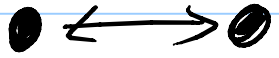
Collisions

PHYS519

Note Title 4/19/2011

Sources: Sakurai, Pethick and Smith, Heinzen's lecture notes (Fermi Summer School, 1998), Brandsen & Jochain, Meystre – Atom Optics, Foot (simple, but cogent)

What do the interactions between atoms look like?



r – internuclear distance

* start by considering elastic collisions

- two ground state neutral atoms: $V = -\frac{C_6}{r^6}$
  (Van der Waals induced dipole–induced dipole interaction)
- ion–neutral (both in ground state): $V = \frac{-\alpha_1 q_B^2}{r^4}$

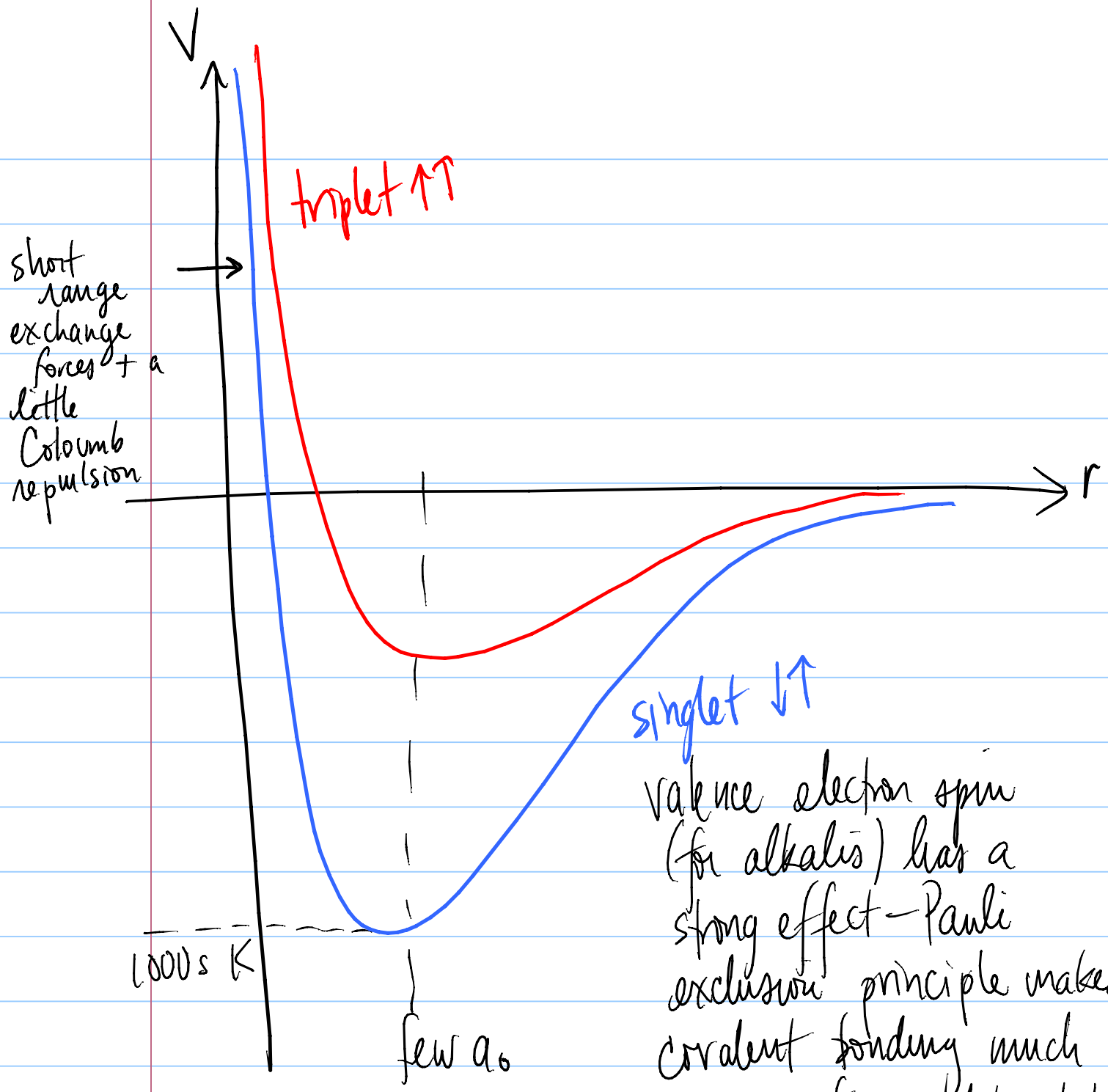
(charge – induced dipole interaction –
α_A: polarizability of neutral,
q_B: charge of ion)

* excited neutral – ground neutral: $V = \frac{-C_3}{r^3}$
(important esp. in MOTs)

It's very hard to calculate much about these potentials. You usually start with a semi-stationary approach – electrons adiabatically follow their ground state configuration as r changes.

Specialize to $1/r^6$ interactions in what follows...

The real, complete potential looks like:
(and is pretty well fit to – based on data – $V = h(r)e^{-\beta r} - \frac{C_6}{r^6}$)

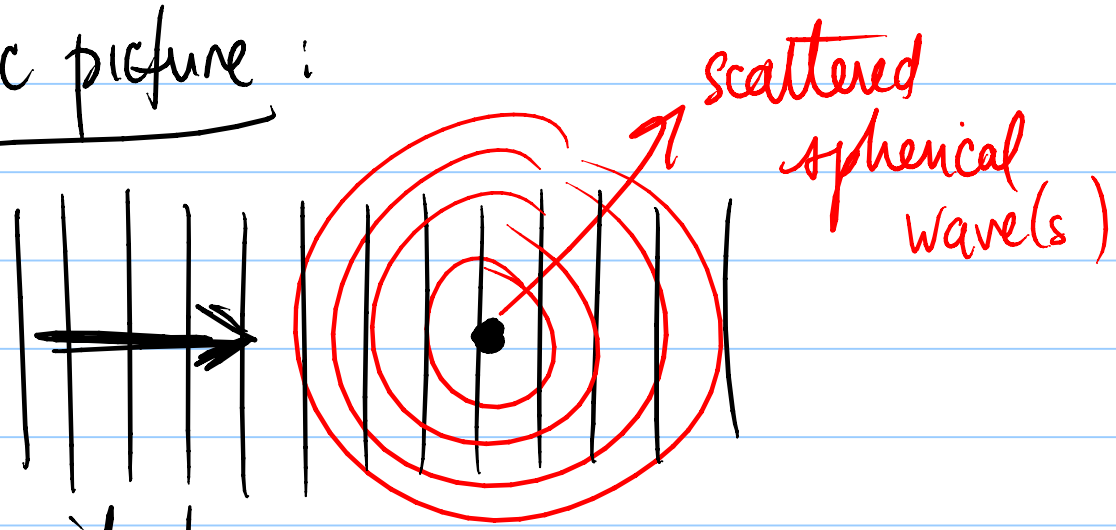


valence electron spin (for alkalis) has a strong effect - Pauli exclusion principle makes covalent bonding much stronger for singlet state!

We're mostly going to ignore spin in what follows... and consider very basic quantum scattering theory. This means that interference effects can play a big role

(e.g., shape resonances, Feshbach resonances, etc.)

Basic picture:



The goal in quantum scattering theory is to find the scattered wave. We use time independent theory ($\psi = \psi(\vec{r}) e^{-iEt/\hbar}$), which may seem a little strange, but is the only tractable approach. This just means that the incident and scattered waves have been present for a long time.

Start with Schrödinger's equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\vec{r}) = E\psi(\vec{r})$$

*key points and equations are marked in green

- assume a central potential, and elastic scattering $\boxed{E = \hbar^2 k^2 / 2m}$

Now, write: $\boxed{\psi \propto e^{ikz} + f(k,\Omega)\frac{e^{ikr}}{r}}$

e^{ikz}: incident wave ψ_{in}

$f(k,\Omega)\frac{e^{ikr}}{r}$: scattered wave, where f is the scattering amplitude ψ_{out}

Our goal is to find f

Since we have a central potential, do a "partial wave expansion":

$$\boxed{\psi = \sum_\ell R_\ell(k,r) P_\ell(\cos\theta)}$$

ℓ: angular momentum quantum #

where R satisfies the usual radial equation:

$$\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\ell(\ell+1)}{r^2}-V(r)+k^2\right]R_\ell(k,r)=0$$

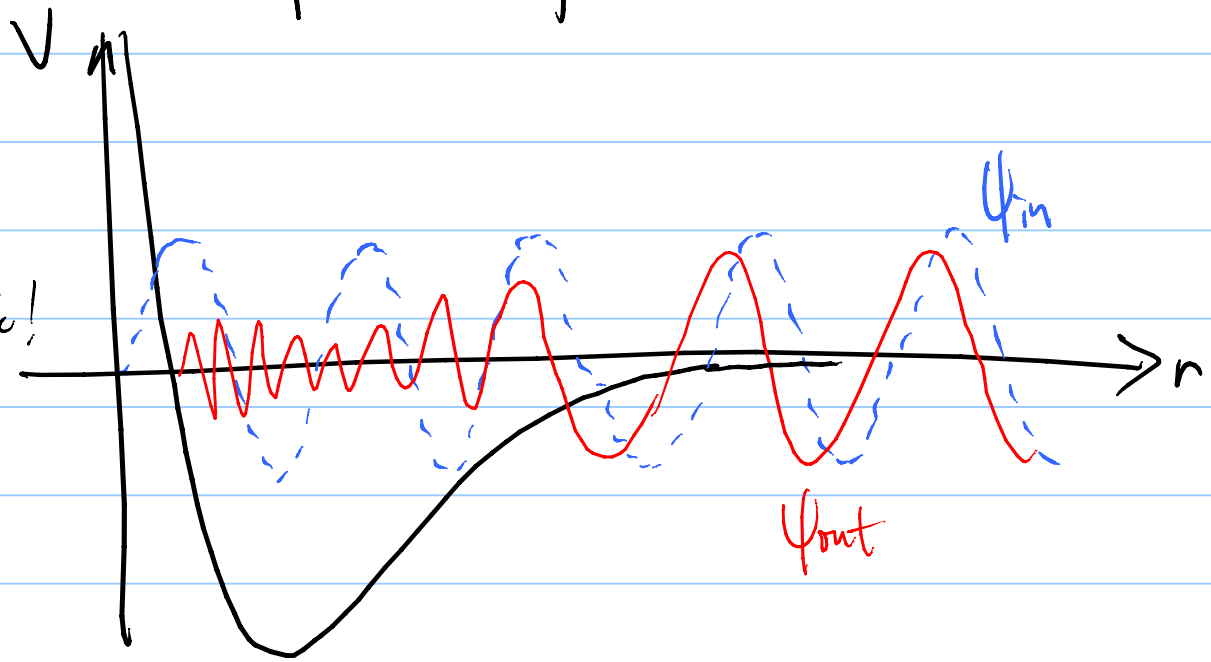
effective potential, including the centrifugal barrier

Asymptotically ($r\to\infty$) one finds:

$$R\propto\frac{1}{kr}\sin\left[kr-\ell\pi/2+\delta_\ell(r)\right]$$

$\delta_\ell(r)$: scattering phase shift

We should have expected that the only free parameter in R at large r is a phase shift!



*note: this picture is somewhat schematic!

At large r, there can only be a phase shift by conservation of probability!

With a lot more math, one can show:

$$f(k,\theta) = \sum_\ell f_\ell(k) P_\ell(\cos\theta)$$

$$f_\ell(k) = \frac{2\ell+1}{k} e^{i\delta_\ell(k)} \sin\delta_\ell(k)$$

note - this is not a solution. Using Green's functions and the Lippman-Schwinger equation,

$$f(k,\theta) \propto \int e^{-i\vec{k}\cdot\vec{r}'} V(r') \psi_k^{out}(\vec{r}') d^3\vec{r}'$$

uh-oh!

You can make progress on solving that equation using the 1st Born approximation:

put $\psi^{out} = \psi^{in}$ into the equation for $f(k,\theta)$

What is all of this useful for?

finding the collision cross section!

definition: $\frac{d\sigma}{d\Omega} d\Omega = \frac{\#\text{ particles scattered into } d\Omega \text{ per unit time}}{\#\text{ incident particles crossing unit area per unit time}}$

to evaluate this, remember that the probability current density is:

$$\vec{j} = \frac{\hbar}{2mi}\left[\psi^* \vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right]$$

at large r: $\vec{j}_{sc} \cdot \hat{r} \propto \frac{\hbar k}{m} |f|^2 / r^2$

and: $j_{in} \propto \hbar k / m$

then: $\frac{d\sigma}{d\Omega} d\Omega = \frac{r^2 |\vec{j}_{sc}| d\Omega}{j_{in}}$

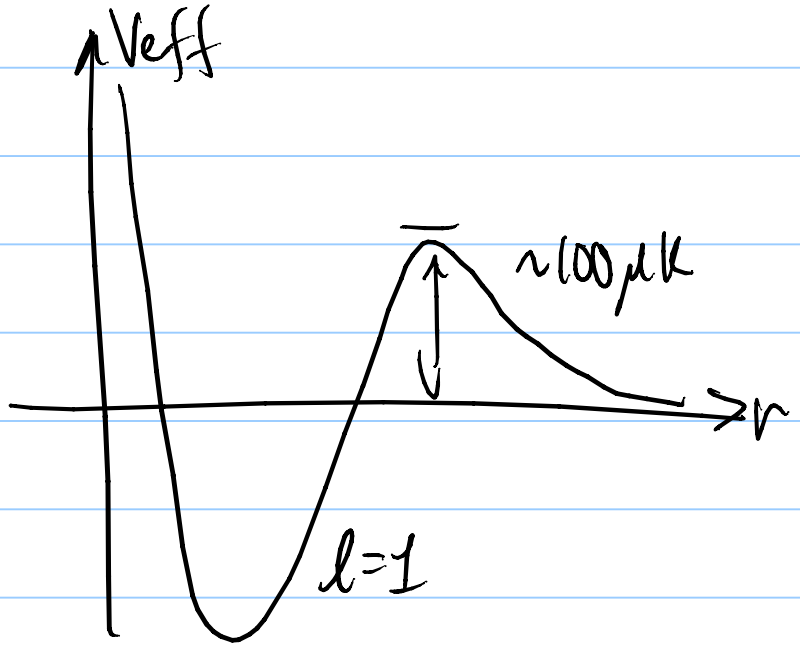
giving: $\boxed{\frac{d\sigma}{d\Omega} = |f|^2}$

$$\boxed{\sigma = \frac{4\pi}{k^2} \sum_\ell (2\ell+1) \sin^2 \delta_\ell}$$

Note, for $\ell=0$, the biggest the cross section can be is $\sigma = 4\pi/k^2$ — this is the "unitarity limit" (i.e, what is consistent with conservation of probability)

Many people like to think in terms of a "scattering length" rather than phase shifts.

Also — we will primarily consider $\ell=0$ from here on. Why? For $T \lesssim 100\,\mu K$, higher partial waves suppressed by the centrifugal barrier:



Consider now the asymptotic solution for $l=0$

$$R \propto \frac{1}{kr} \sin(kr + \delta_0)$$

we can rewrite this as: $R \propto \sin[k(R-a)]$

where $$a = -\lim_{k \to 0} \frac{\delta_0(k)}{k}$$

we have just traded a phase shift for a length!

then: $$\boxed{\sigma_{k \to 0} = 4\pi a^2}$$

From "effective range theory" (see Jochain, Quantum Collision Theory), one can show:

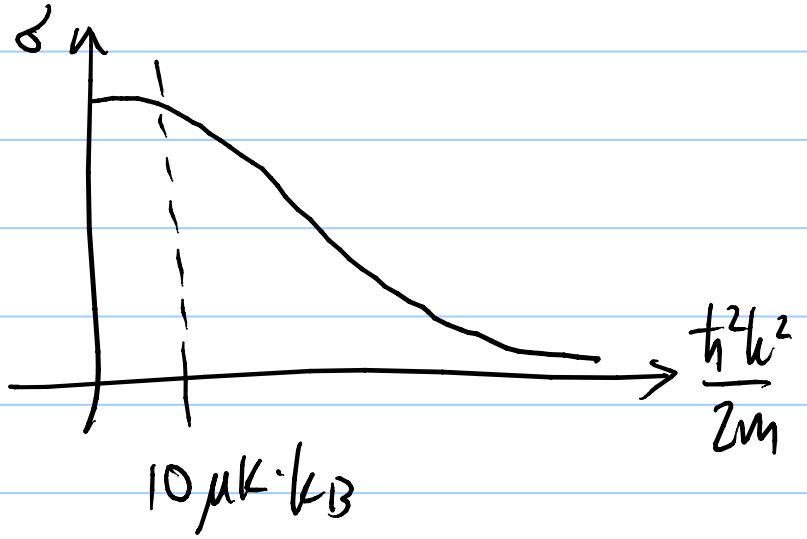
$$\boxed{\sigma = \frac{4\pi a^2}{\left(1 - \frac{1}{2} k^2 a r_e\right)^2 + k^2 a^2}}$$

where r_e is the range of the potential

note that, for any finite k, as $|a| \to \infty$,

$\sigma \to 4\pi/k^2$

also:



Even though σ is roughly fixed at low energy, it decreases at higher energy (consistent with unitarity limit)

Note that a can take on any value from $+\infty \to -\infty$

This is usually understood by considering scattering from a square well:

$$V = \begin{cases} -V_0, & r < r_0 \\ 0, & r > r_0 \end{cases}$$

at zero energy ($k=0$),

Schrodinger's equation is:

$$\frac{d^2u}{dr^2} = 0 \quad \text{for } r > r_e, \text{ where } u = rR$$

this is solved by $u \propto r - a$, which is just an infinitely long wavelength sinusoidal function (a here is an integration constant, chosen to coincide with the scattering length)

for $r < r_e$, we have:

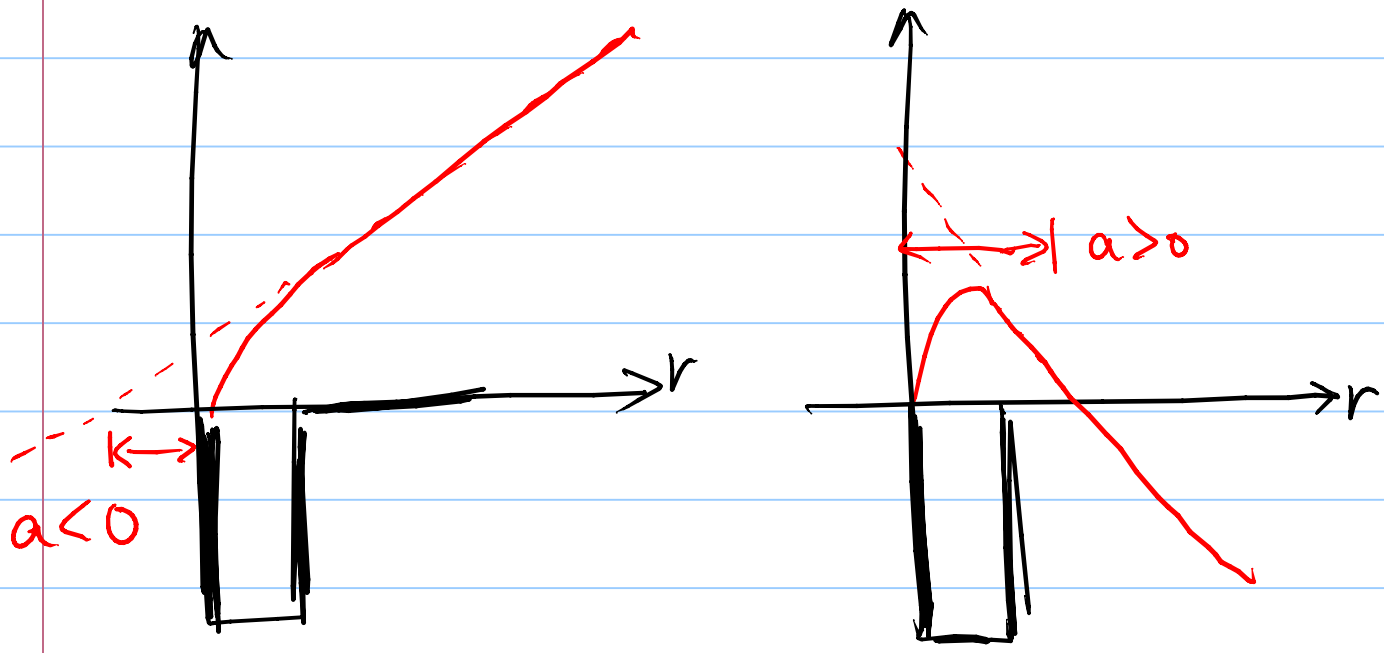
$$\frac{d^2u}{dr^2} = -V_0$$

which is solved by

$$u \propto \sin Kr \quad \text{, for } r < r_e$$

with: $K = \sqrt{\frac{2mV_0}{\hbar}}$

Now, we have to match the inside and outside solutions — there are two outcomes, depending on K



→ a depends on the slope of the inside wavefunction at r=re!

→ a can be positive or negative, depending on the sign of that slope, and potentially very large if that slope is small

This is often understood as having to do with bound states of the potential... the argument goes something like this:

- for a large and $a>0$ (and $E>0$), the outside wavefunction is very flat and similar to $u \propto e^{-\kappa r}$
- but, that's just what we get for a bound state at $r>r_e$ (and $E<0$)
- if we equate the logarithmic derivatives for the inside wavefunctions with and without a bound state at the boundary, we find:

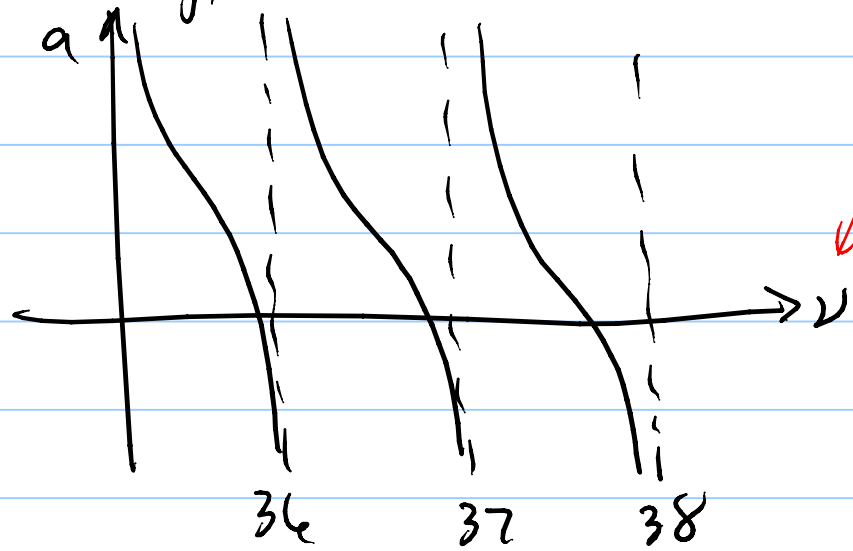
$$\left.\frac{-\kappa e^{-\kappa r}}{e^{-\kappa r}}\right|_{r=r_e} = \left.\frac{1}{r-a}\right|_{r=R} \quad \left(= \frac{du/dr}{u}\right)$$

for $r_e \ll a$, $\kappa \simeq 1/a$

and $\frac{\hbar^2\kappa^2}{2m} = \frac{\hbar^2}{2ma^2}$ = binding energy

- so, if the potential is just shy of supporting a bound state, then $a<0$ and a bit large
- if the potential just barely supports the last bound state, then $a>0$ and large

- generally, one can show that:



really the depth of the potential — non-integer v does not make sense

v: quantum number of last bound state

define $\bar{\Phi} = (v + \frac{1}{2})\pi$

then $a = a_{sc}(1 + \tan\bar{\Phi})$

where $a_{sc} \propto C_6^{1/4}$

Many different values of a for the alkalis

H: known from first principles

$a_t = 1.2 a_0$ "triplet scattering length"

$a_s = 0.41 a_0$ "singlet scattering length"

you have to decompose the (long range) m_F states into (valence electron) singlet and triplet — remember that there are different potentials

^{87}Rb: $a_t \approx a_s \approx 100\, a_0$

^{40}K: $a_t \approx 150\, a_0$
$a_s \approx 100\, a_0$

^{23}Na: $a_t \approx 70\, a_0$
$a_s \approx 20\, a_0$

^{133}Cs: $a_t \approx -3000\, a_0$ — if the potential was a little bit deeper, there'd be another bound state

Identical particles

two particle wavefunction should actually obey exchange symmetry...

one way to ensure this is to write:

$$\psi \propto \left(e^{ikz} \pm e^{-ikz}\right) + \left[f(\theta) \pm f(\pi-\theta)\right]\frac{e^{ikr}}{r}$$

+: bosons
−: fermions

recall, exchange corresponds to:

$$r \to r,\ \theta \to \pi-\theta,\ \varphi \to \pi+\varphi$$

and, $\cos\theta \to \cos(\pi-\theta) \to -\cos\theta$

now, with $f = \sum_\ell f_\ell P_\ell(\cos\theta)$

even ℓ: $P_\ell(-\cos\theta) = P_\ell(\cos\theta)$
odd ℓ: $P_\ell(-\cos\theta) = -P_\ell(\cos\theta)$

This means that:

bosons: ℓ even, $f(\theta)+f(\pi-\theta) \to 2f(\theta)$ collisions!
ℓ odd, $f(\theta)+f(\pi-\theta) \to 0$ no collisions!

fermions: ℓ even: $f(\theta)-f(\pi-\theta) \to 0$ no collisions!
ℓ odd: $f(\theta)-f(\pi-\theta) \to 2f(\theta)$ collisions!

identical bosons: $\ell = 0$ (low temperature collisions) allowed

identical fermions: $\ell = 0$ (low temperature collisions) not allowed

You can show that $\boxed{\sigma = 8\pi a^2}$ for identical bosons — there are multiple factors of 2 that you have to be careful about — see DeMarco's and Burke's theses from JILA.

How do you get fermions to collide (which is necessary for cooling)? Use two spin states!

$$\psi = \left\{ \left(e^{ikz} + e^{-ikz}\right) + \left[f(\theta) + f(\pi - \theta)\right] \frac{e^{ikr}}{r} \right\} \chi$$

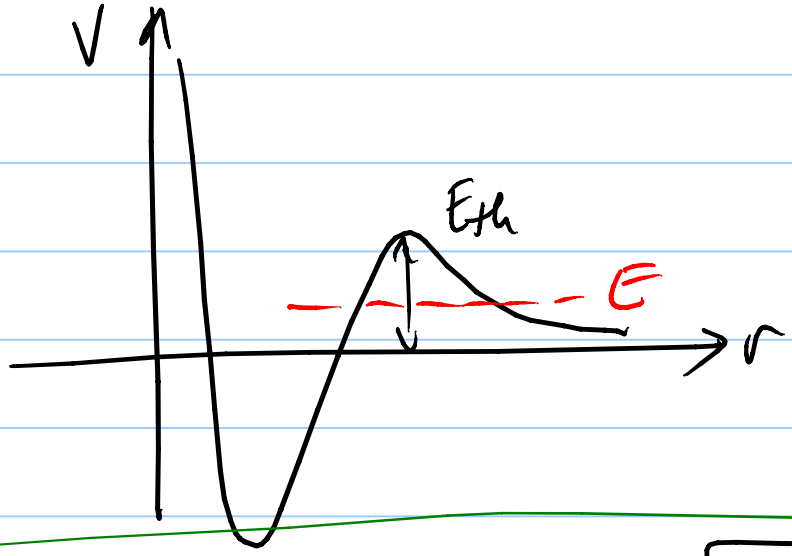
χ: 2 component spinor

- with $\chi = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$, ψ is properly symmetrized for exchange! This means

that all colliding pairs must be in a spin singlet

- again, after dealing with many factors of 2, you can show that $\sigma = 4\pi a^2$ for 2 spin states of a fermionic atom

An aside — for any collision that is classically forbidden by the centrifugal barrier (such as p-wave for identical fermions at low temp), the "Wigner threshold law" applies

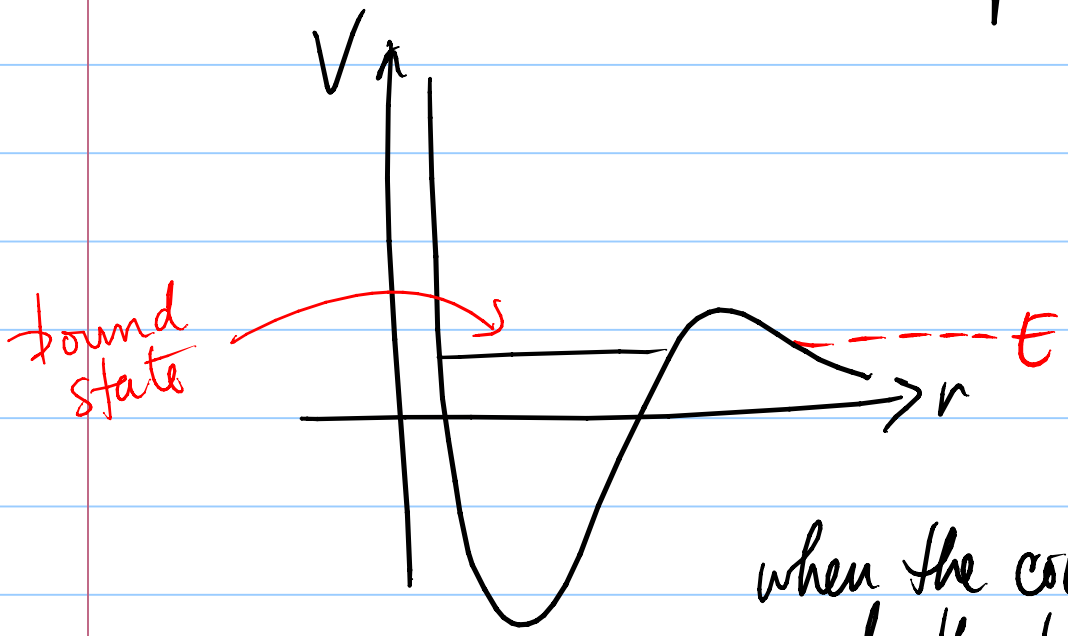


$$E_{th} = \frac{\hbar^2 \ell(\ell+1)}{2mb^2} - \frac{C_6}{b^6} \qquad b^2 = \sqrt{\frac{6C_6 m}{\hbar^2 \ell(\ell+1)}}$$

if $E < E_{th}$, then $\delta_\ell \sim k^{2\ell+1}$

or $\boxed{\sigma \propto E^{2\ell}}$

Note – somewhat related are "shape resonances"



when the collision energy equals the bound state energy you get enhanced scattering – this happens for $\ell=1$ collisions in ^{40}K and $\ell=2$ collisions in ^{87}Rb

Inelastic Collisions

Often play an important role in experiments! (Usually are a problem, but are occasionally useful)

Spin exchange

preserve total m_F

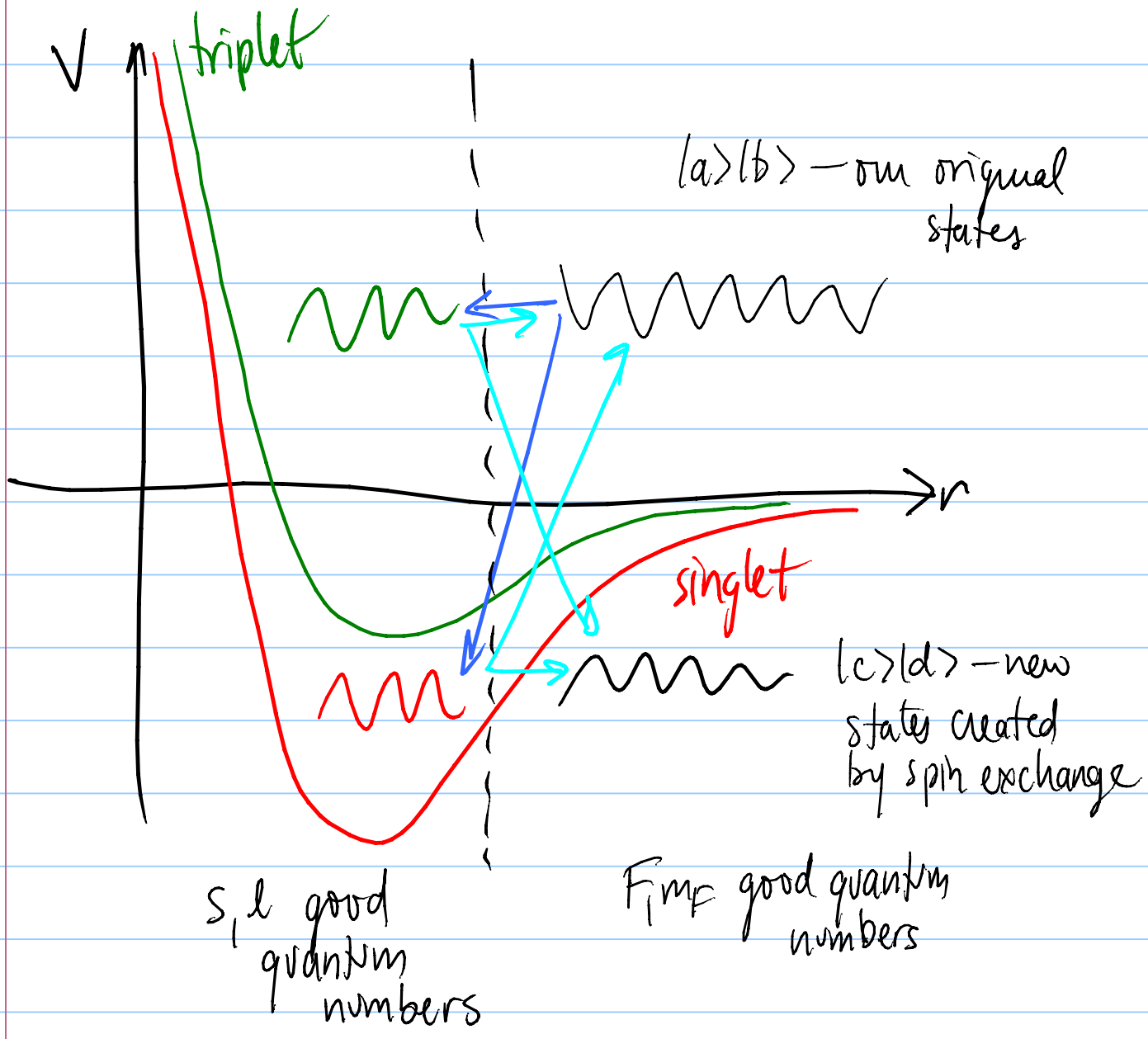
ex: ^{87}Rb: $F=1, m_F=0 + F=1, m_F=0 \rightarrow$

$F=1, m_F=-1 + F=1, m_F=+1$

This happens because F, m_F are good quantum numbers at long range, but not at short range.

As the particles accelerate inward, they project onto the singlet and triplet potentials.

As they accelerate outwards, they recombine into F, m_F states, but with different phases between the triplet and singlet components — hence we can get some new F, m_F states.



Dipolar relaxation

arises from dipole-dipole interaction between the electron spins in each atom

We can write the dipole-dipole interaction as:

$$V_d = \frac{-\mu_0}{4\pi}\frac{\mu_0^2}{r^3}\sum_{\mu=-2}^{2}\frac{4\pi}{5}Y_2^{\mu}(\hat{r})\underbrace{A(s_1,s_2)}$$

rank-2 tensor formed from the two spins

this is not a central force, and therefore can couple the orbital and spin angular momentum!

It does conserve $m_F^{(1)} + m_F^{(2)} + m_\ell$, where m_ℓ is the projection of the orbital angular momentum (of the colliding pair) onto the collision axis.

Example: ^{87}Rb $F=2, m_F=2 + F=2, m_F=2 \rightarrow$

at low temp, we always have $\ell=0$, and $m_\ell=0$

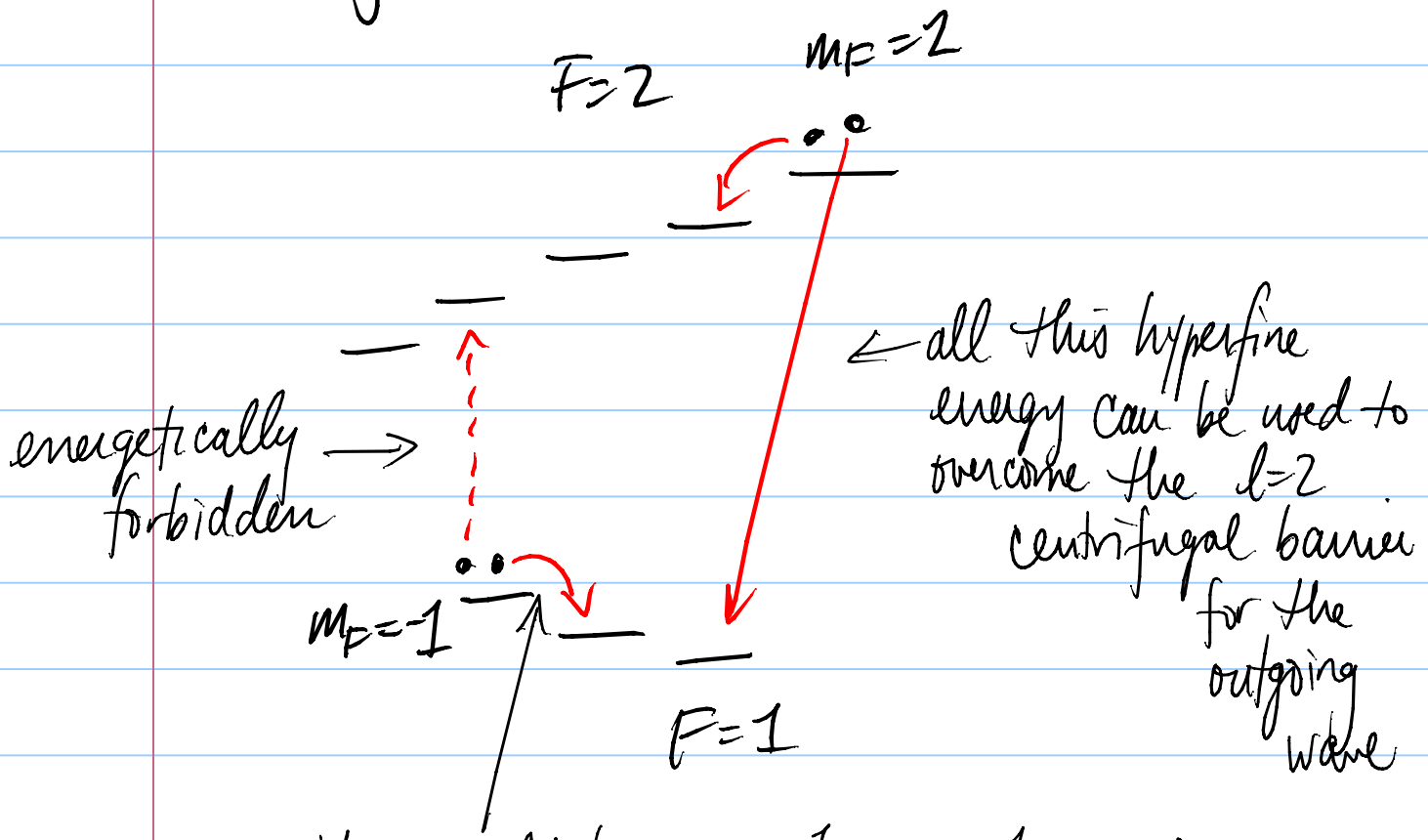
$\rightarrow m_\ell=0 \rightarrow$

$F=2, m_F=2 + F=1, m_F=1 \rightarrow$

$m_\ell=1$ ← outgoing partial wave $\ell>0$!

Because of the Y_2^m in V_d, we require $\Delta l = 0, \pm 2$ in the collision. Now, since $l = 0$ at fixed temp, dipolar relaxation generally involves an $l = 2$ outgoing partial wave.

This is why $|2,2\rangle$ is a worse choice than $|1,-1\rangle$ for magnetic trapping and evaporative cooling in ^{87}Rb...



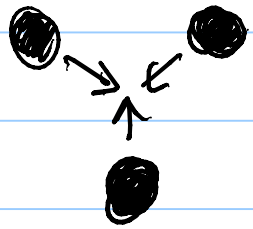
this would be $m_F=-1 + m_F=-1 + m_e=0 \rightarrow$ $m_F=-1 + m_F=0 + m_e=-1$. At low magnetic field, the Zeeman energy can be too small to overcome the $l=2$ centrifugal

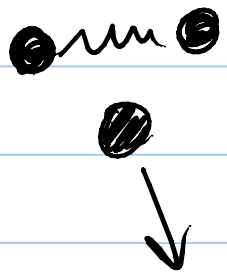
barrier for the outgoing wave, thus suppressing dipolar relaxation

Three-body recombination

Usually a problem at BEC densities...

Just the beginning of the process of solid formation — alkali atoms should be a solid at room temperature!





carries away the binding energy — 3 particles are required to conserve energy and momentum!

Elastic collisions – pseudopotentials

As we start thinking about quantum gases, we need to find a way to take into account the interaction energy present because of these inter-atomic potentials.

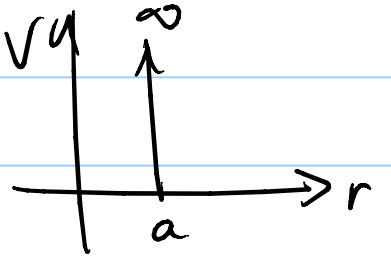
It would be nice if we could ignore all the complication of the real potential and cheat!

We can – by considering an exactly solvable short-range potential that gets all of the long-range physics (and hence a and the interaction energy) right.

This idea is attributed to Fermi!

Most common pseudopotential: hard core

$$V = \begin{cases} \infty, & r < a \\ 0, & r > a \end{cases}$$



the exact solution is $\psi_{k\to 0} \propto 1 - a/r$ (or $u = rR \propto r - a$) for $r > a$ and $\psi = 0$ for $r < a$. This seems great! It gets the long range behavior exactly right!

But, we have to be more careful. We can't use this potential to calculate and interaction energy. Better would be to follow the approach used in electrostatics — put something like a set of multipoles at the origin, and then solve for the potential (in this case the wavefunction) away from any real sources. Said another way — we just want to create something integrable that gets the boundary condition ($\psi \to 0$ at $r = a$) right.

Here's the way this story is usually told...

We introduce an "extended wavefunction" ψ_{ex} that solves:

$$(\nabla^2 + k^2)\psi_{ex} = 0 \quad \text{with} \quad \psi_{ex}(a) = 0$$

(this is just Schrodinger's equation with $V=0$ and $E = \hbar^2 k^2 / 2m$)

Our goal is to eliminate the unphysical condition $\psi(r<a)=0$, while keeping $\psi(r=a)=0$.

For this equation, as $k \to 0$, $\psi_{ex} \to \chi(1 - a/r)$ everywhere but $r=0$. Here, $\chi = \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}$ — see Huang's book for details.

How do we fix $r=0$? Well, with $k=0$, we have $\nabla^2 \psi_{ex} = 0$. Using Gauss' theorem $\left(\nabla^2 \frac{1}{r} = -4\pi\delta(r)\right)$, we have:

$$\nabla^2 \psi_{ex}\big|_{r=0} = 4\pi a \delta(r) \left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}.$$ So, we can rewrite Schrodinger's equation

as:

$$(\nabla^2 + k^2)\psi_{ex} = \overbrace{4\pi a\, \delta(r)\left[\frac{\partial}{\partial r}(r\psi_{ex})\right]_{r=0}}^{\text{pseudopotential}}$$

only non-zero at the origin

This looks just like Schrodinger's equation with a potential at the origin!

Consider:

$$\left(\frac{-\hbar^2}{2\mu}\nabla^2 + V\right)\psi = E\psi \qquad \mu = \frac{m}{2} \text{ - reduced mass}$$

$$\left(\frac{-\hbar^2}{2\mu}\nabla^2 + V\right)\psi = \frac{\hbar^2 k^2}{2m}\psi$$

$$(\nabla^2 + k^2)\psi = \frac{2\mu}{\hbar^2} V\psi = \frac{m}{\hbar^2} V\psi$$

whatever appears here is $\frac{m}{\hbar^2}V$

So, our pseudopotential is

$$V = \frac{4\pi a \hbar^2}{m}\delta(r)\underbrace{\left[\frac{\partial}{\partial r} r\right]_{r=0}}$$

typically this is ignored

why?

Well, $\frac{\partial}{\partial r}(r\psi_{ex})\Big|_{r=0} = \psi_{ex}(r=0) + \left(r\frac{\partial}{\partial r}\psi_{ex}\right)\Big|_{r=0}$

As long as ψ is "well behaved" at $r=0$ (i.e., it has slope $=0$), then $\left(\frac{\partial}{\partial r}\psi_{ex}\right)\Big|_{r=0} = 0$, and $\frac{\partial}{\partial r}(r\psi_{ex})\Big|_{r=0} = \psi_{ex}(r=0)$, which is like saying $\frac{\partial}{\partial r} r = 1$.

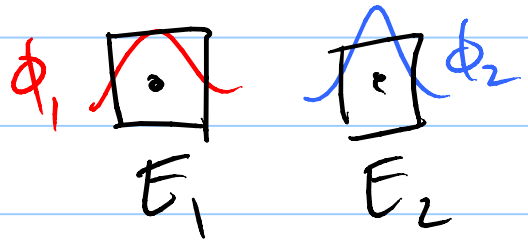
And, so, we write

$$\boxed{V = \frac{4\pi a \hbar^2}{m}\delta(r)}$$

This is great! First — it has $\psi(a)=0$, while allowing ψ to be finite everywhere. And — it's integrable.

Look at how we can calculate the interaction energy for 2 particles:

start with 2 independent particles:



and ask:

what is E_{12}?

- assume ϕ_1 and ϕ_2 unchanged by the interaction

$$E_{12} = E_1 + E_2 + \langle H_{int} \rangle$$

$$H_{int} = \frac{4\pi a \hbar^2}{m} \delta(r_1 - r_2)$$

$$\langle H_{int} \rangle = \int d^3\vec{r}_1 \int d^3\vec{r}_2 \, \phi_1^*(\vec{r}_1) \phi_2^*(\vec{r}_2) \frac{4\pi a \hbar^2}{m} \delta(\vec{r}_1 - \vec{r}_2)$$

$$\phi(r_1)\phi(r_2)$$

$$\langle H_{int} \rangle = \frac{4\pi a \hbar^2}{m} \int d^3r \, |\phi_1(\vec{r})|^2 |\phi_2(\vec{r})|^2$$

$n_1(r)$ $n_2(r)$

basically the density

the upshot: $\langle t_{hint} \rangle \propto a$

This means that:

$a > 0$: interactions effectively repulsive

$a < 0$: interactions effectively attractive