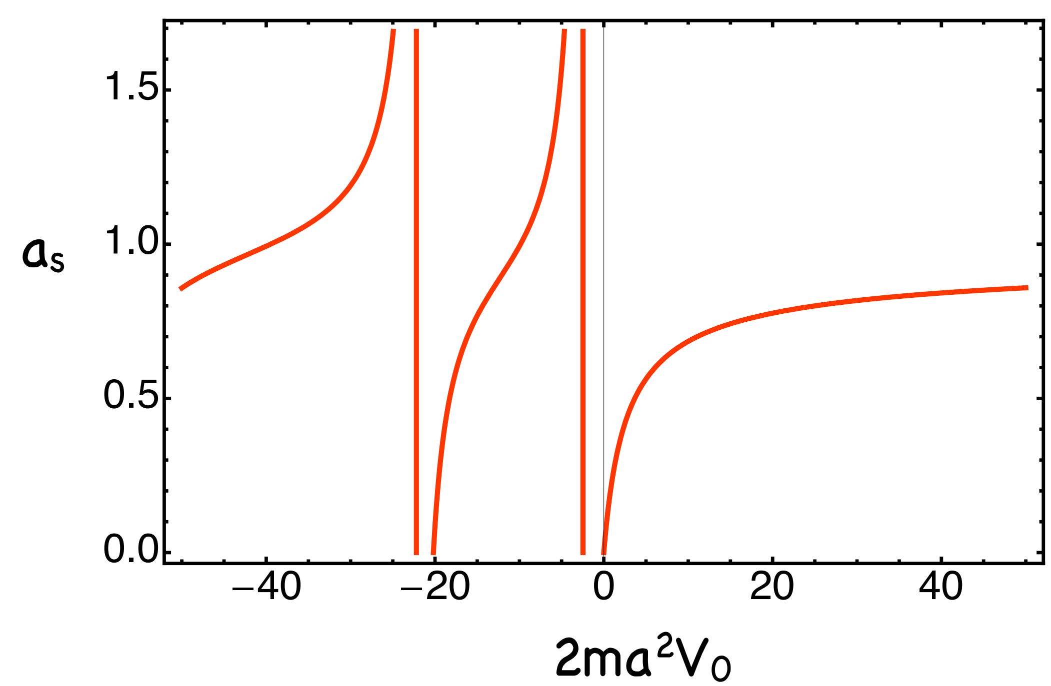
a_s diverges when $qa = (2n+1)\,\pi/2$

Scattering Cross-Section $\sigma_0 = 4\pi a_s^2$

Scattering Amplitude $f_0(p) = \frac{1}{p\cot\delta_0(p) - ip} = \frac{-1}{\frac{1}{a_s} + ip} = -\frac{a_s}{1+ipa_s}$ $f_0(0) = -a_s$

f_0 does not diverge when $qa = (2n+1)\,\pi/2$, f_0 is $-1/ip$ at this point --- Unitary limit



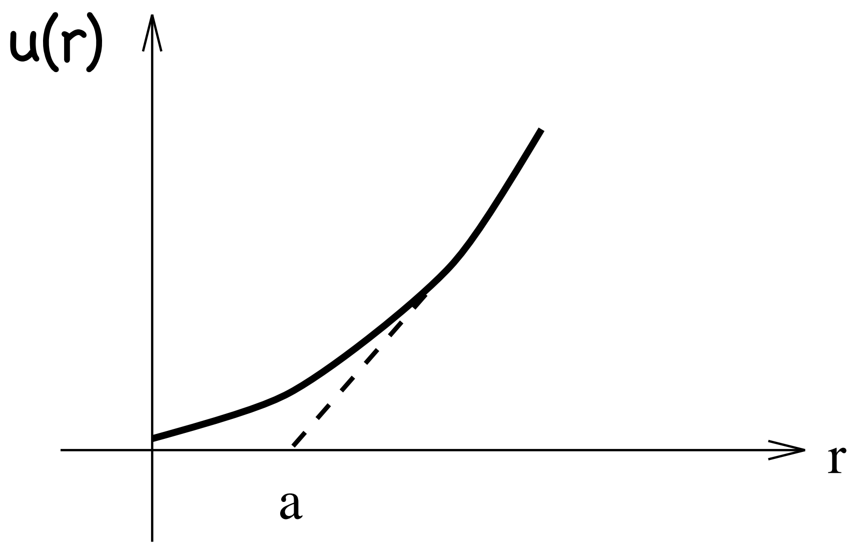


s-wave Scattering Length

For large r $u_0(r) \sim e^{i\delta_0} \sin(pr + \delta_0) \sim e^{i\delta_0} \sin p(r - a_s) \sim e^{i\delta_0} p(r - a_s)$

So a_s has the interpretation of the first point in space where the extrapolation of the far solution hits zero. Note that it is not a zero of the actual solution.

$$-\frac{d^2 u_l(r)}{dr^2} + \left[2mV(r) - p^2 + \frac{l(l+1)}{r^2}\right] u_l(r) = 0$$



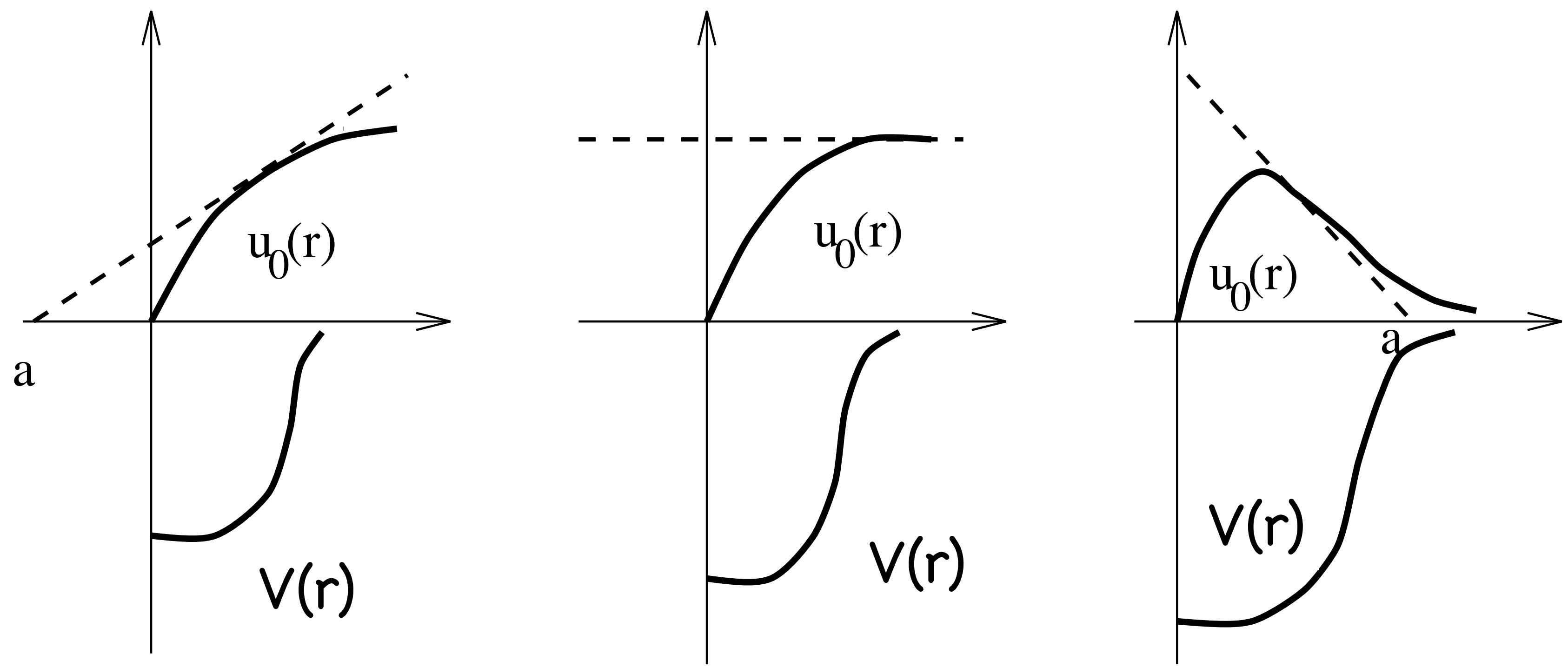
Consider p=0, l=0

For purely repulsive potential
curvature is away from axis.
Scattering Length is always positive

s-wave Scattering Length

For large r $u_0(r) \sim e^{i\delta_0}\sin(pr+\delta_0) \sim e^{i\delta_0}\sin p(r-a_s) \sim e^{i\delta_0}p(r-a_s)$

So as has the interpretation of the first point in space where the extrapolation of the far solution hits zero. Note that it is not a zero of the actual solution.



For attractive potential wells, the scattering length is initially negative

As we increase the well depth,the scattering length becomes more and more negative till it reaches -∞

Beyond this point, the scattering length starts at + ∞ and keeps decreasing

This is the point where we have the first bound state in the system

Effective Range Expansion

H. A. Bethe, Phys. Rev. **76**, 38 (1949)

What happens when we go to larger energies, aka what is the next term in f

$$f_0(p) = \frac{1}{p\cot\delta_0(p) - ip} = \frac{-1}{\frac{1}{a_s} + ip} = -\frac{a_s}{1 + ipa_s}$$

Schrodinger Eqn for 2 different momenta

$$-\frac{d^2u_l(r)}{dr^2} + \left[2mV(r) - p^2 + \frac{l(l+1)}{r^2}\right]u_l(r) = 0$$

$$\frac{d^2u_1}{dr^2} + [p_1^2 - V(r)]u_1(r) = 0 \qquad \frac{d^2u_2}{dr^2} + [p_2^2 - V(r)]u_2(r) = 0$$

$$u_2\frac{d^2u_1}{dr^2} - u_1\frac{d^2u_2}{dr^2} = (p_1^2 - p_2^2)u_1u_2 \longrightarrow u_2\frac{du_1}{dr} - u_1\frac{du_2}{dr}\bigg|_0^R = (p_1^2 - p_2^2)\int_0^R dr u_1 u_2$$

Consider the asymptotic form of the solutions at large r

$$\psi_p(r) = \frac{\sin[pr + \delta_0(p)]}{\sin\delta_0(p)}$$

The asymptotic soln. also follows similar eqns as u

$$\psi_2\frac{d\psi_1}{dr} - \psi_1\frac{d\psi_2}{dr}\bigg|_0^R = (p_1^2 - p_2^2)\int_0^R dr\psi_1\psi_2$$

Effective Range Expansion

H. A. Bethe, Phys. Rev. **76**, 38 (1949)

Subtract the equations for u and ψ,

$$\psi_2 \frac{d\psi_1}{dr} - u_2 \frac{du_1}{dr} - \psi_1 \frac{d\psi_2}{dr} + u_1 \frac{du_2}{dr}\bigg|_0^R = (p_1^2 - p_2^2)\int_0^R dr \psi_1\psi_2 - u_1 u_2$$

At r=R, LHS vanishes by continuity eqn.s.
At r=0, terms in LHS involving u vanish as u(0)=0.

$$\psi_1 \frac{d\psi_2}{dr} - \psi_2 \frac{d\psi_1}{dr}\bigg|_0 = (p_1^2 - p_2^2)\int_0^\infty dr \psi_1\psi_2 - u_1 u_2$$

Int extended to ∞ since the integrand vanishes outside the range of potential

Using explicit form ψ at r=0, $p_2 \cot\delta_0(p_2) - p_1 \cot\delta_0(p_1) = (p_1^2 - p_2^2)\int_0^\infty dr \psi_1\psi_2 - u_1 u_2$

$$p_1 \to 0, \quad p_2 \to p \qquad p\cot\delta_0(p) = -\frac{1}{a_s} - p^2 \int_0^\infty dr \psi_0\psi_p - u_0 u_p$$

$$\simeq -\frac{1}{a_s} - p^2 \underline{\int_0^\infty dr \psi_0^2 - u_0^2}$$

Effective range of potential r_0

$$p\cot\delta_0(p) = \frac{-1}{a_s} - r_0 p^2 \qquad f_0(p) = \frac{-1}{\frac{1}{a_s} + ip + r_0 p^2}$$

Effective range expansion

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.