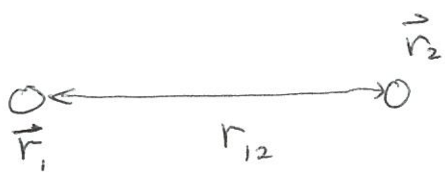
Ultracold collisions

Lecture #19
PHYS 598 AQG
Fall 2017, 10/31/17

How do we describe the interactions between cold atom?

First, what's the physical form of the two-atom interaction?

(~~...~~ i.e. for elastic interactions)



This case will be what we mostly care about

$\boxed{\text{2 Neutral atoms}}$ – induced dipole-induced dipole interactions, i.e. Van der Waals interactions

$$V = -\frac{C_6}{r_{12}^6}$$ @ large r_{12} (internuclear separation)

2 ions

$$V = \frac{K q_A q_B}{r_{12}^2}$$

neutral (ground) + neutral (excited)

$$V = -\frac{C_3}{r^3}$$

important in MOTs, when many atoms are excited

ion + neutral

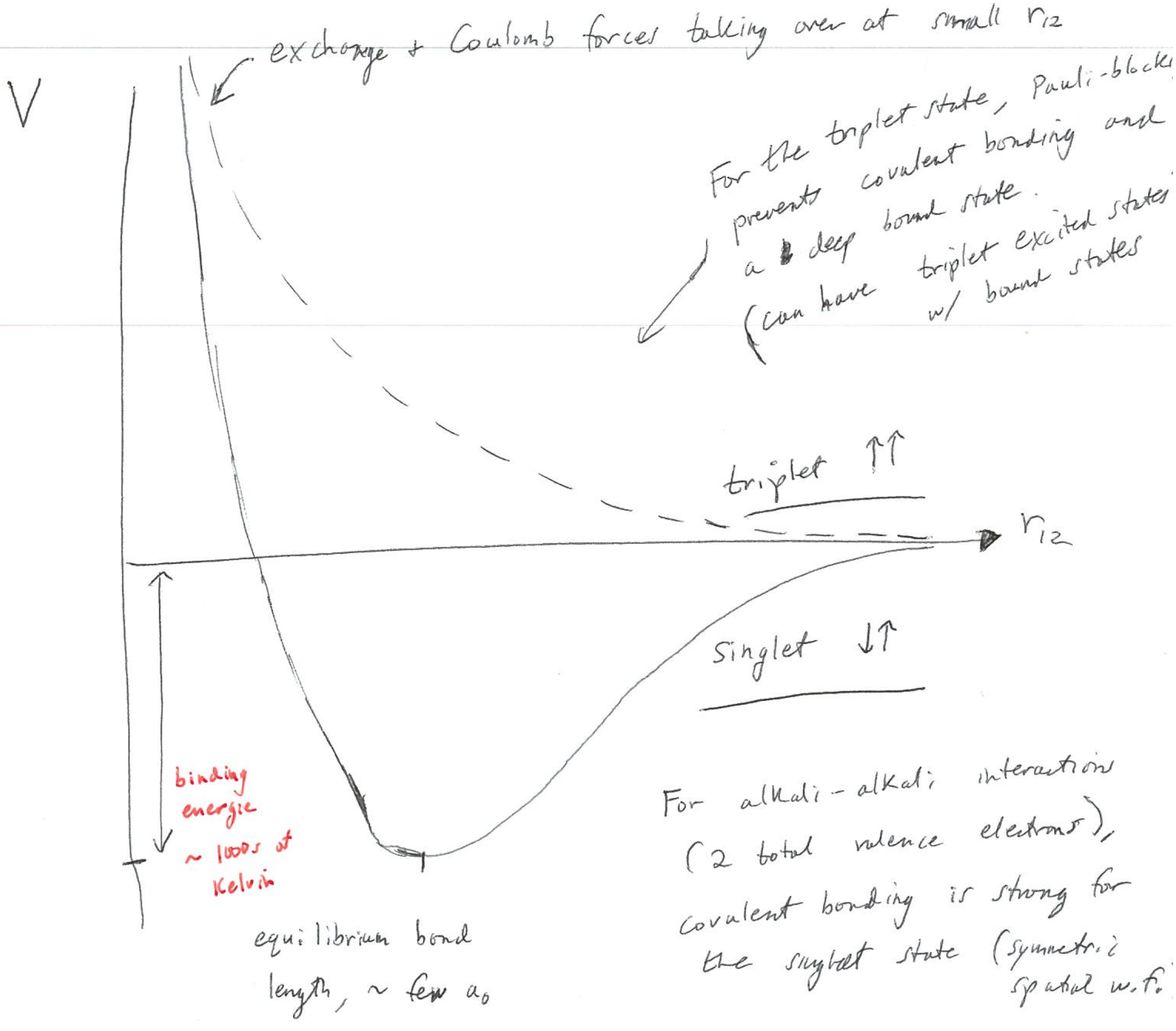
(both in ground electronic state)

$$V = -\frac{\alpha_A q_B^2}{r_{12}^4}$$

α_A = polarizability of neutral

charge-induced dipole interaction

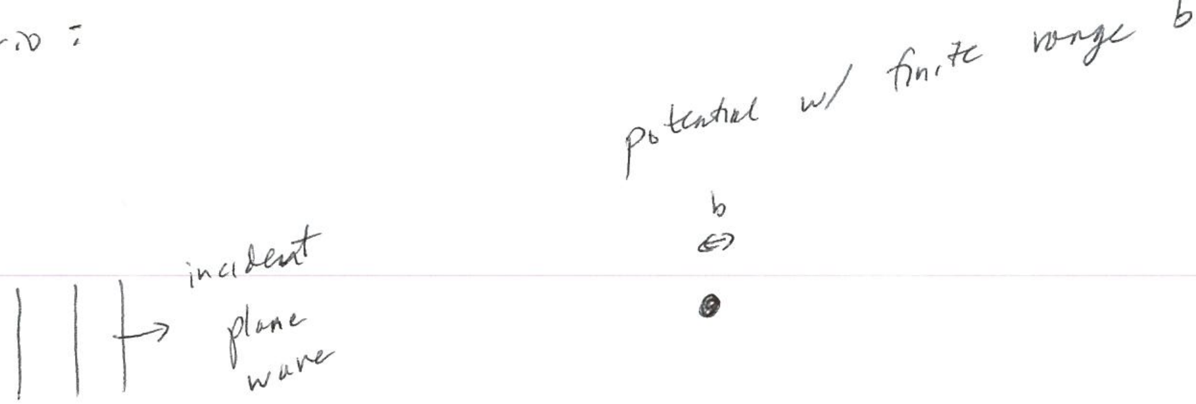
For neutral-neutrals, the real potential looks roughly like $V(r_{12}) = h(r_{12})\, e^{-\beta r_{12}} - \frac{C_6}{r_{12}^6}$, where the values of β, C_6, and form of $h(r_{12})$ would be determined from data for most atoms.



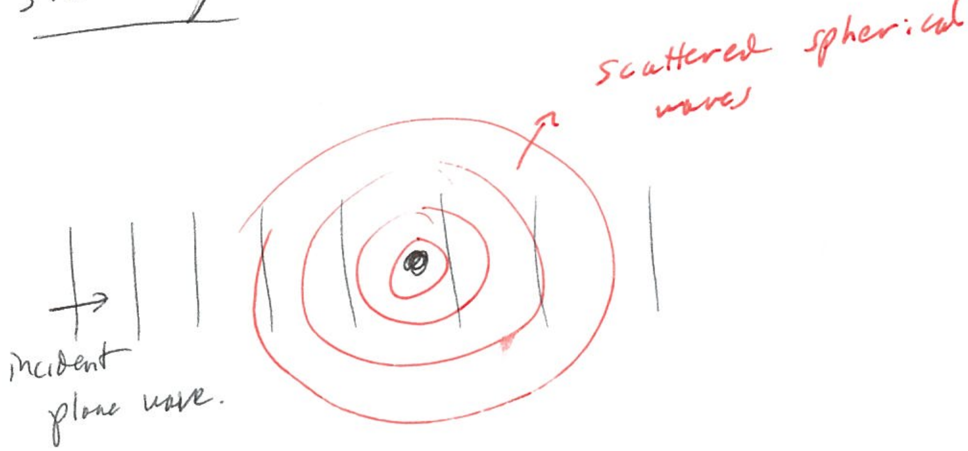
energy splittings are large (electrons are light), typically atoms follow the ground state potential during collision (as r_{12} changes), and do not make non-adiabatic transitions.

We'll take a step back now and consider some basic quantum scattering theory. One key point regarding this elastic neutral-neutral interaction — it's a <u>central</u> internuclear potential (only depends on r_{12}).

We want to find the form of the scattered wave in the following scenario:



one tractable way to treat this problem is to solve for <u>stationary</u> solutions of the form as shown.



solutions to
$$\left(\frac{\vec{p}^{\,2}}{2\mu} + V(\vec{r}_{12})\right)\Psi_K = E_K \Psi_K$$

$\mu = \frac{m}{2}$, $\vec{p} = \vec{p}_1 - \vec{p}_2$

we care about the form of $\psi_K(\vec{r})$ away from the potential (ignore short-range physics), of the form

valid for $E \ll \frac{\hbar^2}{2\mu b^2}$ or $\lambda_{dB} \gg b$

$$\psi_K(\vec{r}) \propto \underbrace{e^{i\vec{K}\cdot\vec{r}}}_{\text{incident wave in, set to } e^{iKz}} + \underbrace{f(K,\Omega)\frac{e^{iKr}}{r}}_{\text{scattered wave, } f(K,\Omega) \text{ relates to scattering amplitude}}$$

☆ We care about finding f, relates to probability to scatter during ~~...~~ collision. [and related quantities].

f depends on energy (through K) and scattering angle (through Ω) in general.

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to note - we care about ~~...~~ form of f (ψ_K) for far scattering region ($|r| \gg b$), but this is intimately related to form in the scattering region.

$$f(K,\Omega) = -\frac{\mu}{2\pi\hbar^2}\int e^{-iK\frac{\vec{r}}{r}\cdot\vec{r}'} V(\vec{r}')\,\psi_K(\vec{r}')\,d^3r'$$

w/ $\frac{\vec{r}}{r}$ normalized vector ~~angle~~ of scattered wave

Because we have a central potential, symmetry allows us to solve for ψ_k of the form

$$\underbrace{\boxed{\psi_k = \sum_\ell R_\ell(k,r)\, P_\ell(\cos\theta)}}_{\text{i.e. partial wave expansion}}$$

w/ ℓ the angular quantum number.

The $R_\ell(k,r)$ satisfy the radial wave equation for $V(r)$,

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} \underbrace{- \frac{\ell(\ell+1)}{r^2} - U(r)}_{\text{effective potential} = V(r) + \text{centrifugal barrier}} + k^2\right] R_\ell(k,r) = 0$$

$$U(r) = \frac{2\mu V(r)}{\hbar^2}$$

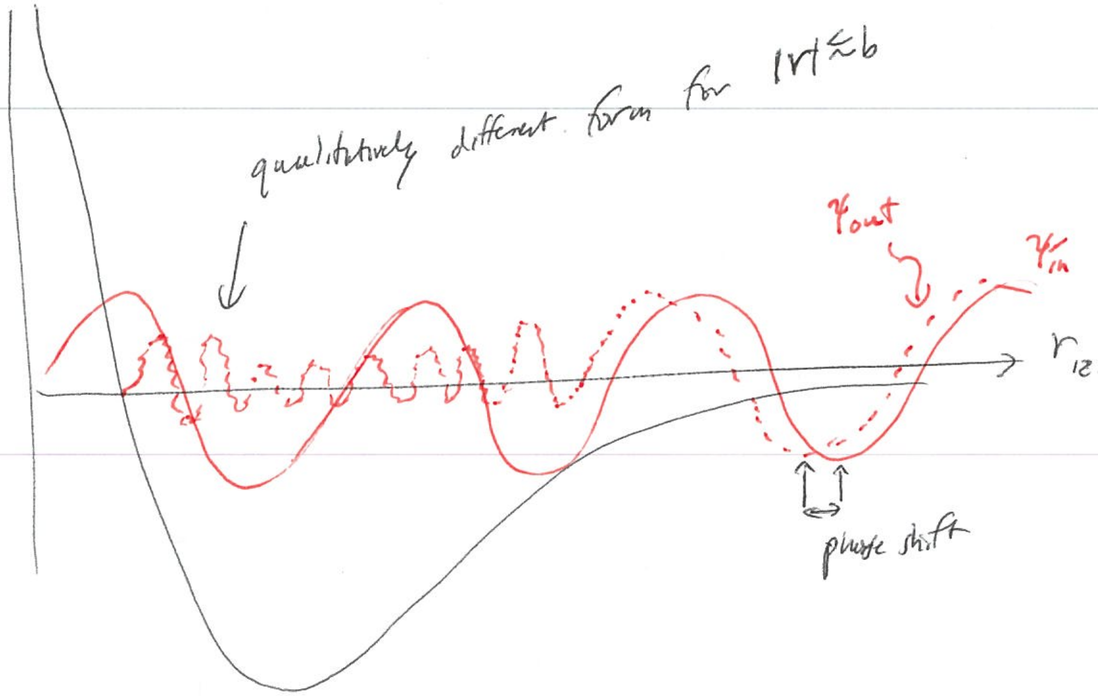
asymptotically ($r \to \infty$), we find solutions of the form

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

$\uparrow$ scattering phase shift.

at large $|r| >> b$, the incident and scattered waves are identical up to this phase shift $\delta_\ell(r)$.

Roughly



Physical reason for only a ~~[illegible]~~ phase shift at large r: conservation of probability!

One can show that

$$\boxed{\begin{aligned} f(K,\theta) &= \sum_\ell f_\ell(K)\, P_\ell[\cos\theta] \\ \text{w/}\quad f_\ell(K) &= \frac{2\ell+1}{K}\, e^{i\delta_\ell(K)} \sin(\delta_\ell(K)) \end{aligned}}$$

This is not yet a solution of $f(K,\theta)$ for some given $V(r)$, rather, looking back at our earlier form,

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

oh no

ψ at large r depends on ψ at small r

ways to treat this

first Born approximation (valid for weak scattering, $V \ll \frac{p^2}{2m}$) $\rightarrow$ assume ψ^{out} on RHS is equal to ψ^{in}.

Once we've found $f(K,\theta)$ and $f_\ell(K)$ we can find σ, the total collision cross section

$$\text{physically } \sigma = \int \underbrace{\frac{d\sigma}{d\Omega}}_{\text{differential scattering cross section}} d\Omega \rightarrow \frac{\text{\# of particles scattered into } d\Omega \text{ per unit time}}{\text{\# of incident particles per unit area per unit t}}$$

where $\boxed{\frac{d\sigma}{d\Omega} = |f(K,\theta)|^2}$ and $\boxed{\sigma = \frac{4\pi}{K^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell}$

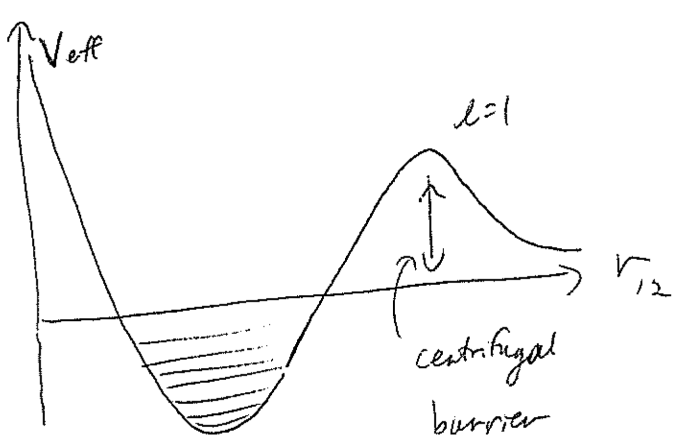
ultracold collisions

From here on out, we'll mostly be considering the $l=0$ (s-wave) scattering channel. Why? There's a centrifugal barrier for higher partial waves ($l \geq 1$), w/ barrier heights $\sim$ hundreds of microKelvin

for $T \ll 100\,\mu K$, the range of collision energies of particles in the sample $\left(\frac{|\vec{p}_1 - \vec{p}_2|^2}{2\mu}\right)$ is too small to overcome this barrier and "sample" the short-range interatomic potential $V(r)$.

One note: for $l=0$, the biggest the cross-section can be is $\sigma_{unit} = \frac{4\pi}{K^2} \rightarrow$ unitarity limit

this is the value consistent w/ conservation of probability.



$$V_{eff}(r) = \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{C_6}{r^6}$$

evaluate @ $r \sim b^*$

$$\text{w/ } (b^*)^4 = \frac{6 C_6}{\hbar^2 l(l+1)}$$

Normally, people talk about low-energy collisions in terms of a scattering length as opposed to the scattering phase shift.

We can take our form of $R \propto \frac{1}{Kr} \sin(Kr + \delta_0)$

for $l = 0$

and write as

$$R \propto \sin(K(r-a))$$

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

This is the extremely low-energy limit of the scattering, where it becomes effectively energy-independent. This yields

$$\boxed{\sigma_{K \to 0} = 4\pi a^2}$$

Taking into account corrections due to finite K-values,

(still $l = 0$)

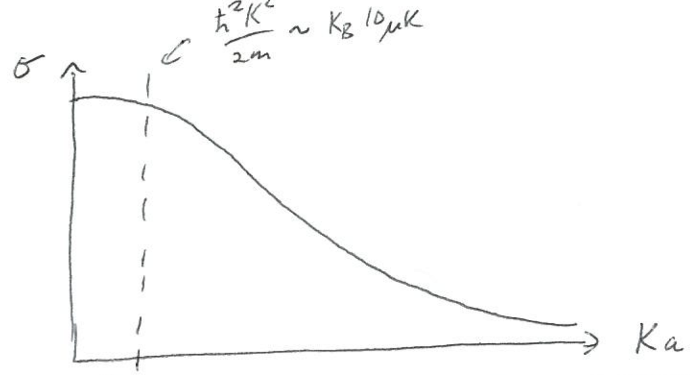
$$\sigma(K) \approx \frac{4\pi a^2}{1 + K^2 a^2}$$

Note: further accounting for so-called "effective range" effects, one has

$$\sigma = \frac{4\pi a^2}{\left(1 - \frac{K^2 a r_{eff}}{2}\right)^2 + K^2 a^2}$$

where $r_{eff} \approx b$ is the range of the potential

For low energies, σ roughly constant at $4\pi a^2$



experiments typically performed here

fixed to $\sigma_0 = 4\pi a^2$ at low collision energy

In principle, a can take on values from $-\infty$ to $+\infty$ (more later on how to control this)

What are typical scattering lengths?

Hydrogen (calculated from first principles)

$$\begin{cases} a_s = 0.41\, a_0 \\ a_t = 1.2\, a_0 \end{cases}$$

Bohr radius $a_0 \simeq 5.3 \times 10^{-11}$ m

^{87}Rb $\quad a_t \simeq a_s \simeq 100\, a_0$ $\rightarrow$ consequence, nearly all $|F^A, m_F^A, F^B, m_F^B\rangle$ combinations have identical scattering properties

$|m_F^A, m_F^B\rangle$ states get projected onto singlet, triplet states to determine scattering length

normally, instead of $a_{triplet}$ and $a_{singlet}$, one talks about

Scattering length between lowest energy internal states (always stable

a_{aa} where "a" stands for the lowest energy state when a B-field / Zeeman shift is applied.

example "a" $\Rightarrow |F, m_F\rangle = |1, 1\rangle$ for $I = 3/2$ atoms (^{23}Na, ^{87}Rb, ^{39}K

Some typical background values of a_{aa} for the alkalis

$^{87}Rb \rightarrow 100\, a_0 \sim 5\text{ nm}$

$^{23}Na \rightarrow 62\, a_0 \sim 3\text{ nm}$

$^{7}Li \rightarrow -25\, a_0$

$^{39}K \rightarrow -29\, a_0$

$^{85}Rb \rightarrow -443\, a_0$

$^{133}Cs \rightarrow 1720\, a_0 \sim 100\text{ nm}$

Compare these to other length scales in cold gases

optical wavelengths: $\frac{\lambda}{2} \sim$ 200-800 nm

system size: $\sim$ tens to 100's of μm ($\sim 10^4$ nm)

typical interparticle spacing:

for $n \sim 10^{12} - 10^{14}\text{ cm}^{-3}$,

$\bar{r}_{12} \sim (1.0 - 0.2)\,\mu\text{m}$

dilute $\longleftrightarrow$ dense

Some questions: what's a "good" value for making "quantum gases"?

- what considerations are important?
  - $\rightarrow$ thermalization ($n\sigma\bar{v}$) $\propto a^2$
  - $\rightarrow$ loss?
  - $\rightarrow$ stability?

- why have we just shown bosons?

Collisions of identical particles $\Rightarrow$ bosons + fermions

the collision is a two-body process, and the two-particle wave function describing the scattering state should obey the exchange symmetry of the particles you're considering.

Let's consider two colliding particles (plane-wave states) along $\overrightarrow{e^{ikz}}$ and $\overleftarrow{e^{-ikz}}$

for identical bosons / fermions, symmetrized / antisymmetri[zed] by hand.

at large $|r_{12}|$, the state should look like

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

"+" for bosons

"−" for fermions

exchange of particle indices gives

$r \to r$

$\theta \to \pi - \theta$

$\varphi \to \pi + \varphi$

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

taking into account

Legendre polynomial

$$f(k,\theta) = \sum_{\ell} f_\ell(k)\, P_\ell[\cos\theta]$$

for even ℓ, $P_\ell(-\cos\theta) = P_\ell(\cos\theta)$

for odd ℓ, $P_\ell(-\cos\theta) = -P_\ell(\cos\theta)$

Consequence

For identical bosons

l even, $f(\theta) + f(\pi - \theta) \to 2f(\theta)$ collisions ($\times 2$)!

l odd, $f(\theta) + f(\pi - \theta) \to 0$ no collisions

For identical fermions

l even, $f(\theta) - f(\pi - \theta) \to 0$ no collisions

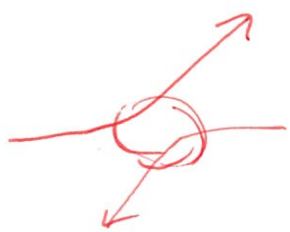
l odd, $f(\theta) - f(\pi - \theta) \to 2f(\theta)$ collisions ($\times 2$)!

At low temperatures ($K_B T \ll$ centrifugal barrier $\sim K_B\, 100\,\mu K$), identical bosons can collide ($l = 0$ allowed) while identical fermions <u>cannot</u> ($l = 0$ dissallowed by Fermi statistics)

[for the bosons, as $K \to 0$, $\underline{\sigma = 8\pi a^2}$ if the particles are identical

extra factor of 2 due to exchange statistics

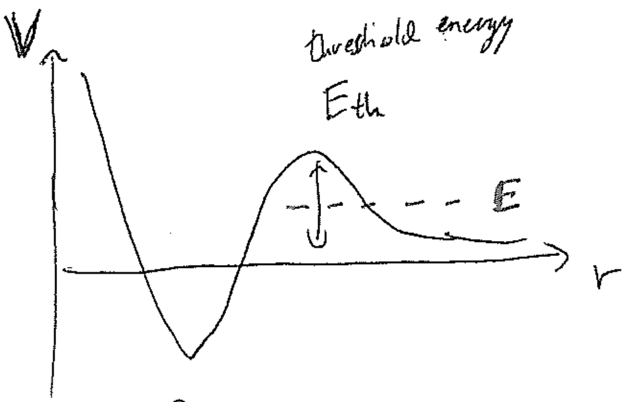
separate short-range trajectories not well-defined for identical particles



or

OK, so how can we get fermionic atoms to collide / thermalize?

Even identical (spin-polarized) fermions will collide if $E_{coll} \sim E_{centrifugal}$. Even when classically forbidden, i.e. $E_{coll} < E_{centr}$, still some probability to tunnel through barrier.



shown for, ie, p-wave collisions ($\ell = 1$)

still some scattering phase shift

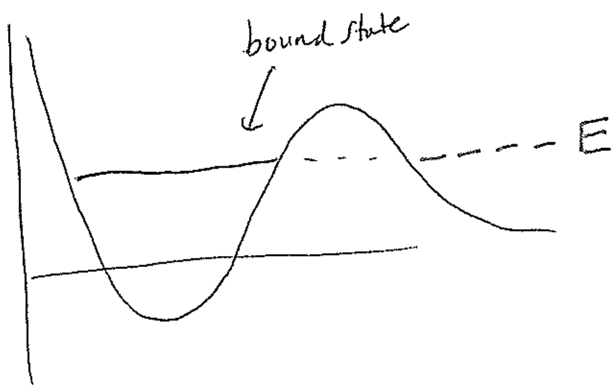
$$\boxed{\delta_\ell \propto k^{2\ell+1}} \quad \text{for } E < E_{th}$$

this relates to

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

$$\sigma_{\ell=0}(k) = \frac{8\pi}{k^2}(2\ell+1)\sin^2\delta_\ell \propto k^{4\ell} \quad \text{as } k \to 0$$

Note, because this is quantum scattering, can get interference effects



so called "shape resonces," leading to enhancement (or general alteration) to scattering when $E_{coll} \sim E_{bound}$

[occurs for 40K @ moderate T for $\ell = 1$]

These temperature-dependent scattering processes break down at low temperature. If we want fermions to collide, need them in <u>different spin states</u>.

Specifically, w/ antisymmetric (singlet) spin state

$$\chi = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$ for the two spin/internal states,

the spatial wave function of the colliding pair can be symmetric ($\ell = 0$) while obeying Fermi exchange statistics.

$$\Psi_{tot} = \Psi_{spatial} \otimes \Psi_{internal} \propto \left\{ \left(e^{ikz} + e^{-ikz}\right) + \left[f(\theta) + f(\pi-\theta)\right]\frac{e^{ikr}}{r} \right\} \otimes \chi$$

$\rightarrow$ get $\sigma = 4\pi a^2$ for 2 fermionic spin states.

for $^6Li \rightarrow a \sim -1500\, a_0$ $\longleftarrow$ compared to bosons, will ^6Li be more stable w.r.t. 3-body loss / collapse?

$^{40}K \rightarrow a \sim 174\, a_0$