* INTERPARTICLE INTERACTIONS

* In the previous sections we discussed the ideal quantum gases, in which we neglected the interparticle interactions. However, in spite of the extreme diluteness of these gases, interparticle interactions play actually a fundamental role. In this lecture we will briefly review some basics of scattering theory, and the crucial idea of Feshbach resonance.

• BASICS OF SCATTERING THEORY

. Under typical conditions we may reduce the analysis of the interparticle interactions to the problem of binary collisions. The problem of calculating the scattering amplitude of 2 colliding particles reduces to the solution of the time-independent Schrödinger equation

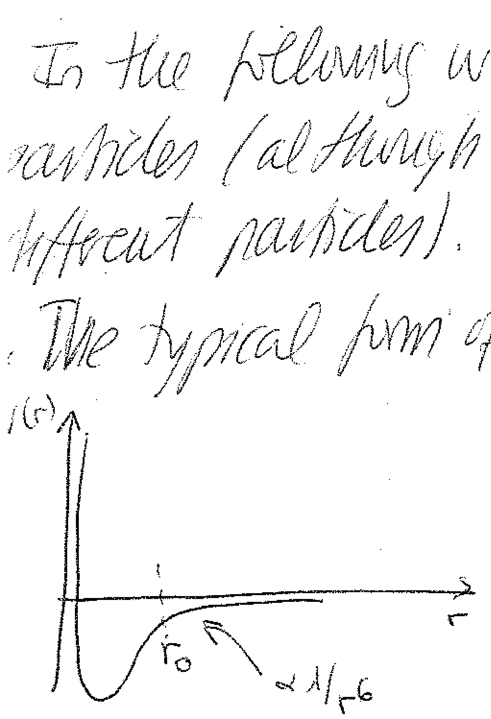
$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi(\vec{r}) = E\,\psi(\vec{r})$$

Note: $V(r)$ is the interparticle potential which is supposed to be central

where μ is the reduced mass.

In the following we consider the collision of 2 identical particles (although the problem may be easily extended to different particles).

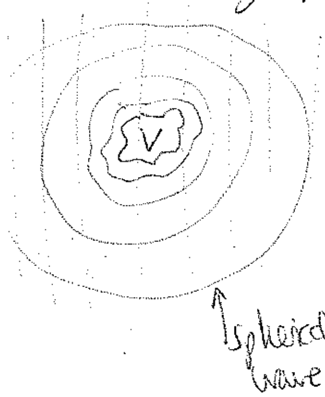
. The typical form of the interparticle potential $V(r)$ is



where r_0 = range of the potential $V(r)$.

($V(r)$ is a central potential)

* We are interested in the solution of the Schrödinger equation in the asymptotic region $r >> r_0$:



incoming wave $\vec{z}$

$$\psi(\vec{r}) = \underbrace{e^{ikz}}_{\text{incoming plane wave}} + \underbrace{f(\theta)}_{\substack{\text{scattering amplitude for an} \\ \text{angle } \theta \text{ between } \vec{r} \text{ and } z}} \underbrace{\frac{e^{ikr}}{r}}_{\text{scattered spherical wave}}$$

* The scattering amplitude is in general a function of the energy E, and determines the scattering cross-section

$$d\sigma = |f(\theta)|^2 d\Omega$$ (i.e. the probability to be scattered in a given solid angle between Ω and $\Omega + d\Omega$)

Actually this expression is only valid for non-identical particles. For identical particles the orbital part of the wave function must be symmetric or antisymmetric depending on whether the total spin of the pair is even or odd and the particles are bosons or fermions:

$$d\sigma = |f(\theta) \pm f(\pi-\theta)|^2 d\Omega \qquad \theta \in [0, \pi/2]$$

$+ \equiv$ bosons (total spin even)

$- \equiv$ fermions (total spin odd)

* We expand the wave function in the form:

$$\psi(\vec{r}) = \sum_{l=0}^{\infty} P_l(\cos\theta) \frac{\chi_{kl}(r)}{kr}$$ $P_l \equiv$ Legendre polynomials

* then, substituting into the Schrödinger equation

$$\frac{d^2}{dr^2}\chi_{k\ell}(r) - \underbrace{\frac{\ell(\ell+1)}{r^2}\chi_{k\ell}(r)}_{\text{Centrifugal barrier}} + \frac{2m}{\hbar^2}(E - V(r))\,\chi_{k\ell}(r) = 0$$

(This is the radial equation)

For $r >> r_0$, we may neglect $V(r)$ and the centrifugal barrier and $\frac{d^2}{dr^2}\chi_{k\ell}(r) + \frac{2mE}{\hbar^2}\chi_{k\ell}(r) = 0$

$$\Longrightarrow \chi_{k\ell}(r) = A_\ell \sin\left(kr - \frac{\pi\ell}{2} + \delta_\ell\right)$$

where we have introduced the dephases δ_ℓ for the channel with total angular momentum ℓ.

* Without entering into all details, we may write the final result for the scattering amplitude as a function of the relative momentum k and the dephases δ_ℓ:

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)\,P_\ell(\cos\theta)\left[e^{2i\delta_\ell} - 1\right] = \sum_{\ell=0}^{\infty} f_\ell(\theta)$$

Note that all the information of the scattering is now in the dephases δ_ℓ.

Note also that since $P_\ell(\cos(\pi-\theta)) = P_\ell(-\cos\theta) = +(-1)^\ell P_\ell(\cos\theta)$

Then: • for identical bosons only even ℓ contribute $\begin{pmatrix} \ell=0 \to s\text{-wave} \\ \ell=2 \to d\text{-wave} \\ \vdots \end{pmatrix}$

• for identical fermions only odd ℓ contribute $\begin{pmatrix} \ell=1 \to p\text{-wave} \\ \vdots \end{pmatrix}$

This restriction has of course very important consequences, as we will see later.

* As we mentioned above the scattering information is in the phase shifts δ_ℓ. To calculate them we need to solve the Schrödinger equation. The situation is simpler for low energies ($kr_0 \ll 1$)

For $r \ll 1/k$ we can set $E \simeq 0$ in the radial equation.

For $l=0$ (s-wave):

$$\frac{d^2}{dr^2}\chi_{k0}(r) - \frac{2m}{\hbar^2}V(r)\,\chi_{k0} = 0$$

For $r_0 \ll r \ll 1/k \longrightarrow V(r) \simeq 0$

$$\frac{d^2}{dr^2}\chi_{k0}(r) = 0 \longrightarrow \chi_{k0}(r) = C_0(1-\kappa r)$$

(Note: that for $r \gg r_0$ $\chi_{k0}(r) \overset{r\gg r_0\ (p.88)}{\simeq} A_0 \sin[kr+\delta_0] = A_0[\sin kr \cos\delta_0 + \cos kr \sin\delta_0]$
$\underset{\text{Taylor expansion}}{\cong} A_0 \sin\delta_0 \,[1+(k\cot\delta_0)r] \longrightarrow \boxed{\kappa = -k\cot\delta_0}$)

For the s-wave:

$$f_0(\theta) = \frac{1}{2ik}\left(e^{2i\delta_0}-1\right)$$

$\tan\delta_0 = \frac{-k}{\kappa} \ll 1 \to \tan\delta_0 \simeq \delta_0$

For $k \to 0 \Rightarrow \cot\delta_0 = \frac{-\kappa}{k} \xrightarrow{k\to 0} \delta_0 \simeq \frac{-k}{\kappa}$

$$\longrightarrow e^{2i\delta_0} - 1 \simeq -2i\frac{k}{\kappa} \longrightarrow f_0(\theta) \simeq -\frac{1}{\kappa}$$

We introduce here the so-called <u>s-wave scattering length</u>

$$a = 1/\kappa \longrightarrow \boxed{\delta_0 = -ak}$$

Note: Hence asymptotically $\chi_{k0} = C_0[1 - r/a]$ $\longrightarrow \psi(\vec{r}) \propto 1 - a/r$. We will employ this form later in p. 97

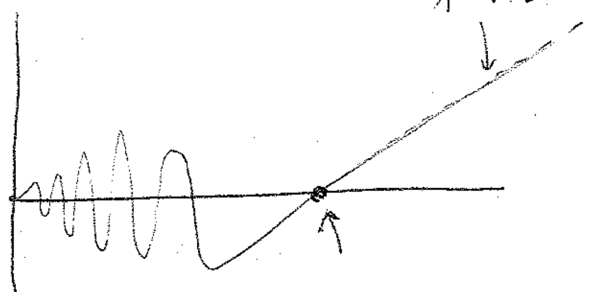
* The phase shifts for $l>0$ behave as $\delta_l \propto k^{2l}$.
Hence the vanish quickly for $k \to 0$.
<u>Note</u>: this isn't surprising. For $l>0$, the centrifugal barrier prevents the particles to get close enough to see the potential if k is very low).

Hence for $k \to 0$: $f(\theta) \simeq f_0(\theta) = -a$.

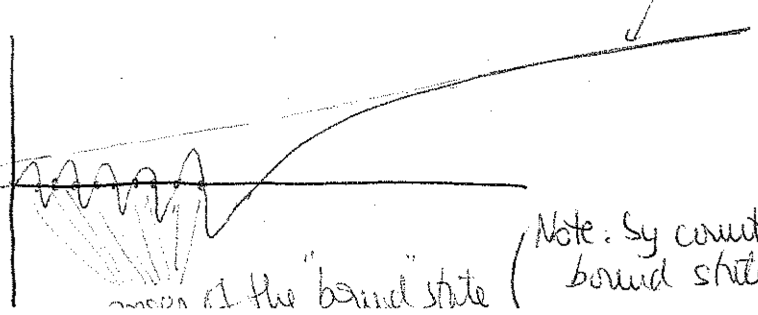
Thus: $$\sigma = \begin{cases} 8\pi a^2 & \text{for bosons} \\ 0 & \text{for fermions} \end{cases}$$ (the factor 4π comes from $\int d\Omega$, and the extra 2 from the $f(\theta)+f(\pi-\theta)$)

<u>Note</u>: we used this result already in p.(49) when we discussed evaporative cooling).

* The s-wave scattering length plays a <u>crucial role</u> in the physics of ultracold gases, as we will see later in these lectures. We may get a feeling of the intuitive meaning of the s-wave scattering length by having a look to the form of $\chi_0(r)$ when $k \to 0$.



In the first example, if we take the asymptotic $1-r/a$ and see the cut we get $a>0$. In the 2nd example we get $a<0$.



Hence a can be understood as the zero of the asymptotic line.

(Note: by counting the nodes you can know how many bound states has the potential $V(r)$)

* The scattering length "a" can then attain positive and negative values. This is particularly important, as we will see later. We may see as well that $|a|$ can take values from 0 to ∞, i.e. from ideal gas into extremelly interacting gas. We will come back to this point in a moment.

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* Note that the whole scattering is characterized by the scattering length a. The details of the potential are actually not important. We can actually substitute the potential by whatever as long as it provides the same scattering length.

In particular we will employ the so-called <u>pseudopotential</u>

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

which provides also a scattering length.

<u>Note</u>: the discussion on the pseudopotential is slightly subtle. For a more detailed discussion, see e.g. K. Huang, "Statistical mechanics".)

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* From the cartoons of p. 90 you can perhaps guess that something may happen if you alter the bound states of the scattering potential (the zeroes of the $\chi_0(r)$ wavefunction). In particular you may change $a>0$ into $a<0$ or viceversa, and make $|a|$ from 0 to ∞, actually in a resonant manner. This brings us to the discussion of the <u>Feshbach resonances</u>.

- ## FESHBACH RESONANCES

* As mentioned above if one could change $V(\vec{r})$ and change the number of bound states, we could actually change the scattering length resonantly between $-\infty$ to $+\infty$.

* In practice what one does is slightly more subtle. One employs two scattering channels (corresponding e.g. to two internal states of the colliding particles). One channel is open (and is where the collision is produced) and the other is closed. The only relevant feature of the closed channel is that it has a bound state ($\varphi(\vec{r})$) with energy $\hbar\Delta$ (see fig. in page 93)

* We then consider a collision between two atoms, but we consider (and this is crucial) the possibility of forming an intermediate molecular state.

~~For simplicity we forget any dispersion of the closed channel.~~

- For simplicity of our discussion we consider no scattering in absence of coupling between the closed and the open channel i.e. in absence of coupling $a=0$).

* In the reference system of the center-of-mass the Hamiltonian of the system is hence

$$\hat{H} = \hat{H}_0 + \hat{W}, \quad \text{where} \quad \hat{H}_0 \equiv \begin{pmatrix} -\frac{\hbar^2}{2\mu}\nabla^2 & 0 \\ 0 & \hbar\Delta \end{pmatrix}$$

$$\hat{W} \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \hbar\Omega(r)$$

where $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow$ open channel, $\begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow$ closed channel.

* So, we have like a two-level atom again, where we have also a coupling potential $\hat{W}$ with an effective "Rabi-like" frequency $\Omega(r)$. Physically this coupling may have different origins. Typically the electronic and nuclear spins of one of the colliding atoms are flipped by the hyperfine interaction, bringing the collisional pair from the ~~closed~~ open to the closed channel (and back again).

Then the bound state $\varphi(\vec{r})$ is a state with a different spin than the open channel, and as a consequence it possesses a different magnetic moment. Hence the difference Δ may be tuned by means of a magnetic field due to the different Zeeman effect.

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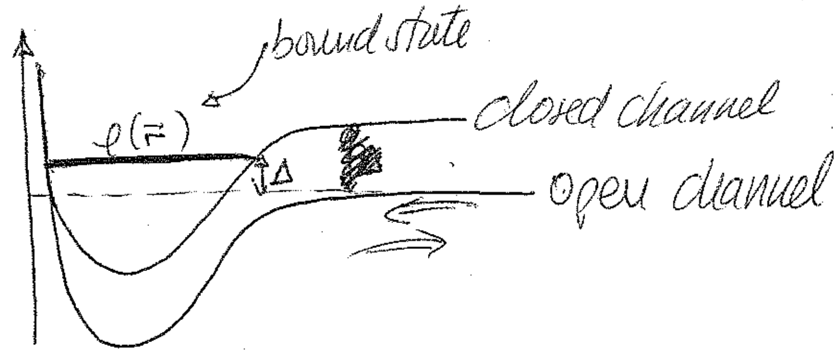


* We look for a stationary state $|\psi_+\rangle = \begin{pmatrix} \psi_+(\vec{r}) \\ \gamma\varphi(\vec{r}) \end{pmatrix}$, which is an admixture of the open and closed channel (due to the coupling $\hat{W}$). This state has an energy E.

The corresponding eigenstate of $\hat{H}_0$ (with energy E) associated to $|\psi_+\rangle$ is $|\psi_0\rangle = \dfrac{e^{i\vec{k}\vec{r}}}{\sqrt{L^3}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Note: We will be later interested in the case $E \to 0$.

Note that $(E - H_0)|\psi_0\rangle = 0$, $E = \dfrac{\hbar^2 k^2}{2m}$

* One may then write $|\Psi_+\rangle$ in the convenient form

$$|\Psi_+\rangle = |\Psi_0\rangle + \frac{1}{E-\hat{H}_0+i\varepsilon}\hat{W}|\Psi_+\rangle \qquad (\varepsilon \to 0)$$

Note that $(E-\hat{H}_0)|\Psi_+\rangle = \hat{W}|\Psi_+\rangle \to E|\Psi_+\rangle = \hat{H}|\Psi_+\rangle$

and also that if $\hat{W}=0 \longrightarrow |\Psi_+\rangle = |\Psi_0\rangle$ as it should.

* let's iterate once:

$$|\Psi_+\rangle = |\Psi_0\rangle + \frac{1}{E-\hat{H}_0+i\varepsilon}\hat{W}|\Psi_0\rangle + \frac{1}{E-\hat{H}_0+i\varepsilon}\hat{W}\frac{1}{E-\hat{H}_0+i\varepsilon}\hat{W}|\Psi_+\rangle$$

* We multiply (from the left) by $(0, \varphi(r))$ and integrate

$$\int d^3r\,(0,\varphi(r))\begin{pmatrix}\Psi_+(r)\\ \varphi(r)\gamma\end{pmatrix} = \left[\int d^3r\,\varphi(r)^2\right]\gamma = \gamma$$

$$\| $$

$$\cancel{\int d^3r\,(0,\varphi(r))\begin{pmatrix}e^{i\vec{k}\vec{r}}/\sqrt{L^3}\\ 0\end{pmatrix}} + \int d^3r\,(0,\varphi(r))\frac{1}{E-\hat{H}_0+i\varepsilon}\hbar\Omega(r)\begin{bmatrix}\\ \frac{e^{i\vec{k}\vec{r}}}{\sqrt{L^3}}\end{bmatrix}$$

$$+\int d^3r\,(0,\varphi(r))\frac{1}{E-\hat{H}_0+i\varepsilon}\hbar\Omega(r)\begin{pmatrix}0&1\\1&0\end{pmatrix}\frac{1}{E-\hat{H}_0+i\varepsilon}\hbar\Omega(r)\begin{bmatrix}\varphi(\vec{r})\gamma\\ \Psi_+(\vec{r})\end{bmatrix}$$

$$= \frac{1}{E-\hbar\Delta+i\varepsilon}\int d^3r\,\varphi(r)\hbar\Omega(r)\frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{L^3}}$$

$$+\int d^3r\,(0,\varphi(r))\frac{1}{E-\hat{H}_0+i\varepsilon}\hbar\Omega(r)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{bmatrix}\frac{1}{E+\hbar^2\nabla^2/2m+i\varepsilon}[\hbar\Omega(r)\varphi(r)\gamma]\\ \frac{1}{E-\hbar\Delta+i\varepsilon}\hbar\Omega(r)\Psi_+(r)\end{bmatrix}$$

$$= \frac{1}{E-\hbar\Delta+i\epsilon} \int d^3r\, \rho(r)\, \hbar\Omega(r)\, e^{i\vec{k}\vec{r}}/\sqrt{L^3}$$

$$+ \frac{1}{E-\hbar\Delta+i\epsilon} \int d^3r\, \rho(r)\, \hbar\Omega(r) \frac{1}{E+\frac{\hbar^2\nabla^2}{2\mu}+i\epsilon} \hbar\Omega(r)\rho(r)\, \gamma$$

* Let $f(\vec{r}) = \frac{1}{\sqrt{2}} \hbar\Omega(\vec{r})\rho(\vec{r})$

$$g(\vec{k}) = \int d^3r\, f(\vec{r})\, e^{-i\vec{k}\cdot\vec{r}}$$

Then $\int d^3r\, \sqrt{2}\, f(r) \frac{1}{E+\frac{\hbar^2\nabla^2}{2\mu}+i\epsilon} f(\vec{r})\sqrt{2}\,\gamma$

$$= 2\gamma \int d^3r \left[\int \frac{d^3k'}{(2\pi)^3} g(\vec{k}')^* e^{i\vec{k}'\vec{r}}\right] \int \frac{d^3k}{\left[E+\frac{\hbar^2k'^2}{2\mu}+i\epsilon\right]} g(k'') e^{i\vec{k}'\cdot\vec{r}}$$

$$= 2\gamma \int \frac{d^3k'}{(2\pi)^3} |g(k')|^2 \frac{1}{E-\frac{\hbar^2k'^2}{2\mu}+i\epsilon} = \frac{2\gamma}{2\pi^2} \int dk'\, g(k')^2 \frac{k'^2}{E-\frac{\hbar^2k'^2}{2\mu}+i\epsilon}$$

Then

$$\int d^3r\, \rho(r)\hbar\Omega(r) \frac{1}{E+\frac{\hbar^2\nabla^2}{2\mu}+i\epsilon} \hbar\Omega(r)\rho(r)\,\gamma = \frac{\gamma}{\pi^2} \int dk' \frac{g(k')^2 k'^2}{E-\frac{\hbar^2k'^2}{2\mu}+i\epsilon}$$

* We are actually interested in our scattering analysis in the stationary state with $E=0$ $(k=0)$. Then:

$$\gamma = \frac{+\sqrt{2}}{-\hbar\Delta+i\epsilon} \frac{g(0)}{\sqrt{L^3}} + \frac{\gamma/\pi^2}{(-\hbar\Delta+i\epsilon)} \int dk' \frac{g(k')^2}{i\epsilon - \hbar^2k'^2/2\mu}$$

$$\xrightarrow[\epsilon\to 0]{} \frac{-g(0)\sqrt{2}}{\hbar\Delta\sqrt{L^3}} + \frac{2\mu}{\pi^2\hbar^2} \frac{1}{(\hbar\Delta)} \int dk'\, g(k')^2$$

Let $\boxed{\Delta_0 = \frac{2\mu}{\pi^2\hbar^3}\int_0^{\infty} g^2(k)\,dk}$

Then: $\gamma = \frac{-g(0)\sqrt{2}}{\Delta\sqrt{L^3}} + \frac{\Delta_0}{\Delta}\gamma$

$$\sqrt{L^3}\,\gamma = \frac{\sqrt{2}\,g(0)}{\hbar(\Delta_0-\Delta)}$$

* Since: $|\psi_+\rangle = |\psi_0\rangle + \frac{1}{E-H_0+i\varepsilon} W|\psi_+\rangle$

$$\begin{pmatrix}\psi_+(r)\\ \gamma\rho(r)\end{pmatrix} = \begin{pmatrix}1/\sqrt{L^3}\\ 0\end{pmatrix} + \frac{1}{-H_0+i\varepsilon}\hbar\Omega(r)\begin{pmatrix}\gamma\rho(r)\\ \psi_+(r)\end{pmatrix}$$

Then $\psi_+(r) = \frac{1}{\sqrt{L^3}} + \frac{1}{(i\varepsilon+\hbar^2\nabla^2/2\mu)}\hbar\Omega(r)\rho(r)\,\gamma$

$$= \frac{1}{\sqrt{L^3}} + \int\frac{d^3k'}{(2\pi)^3}\sqrt{2}\,\gamma\left(\frac{1}{i\varepsilon-\frac{\hbar^2k'^2}{2\mu}}\right)g(k')\,e^{-i\vec{k}'\cdot\vec{r}}$$

$$= \frac{1}{\sqrt{L^3}} + \frac{\sqrt{2}\,\gamma}{(2\pi)^3}\int_0^{\infty}dk'\,\frac{2\mu}{\hbar^2}\,g(k')\int e^{-i\vec{k}'\cdot\vec{r}}\,d\Omega$$ solid angle

$$= \frac{1}{\sqrt{L^3}} + \sqrt{2}\,\gamma\left(\frac{-\mu}{\pi^2\hbar^2}\right)\int_0^{\infty}dk'\,g(k')\,\frac{\sin(k'r)}{(k'r)} \simeq$$ r large

$$= \frac{1}{\sqrt{L^3}} + \sqrt{2}\,\gamma\left(\frac{-\mu}{2\pi\hbar^2}\right)\frac{1}{r}\,g(0)$$

$$\sqrt{L^3}\,\psi_+(r) = 1 + \sqrt{2}\left(\sqrt{L^3}\,\gamma\right)\left(\frac{-\mu}{2\pi\hbar^2}\right)\frac{g(0)}{r}$$

Hence

$$\sqrt{L^3}\,\psi_+(r) = 1 - \frac{2g(0)}{\hbar(\Delta_0-\Delta)}\,\frac{\mu}{2\pi\hbar^2}\,\frac{g(0)}{r}$$

$$= 1 - \left[\frac{\mu\, g(0)^2}{(\Delta_0-\Delta)\pi\hbar^3}\right]\frac{1}{r}$$

* For large r, remember that

$$\sqrt{L^3}\,\psi_+(r) \simeq 1 - a/r$$

(**Note**: we showed in p. 89 that $\chi_{k0}(r) = c_0(1 - r/a)$, but $\psi_+(r) \sim \chi_{k0}(r)/r \longrightarrow \sim 1 - a/r$)

* Hence the effective scattering length for the open channel is of the form:

$$\boxed{a = \frac{+\mu\, g(0)^2}{\pi\hbar^3(\Delta_0-\Delta)}}$$

* Note that since Δ depends linearly on B due to the Zeeman effect, then we may re-express in the form:

$$\boxed{a = \frac{a_0\,\Delta B}{B_0 - B}}$$

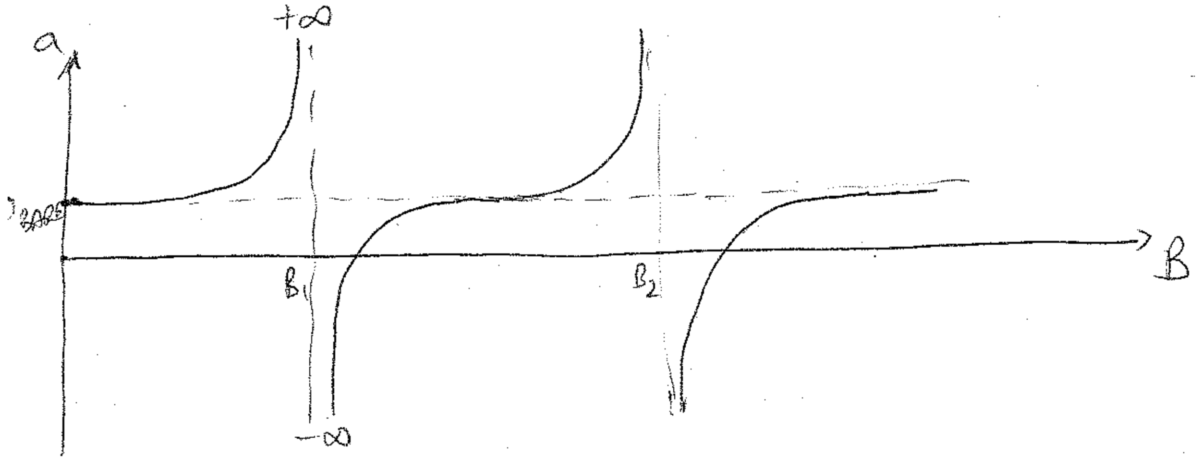
Hence, as a result of the coupling with the closed channel we may have a 'very large modification of the scattering properties. Note that if $\Delta \Rightarrow \Delta_0 \Rightarrow a$ tends to $\pm\infty$ (!!)

This is a <u>Feshbach resonance</u>

* If, in absence of coupling, there's scattering, then, at the m^{th} resonance

$$a = a_{Bare}\left[1 - \frac{\Delta B}{B - B_m}\right]$$

where B_m is the magnetic field associated to the m^{th} Feshbach resonance.



* Hence, by properly switching the magnetic field to an appropriated value we may change the scattering properties basically at will.

This is indeed a very important and useful tool for the manipulation of cold atoms, which has been extensively used, and has became a standard experimental tool.

* There are many subtleties related to Feshbach resonances which we won't cover here. For more details, see e.g. Timmermans et al., Physics Reports 315, 199 (1999).