# Atom-Atom Interactions in Ultracold Quantum Gases

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# Lecture 1

# Quantum description of elastic collisions between ultracold atoms

The basic ingredients for a mean-field description of gaseous Bose Einstein condensates

# Lecture 2

#### **Quantum theory of Feshbach resonances**

How to manipulate atom-atom interactions in a quantum ultracold gas

## A few general references

- 1 L.Landau and E.Lifshitz, Quantum Mechanics, Pergamon, Oxford (1977)
- 2 A.Messiah, Quantum Mechanics, North Holland, Amsterdam (1961)
- 3 C.Cohen-Tannoudji, B.Diu and F.Laloë, Quantum Mechanics, Wiley, New York (1977)
- 4 C.Joachain, Quantum collision theory, North Holland, Amsterdam (1983)
- 5 J.Dalibard, in *Bose Einstein Condensation in Atomic Gases*, edited by M.Inguscio, S.Stringari and C.Wieman, International School of Physics Enrico Fermi, IOS Press, Amsterdam, (1999)
- 6 Y. Castin, in 'Coherent atomic matter waves', Lecture Notes of Les Houches Summer School, edited by R. Kaiser, C. Westbrook, and F. David, EDP Sciences and Springer-Verlag (2001)
- 7 C.Cohen-Tannoudji, Cours au Collège de France, Année 1998-1999 http://www.phys.ens.fr/cours/college-de-france/
- 8 C.Cohen-Tannoudji, Compléments de mécanique quantique, Cours de 3<sup>ème</sup> cycle, Notes de cours rédigées par S.Haroche <u>http://www.phys.ens.fr/cours/notes-de-cours/cct-dea/index.html/</u>
- 9 T.Köhler, K.Goral, P.Julienne, Rev.Mod.Phys. 78, 1311-1361 (2006)

# **Outline of lecture 2**

## <u>1 - Introduction</u>

## 2 - Collision channels

- Spin degrees of freedom.
- Coupled channel equations
- Strong couplings and weak couplings between channels

## 3 - Qualitative interpretation of Feshbach resonances

## 4 - Two-channel model

- Two-channel Hamiltonian
- What we want to calculate

## 5 - Scattering states of the 2-channel Hamiltonian

- Calculation of the outgoing scattering states
- Asymptotic behavior. Scattering length
- Feshbach resonance

## 5 - Bound states of the 2-channel Hamiltonian

- Calculation of the energy of the bound state
- Calculation of the wave function

#### Importance of Feshbach resonances

Give the possibility to manipulate the interactions between ultracold atoms, just by sweeping a static magnetic field

- Possibility to change from a repulsive gas to an attractive one and vice versa
- Possibility to turn off the interactions  $\rightarrow$  perfect gas
- Possibility to study a regime of strong interactions and correlations
- Possibility to associate pairs of ultracold atoms into molecules and vice versa

Example of a recent breakthrough using Feshbach resonances (MIT) Investigation of the BEC-BCS crossover

Ultracold atoms with interactions manipulated by Feshbach resonances become a very attractive system for getting a better understanding of quantum many body systems

# **Purpose of this lecture**

- Provide a physical interpretation of Feshbach resonances in terms of a resonant coupling of the state of a colliding pair of atoms to a metastable bound state belonging to another collision channel
- Present a simple two-channel model allowing one to get analytical predictions for the scattering states and the bound states of the two colliding atoms near a Feshbach resonance
  - How does the scattering length behave near a resonance?
  - When can we expect broad resonances or narrow resonances?
  - Are there bound states near the resonances? What are their binding energies and wave functions?
- In addition to their interest for ultracold atoms, Feshbach resonances are a very interesting example of resonant effect in collision processes deserving to be studied for themselves

This lecture will closely follow the presentation of Ref.9: T.Köhler, K.Goral, P.Julienne, Rev.Mod.Phys. 78, 1311-1361 (2006) See also the references therein

# **Microscopic atom-atom interactions**

## Case of two identical alkali atoms

Unpaired electrons for each atom with spins  $\vec{S}_1$ ,  $\vec{S}_2$ Nuclear spins  $\vec{I}_1$ ,  $\vec{I}_2$ Hyperfine states  $f_1$ ,  $m_{f1}$ ;  $f_2$ ,  $m_{f2}$ 

# Born Oppenheimer potentials (2 atoms fixed at a distance r)



2 potential curves:  $V_T(r)$  for the triplet state S=1  $V_S(r)$  for the singlet state S=0

S : quantum number for the total spin  $\vec{S} = \vec{S}_1 + \vec{S}_2$ 

 $V(r) = V_{S}(r)P_{S} + V_{T}(r)P_{T}$  (2.1)

 $P_S$ : Projector on S = 0 states  $P_T$ : Projector on S = 1 states

# Microscopic atom-atom interactions (continued)

#### **Electronic interactions**

$$V_{el}(\mathbf{r}) = V_{s}(\mathbf{r})P_{s} + V_{T}(\mathbf{r})P_{T}$$
  
=  $\frac{1}{4}V_{s}(\mathbf{r}) + \frac{3}{4}V_{T}(\mathbf{r}) + \frac{1}{2\hbar^{2}}\left[V_{T}(\mathbf{r}) - V_{s}(\mathbf{r})\right]\vec{S}_{1}.\vec{S}_{2}$  (2.2)

This interaction depends on the electronic spins because of Pauli principle (electrostatic interaction between antisymmetrized states). It is called also "exchange interaction"

Does not depend on the orientation in space of the molecular axis (line joining the nuclei of the 2 atoms)

## <u>Magnetic spin-spin interactions</u> $V_{ss}$

Dipole-dipole interactions between the 2 electronic spin magnetic moments. Depends on the orientation in space of the molecular axis

## Interaction Hamiltonian

$$V^{\text{int}} = V_{\text{el}} + V_{ss}$$

 $V_{\rm el}$  is much larger than  $V_{ss}$ 

(2.3)

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  - What we want to calculate

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## Channels

Two atoms entering a collision in a s-wave ( $\ell = 0$ ) and in well defined hyperfine and Zeeman states. This defines the "entrance channel"  $\alpha$  defined by the set of quantum numbers:

$$\alpha : \{f_1, m_{f_1}, f_2, m_{f_2}, \ell = 0\}$$

The eigenstates of the total Hamiltonian with eigenvalues E can be written:

$$|\psi\rangle = \sum_{\alpha} |\alpha\rangle \psi_{\alpha}(\vec{r})$$
 (2.4)

where  $\psi_{\alpha}(\mathbf{r})$  is the wave function in channel  $\alpha$  whose radial part is of the form:

$$\frac{F_{\alpha}(r, E)}{r}$$

Because the interaction has off diagonal elements between different channels, the  $F_{\alpha}$  do not evolve independently from each other

# **Coupled channel equations**

The coupled equations of motion of the  $F_{\alpha}$  are of the form:

$$\frac{\partial^2}{\partial \boldsymbol{r}^2} \boldsymbol{F}_{\alpha}(\boldsymbol{r}, \boldsymbol{E}) + \frac{2\mu}{\hbar^2} \sum_{\beta} \left[ \boldsymbol{E} \ \delta_{\alpha\beta} - \boldsymbol{V}_{\alpha\beta} \right] \boldsymbol{F}_{\beta}(\boldsymbol{r}, \boldsymbol{E}) = 0 \quad (2.5)$$
$$\boldsymbol{V}_{\alpha\beta} = \left[ \boldsymbol{E}_{f_i, \boldsymbol{m}_{f_1}} + \boldsymbol{E}_{f_2, \boldsymbol{m}_{f_2}} + \frac{\ell(\ell + 1)\hbar^2}{2\mu \boldsymbol{r}^2} \right] \delta_{\alpha\beta} + \boldsymbol{V}_{\alpha\beta}^{\text{int}}(\boldsymbol{r}) \quad (2.6)$$

Solving numerically these coupled differential equations gives the asymptotic behavior of  $F_{\alpha}$  for large r from which one can determine the phase shift  $\delta_0$  and the scattering length in channel  $\alpha$ .

## Importance of symmetry considerations

The symmetries of  $V_{el}(r)$  and  $V_{ss}$  determine if 2 channels can be coupled by the interaction. In particular, if 2 channels can be coupled by  $V_{el}$ , the Feshbach resonance which can appear due to this coupling will be broad because  $V_{el}$  is large. If the symmetries are such that only  $V_{ss}$  can couple the 2 channels, the Feshbach resonance will be narrow.

# **Examples of symmetry considerations**

If the magnetic field  $B_0$  is the only external field, the projection M of the total angular momentum along the z-axis of  $B_0$  is conserved.

$$\boldsymbol{M} = \boldsymbol{m}_{f1} + \boldsymbol{m}_{f2} + \boldsymbol{m}_{\ell}$$

Only states with the same value of  $m_{f1} + m_{f2} + m_{\ell}$  can be coupled by the interaction Hamiltonian

The s-wave entrance channel can be coupled to  $\ell \neq 0$  channels only by  $V_{ss}$  because  $V_{el}$ , which depends only on the distance *r* between the 2 atoms, commutes with the molecule orbital angular momentum  $\vec{L}$ 

Consider the various states  $M = m_{f1} + m_{f2} + m_{\ell}$  with a fixed value of M. They can be also classified by the eigenvalues of  $\vec{F}^2$ ,  $F_z$ , where  $\vec{F} = \vec{F}_1 + \vec{F}_2$ . This gives the states  $\{f_1, f_2, F, M_F, m_\ell\}$  with  $M_F + m_\ell = M$ . Since  $\vec{S}_1 \cdot \vec{S}_2$ , and thus  $V_{el}$ , commutes with  $\vec{F} = \vec{S}_1 + \vec{S}_2 + \vec{I}_1 + \vec{I}_2$  and  $\vec{L}$ ,  $V_{el}$  can couple only states with the same value of F and  $\ell$ .

Examples of application of these symmetry considerations to the identification of broad Feshbach resonances will be give later on

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# **Open channel and closed channel**



The 2 atoms collide with a very small positive energy E in an channel which is called "open"

The energy of the dissociation threshold of the open channel is taken as the zero of energy

There is another channel above the open channel where scattering states with energy E cannot exist because E is below the dissociation threshold of this channel which is called "closed"

There is a bound state in the closed channel whose energy  $E_{res}$  is close to the collision energy E in the open channel

## Physical mechanism of the Feshbach resonance

The incoming state with energy E of the 2 colliding atoms in the open channel is coupled by the interaction to the bound state  $\phi_{res}$  in the closed channel.

The pair of colliding atoms can make a virtual transition to the bound state and come back to the colliding state. The duration of this virtual transition scales as  $\hbar / I E_{res}$ -*E* I, i.e. as the inverse of the detuning between the collision energy E and the energy  $E_{res}$  of the bound state.

When *E* is close to  $E_{res}$ , the virtual transition can last a very long time and this enhances the scattering amplitude

Analogy with resonant light scattering when an impinging photon of energy hv can be absorbed by an atom which is brought to an excited discrete state with an energy  $hv_0$  above the initial atomic state and then reemitted. There is a resonance in the scattering amplitude when v is close to  $v_0$ 

# Sweeping the Feshbach resonance

The total magnetic moment of the atoms are not the same in the 2 channels (different spin configurations). The energy difference between the 2 channels can thus be varied by sweeping a magnetic field



## Shape resonances



Can appear in a  $\ell \neq 0$  channel where the sum of the potential and the centrifugal barrier gives rise to a potential well

The 2 colliding atoms arrive in a state with positive energy

In the potential well, there are quasi-bound states with positive energy which can decay by tunnel effect through the potential barrier due to the centrifugal potential. This is why they are metastable If the energy of the incoming state is close to the energy of the metastable state, there is a resonance in the scattering amplitude These resonances are different from the zero-energy resonances studied in this lecture. They explain how scattering in  $\ell \neq 0$  waves can become as important as s-wave scattering at low temperatures

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## **Two-channel model**

Only two channels are considered, one open and one closed

## State of the atomic system

$$\mathsf{op} \left\langle \varphi_{\mathsf{op}}(\vec{r}) + \left| \mathsf{cl} \right\rangle \varphi_{\mathsf{cl}}(\vec{r}) \right\rangle$$
(2.7)

The wave function has two components, one in each channel

## <u>Hamiltonian</u>

$$\boldsymbol{H}_{2-\text{channel}} = \begin{pmatrix} \boldsymbol{H}_{\text{op}} & \boldsymbol{W}(\boldsymbol{r}) \\ \boldsymbol{W}(\boldsymbol{r}) & \boldsymbol{H}_{\text{cl}} \end{pmatrix} (2.8) \qquad \qquad \boldsymbol{H}_{\text{op}} = -\frac{\hbar^{2}}{2\mu}\Delta + \boldsymbol{V}_{\text{op}} \\ \boldsymbol{H}_{\text{cl}} = -\frac{\hbar^{2}}{2\mu}\Delta + \boldsymbol{V}_{\text{cl}} \qquad (2.9)$$

#### Resonant bound state in the closed channel

$$\boldsymbol{H}_{cl} \varphi_{res}(\boldsymbol{r}) = \boldsymbol{E}_{res} \varphi_{res}(\boldsymbol{r}) \qquad \boldsymbol{E}_{res} = \hbar \Delta \qquad (2.10)$$

The energy  $E_{\text{res}}$  of this state, denoted also  $\hbar\Delta$ , is close to the energy  $E \simeq 0$  of the colliding atoms in the open channel

# What we want to calculate

We want to calculate the eigenstates and eigenvalues of H<sub>2-channel</sub>

$$\begin{pmatrix} \boldsymbol{H}_{op} & \boldsymbol{W}(\boldsymbol{r}) \\ \boldsymbol{W}(\boldsymbol{r}) & \boldsymbol{H}_{cl} \end{pmatrix} \begin{pmatrix} \varphi_{op} \\ \varphi_{ol} \end{pmatrix} = \boldsymbol{E} \begin{pmatrix} \varphi_{op} \\ \varphi_{cl} \end{pmatrix}$$
(2.11)  
$$\boldsymbol{H}_{op} \ \varphi_{op}(\vec{r}) + \boldsymbol{W}(\boldsymbol{r})\varphi_{cl}(\vec{r}) = \boldsymbol{E} \ \varphi_{op}(\vec{r})$$
(2.12)  
$$\boldsymbol{W}(\boldsymbol{r}) \ \varphi_{op}(\vec{r}) + \boldsymbol{H}_{cl} \ \varphi_{cl}(\vec{r}) = \boldsymbol{E} \ \varphi_{cl}(\vec{r})$$

#### **Eigenstates with positive eigenvalues E>0**

They describe the scattering states of the 2 atoms in the presence of the coupling W. In particular, we are interested in the behavior of the scattering length when  $E_{res}$  is swept around 0

The 2 components of the scattering state corresponding to an incoming wave  $\vec{k}$  are denoted  $\varphi_{\rm op}^{\vec{k}}$  and  $\varphi_{\rm cl}^{\vec{k}}$ 

#### Eigenstates with negative eigenvalues E<sub>b</sub><0

They describe the bound states of the 2 atoms in the presence of W Their 2 components are denoted  $\varphi_{op}^{b}$  and  $\varphi_{cl}^{b}$ 

# Single resonance approximation

We will neglect all eigenstates of  $H_{cl}$  other than  $\varphi_{res}$ Near the resonance we want to study ( $E_{res}$  close to 0), they are too far from E=0 and their contribution is negligible

We will use the following expression for the Hamiltonian of the closed channel

$$\boldsymbol{H}_{cl} = \boldsymbol{E}_{res} \left| \boldsymbol{\varphi}_{res} \right\rangle \left\langle \boldsymbol{\varphi}_{res} \right|$$
(2.13)

The resolvent operator (or Green function) of  $H_{cl}$  will be thus given by:

$$G_{cl}(z) = \frac{1}{z - H_{cl}} = \frac{\left|\varphi_{res}\right\rangle \left\langle\varphi_{res}\right|}{z - E_{res}}$$
(2.14)

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## Scattering states of the two-channel Hamiltonian H<sub>2-channel</sub>

## Open channel component of the scattering state of H<sub>2-channel</sub>

The first equation (2.12) can be written

$$\left(\boldsymbol{E} - \boldsymbol{H}_{\rm op}\right)\varphi_{\rm op}^{\vec{k}}(\vec{r}) = \boldsymbol{W}(\boldsymbol{r}) \varphi_{\rm cl}^{\vec{k}}(\vec{r})$$
(2.15)

Its solution is the sum of a solution of the equation without the rightside member and a solution of the full equation with the right-side member considered as a source term.

$$\varphi_{\rm op}^{\vec{k}} = \varphi_{\vec{k}}^{+} + G_{\rm op}^{+}(E) W \varphi_{\rm cl}^{\vec{k}} \qquad G_{\rm op}^{+}(E) = \frac{1}{E - H_{\rm op}} + i \varepsilon$$
 (2.16)

In (2.16),  $G^+_{op}(E)$  is a Green function of  $H_{op}$ . The term +i $\varepsilon$ , where  $\varepsilon$  is a positive number tending to 0, insures that the second term of (2.16) has the asymptotic behavior of an outgoing scattered state for r $\rightarrow \infty$ .

The first term of (2.16), involving only  $H_{op}$ , is chosen as an outgoing scattering state of  $H_{op}$ , in order to get the good behavior for  $r \rightarrow \infty$ .

$$\varphi_{\vec{k}}^{+}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \left[ \mathbf{e}^{i\,\vec{k}.\vec{r}} + \frac{1}{\mathbf{E} - \mathbf{T} + i\varepsilon} \mathbf{V}_{\text{op}} \,\varphi_{\vec{k}}^{+}(\vec{r}) \right] \qquad \mathbf{T} = \frac{\vec{p}^{2}}{2\mu} \quad (2.17)$$

# Scattering states of the two-channel Hamiltonian H<sub>2-channel</sub> (continued)

## Closed channel component of the scattering state of H<sub>2-channel</sub>

The second equation (2.12) can be written:

$$\left(\boldsymbol{E} - \boldsymbol{H}_{cl}\right)\varphi_{cl}^{\vec{k}}(\vec{r}) = \boldsymbol{W}(\boldsymbol{r}) \varphi_{op}^{\vec{k}}(\vec{r}) \qquad (2.18)$$

Its solution can be written in terms of the Green function of  $H_{cl}$ :

$$\varphi_{cl}^{\vec{k}} = G_{cl}(E) W \varphi_{op}^{\vec{k}} \qquad G_{cl}(E) = (E - H_{cl})^{-1}$$
 (2.19)

Using the single resonance approximation (2.14), we get:

$$\varphi_{cl}^{\vec{k}}(\vec{r}) = \varphi_{res}(\vec{r}) \frac{\left\langle \varphi_{res} \middle| W \middle| \varphi_{op}^{\vec{k}} \right\rangle}{E - E_{res}}$$
(2.20)

The closed channel component  $\varphi_{cl}^{\kappa}$  is thus proportional to  $\varphi_{res}$ 

#### **Dressed states and bare states**

The 2 components  $\varphi_{op}^{\vec{k}}$  and  $\varphi_{cl}^{\vec{k}}$  of the scattering states of  $H_{2-channel}$  are called dressed states because they include the effect of W. The eigenstates  $\varphi_{\vec{k}}^{+}$  and  $\varphi_{res}$  of  $H_{op}$  and  $H_{cl}$  are called bare states

# Open channel components of the scattering states of $H_{2-channel}$ in terms of bare states

Inserting (2.20) into (2.16), we get:

$$\left| \varphi_{\mathsf{op}}^{\vec{k}} \right\rangle = \left| \varphi_{\vec{k}}^{+} \right\rangle + G_{\mathsf{op}}^{+}(E) W \left| \varphi_{\mathsf{res}} \right\rangle \frac{\left\langle \varphi_{\mathsf{res}} \left| W \right| \varphi_{\mathsf{op}}^{\vec{k}} \right\rangle}{E - E_{\mathsf{res}}}$$
(2.21)

In order to eliminate  $\varphi_{op}^{\vec{k}}$  in the right side, we multiply both sides of (2.21) by  $\langle \varphi_{res} | W$ , which gives:

$$\frac{\left\langle \varphi_{\text{res}} \middle| W \middle| \varphi_{\text{op}}^{\vec{k}} \right\rangle}{E - E_{\text{res}}} = \frac{\left\langle \varphi_{\text{res}} \middle| W \middle| \varphi_{\vec{k}}^{+} \right\rangle}{E - E_{\text{res}} - \left\langle \varphi_{\text{res}} \middle| W G_{\text{op}}^{+}(E) W \middle| \varphi_{\text{res}} \right\rangle}$$
(2.22)

Inserting (2.22) into (2.21), we finally get:

$$\left| \varphi_{\mathsf{op}}^{\vec{k}} \right\rangle = \left| \varphi_{\vec{k}}^{+} \right\rangle + G_{\mathsf{op}}^{+}(E) \frac{W}{E - E_{\mathsf{res}} - \left\langle \varphi_{\mathsf{res}} \right| W G_{\mathsf{op}}^{+}(E) W \left| \varphi_{\mathsf{res}} \right\rangle} \left| \varphi_{\vec{k}}^{+} \right\rangle (2.23)$$

Only the bare states appear in the right side of (2.23).

# **Connection with two-potential scattering**

Equation (2.23) can be rewritten in a more suggestive way. If we introduce the effective coupling  $V_{eff}$  defined by:

$$\boldsymbol{V}_{\text{eff}} = \boldsymbol{W} \frac{\left|\boldsymbol{\varphi}_{\text{res}}\right\rangle \left\langle \boldsymbol{\varphi}_{\text{res}} \right|}{\boldsymbol{E} - \boldsymbol{E}_{\text{res}} - \left\langle \boldsymbol{\varphi}_{\text{res}} \right| \boldsymbol{W} \boldsymbol{G}_{\text{op}}^{+}(\boldsymbol{E}) \boldsymbol{W} \left| \boldsymbol{\varphi}_{\text{res}} \right\rangle} \boldsymbol{W}$$
(2.24)

we get, by inserting (2.24) into (2.23):

$$\left| \varphi_{\rm op}^{\vec{k}} \right\rangle = \left| \varphi_{\vec{k}}^{+} \right\rangle + \frac{1}{E - H_{\rm op}} + i \varepsilon V_{\rm eff} \left| \varphi_{\vec{k}}^{+} \right\rangle$$
(2.25)

 $V_{\rm eff}$  acts only, like  $V_{\rm op}$ , inside the open channel space. It describes the effect of virtual transitions to the closed channel subspace. The twochannel scattering problem can thus be reformulated in terms of a single-channel scattering problem (in the open channel), but with a new potential  $V_{\rm tot}$  in this channel, which is the sum of 2 potentials

$$\boldsymbol{V}_{\text{tot}} = \boldsymbol{V}_{\text{op}} + \boldsymbol{V}_{\text{eff}}$$
(2.26)

Equation (2.25) then appears as the scattering produced by  $V_{eff}$  on waves "distorted" by  $V_{op}$ . (Generalized Lippmann-Schwinger equation) (see for example ref.4, Chapter 17) 26

# Asymptotic behavior of the scattering states of H<sub>2-channel</sub>

Let us come back to (2.23). Only the asymptotic behavior of the open channel component is interesting because the closed channel component, proportional to  $\varphi_{res}$  vanishes for large r.

We expect the asymptotic behavior of  $\varphi_{op}^{\vec{k}}$  to be of the form:

$$\varphi_{\rm op}^{\vec{k}}(\vec{r}) \simeq_{r \to \infty} \frac{1}{(2\pi)^{3/2}} \left[ e^{i\,\vec{k}.\vec{r}} + f(k,\,\vec{n}) \,\frac{e^{i\,k\,r}}{r} \right] \qquad \vec{n} = \vec{r} \,/\,r \qquad (2.27)$$

In the limit  $k \rightarrow 0$ , the scattering amplitude becomes spherically symmetric and gives the scattering length we want to calculate

$$f(k, \vec{n}) \underset{k \to 0}{\to} -a$$
 (2.28)

The asymptotic behavior of the first term of (2.23) describes the scattering in the open channel without coupling to the closed channel. It gives the scattering length  $a_{op}$  in the open channel alone (W = 0). This scattering length is often called the background scattering length.

$$\boldsymbol{a}_{\rm op} = \boldsymbol{a}_{\rm bg} \tag{2.29}$$

# **Position of the resonance**

The second term of (2.23) is the most interesting since it gives the effects due to the coupling W.

The scattering amplitude given by its asymptotic behavior becomes large if the denominator of the second term of (2.23) vanishes, *i.e.* if:

$$\boldsymbol{E} = \boldsymbol{E}_{\text{res}} + \left\langle \varphi_{\text{res}} \middle| \boldsymbol{W} \; \boldsymbol{G}_{\text{op}}^{+}(\boldsymbol{E}) \; \boldsymbol{W} \middle| \varphi_{\text{res}} \right\rangle$$
(2.30)

When E is close to 0, the last term of (2.30) is equal to:

$$\langle \varphi_{\text{res}} | W G_{\text{op}}^{+}(0) W | \varphi_{\text{res}} \rangle = \sum_{\vec{k}} \frac{\left| \langle \varphi_{\text{res}} | W | \varphi_{\vec{k}}^{+} \rangle \right|^{2}}{-E_{\vec{k}} + i \varepsilon} = \hbar \Delta_{0}$$
 (2.31)

Its interpretation is clear. It gives the shift  $\hbar\Delta_0$  of  $\varphi_{res}$  due to the second order coupling induced by W between  $\varphi_{res}$  and the continuum of  $H_{op}$  We thus predict that the scattering amplitude, and then the scattering length, will be maximum (in absolute value), not when  $E_{res}$  is close to 0, but when the shifted energy of  $\varphi_{res}$ 

$$\tilde{\boldsymbol{E}}_{\text{res}} = \boldsymbol{E}_{\text{res}} + \hbar \Delta_0 \qquad (2.32)$$

is close to the energy  $E \simeq 0$  of the incoming state

## <u>Remark</u>

Strictly speaking, the Green function  $G_{op}^+(E) = (E - E_{\vec{k}} + i \varepsilon)^{-1}$ appearing in (2.30) is equal to:

$$\frac{1}{\boldsymbol{E} - \boldsymbol{E}_{\vec{k}} + \boldsymbol{i} \varepsilon} = \mathcal{P}\left(\frac{1}{\boldsymbol{E} - \boldsymbol{E}_{\vec{k}}}\right) - \boldsymbol{i} \pi \delta\left(\boldsymbol{E} - \boldsymbol{E}_{\vec{k}}\right)$$
(2.33)

where  $\mathcal{P}$  means principal part.

Because of the last term of (2.33), equation (2.31) should also contain an imaginary term describing the damping of  $\varphi_{res}$  due to its coupling induced by W with the continuum of  $H_{op}$ .

But we are considering here the limit of ultracold collisions  $E \to 0$ and the density of states of the continuum of  $H_{op}$  vanishes near  $E_{\vec{k}} = 0$ , which means that the damping of  $\varphi_{res}$  can be ignored in the limit  $E \to 0$ .

For large values of  $E_{res}$ , the imaginary term of (2.33) can no longer be ignored, and it can be shown that it gives rise to an imaginary term in the scattering amplitude, proportional to *k*.

# Variations of $E_{res}$ and $\tilde{E}_{res}$ with B

The spin configurations of the two channels have different magnetic moments. The energies of the states in these channels vary differently when a static magnetic field *B* is applied and scanned. If  $\xi$  is the difference of magnetic moments in the 2 channels, the difference between the energies of 2 states belonging to the channels varies linearly with *B* with a slope  $\xi$ .

If we take the energy of the dissociation threshold of the open channel as the zero of energy, the energy  $E_{\rm res}$  of  $\varphi_{\rm res}$  is equal to:

$$\boldsymbol{E}_{\text{res}} = \boldsymbol{\xi} \left( \boldsymbol{B} - \boldsymbol{B}_{\text{res}} \right)$$
(2.34)

 $E_{\rm res}$  is degenerate with the energy of the ultracold collision state when  $B=B_{\rm res}$ 

In fact, the position of the Feshbach resonance is given, not by the zero of  $E_{\rm res}$ , but by the zero of  $\tilde{E}_{\rm res}$ 

$$\tilde{\boldsymbol{E}}_{\text{res}} = \boldsymbol{E}_{\text{res}} + \hbar \Delta_0 = \xi \left( \boldsymbol{B} - \boldsymbol{B}_0 \right)$$
(2.35)

This equation gives the correct value,  $B_0$ , at which we expect a divergence of the scattering length.



We suppose here  $\xi < 0$ Since  $\Delta_0$  is also negative according to (2.31),  $B_0$  is smaller than  $B_{res}$ .

# Contribution of the inter channel coupling W to the scattering length

Asymptotic behavior of the W-dependent term of  $\varphi_{op}^{\tilde{k}}$ 

Using (2.30) and (2.32), we can rewrite (when  $E\simeq 0$ ) equation (2.23):

$$\left|\varphi_{\mathsf{op}}^{\vec{k}}\right\rangle = \left|\varphi_{\vec{k}}^{+}\right\rangle + G_{\mathsf{op}}^{+}(E) \frac{W\left|\varphi_{\mathsf{res}}\right\rangle\left\langle\varphi_{\mathsf{res}}\right|W}{E - \tilde{E}_{\mathsf{res}}}\right|\varphi_{\vec{k}}^{+}\right\rangle$$
(2.36)

To find the contribution of W to the scattering length, we have to find the asymptotic behavior for r large of the wave function of the last term

$$\left\langle \vec{r} \mid \boldsymbol{G}_{op}^{+}(\boldsymbol{E}) \frac{\boldsymbol{W} \mid \varphi_{res} \left\langle \varphi_{res} \mid \boldsymbol{W} \right\rangle}{\boldsymbol{E} - \tilde{\boldsymbol{E}}_{res}} \left| \varphi_{\vec{k}}^{+} \right\rangle =$$

$$\int d^{3}\boldsymbol{r}' \left\langle \vec{r} \mid \boldsymbol{G}_{op}^{+}(\boldsymbol{E}) \mid \vec{r}' \right\rangle \left\langle \vec{r}' \mid \frac{\boldsymbol{W} \mid \varphi_{res} \left\langle \varphi_{res} \mid \boldsymbol{W} \right\rangle}{\boldsymbol{E} - \tilde{\boldsymbol{E}}_{ros}} \left| \varphi_{\vec{k}}^{+} \right\rangle$$

$$(2.37)$$

We need for that to know the asymptotic behavior for *r* large of the Green function of  $H_{op}$ 

$$G_{\rm op}^{+}\left(E,\vec{r},\vec{r}'\right) = \left\langle \vec{r} \right| \frac{1}{E - H_{\rm op}} + i \varepsilon \left| \vec{r}' \right\rangle \qquad (2.38)$$

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# Contribution of the inter channel coupling W to the scattering length (continued)

One can show (see Appendix) that:

$$G_{\rm op}^{+}\left(\boldsymbol{E}, \boldsymbol{\vec{r}}, \boldsymbol{\vec{r}}'\right) \underset{r \to \infty}{\simeq} - \frac{e^{i\,k\,r}}{r} \frac{2\mu}{\hbar^2} \sqrt{\frac{\pi}{2}} \left[\varphi_{k\,\vec{n}}^{-}\left(\boldsymbol{\vec{r}}'\right)\right]^{*} \qquad \vec{n} = \vec{r} / r \quad (2.39)$$

Using  $\left[\varphi_{k\vec{n}}(\vec{r}')\right]^* = \left\langle \varphi_{k\vec{n}}(\vec{r}') \right\rangle^*$  and the closure relation for  $\vec{r}'$ , we get for the asymptotic behavior of (2.37):

$$-\frac{\mathbf{e}^{i\,k\,r}}{r}\frac{2\mu}{\hbar^2}\,2\pi^2\,\frac{\left\langle \varphi_{k\,\vec{n}}^{-} \middle| \mathbf{W} \middle| \varphi_{\mathrm{res}} \right\rangle \left\langle \varphi_{\mathrm{res}} \middle| \mathbf{W} \middle| \varphi_{\vec{k}}^{+} \right\rangle}{\mathbf{E}\,-\,\tilde{\mathbf{E}}_{\mathrm{res}}} \tag{2.40}$$

In the limit  $\mathbf{k} \to 0$ ,  $\mathbf{E} \to 0$ ,  $\varphi_{\vec{k}}^+ \to \varphi_{\vec{0}}^+$  and  $\varphi_{\vec{k}\,\vec{n}}^- \to \varphi_{\vec{0}}^- = \varphi_{\vec{0}}^+$  since  $e^{\pm i\,kr} / r \to 1 / r$  so that (2.40) can be also written, using (2.35):  $-\frac{1}{r}\frac{2\mu}{\hbar^2}2\pi^2 \frac{\left|\left\langle \varphi_{\vec{0}}^+ \left| \mathbf{W} \right| \varphi_{\text{res}} \right\rangle\right|^2}{0 - \tilde{E}_{\text{res}}} = +\frac{1}{r}\frac{2\mu}{\hbar^2}2\pi^2 \frac{\left|\left\langle \varphi_{\vec{0}}^+ \left| \mathbf{W} \right| \varphi_{\text{res}} \right\rangle\right|^2}{\xi \left(\mathbf{B} - \mathbf{B}_0\right)}$  (2.41)

The coefficient of -1/r in (2.41) gives the contribution of the interchannel coupling to the scattering length

# **Scattering length**

The asymptotic behavior of the first term of (2.23) gives the background scattering length. Adding the contribution of the second term we have just calculated, we get for the total scattering length:

$$\boldsymbol{a} = \boldsymbol{a}_{bg} - \frac{2\mu}{\hbar^2} 2\pi^2 \frac{\left|\left\langle \varphi_{\bar{0}}^+ \mid \boldsymbol{W} \mid \varphi_{res} \right\rangle\right|^2}{-\xi \left(\boldsymbol{B} - \boldsymbol{B}_0\right)} = \boldsymbol{a}_{bg} \left[1 - \frac{\Delta \boldsymbol{B}}{\boldsymbol{B} - \boldsymbol{B}_0}\right] \quad (2.42)$$
where:  

$$\Delta \boldsymbol{B} = \frac{2\mu}{\hbar^2} 2\pi^2 \frac{\left|\left\langle \varphi_{\bar{0}}^+ \mid \boldsymbol{W} \mid \varphi_{res} \right\rangle\right|^2}{\xi \boldsymbol{a}_{bg}} \quad (2.43)$$

This is the main result of this lecture.

- The scattering length diverges when  $B = B_0$
- It changes sign when B is scanned around  $B_0$
- It vanishes for  $B B_0 = \Delta B$

The variations of the scattering length with the static field are represented in the next figure

# Scattering length versus magnetic field



Figure corresponding to two colliding  $Rb^{85}$  atoms each in the state f = 2,  $m_f = -2$  in a s-wave ( $\ell = 0$ ). In this case, we have  $a_{bg} < 0$  and  $\xi < 0$  35

## **Examples of broad and narrow Feshbach resonances**



Zeeman and hyperfine levels of Rb<sup>85</sup> (Figure taken from Ref.9)

- Entrance channel : ee  $f_1 = 2, m_{f_1} = -2, f_2 = 2, m_{f_2} = -2, \ell = m_{\ell} = 0$   $M = m_{f_1} + m_{f_2} + m_{\ell} = -4$ 
  - Other channels with the same M=-4  $\ell=m_\ell=0$  gg, fh eg,df

They are open because they are above the entrance channel. They have the same negative slope  $\xi$ with respect to ee when *B* is varied

Classification by other quantum numbers  $(f_1, f_2)F, M, \ell = m_\ell = 0$   $(\vec{F} = \vec{f_1} + \vec{f_2})$ If  $f_1 = f_2 = 2, F = 0, 2, 4$  (Odd values of *F* are forbidden for identical bosons) Only F = 4 can give  $M = -4 \Rightarrow$  Channel ee corresponds to (22), F = 4, M = -4If  $f_1 = f_2 = 3, F = 0, 2, 4, 6$  (Odd values of *F* are forbidden for identical bosons) Only F = 4, 6 can give  $M = -4 \Rightarrow$  Channel gg and fh give rise to 2 types of states (33), F = 4, M = -4 and (33), F = 6, M = -4

## Feshbach resonances associated with gg and fh



In the potential wells of the channels (33) F = 6 or 4, M = - 4, there are vibrational levels v = -1, -2, -3, ... staring from the highest one v = -1

#### The energy level

(33) F = 4, M = -4, v = -3crosses the energy (~0) of the entrance channel around B=155 G The energy level

(33) F = 6, M= - 4,v = -3
crosses E~0) around B=250 G
(Lower part of the figure)

The 2 levels which cross at B=155 G correspond to the same value of *F* and can thus be coupled by the strong interaction  $V_{el}$ . This is why the corresponding Feshbach resonance is broad The 2 levels which cross at B=250 G correspond to different values of *F* and can thus be coupled only by the weak interaction  $V_{ss}$ . This is why the corresponding Feshbach resonance is narrow (Upper part of the figure)

# **Outline of lecture 2**

## 1 - Introduction

- 2 Collision channels
  - Spin degrees of freedom.
  - Coupled channel equations
  - Strong couplings and weak couplings between channels

## 3 - Qualitative interpretation of Feshbach resonances

- 4 Two-channel model
  - Two-channel Hamiltonian
  - What we want to calculate

## 5 - Scattering states of the 2-channel Hamiltonian

- Calculation of the outgoing scattering states
- Asymptotic behavior. Scattering length
- Feshbach resonance

#### 5 - Bound states of the 2-channel Hamiltonian

- Calculation of the energy of the bound state
- Calculation of the wave function

# Bound states of the two-channel Hamiltonian H<sub>2-channel</sub>

Are there bound states for  $H_{2-\text{channel}}$  for *B* close to  $B_0$ ? How are they related to the bound state  $\varphi_{\text{res}}$  of  $H_{\text{cl}}$ ? How do their energy  $E_{\text{b}}$  and wave function vary with B?

We denote such a bound state

$$\mathsf{op} \left\langle \varphi_{\mathsf{op}}^{\mathsf{b}}(\vec{r}) + \left| \mathsf{cl} \right\rangle \varphi_{\mathsf{cl}}^{\mathsf{b}}(\vec{r}) \right\rangle$$
(2.44)

 $\varphi_{op}^{b}$  and  $\varphi_{cl}^{b}$  are the components of the bound state in the open channel and the closed channel, respectively, obeying the normalization condition:

$$\left\langle \varphi_{\rm op}^{\rm b} \mid \varphi_{\rm op}^{\rm b} \right\rangle + \left\langle \varphi_{\rm cl}^{b} \mid \varphi_{\rm cl}^{b} \right\rangle = 1$$
 (2.45)

Expressing that the state (2.44) is an eigenstate of the Hamiltonian (2.8) with eigenvalue  $E_{\rm b}$ , we get the following 2 equations:

$$H_{op} \varphi_{op}^{b}(\vec{r}) + W(r) \varphi_{cl}^{b}(\vec{r}) = E_{b} \varphi_{op}^{b}(\vec{r})$$

$$W(r) \varphi_{op}^{b}(\vec{r}) + H_{cl} \varphi_{cl}^{b}(\vec{r}) = E_{b} \varphi_{cl}^{b}(\vec{r})$$
(2.46)

# Bound states of the two-channel Hamiltonian H<sub>2-channel</sub> (continued)

To solve equation (2.46), we can use the Green functions of  $H_{op}$  and  $H_{cl}$  without the i $\varepsilon$  term because  $E_{b}$  is negative (below the threshold of  $V_{op}$ )

$$\begin{array}{l} \left| \varphi_{\text{op}}^{\text{b}} \right\rangle = \left| G_{\text{op}}(E_{b}) W \right| \left| \varphi_{\text{cl}}^{b} \right\rangle \\ \left| \varphi_{\text{cl}}^{b} \right\rangle = \left| G_{\text{cl}}(E_{b}) W \right| \left| \varphi_{\text{op}}^{b} \right\rangle \end{array}$$

$$(2.47)$$

As above, we can use the single resonance approximation for  $G_{cl}$ :

$$G_{cl}(E_b) = \frac{\left|\varphi_{res}\right\rangle \left\langle\varphi_{res}\right|}{E_b - E_{res}}$$
(2.48)

Inserting (2.48) into the second equation (2.47) shows that  $\varphi_{cl}^{b}$  is proportional to  $\varphi_{res}$ , so that we can write:

$$\begin{pmatrix} \varphi_{\rm op}^{\rm b} \\ \varphi_{\rm cl}^{\rm b} \end{pmatrix} = \frac{1}{N_{b}} \begin{pmatrix} G_{\rm op}(E_{b}) W \varphi_{\rm res} \\ \varphi_{\rm res} \end{pmatrix}$$
(2.49)

where  $N_{\rm b}$  is a normalization factor

$$N_{b} = \sqrt{1 + \left\langle \varphi_{\text{res}} \middle| W \: G_{\text{op}}^{2}(E_{b})W \middle| \varphi_{\text{res}} \right\rangle}$$
(2.50) (2.50)

## Implicit equation for the energy $E_{\rm b}$

Inserting (2.48) into the second equation (2.47) gives:

$$\left| \varphi_{cl}^{b} \right\rangle = \frac{1}{E_{b} - E_{res}} \left| \varphi_{res} \right\rangle \left\langle \varphi_{res} \left| W \right| \varphi_{op}^{b} \right\rangle$$
(2.51)

which, inserted into the first equation (2.47) leads to:

$$\left| \varphi_{\rm op}^{\rm b} \right\rangle = \frac{1}{E_{b} - E_{\rm res}} G_{\rm op}(E_{b}) W \left| \varphi_{\rm res}^{\rm c} \right\rangle \left\langle \varphi_{\rm res}^{\rm c} \left| W \right| \varphi_{\rm op}^{\rm b} \right\rangle$$
(2.52)

As for equation (2.21), we can eliminate the dressed state  $\varphi_{op}^{b}$  by multiplying both sides of this equation at left by  $\langle \varphi_{res} | W$ . This gives:  $E = E_{res} = \langle \varphi_{res} | W G_{res} \rangle = \langle \varphi_{res} \rangle = \langle \varphi_{res} \rangle$ 

$$\boldsymbol{E}_{b} - \boldsymbol{E}_{\text{res}} = \left\langle \varphi_{\text{res}} \middle| \boldsymbol{W} \; \boldsymbol{G}_{\text{op}}(\boldsymbol{E}_{b}) \; \boldsymbol{W} \middle| \varphi_{\text{res}} \right\rangle$$
(2.53)

Now, using the identity

$$G_{\rm op}(E_b) = \frac{1}{E_b - H_{\rm op}} = -\frac{1}{H_{\rm op}} + E_b \frac{1}{H_{\rm op}} \frac{1}{E_b - H_{\rm op}}$$
(2.54)

we can rewrite (2.53) as:

$$\boldsymbol{E}_{b} = \boldsymbol{E}_{\text{res}} + \left\langle \varphi_{\text{res}} \middle| \boldsymbol{W}\boldsymbol{G}_{\text{op}}(0)\boldsymbol{W} \middle| \varphi_{\text{res}} \right\rangle - \boldsymbol{E}_{b} \left\langle \varphi_{\text{res}} \middle| \boldsymbol{W}\boldsymbol{G}_{\text{op}}(0)\boldsymbol{G}_{\text{op}}(\boldsymbol{E}_{b})\boldsymbol{W} \middle| \varphi_{\text{res}} \right\rangle$$

$$(2.55)$$

$$(2.55)$$

# Implicit equation for the energy $E_{\rm b}$ (continued)

The second term of the right side of (2.55) is the shift  $\hbar\Delta_0$  of  $\varphi_{\rm res}$ . Adding it to  $E_{\rm res}$ , we get  $\tilde{E}_{\rm res}$ , so that (2.55) can be rewritten:

$$\boldsymbol{E}_{b} = \tilde{\boldsymbol{E}}_{res} - \boldsymbol{E}_{b} \left\langle \varphi_{res} \middle| \boldsymbol{W} \; \boldsymbol{G}_{op}(0) \; \boldsymbol{G}_{op}(\boldsymbol{E}_{b}) \; \boldsymbol{W} \middle| \varphi_{res} \right\rangle$$
(2.56)

To go further, we introduce the spectral decomposition of  $G_{op}(z)$ 

$$G_{\rm op}(z) = \int d^3k \, \frac{\left| \varphi_{\vec{k}}^+ \right\rangle \left\langle \varphi_{\vec{k}}^+ \right|}{z - \hbar^2 k^2 / 2\mu} + G_{\rm op}^{\rm b}(z) \tag{2.57}$$

The last term of (2.57) gives the contribution of the bound states of  $H_{op}$ . Se suppose here that their energy if far below E = 0, so that we can ignore this term. Using (2.57), we can then write (2.56) as:

$$\boldsymbol{E}_{\boldsymbol{b}} = \boldsymbol{\tilde{E}}_{\text{res}} - (2\mu)^{2} \boldsymbol{E}_{\boldsymbol{b}} \int d^{3}\boldsymbol{k} \frac{\left|\left\langle \varphi_{\text{res}} \mid \boldsymbol{W} \mid \varphi_{\boldsymbol{k}}^{+} \right\rangle\right|^{2}}{\hbar^{2}\boldsymbol{k}^{2} \left(\hbar^{2}\boldsymbol{k}^{2} + 2\mu \left|\boldsymbol{E}_{\boldsymbol{b}}\right|\right)}$$
(2.58)

This is an implicit equation for  $E_{\rm b}$  that we will try now to solve

# Calculation of the energy $E_{\rm b}$

To calculate the integral of (2.58), we introduce the new variable:

$$\boldsymbol{u} = \frac{\hbar \boldsymbol{k}}{\sqrt{2\mu \left|\boldsymbol{E}_{\boldsymbol{b}}\right|}} \tag{2.59}$$

which allows one to rewrite, after angular integration, the integral of (2.58) as:

$$\frac{1}{\hbar^3} \frac{4\pi}{\sqrt{2\mu |\boldsymbol{E}_b|}} \int_0^\infty d\boldsymbol{u} \, \frac{\left| \left\langle \varphi_{\text{res}} \mid \boldsymbol{W} \mid \varphi_{\vec{k}}^+ \right\rangle \right|^2}{\left( \boldsymbol{u}^2 + 1 \right)} \tag{2.60}$$

Let  $k_0$  be the width of  $|\langle \varphi_{\text{res}} | W | \varphi_{\vec{k}}^+ \rangle|^2$  considered as a function of k. This defines a value  $u_0$  of u

$$\boldsymbol{u}_{0} = \frac{\hbar \boldsymbol{k}_{0}}{\sqrt{2\mu \left|\boldsymbol{E}_{b}\right|}}$$
(2.61)

characterizing the width in u of the numerator of the integral of (2.60). Two different limits can then be considered:  $u_0 \gg 1$  and  $u_0 \ll 1$ ? Calculation of the energy  $E_{\rm b}$  (continued)

# **<u>First limit</u>** $\boldsymbol{u}_0 \gg 1 \quad \Leftrightarrow \quad \left| \boldsymbol{E}_{\boldsymbol{b}} \right| \ll \hbar^2 \boldsymbol{k}_0^2 / 2\mu$

The denominator of the integral of (2.60) varies more rapidly with *u* than the numerator which can be replaces by its value for  $\vec{k} = \vec{0}$ Equation (2.60) can then be approximated by:

$$\frac{1}{\hbar^{3}} \frac{4\pi}{\sqrt{2\mu \left|\boldsymbol{E}_{\boldsymbol{b}}\right|}} \left| \left\langle \boldsymbol{\varphi}_{\text{res}} \left| \boldsymbol{W} \right| \boldsymbol{\varphi}_{\bar{0}}^{+} \right\rangle \right|^{2} \underbrace{\int_{0}^{\infty} \frac{d\boldsymbol{u}}{\boldsymbol{u}^{2} + 1}}_{=\pi/2} \qquad (2.62)$$

Replacing the integral of (2.58) by (2.62) then leads to:

$$\boldsymbol{E}_{\boldsymbol{b}} = \tilde{\boldsymbol{E}}_{\text{res}} + \sqrt{\left|\boldsymbol{E}_{\boldsymbol{b}}\right|} \frac{2\pi^{2} \left(2\mu\right)^{3/2}}{\hbar^{3}} \left|\left\langle \varphi_{\text{res}} \mid \boldsymbol{W} \mid \varphi_{\bar{0}}^{+}\right\rangle\right|^{2}$$
(2.63)

One can then reexpress  $|\langle \varphi_{\text{res}} | W | \varphi_{\bar{0}}^{+} \rangle|^{2}$  in terms of  $\Delta B$  thanks to (2.43) and  $\tilde{E}_{\text{res}}$  in terms of  $\xi(B - B_{0})$  thanks to (2.35) and finally use (2.43) to show that the solution of (2.6) is, to a good approximation:

$$\boldsymbol{E}_{\boldsymbol{b}} = -\frac{\hbar^2}{2\mu a^2} \tag{2.64}$$

# Calculation of the energy $E_{\rm b}$ (continued)

# **Second limit** $\boldsymbol{u}_0 \ll 1 \quad \Leftrightarrow \quad \left| \boldsymbol{E}_{\boldsymbol{b}} \right| \gg \hbar^2 \boldsymbol{k}_0^2 / 2\mu$

The numerator of the integral of (2.60) varies more rapidly with u than the denominator, so that we can neglect the term  $u^2$  in the denominator.

In fact, this approximation amounts to neglecting  $\hbar^2 k^2$  compared to  $2\mu |E_b|$  in the denominator of the integral of (2.58)

This approximation allows one to transform (2.58) into:

$$E_{b} = \tilde{E}_{res} + (2\mu)^{2} \int d^{3}k \frac{\left|\left\langle \varphi_{res} \mid W \mid \varphi_{\bar{k}}^{+} \right\rangle\right|^{2}}{2\mu \hbar^{2}k^{2}}$$
$$= \tilde{E}_{res} + \int d^{3}k \frac{\left|\left\langle \varphi_{res} \mid W \mid \varphi_{\bar{k}}^{+} \right\rangle\right|^{2}}{\hbar^{2}k^{2} / 2\mu}$$
$$= \tilde{E}_{res} - \hbar\Delta_{0} = E_{res} = \xi \left(B - B_{res}\right)$$
(2.65)

We have used the expression (2.31) of  $\hbar\Delta_0$  and equation (2.35)



- The bound state of  $H_{2-channel}$  appears for  $B > B_0$ , in the region a>0.
- $E_{\rm b}$  first decreases quadratically with B- $B_0$  and then tends to the unperturbed energy  $E_{\rm res}$  of the bound state  $\varphi_{\rm res}$  of the closed channel
- If  $B_0$  is swept through the Feshbach resonance from the region a<0 to the region a>0, a pair of ultracold atoms can be transformed into a molecule

# Wave function of the bound state

## Weight of the closed channel component of the bound state

According to (2.49) and (2.50), the relative weight of  $\varphi_{cl}^{b}$  in the (normalized) wave function of  $H_{2-channel}$  is given by:

 $\left\langle \varphi_{cl}^{b} \middle| \varphi_{cl}^{b} \right\rangle = \frac{1}{N_{b}^{2}} \qquad N_{b}^{2} = 1 + \left\langle \varphi_{res} \middle| W \ G_{op}^{2}(E_{b})W \middle| \varphi_{res} \right\rangle \qquad (2.66)$ Using

$$G_{\rm op}(E_b) = \frac{1}{E_b - H_{\rm op}} \implies \frac{\partial}{\partial E_b} G_{\rm op}(E_b) = -\frac{1}{\left(E_b - H_{\rm op}\right)^2} = -G_{\rm op}^2(E_b)$$
(2.67)

we can rewrite the second equation (2.66) as:

$$N_{b}^{2} = 1 - \frac{\partial}{\partial E_{b}} \left\langle \varphi_{\text{res}} \middle| W G_{\text{op}}(E_{b}) W \middle| \varphi_{\text{res}} \right\rangle$$
(2.68)

The last term of (2.68) can be transformed using (2.53)

$$\boldsymbol{E}_{b} = \underbrace{\boldsymbol{E}_{\text{res}}}_{=\xi(\boldsymbol{B}-\boldsymbol{B}_{\text{res}})} + \left\langle \varphi_{\text{res}} \middle| \boldsymbol{W} \; \boldsymbol{G}_{\text{op}}(\boldsymbol{E}_{b}) \boldsymbol{W} \middle| \varphi_{\text{res}} \right\rangle$$
(2.69)

# Wave function of the bound state (continued)

Taking the derivative of (2.69) with respect to *B*, we get:

$$\frac{\partial E_{b}}{\partial B} = \xi + \frac{\partial}{\partial E_{b}} \left\langle \varphi_{\text{res}} \middle| W G_{\text{op}}(E_{b})W \middle| \varphi_{\text{res}} \right\rangle \frac{\partial E_{b}}{\partial B}$$
(2.70)  
This finally gives:  
$$\frac{1}{N_{b}^{2}} = \frac{\partial E_{b} \middle/ \partial B}{\xi}$$
(2.71)

The weight of the closed channel component in the wave function of the bound state, for a given value of *B*, is thus equal to the slope of the curve giving  $E_b(B)$  versus *B*, divided by the slope  $\xi$  of the asymptote of the curve giving  $E_b(B)$  versus *B* (see Figure page 46)

## **Conclusion**

When the bound state of the 2-channel Hamiltonian appears near  $B=B_0$  in the region a > 0, the slope of the curve  $E_b(B)$  is equal to 0 and the weight of the closed channel component in its wave function is negligible. For larger values of B, near the asymptote of  $E_b(B)$ , this weight tends to 1 48

# Wave function of the bound state (continued)

## Expression of the wave function of the bound state

The previous conclusion means that, near the Feshbach resonance, the coupling with the closed channel can be neglected for calculating the wave function of the bound state and that we can thus look for the eigenfunction of  $H_{op}$  with an eigenvalue  $-\hbar^2/2\mu a^2$ .

The asymptotic behavior of this wave function (at distances larger than the range of  $V_{op}$ ) can be obtained by solving the 1D radial Schrödinger equation for  $u_0(r)$  with  $V_{op}=0$ .

$$-\frac{\hbar^2}{2\mu}\frac{d^2 u_0(r)}{dr^2} = -\frac{\hbar^2}{2\mu a^2}u_0(r)$$
(2.72)

The 3D wave function of the bound state thus behaves asymptotically as

$$\frac{\exp\left(-r \ / \ a\right)}{r} \tag{2.73}$$

#### **Comparison with quantitative calculations**



Note the logarithmic scale of the r-axis

When one gets closer to the Feshbach resonance, the extension of the wave function becomes bigger and the weight of the closed channel component smaller:

4.7 % at B=160 G 0.1 % at B=155.5 G

Figure taken from Ref. 9

# Conclusion

The coupling between the collision state of 2 ultracold atoms and a bound state of these 2 atoms in another closed collision channel gives rise to resonant variations of the scattering length a when the energy of the bound state is varied around the threshold of the closed channel by sweeping a static magnetic field B.

The scattering length a diverges for the value  $B_0$  of B for which the energy of the bound state in the closed channel, perturbed by its coupling with the continuum of collision states in the open channel, coincides with the threshold of the open channel.

The scattering length can thus take positive or negative values, very large values. It vanishes for a certain value of B depending on the background scattering length in the open channel.

By choosing the value of B, one can thus obtain an attractive gas, a repulsive one, a perfect gas without interactions (a=0), a gas with very strong interactions (a very large, corresponding to the unitary limit).

# **Conclusion (continued)**

The width of the resonance, given by the distance between the value of B for which a diverges and the value of B for which it vanishes, depends on the strength of the coupling between the 2 channels. The resonance is broad if the 2 channels are coupled by the spin exchange interaction, narrow if they can be coupled only by the magnetic dipole-dipole spin interactions.

Near B=B<sub>0</sub>, in the region a>0, the two-atom system has a bound state, with a very weak binding energy, equal to  $\hbar^2/2\mu a^2$ . The wave function of this bound state has a very large spatial extent of the order of a. Its closed channel component is negligible compared to the open channel component.

By sweeping B near  $B_0$ , one can transform a pair of colliding atoms into a molecule or vice versa.

A few problems not considered here:

- Influence of the speed at which B is scanned.
- Stability of the "Feshbach molecules". How do inelastic and 3-body collisions limit their lifetime. Bosonic versus fermionic molecules.

D.Petrov, C.Salomon, G.Shlyapnikov, Phys.Rev.Lett. 93, 090404 (2004)