Atom-Atom Interactions in Ultracold Quantum Gases

Claude Cohen-Tannoudji

Lectures on Quantum Gases
Institut Henri Poincaré, Paris, 25 April 2007

1530
Collège de France

CNRS CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE

Institut Francilien de Recherche sur les Atomes Froids
IFRAF

Lecture 1 (25 April 2007)

Quantum description of elastic collisions between ultracold atoms

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

Lecture 2 (27 April 2007)

Quantum theory of Feshbach resonances

How to manipulate atom-atom interactions in a ultracold quantum 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.Joachin, 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 3ème cycle, Notes de cours rédigées par S.Haroche http://www.phys.ens.fr/cours/notes-de-cours/cct-dea/index.html/

9 – T.Köhler, K.Goral, P.Julienne, Rev.Mod.Phys. 78, 1311-1361 (2006)

Outline of lecture 1

1 - Introduction

2 - Scattering by a potential. A brief reminder

- Integral equation for the wave function
- Asymptotic behavior. Scattering amplitude
- Born approximation

3 - Central potential. Partial wave expansion

- Case of a free particle
- Effect of the potential. Phase shifts
- S-Matrix in the angular momentum representation

4 - Low energy limit

- Scattering length a
- Long range effective interactions and sign of a

5 - Model used for the potential. Pseudo-potential

- Motivation
- Determination of the pseudo-potential
- Scattering and bound states of the pseudo-potential
- Pseudo-potential and Born approximation

Interactions between ultracold atoms

At low densities, 2-body interactions are predominant and can be described in terms of collisions. We will focus here on elastic collisions (although inelastic collisions and 3-body collisions are also important because they limit the achievable spatial densities of atoms).

Collisions are essential for reaching thermal equilibrium

At very low temperatures, mean-field descriptions of degenerate quantum gases depend only on a very small number of collisional parameters. For example, the shape and the dynamics of Bose Einstein condensates depend only on the scattering length

Possibility to control atom-atom interactions with Feshbach resonances. This explains the increasing importance of ultracold atomic gases as simple models for a better understanding of quantum many body systems

Purpose of these lectures: Present a brief review of the concepts of atomic and molecular physics which are needed for a quantitative description of interactions in ultracold atomic gases.

Notation

Two atoms, with mass m, interacting with a 2-body interaction potential $V(\vec{r}_1 - \vec{r}_2)$

In lecture 1, we ignore the spins degrees of freedom. They will be taken into account in lecture 2.

Hamiltonian

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(\vec{r}_1 - \vec{r}_2) \qquad (1.1)$$

Change of variables

$\vec{R}_G = \left(\vec{r}_1 + \vec{r}_2\right)/2 \qquad \vec{P}_G = \vec{p}_1 + \vec{p}_2$ Center of mass variables

$M = m_1 + m_2 = 2m$ Total mass

$\vec{r} = \vec{r}_1 - \vec{r}_2 \qquad \vec{p} = \left(\vec{p}_1 - \vec{p}_2\right)/2$ Relative variables

$\mu = m_1 m_2 / \left(m_1 + m_2\right) = m/2$ Reduced mass

$$H = \underbrace{\vec{P}_G^2 / 2M}_{H_{CM}} + \underbrace{\left(\vec{p}^2 / 2\mu\right) + V\left(\vec{r}\right)}_{H_{rel}} \qquad (1.2)$$

Hamiltonian of a free particle with mass M

Hamiltonian of a "fictitious" particle with mass μ, moving in $V(\mathbf{r})$

Finite range potential

Simple case where $V\left(\vec{r}\right) = 0$ for $r > b$

b is called the range of the potential

One can extend the results obtained in this simple case to potentials decreasing fast enough with *r* at large distances.

For example, for the Van der Waals interactions between atoms decreasing as C_6 / r^6 for large *r*, one can define an effective range

$$\boldsymbol{b}_{\mathrm{VdW}} = \left(\frac{2\mu \boldsymbol{C}_6}{\hbar^2}\right)^{1/4} \qquad (1.3)$$

See for example Ref. 5

Outline of lecture 1

1 - Introduction

2 - Scattering by a potential. A brief reminder

- Integral equation for the wave function
- Asymptotic behavior. Scattering amplitude
- Born approximation

3 - Central potential. Partial wave expansion

- Case of a free particle
- Effect of the potential. Phase shifts
- S-Matrix in the angular momentum representation

4 - Low energy limit

- Scattering length a
- Long range effective interactions and sign of a

5 - Model used for the potential. Pseudo-potential

- Motivation
- Determination of the pseudo-potential
- Scattering and bound states of the pseudo-potential

Scattering by a potential. A brief reminder

Shrödinger equation for the relative particle (with E>0)

$$\left[-\frac{\hbar^2}{2\mu}\Delta+V\left(\vec{r}\right)\right]\psi(\vec{r})=E\psi(\vec{r}) \qquad E=\frac{\hbar^2k^2}{2\mu} \tag{1.4}$$

$$\left[\Delta+\boldsymbol{k}^2\right]\psi\left(\vec{\boldsymbol{r}}\right)=\frac{2\mu}{\hbar^2}\boldsymbol{V}\left(\vec{\boldsymbol{r}}\right)\psi\left(\vec{\boldsymbol{r}}\right)$$

Green function of Δ + k²

$$\left[\Delta+\boldsymbol{k}^2\right]\boldsymbol{G}\left(\vec{\boldsymbol{r}}\right)=\delta\left(\vec{\boldsymbol{r}}\right) \tag{1.5}$$

The boundary conditions for *G* will be chosen later on (1.6)

Integral equation for the solution of Shrödinger equation

$\varphi_0\left(\vec{\boldsymbol{r}}\right)$: Solution of the equation without the right member

$$\left[\Delta+\boldsymbol{k}^2\right]\varphi_0\left(\vec{\boldsymbol{r}}\right)=0 \tag{1.7}$$

$$\psi\left(\vec{\boldsymbol{r}}\right)=\varphi_0\left(\vec{\boldsymbol{r}}\right)+\int \mathrm{d}^3\boldsymbol{r}'\,\boldsymbol{G}\left(\vec{\boldsymbol{r}}-\vec{\boldsymbol{r}}'\right)\boldsymbol{V}\left(\vec{\boldsymbol{r}}'\right)\psi\left(\vec{\boldsymbol{r}}'\right) \tag{1.8}$$

Choice of boundary conditions

We choose for φ_0 a plane wave with wave vector **k**

$$\varphi_0\left(\vec{r}\right) = \mathrm{e}^{i\,\vec{k}.\vec{r}} = \mathrm{e}^{i\,k\,\vec{\kappa}.\vec{r}} \qquad \vec{\kappa} = \vec{k}\,/\,k \tag{1.9}$$

and we choose, for the Green function G, boundary conditions corresponding to an outgoing spherical wave (see Ref.2, Chap.XIX)

$$G_+(\vec{r}-\vec{r}\,') = -\frac{1}{4\pi}\frac{\mathrm{e}^{i\,k\left|\vec{r}-\vec{r}\,'\right|}}{\left|\vec{r}-\vec{r}\,'\right|} \tag{1.10}$$

We thus get the following solution for Schrödinger equation

$$\psi^+_{\vec{k}}(\vec{r}) = \mathrm{e}^{i\,\vec{k}.\vec{r}} - \frac{1}{4\pi}\int \mathrm{d}^3 r'\,\frac{\mathrm{e}^{i\,k\left|\vec{r}-\vec{r}\,'\right|}}{\left|\vec{r}-\vec{r}\,'\right|} V(\vec{r}\,')\,\psi^+_{\vec{k}}(\vec{r}\,') \tag{1.11}$$

If V has a finite range b, the integral over r’ is restricted to a finite range and we can write:

If $r \gg b,\ \left|\vec{r}-\vec{r}\,'\right| \simeq r - \vec{r}\,'.\vec{n}$ with $\vec{n} = \vec{r}\,/\,r$

$$\psi^+_{\vec{k}}(\vec{r}) \simeq \mathrm{e}^{i\,\vec{k}.\vec{r}} - f(k,\vec{\kappa},\vec{n})\frac{\mathrm{e}^{i\,kr}}{r}$$

$$f(k,\vec{\kappa},\vec{n}) = -\frac{2\mu}{4\pi\hbar^2}\int \mathrm{d}^3 r'\,\mathrm{e}^{-i\,k\,\vec{n}.\vec{r}\,'}\,V(\vec{r}\,')\,\psi^+_{\vec{k}}(\vec{r}\,') \tag{1.12}$$

Scattering state with an outgoing spherical wave

Asymptotic behavior for large r

The state $\psi^+_{\vec{k}}(\vec{r})$ is a solution of the Schrodinger equation behaving for large r as the sum of an incoming plane wave $\exp\left(i\,\vec{k}.\vec{r}\right)$ and of an outgoing spherical wave $f(k,\vec{\kappa},\vec{n})\exp(i\,k\,r)\,/\,r$

Scattering amplitude f

$$f(k,\vec{\kappa},\vec{n}) = -\frac{2\mu}{4\pi\hbar^2}\int \mathrm{d}^3r'\,\mathrm{e}^{-i\,\vec{k}'.\vec{r}'}\,V(\vec{r}')\,\psi^+_{\vec{k}}(\vec{r}') \qquad (1.13)$$

We have put $\vec{k}' = k\,\vec{n} = k\,\vec{r}\,/\,r$

$f(k,\vec{\kappa},\vec{n})$ is the amplitude of the outgoing spherical wave in the direction of $\vec{k}' = k\,\vec{n} = k\,\vec{r}\,/\,r$. It depends only on k and on the polar angles θ and φ of $\vec{k}'$ with respect to $\vec{k}$

Differential cross section

Comparing the fluxes along ***k*** and ***k'***, one gets :

$$\mathrm{d}\sigma\,/\,\mathrm{d}\Omega = \left|f(k,\vec{\kappa},\vec{n})\right|^2 \qquad (1.14)$$

Born approximation

In the scattering amplitude, the potential *V* appears explicitly

$$\boldsymbol{f}(\boldsymbol{k}, \vec{\kappa}, \vec{\boldsymbol{n}}) = -\frac{2\mu}{4\pi\hbar^2} \int \mathrm{d}^3 \boldsymbol{r}' \, \mathrm{e}^{-i\,\vec{k}'.\vec{r}'} \, V(\vec{\boldsymbol{r}}') \, \psi^{+}_{\vec{k}}(\vec{\boldsymbol{r}}') \tag{1.15}$$

To lowest order in V, one can thus replace $\psi^{+}_{\vec{k}}(\vec{r}')$ by the zeroth order solution of the Schrodinger equation $\exp(i\,\vec{k}.\vec{r})$

$$\boldsymbol{f}(\boldsymbol{k}, \vec{\kappa}, \vec{\boldsymbol{n}}) = -\frac{2\mu}{4\pi\hbar^2} \int \mathrm{d}^3 \boldsymbol{r}' \, \mathrm{e}^{\,i\,(\vec{k}-\vec{k}').\vec{r}'} \, V(\vec{\boldsymbol{r}}') \tag{1.16}$$

This is the Born approximation

In this approximation, the scattering amplitude is proportional to the spatial Fourier transform of the potential

Low energy limit

The presence of *V(r')* in the scattering amplitude

$$f(k,\vec{\kappa},\vec{n}) = -\frac{2\mu}{4\pi\hbar^2}\int \mathrm{d}^3 r' \, \mathrm{e}^{-i\,\vec{k}'.\vec{r}'}\, V(\vec{r}')\,\psi^+_{\vec{k}}(\vec{r}') \qquad (1.17)$$

restricts the integral over *r'* to a finite range *r'* < *b*

If $kb \ll 1$, one can replace $\mathrm{e}^{-i\,k'.\vec{r}'}$ by 1. The scattering amplitude

$$f(k,\vec{\kappa},\vec{n}) = -\frac{2\mu}{4\pi\hbar^2}\int \mathrm{d}^3 r' V(\vec{r}')\psi^+_{\vec{k}}(\vec{r}') \qquad (1.18)$$

then no longer depends on the direction of the scattering vector $\vec{k}'$.
It is spherically symmetric even if $V(\vec{r})$ is not.

When $k \rightarrow 0, \quad f(k,\vec{\kappa},\vec{n}) \rightarrow -a$

$$\psi^+_{\vec{k}}(\vec{r}) \simeq \mathrm{e}^{i\,\vec{k}.\vec{r}} - a\,\frac{\mathrm{e}^{i\,k\,r}}{r} \rightarrow 1 - \frac{a}{r} \qquad (1.19)$$

a is a constant, called “scattering length”, which will be discussed in more details later on

Another interpretation of the outgoing scattering state

Another expression for this state (see refs. 4 and 8)

$$\left|\psi^{+}_{\vec{k}}\right\rangle = \left|\varphi_{\vec{k}}\right\rangle + \operatorname{Lim}_{\varepsilon\to 0_+} \frac{1}{E - T + i\varepsilon} V \left|\psi^{+}_{\vec{k}}\right\rangle \qquad T = p^2 / 2\mu \tag{1.20}$$

For ε non zero but very small, $\left|\psi^{+}_{\vec{k}}\right\rangle$ appears as the state obtained at $t = 0$ by starting from the free state $\left|\varphi_{\vec{k}}\right\rangle$ at $t = -\infty$ and by switching on slowly V on a time interval on the order of $\hbar / \varepsilon$

Ingoing scattering state

$$\psi^{-}_{\vec{k}}(\vec{r}) = \mathrm{e}^{i\,\vec{k}.\vec{r}} - \frac{1}{4\pi}\int \mathrm{d}^3 r' \, \frac{\mathrm{e}^{-i\,k\left|\vec{r}-\vec{r}\,'\right|}}{\left|\vec{r} - \vec{r}\,'\right|} V(\vec{r}\,')\, \psi^{-}_{\vec{k}}(\vec{r}\,')$$

$$\left|\psi^{-}_{\vec{k}}\right\rangle = \left|\varphi_{\vec{k}}\right\rangle + \operatorname{Lim}_{\varepsilon\to 0_+} \frac{1}{E - T - i\varepsilon} V \left|\psi^{-}_{\vec{k}}\right\rangle \tag{1.21}$$

If one starts from such a state at $t = 0$ and if one switches off V slowly on a time interval on the order of $\hbar / \varepsilon$, one gets the free state $\left|\varphi_{\vec{k}}\right\rangle$ at $t = +\infty$

S - Matrix

Definition

$$S_{ji} = \left\langle \varphi_{\vec{k}_j} \middle| S \middle| \varphi_{\vec{k}_i} \right\rangle = \lim_{\substack{t_1 \to -\infty \\ t_2 \to +\infty}} \left\langle \varphi_{\vec{k}_j} \middle| \tilde{U}(t_2, t_1) \middle| \varphi_{\vec{k}_i,} \right\rangle \qquad (1.22)$$

$\tilde{U}$: evolution operator in interaction representation

One can show that $S_{ji} = \left\langle \psi^-_{\vec{k}_j} \middle| \psi^+_{\vec{k}_i} \right\rangle$ (1.23)

Qualitative interpretation

V is switched on slowly (time scale $\hbar/\varepsilon$) between -∞ and 0, and then switched off slowly (time scale $\hbar/\varepsilon$) between 0 and +∞

One starts from φ_i at t = -∞ and one looks for the probability amplitude to be in φ_j at t = +∞

From $t = -\infty$ to $t = 0$, the initial free state φ_i is transformed into ψ^+_i. Since the evolution operator is unitary, and since $\langle \psi^-_j |$ transforms into $\langle \varphi_j |$ from $t = 0$ to $t = +\infty$, $\langle \psi^-_j | \psi^+_i \rangle$ is the amplitude to find the system in the free state φ_j at $t = +\infty$ if one starts from φ_i at $t = -\infty$.

Outline of lecture 1

Central potential

V depends only on *r*

1D radial Schrödinger equation

One looks for solutions of the form

$$\varphi_{klm}(\vec{r}) = R_{kl}(r) Y_{lm}(\vec{n}) \qquad \vec{n} = \vec{r}/r \tag{1.24}$$

If we put

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} \tag{1.25}$$

with the boundary condition $u_{kl}(0) = 0$ (1.26)

one gets for u_{kl} the following 1D radial equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2} V(r)\right] u_{kl}(r) = 0 \tag{1.27}$$

1D Schrödinger equation for a particle moving in a potential which is the sum of V and of the centrifugal barrier

$$\frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} \tag{1.28}$$

Case of a free particle (V=0)

The solutions of the Schrödinger equation are:

$$\varphi^{(0)}_{k\,l\,m}(\vec{r}) = \sqrt{\frac{2k^2}{\pi}}\, j_l(kr) Y_{l\,m}(\vec{n}) \qquad (1.29)$$

where the j_l are the spherical Bessel functions of order l

$$j_l(kr) \underset{r \to 0}{\simeq} \frac{(kr)^l}{(2l+1)!!} \qquad j_l(kr) \underset{r \to \infty}{\simeq} \frac{1}{kr} \sin\left(kr - l\frac{\pi}{2}\right) \qquad (1.30)$$

For large r we thus have

$$\begin{aligned} \varphi^{(0)}_{k\,l\,m}(\vec{r}) &\underset{r \to \infty}{\simeq} \sqrt{\frac{2}{\pi}}\, Y_{l\,m}(\vec{n}) \frac{\sin(kr - l\pi/2)}{r} \\ &= \sqrt{\frac{2}{\pi}}\, Y_{l\,m}(\vec{n}) \frac{\left[e^{i(kr - l\pi/2)} - e^{-i(kr - l\pi/2)}\right]}{2ir} \\ &= \text{outgoing spherical wave + ingoing spherical wave} \end{aligned} \qquad (1.31)$$

These functions form an orthonormal set (see Appendix)

$$\left\langle \varphi^{(0)}_{k'l'm'} \middle| \varphi^{(0)}_{klm} \right\rangle = \delta(k - k')\delta_{ll'}\delta_{mm'} \qquad (1.32)$$

Expansion of a plane wave in free spherical waves

Plane wave

$$\langle \vec{r} \mid \vec{k} \rangle = (2\pi)^{-3/2} e^{i\,\vec{k}.\vec{r}} \qquad \langle \vec{k}' \mid \vec{k} \rangle = \delta(\vec{k} - \vec{k}') \tag{1.33}$$

The factor $(2\pi)^{-3/2}$ is introduced for the orthonormalization

One can show that:

$$(2\pi)^{-3/2} e^{i\,\vec{k}.\vec{r}} = (2\pi)^{-3/2}\, 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} (i)^l\, Y_{lm}(\vec{n}) Y_{lm}{}^{*}(\vec{\kappa}) j_l(kr)$$
$$= \frac{1}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} (i)^l\, Y_{lm}{}^{*}(\vec{\kappa})\, \varphi_{klm}^{(0)}(\vec{r}) \tag{1.34}$$

with $\vec{\kappa} = \vec{k} / k$

The transformation from the orthonormal basis $\left\{ \mid \vec{k} \rangle \right\}$ to t

he orthonormal basis $\left\{ \mid \varphi_{klm}^{(0)} \rangle \right\}$ is given by the matrix

$$\langle \varphi_{k'l'm'}^{(0)} \mid \vec{k} \rangle = \delta(k - k') \frac{1}{k} Y_{l'm'}{}^{*}(\vec{\kappa}) \tag{1.35}$$

Effect of a potential. Phase shifts

We come back to the Schrödinger equation with $V \neq 0$. Consider, for r large, an incoming wave exp[-i(kr-lπ/2)]. Since the reflection coefficient of V is 1 (conservation of the norm), the reflected outgoing wave has the same modulus and has just accumulated a phase shift with respect to the $V=0$ case. The superposition of the 2 waves is thus a shifted sinusoid.

We conclude that there is a set of solutions of the Schrödinger equation with $V \neq 0$ which behave for large r as:

$$\varphi_{klm}(\vec{r}) \underset{r\to\infty}{\simeq} \sqrt{\frac{2}{\pi}}\, Y_{lm}(\vec{n})\, \frac{\sin\left[kr - l\pi/2 + \delta_l(k)\right]}{r} \qquad (1.36)$$

One can show that these functions are orthonormalized (see Appendix)

$$\left\langle \varphi_{k'l'm'} \middle| \varphi_{klm} \right\rangle = \delta(k - k')\,\delta_{ll'}\,\delta_{mm'} \qquad (1.37)$$

They don't form a basis if there are also bound states in the potential V.

Partial wave expansion of the outgoing scattering state

Consider the linear superposition of the states φ_{klm} with the same coefficients as those appearing in the expansion (1.34) of the plane wave on the $\varphi_{klm}^{(0)}$, each state being multiplied by the phase factor $\exp(i\delta_l)$. We will show that such a state is nothing but the outgoing state $\psi_{\vec{k}}^{+}$ (multiplied by $(2\pi)^{-3/2}$ for having an orthonormalized state)

$$\begin{aligned} \left|\psi_{\vec{k}}^{+}\right\rangle &= \frac{1}{k}\sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}(i)^l\, Y_{lm}^{*}(\vec{\kappa})\, e^{i\delta_l}\left|\varphi_{klm}\right\rangle \\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}\left\langle\varphi_{klm}^{(0)}\middle|\vec{k}\right\rangle e^{i\delta_l}\left|\varphi_{klm}\right\rangle \end{aligned} \qquad (1.38)$$

Before demonstrating this identity, let us discuss its physical meaning.The outgoing scattering state is obtained by switching on slowly V on the free state. Each spherical wave $\varphi_{klm}^{(0)}$ of the expansion of $\vec{k}$ is transformed into φ_{klm} , but in addition it acquires a phase factor $e^{i\delta_l}$ which depends on l and which thus varies from one spherical wave of the expansion to another one.

Demonstration

For large r, the linear superposition introduced in (1.38) behaves as:

$$\frac{1}{k}\sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}(i)^l Y_{lm}^*(\vec{\kappa})\sqrt{\frac{2}{\pi}}\,Y_{lm}(\vec{n})\,\frac{e^{i\left(kr-l\pi/2+2\delta_l\right)}-e^{-i\left(kr-l\pi/2\right)}}{2ir} \tag{1.39}$$

Using $\exp i\left(kr - l\pi/2 + 2\delta_l\right) = \exp i\left(kr - l\pi/2\right)\times\left[1+\left(e^{2i\delta_l}-1\right)\right]$

we get: (1.40)

$$\frac{1}{k}\sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}(i)^l Y_{lm}^*(\vec{\kappa})\sqrt{\frac{2}{\pi}}\,Y_{lm}(\vec{n})\left[\frac{\sin\left(kr-l\pi/2\right)}{r}+\frac{\left(e^{2i\delta_l}-1\right)e^{-il\pi/2}}{2i}\,\frac{e^{ikr}}{r}\right] \tag{1.41}$$

The contribution of the first term of the bracket is nothing but the asymptotic expansion of the plane wave in spherical waves.
The second term gives an outgoing spherical wave

$$(2\pi)^{-3/2}\left[e^{i\vec{k}.\vec{r}}+f(k,\vec{\kappa},\vec{n})\,\frac{e^{ikr}}{r}\right] \tag{1.42}$$

This demonstrates that the state given in (1.38) is an outgoing scattering state and gives in addition the expression of the amplitude f

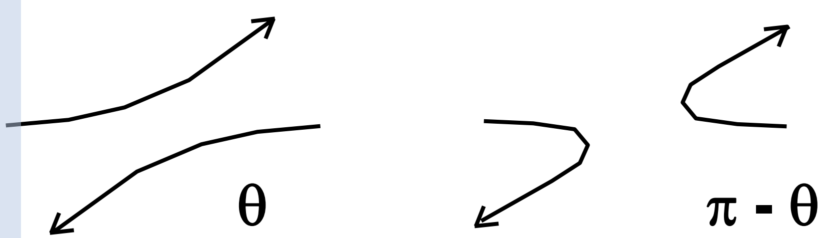
Scattering amplitude in terms of the phase shifts

$$f(k, \vec{\kappa}, \vec{n}) = \frac{4\pi}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} e^{i\delta_l} \sin\delta_l \, Y_{lm}(\vec{n}) Y_{lm}^{*}(\vec{\kappa})$$
$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \, e^{i\delta_l} \sin\delta_l \, P_l(\cos\theta) \qquad (1.43)$$

where $P_l(\cos\theta)$ is a Legendre polynomial and where θ is the angle between $\vec{n}$ and $\vec{\kappa}$. Integrating $|f|^2$ over the polar angles of $\vec{\kappa}$ gives the scattering cross section

$$\sigma(k) = \sum_{l=0}^{\infty} \sigma_l(k) \qquad \sigma_l(k) = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l(k) \qquad (1.44)$$

Scattering of 2 identical particles



Quantum interference between 2 different paths

$$f_k(\theta) \to f_k(\theta) + \varepsilon f_k(\pi - \theta)$$

$\varepsilon = +1 \; (-1)$ for bosons (fermions)

$$\sigma_{\text{total}} = \int_0^{\pi/2} 2\pi \sin\theta \, d\theta \left| f_k(\theta) + \varepsilon f_k(\pi - \theta) \right|^2 \qquad (1.45)$$

Partial wave expansion of the ingoing scattering state

$\psi_{\vec{k}}^{-}$ is given by a linear superposition of the states φ_{klm} analogous to the one introduced for $\psi_{\vec{k}}^{+}$ each state being now multiplied by the phase factor $\exp(-i\delta_l)$ instead of $\exp(i\delta_l)$.

$$\left|\psi_{\vec{k}}^{-}\right\rangle = \frac{1}{k}\sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}(i)^l Y_{lm}{}^{*}(\vec{\kappa})\, \mathrm{e}^{-i\delta_l}\left|\varphi_{klm}\right\rangle = \sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l}\left\langle\varphi_{klm}^{(0)} \middle| \vec{k}\right\rangle \mathrm{e}^{-i\delta_l}\left|\varphi_{klm}\right\rangle \tag{1.46}$$

The demonstration of this identity is similar to the one given above for the outgoing scattering state

If we start from this state and if we switch off V slowly, it transforms into the free state $\vec{k}$. Each wave φ_{klm} is transformed into $\varphi_{klm}^{(0)}$, but in addition its phase factor changes from $\mathrm{e}^{-i\delta_l}$ to 1 which corresponds to acquiring a phase factor $\mathrm{e}^{+i\delta_l}$

Finally, when we go from $t = -\infty$ to $t = +\infty$, switching on and then switching off V slowly, we start from $\varphi_{klm}^{(0)}$ and we end in $\varphi_{klm}^{(0)}$ acquiring a global phase factor $\mathrm{e}^{+i\delta_l} \times \mathrm{e}^{+i\delta_l} = \mathrm{e}^{+2i\delta_l}$

S – Matrix in the angular momentum representation

$$S_{\vec{k}'\,\vec{k}} = \left\langle \vec{k}' \middle| S \middle| \vec{k} \right\rangle = \left\langle \psi^-_{\vec{k}'} \middle| \psi^+_{\vec{k}} \right\rangle \tag{1.47}$$

We use the expansion of $\psi^+_{\vec{k}}$ and $\psi^-_{\vec{k}'}$ in spherical waves

$$\left| \psi^+_{\vec{k}} \right\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \left\langle \varphi^{(0)}_{klm} \middle| \vec{k} \right\rangle \mathrm{e}^{i\delta_l} \left| \varphi_{klm} \right\rangle \qquad \left| \psi^-_{\vec{k}'} \right\rangle = \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=+l'} \left\langle \varphi^{(0)}_{k'l'm'} \middle| \vec{k}' \right\rangle \mathrm{e}^{-i\delta_l} \left| \varphi_{k'l'm'} \right\rangle \tag{1.48}$$

This gives a first expression of $S_{\vec{k}'\,\vec{k}}$

$$S_{\vec{k}'\,\vec{k}} = \left\langle \psi^-_{\vec{k}'} \middle| \psi^+_{\vec{k}} \right\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=+l'} \left\langle \vec{k}' \middle| \varphi^{(0)}_{k'l'm'} \right\rangle \mathrm{e}^{+i\delta_l} \underbrace{\left\langle \varphi_{k'l'm'} \middle| \varphi_{klm} \right\rangle}_{\delta(\vec{k}-\vec{k}')\delta_{l\,l'}\delta_{m\,m'}} \mathrm{e}^{i\delta_l} \left\langle \varphi^{(0)}_{klm} \middle| \vec{k} \right\rangle \tag{1.49}$$

On the other hand, a change of basis gives for $S_{\vec{k}'\,\vec{k}}$

$$S_{\vec{k}'\,\vec{k}} = \left\langle \vec{k}' \middle| S \middle| \vec{k} \right\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=+l'} \left\langle \vec{k}' \middle| \varphi^{(0)}_{k'l'm'} \right\rangle \left\langle \varphi^{(0)}_{k'l'm'} \middle| S \middle| \varphi^{(0)}_{klm} \right\rangle \left\langle \varphi^{(0)}_{klm} \middle| \vec{k} \right\rangle \tag{1.50}$$

Comparing the 2 expressions obtained for $S_{\vec{k}'\,\vec{k}}$, we get

$$\left\langle \varphi^{(0)}_{k'l'm'} \middle| S \middle| \varphi^{(0)}_{klm} \right\rangle = \mathrm{e}^{+2i\,\delta_l}\, \delta(k - k')\, \delta_{l\,l'}\, \delta_{m\,m'} \tag{1.51}$$

which shows that the S-matrix is diagonal in the angular momentum representation, with diagonal elements $\exp(2i\delta_l)$ clearly showing the unitarity of S

Outline of lecture 1

1 - Introduction

2 - Scattering by a potential. A brief reminder

- Integral equation for the wave function
- Asymptotic behavior. Scattering amplitude
- Born approximation

3 - Central potential. Partial wave expansion

- Case of a free particle
- Effect of the potential. Phase shifts
- S-Matrix in the angular momentum representation

4 - Low energy limit

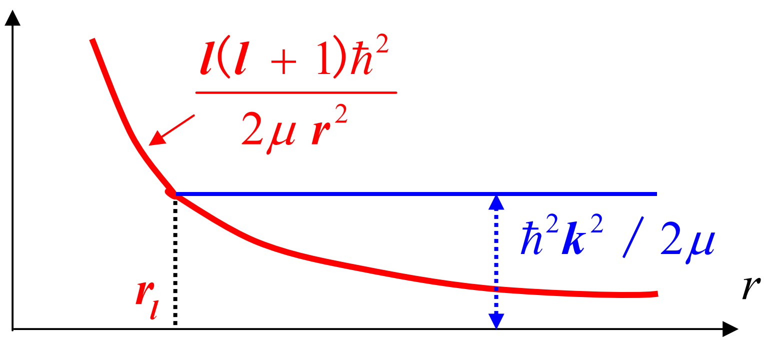
- Scattering length a
- Long range effective interactions and sign of a

5 - Model used for the potential. Pseudo-potential

- Motivation
- Determination of the pseudo-potential
- Scattering and bound states of the pseudo-potential

Central potential. Low energy limit

Suppose first V=0. The centrifugal barrier in the 1D Schrödinger equation prevents the particle from approaching near the region r=0



$$\frac{l(l+1)\hbar^2}{2\mu r_l^2} = \frac{\hbar^2 k^2}{2\mu}$$

$$k\, r_l = \sqrt{l(l+1)}$$

$$r_l = \sqrt{l(l+1)}\, \lambda\!\!\!^{-}_{\mathrm{dB}}$$

If the range b of the potential is small enough, *i.e.* if

$$b \ll \lambda\!\!\!^{-}_{\mathrm{dB}} \qquad (1.52)$$

a particle with $l \neq 0$ cannot feel the potential

Only $l = 0$ wave will feel V. "s-wave scattering"

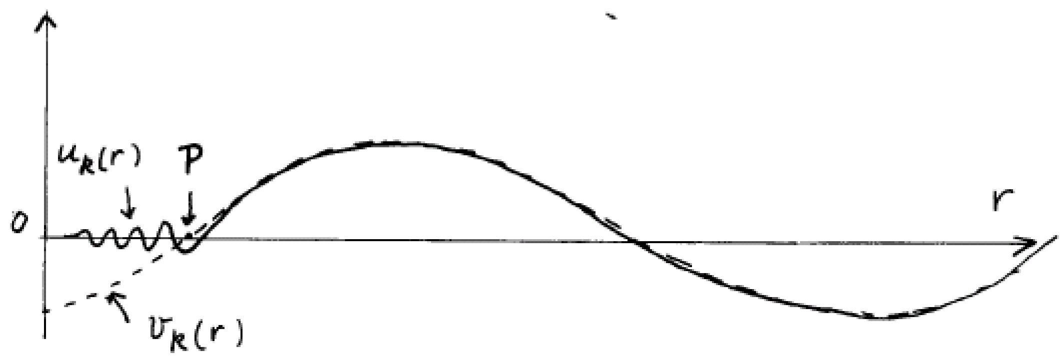
$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{2\mu}{\hbar^2} V(r)\right] u_{k0}(r) = 0 \qquad (1.53)$$

Scattering length

For r large enough, $u_{k0} = u_k$ varies as $\sin\left[kr + \delta_0(k)\right]$

Let v_k be the function $\sin\left[kr + \delta_0(k)\right]$ extending u_k for all r.

Let P be the intersection point of v_k with the r-axis which is the closest from the origin.By definition, the scattering length a is the limit of the abscissa of P when $k \to 0$ (see figure)



Expansion of v_k in powers of kr near $kr = 0$

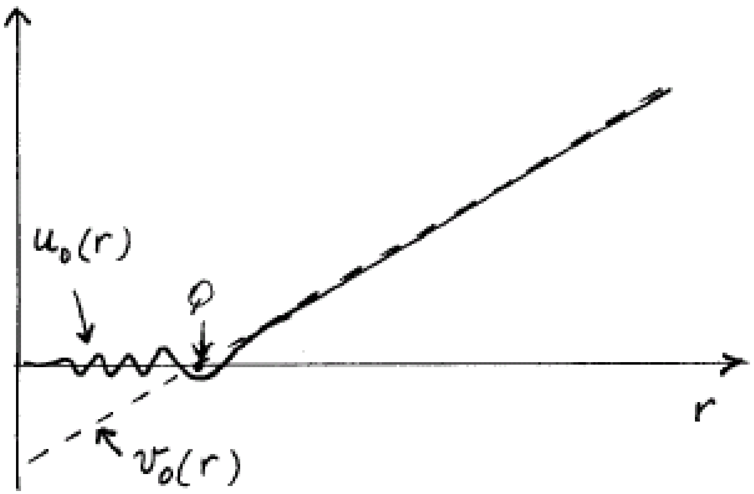
$$v_k(r) = \sin\left[kr + \delta_0(k)\right] \underset{kr \to 0}{\to} \sin\delta_0(k) + kr\cos\delta_0(k) \tag{1.54}$$

Abscissa of P : $-\dfrac{1}{k}\tan\delta_0(k)$

$$a = \lim_{k \to 0} \frac{-\tan\delta_0(k)}{k} \qquad -\frac{\pi}{2} \le \delta_0(k) \le +\frac{\pi}{2} \tag{1.55}$$

Scattering length (continued)

Limit *k=0*



$$\left[\frac{d^2}{dr^2} - \frac{2\mu}{\hbar^2} V(r)\right] u_0(r) = 0 \qquad (1.56)$$

Far from r=o, the solution of the S.E. is a straight line and

$$v_0(r) \propto r - a \qquad (1.57)$$

The abscissa of Q is equal to a

Scattering cross section

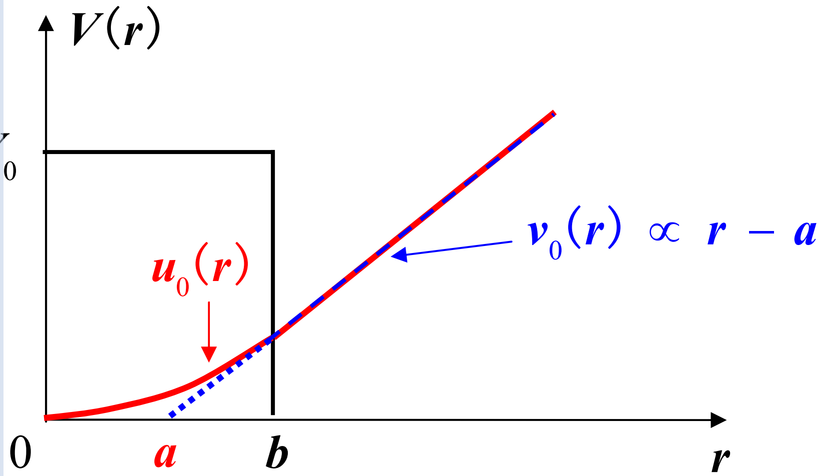
$$\sigma_l(k) = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l(k) \Rightarrow \sigma_{l=0}(k) = 4\pi\frac{\sin^2\delta_0(k)}{k^2} \qquad (1.58)$$

$$\delta_0(k) \underset{k\to 0}{\simeq} -k\,a \Rightarrow \sigma_{l=0}(k) = 4\pi a^2 \qquad (1.59)$$

For identical bosons $\sigma_{l=0}(k) = 8\pi a^2$ (1.60)

Scattering length for square potentials

Square potential barriers



Square barrier of height $V_0 = \hbar^2 k_0^2 / 2\mu$ and width b

For $r > b$ and $k = 0$

$$u_0(r) = v_0(r) \propto r - a$$

For $r < b$ and $k = 0$

$$u_0''(r) = k_0^2 u_0(r)$$

The curvature of u_0 is positive and $u_0(r = 0) = 0$

We conclude that the scattering length is always positive and smaller than the range b of the potential

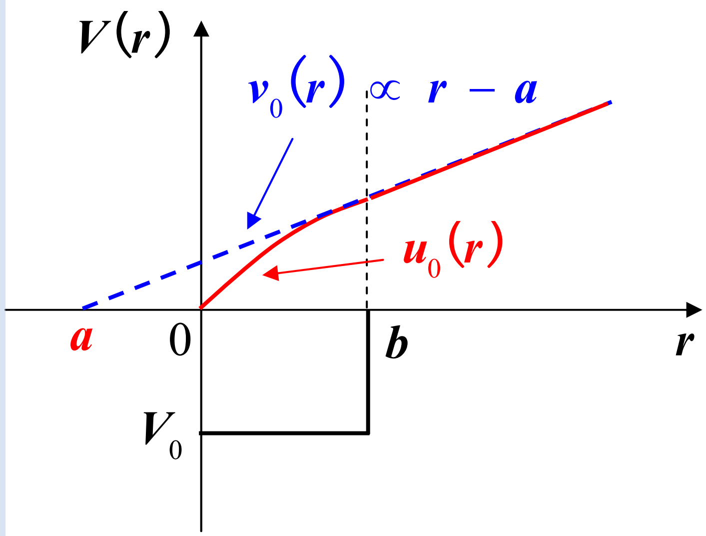
$$0 \leq a \leq b$$

When $V_0 \to \infty$ (hard sphere potential)

$$a \to b$$

Scattering length for square potentials (continued)

Square potential wells



$$V_0 = -\hbar^2 k_0^2 / 2\mu$$

For $r > b$ and $k = 0$

$$u_0(r) = v_0(r) \propto r - a$$

For $r < b$ and $k = 0$

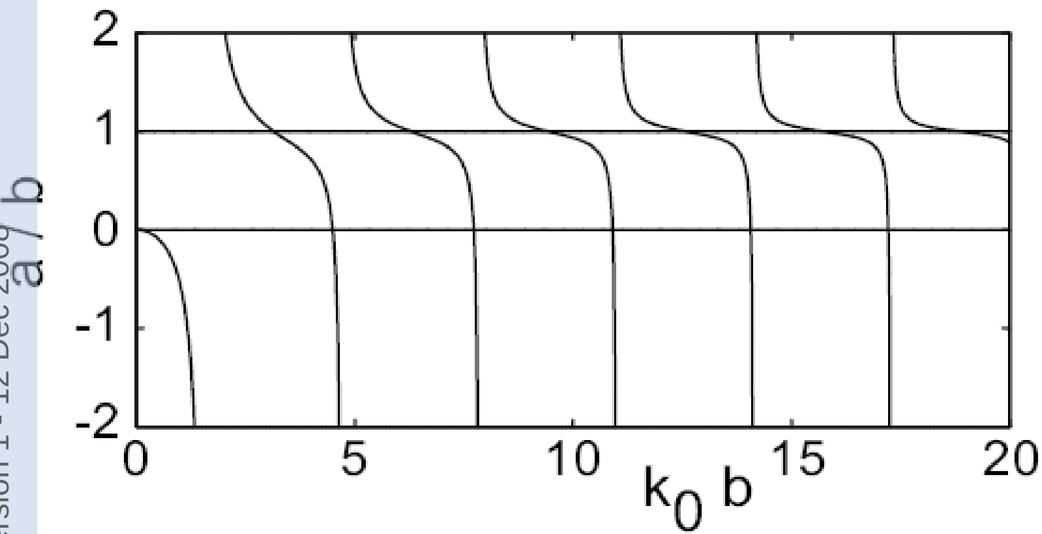
$$u_0''(r) = -k_0^2 u_0(r)$$

The curvature of u_0 is negative and $u_0(r = 0) = 0$

If V_0 is small enough so that there is no bound state in the potential well, the curvature of u_0 for $r < b$ is small and a is negative

When $|V_0|$ increases, the curvature of u_0 for $r < b$ increases in absolute value and $a \to -\infty$. Then a switches suddenly to $+\infty$ and decreases. This divergence of a corresponds to the appearance of the first bound state in the potential well

Square potential wells (continued)



Variations of a with k_0 figure taken from Ref.5

When the depth of the potential well increases, divergences of a occur for all values of V_0 such that $k_0 b = (2n+1)\pi/2$ corresponding to the appearances of successive bound states in the potential well.
These divergences of a which goes from $-\infty$ to $+\infty$ are called "zero-energy" resonances

Long range effective interactions and sign of a

The scattering length determines how the long range behavior of the wave functions is modified by the interactions. To understand how the sign of a is related to the sign of the effective long range interactions, it will be useful to consider the particle enclosed in a spherical box with radius R, so that we have the boundary condition

$$u_0(R) = 0 \qquad (1.61)$$

leading to a discrete energy spectrum

In the absence of interactions (V=0), the normalized eigenstates and the eigenvalues of the 1D Schrödinger equation are:

$$\psi_N^{(0)}(r) = \sqrt{\frac{1}{2\pi R}}\,\frac{\sin(N\pi r / R)}{r} \qquad E_N = \frac{\hbar^2}{2\mu}\frac{N^2\pi^2}{R^2} \qquad N = 1, 2, \ldots \qquad (1.62)$$

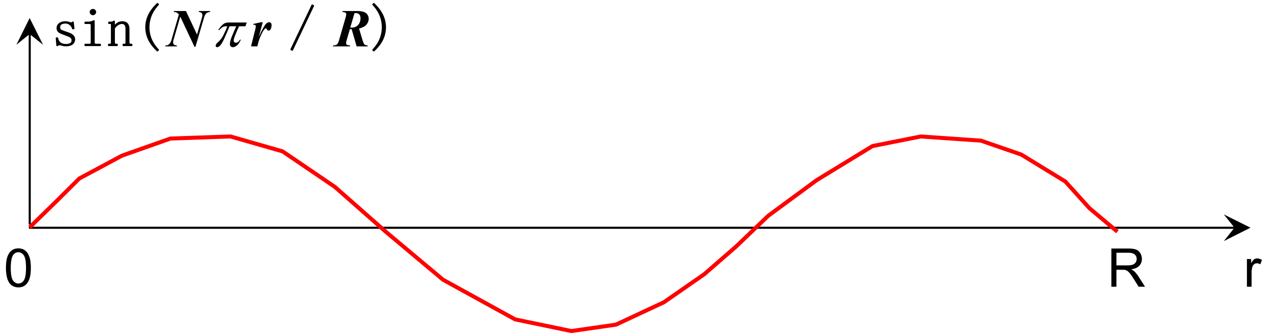
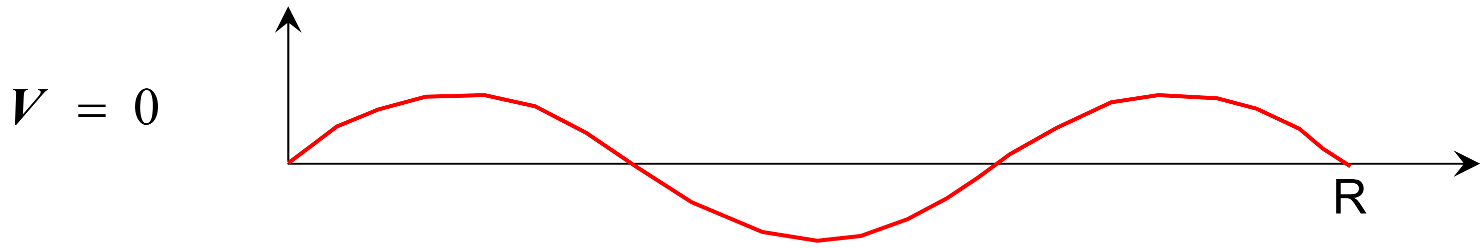
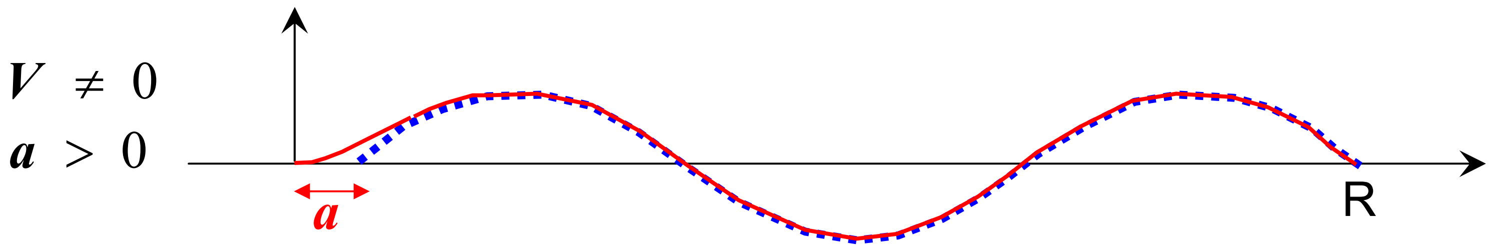
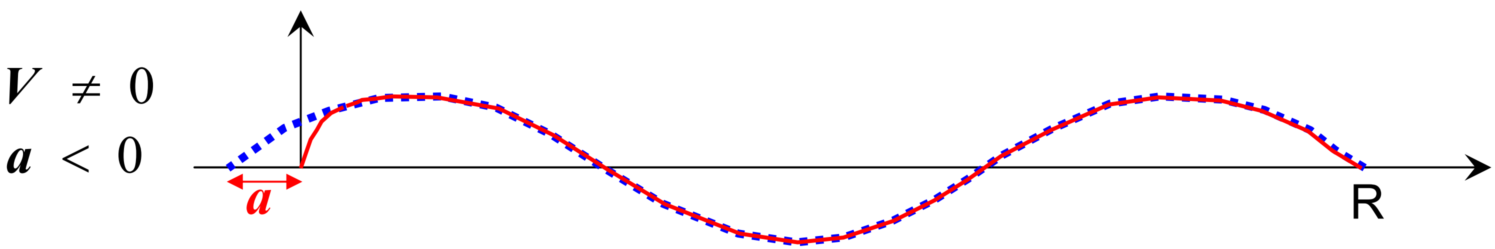


Figure corresponding to N=3



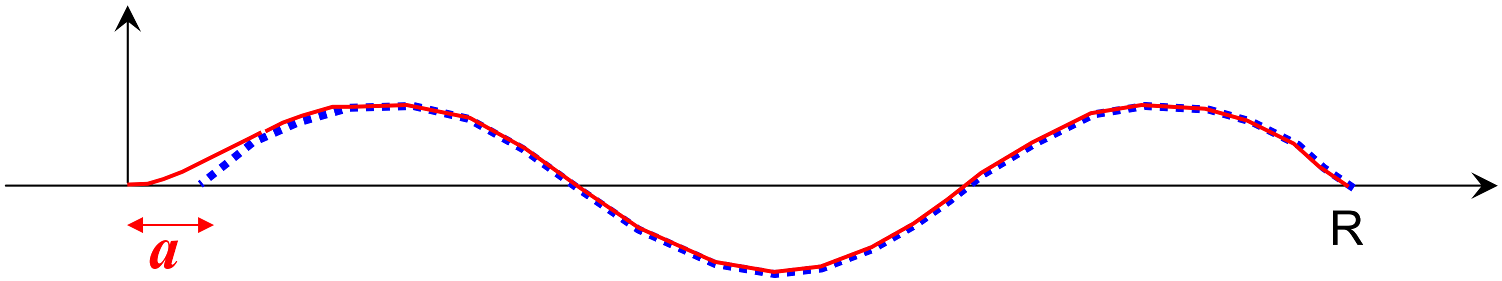


The dotted line is the sinusoid outside the range of the potential
It has a shorter wavelength than for V=0, and thus a larger wave number k.
The kinetic energy in this region, which is also the total energy, is larger



The dotted line is the sinusoid outside the range of the potential
It has a longer wavelength than for V=0, and thus a smaller wave number k.
The kinetic energy in this region, which is also the total energy, is smaller

Correction to the energy to first order in a



For the state $\psi_N^{(0)}$, we have $R = N\lambda / 2$

Because of the interactions, these N half wavelengths occupy now a length $R - a$ so that

$$\lambda = 2R / N \quad \rightarrow \quad \lambda' = 2(R - a) / N$$

$$k = 2\pi / \lambda \quad \rightarrow \quad k' = 2\pi / \lambda' = k\, R / (R - a)$$

$$E_N = \hbar^2 k^2 / 2\mu \quad \rightarrow \quad E'_N = E_N\, k'^2 / k^2 = E_N R^2 / (R - a)^2 \simeq E_N \left(1 + \frac{2a}{R}\right)$$

Finally, we have $\delta E_N = E'_N - E_N = \dfrac{2a}{R} E_N = \dfrac{\hbar^2 \pi^2 N^2}{\mu R^3} a$ (1.63)

Long range effective interactions are - repulsive if $a > 0$

- attractive if $a < 0$

Outline of lecture 1

1 - Introduction

2 - Scattering by a potential. A brief reminder

- Integral equation for the wave function
- Asymptotic behavior. Scattering amplitude
- Born approximation

3 - Central potential. Partial wave expansion

- Case of a free particle
- Effect of the potential. Phase shifts
- S-Matrix in the angular momentum representation

4 - Low energy limit

- Scattering length a
- Long range effective interactions and sign of a

5 - Model used for the potential. Pseudo-potential

- Motivation
- Determination of the pseudo-potential
- Scattering and bound states of the pseudo-potential

Model used for the potential *V(r)*

Why not using the exact potential?

The interaction potential is very difficult to calculate exactly.

A small error in V can introduce a very large error on the scattering length deduced from this potential.

Mean field description of ultracold quantum gases require in general a first order treatment of the effect of V (Born approximation). But Born approximation cannot be in general applied to the exact potential

Approach followed here

The motivation here is not to calculate the scattering length. This parameter is supposed known experimentally. We are interested in the derivation of the macroscopic properties of the gas from a mean field description using a single parameter which is a.

The key idea is to replace the exact potential by a "pseudo-potential" simpler to use than the exact one and obeying 2 conditions:

- It has the same scattering length as the exact potential
- It can be treated with Born approximation so that mean field descriptions of its effects are possible

Determination of the pseudo-potential

Derivation "à la" H.Bethe and R.Peierls (Y.Castin, private communication)

We add to the 3D Schrödinger equation of a free particle (*V*=0) a term proportional to a delta function

$$-\frac{\hbar^2}{2\mu}\Delta\psi(\vec{r}) + C\,\delta(\vec{r}) = \frac{\hbar^2 k^2}{2\mu}\psi(\vec{r}) \qquad (1.64)$$

To determine the coefficient C, we impose to the solution of this equation to coincide with the extension to all r of the asymptotic behavior $\sin\left[kr + \delta_0(k)\right]/r$ of the true wave function $u_0(r)/r$

In particular, for k small enough, one should have:

$$\psi(\vec{r}) \underset{r\to 0}{\simeq} B(r-a)/r \qquad (1.65)$$

Inserting (1.65) into (1.64) and using $\Delta(1/r) = -4\pi\,\delta(r)$, we get an equation containing a delta function multiplied by a coefficient

$$C - \frac{4\pi\hbar^2}{2\mu}a\,B$$

which must vanish. This gives the coefficient C appearing in (1.64)

$$C = g\,B \qquad \text{where} \qquad g = \frac{4\pi\hbar^2}{2\mu}a = \frac{4\pi\hbar^2}{m}a \qquad (1.66)$$

Determination of the pseudo-potential (continued)

It will be more convenient to express $C=gB$, not in terms of the coefficient B appearing in the wave function $\psi = B(r-a)/r$ of equation (1.65), but in terms of the wave function ψ itself. We use for that

$$B = \left[\frac{\mathrm{d}}{\mathrm{d}r} r\psi \right]_{r=0} \tag{1.67}$$

Equation (1) can be rewritten as:

$$-\frac{\hbar^2}{2\mu}\Delta\psi(\vec{r}) + V_{\text{pseudo}}\,\psi(\vec{r}) = \frac{\hbar^2 k^2}{2\mu}\psi(\vec{r}) \tag{1.68}$$

where $$V_{\text{pseudo}}\,\psi(\vec{r}) = g\,\delta(\vec{r})\frac{\mathrm{d}}{\mathrm{d}r}\left[r\,\psi(\vec{r})\right] \tag{1.69}$$

V_{pseudo} is called the pseudo-potential. The term $\left[(\mathrm{d}/\mathrm{d}r)\, r\right]$ regularizes the action of $\delta(\vec{r})$ when it acts on functions behaving as $1/r$ near $r = 0$. For functions which are regular in $r = 0$, V_{pseudo} has the same effect as $g\,\delta(\vec{r})$:

$$\begin{aligned} &\psi(\vec{r}) = u(r)/r \ \text{ with } \ u(0) \neq 0 &&\Rightarrow\quad V_{\text{pseudo}}\,\psi(\vec{r}) = g\,u'(0)\,\delta(\vec{r}) \\ &\psi(\vec{r}) \ \text{ regular in } r = 0 &&\Rightarrow\quad V_{\text{pseudo}}\,\psi(\vec{r}) = g\,\psi(\vec{0})\,\delta(\vec{r}) \end{aligned} \tag{1.70}$$

Scattering states of the pseudo-potential

We are looking for solutions of equation (1.68) with $E > 0$

For $l \neq 0$, the centrifugal barrier prevents the particle from approaching $r = 0$, and one can show that $\psi(\vec{0}) = 0$, so that, according to (1.70), $V_{\text{pseudo}}\psi(\vec{r}) = 0$. V_{pseudo} gives only s-scattering and one can write $\psi(\vec{r}) = u_0(r) / r$ where $u_0(0)$ can be $\neq 0$.

$$\Delta \frac{u_0(r)}{r} = \Delta\left[\frac{u_0(0)}{r} + \frac{u_0(r) - u_0(0)}{r}\right] = -4\pi\, u_0(0)\delta(r) + \frac{1}{r}\frac{\mathrm{d}^2 u_0}{\mathrm{d}r^2} \qquad (1.71)$$

The Schrödinger equation for u_0 becomes:

$$-\frac{\hbar^2}{2\mu}\left[-4\pi\, u_0(0)\delta(\vec{r}) + \frac{u_0''(r)}{r}\right] + g\delta(\vec{r})u_0'(0) = \frac{\hbar^2 k^2}{2\mu}\frac{u_0(r)}{r} \qquad (1.72)$$

Cancelling the term proportional to $\delta(\vec{r})$ and the term independant of $\delta(\vec{r})$, we get 2 equations:

$$\frac{u_0(0)}{u_0'(0)} = -g\frac{\mu}{2\pi\hbar^2} = -a \qquad\qquad u_0''(r) + k^2 u_0(r) = 0 \qquad (1.73)$$

Scattering states of the pseudo-potential (continued)

The solution of the second equation can be written:

$$u_0(r) = \sin\left(k\, r + \delta_0\right) \qquad (1.74)$$

Inserting this solution into the first equation gives:

$$\tan \delta_0 = -k\, a \qquad (1.75)$$

On the other hand, the s-wave scattering amplitude is equal to:

$$f_0(k) = \frac{1}{k}\, e^{i\,\delta_0} \sin \delta_0 \qquad (1.76)$$

Using equation (1.75) giving $\tan\delta_0$ finally gives after simple algebra:

$$f_0(k) = -\frac{a}{1 + i\, k\, a} \qquad (1.77)$$

V_{pseudo} is proportional to a. A first order treatment of V_{pseudo} thus gives the correct result for the scattering amplitude in the zero energy limit $(k\, a = 0)$. This shows that Born approximation can be used with V_{pseudo} for ultracold atoms

The 2 conditions imposed above on V_{pseudo} are thus fulfilled

The unitary limit

From the expression of the scattering amplitude obtained above, we deduce the scattering amplitude for identical bosons

$$\sigma(k) = \frac{8\pi a^2}{1 + k^2 a^2} \tag{1.78}$$

which is valid for all k.

The low energy limit $(ka \ll 1)$ gives the well known result:

$$\sigma(k) \underset{ka \ll 1}{\simeq} 8\pi a^2 \tag{1.79}$$

There is another interesting limit, corresponding to high energy, or strong interaction $(ka \gg 1)$ leading to result independent of a:

$$\sigma(k) \underset{ka \gg 1}{\simeq} \frac{8\pi}{k^2} \tag{1.80}$$

This is the so called “unitary limit”

Bound state of the pseudo-potential

The calculation is the same as for the scattering states, except that we replace the positive energy $\hbar^2 k^2 / 2\mu$ by a negative one $-\hbar^2 \kappa^2 / 2\mu$

The 2 equations derived from the Schrodinger equation are now:

$$\frac{u_0(0)}{u_0'(0)} = -a \qquad u_0''(r) - \kappa^2 u_0(r) = 0 \tag{1.81}$$

The solution of the second equation (finite for $r \to \infty$) is:

$$u_0(r) = e^{-\kappa r} \tag{1.82}$$

which inserted into the first equation gives:

$$\kappa = 1 / a \tag{1.83}$$

The pseudo-potential thus has a bound state with an energy

$$E = -\frac{\hbar^2}{2\mu a^2} \tag{1.84}$$

and a wave function:

$$\exp\left(-\frac{r}{a}\right) \tag{1.85}$$

Energy shifts produced by the pseudo-potential

We come back to the problem of a particle in a box of radius R. We have calculated above the energy shifts of the discrete energy levels of this particle produced by a potential characterized by a scattering length a. To first order in a, we found:

$$\delta E_N = \frac{\hbar^2 \pi^2 N^2}{\mu R^3} a \qquad (1.86)$$

This result was deduced directly from the modification induced by the interaction on the asymptotic behavior of the wave functions and not from a perturbative treatment of V. We show now that:

$$\delta E_N = \left\langle \psi_N^{(0)} \middle| V_{\text{pseudo}} \middle| \psi_N^{(0)} \right\rangle \quad \text{to first order in } V_{\text{pseudo}} \qquad (1.87)$$

which is another evidence for the fact that the effect of the pseudo potential can be calculated perturbatively, which is not the case for the real potential. For example, a hard core potential (V=∞ for r< a) cannot obviously be treated perturbatively, but its scattering length is a , and using a pseudo-potential with scattering length a allows perturbative calculations.

Demonstration

The unperturbed normalized eigenfunctions of the particle in the spherical box are:

$$\psi_N^{(0)}(r) = \sqrt{\frac{1}{2\pi R}}\,\frac{\sin(N\pi r / R)}{r} \tag{1.47}$$

$\psi_N^{(0)}(r)$ is regular in $r = 0$ and

$$\psi_N^{(0)}(0) = \frac{1}{\sqrt{2\pi}}\,N\pi\,\frac{1}{R^{3/2}} \tag{1.88}$$

so that

$$V_{pseudo}\psi_N^{(0)}(r) = g\delta(\vec{r})\,\psi_N^{(0)}(0) \tag{1.89}$$

We deduce that

$$\delta E_N = g\left|\psi_N^{(0)}(0)\right|^2 = g\,\frac{N^2\pi^2}{2\pi R^3} = \frac{\hbar^2\pi^2N^2}{\mu R^3}\,a \tag{1.90}$$

which coincides with the result obtained above in (1.63).

Conclusion

Elastic collisions between ultracold atoms are entirely characterized by a single number, the scattering length

Effective long distance interactions are attractive if $a<0$ and repulsive if $a>0$

Giving the same scattering length as the real potential, the pseudo-potential gives the good asymptotic behavior for the wave function describing the relative motion of 2 atoms, and thus correctly describes their long distance interactions

In a dilute gas, atoms are far apart. The pseudo-potential is proportional to a and can be treated perturbatively. A first order treatment of the pseudo-potential is the basis of mean field description of Bose Einstein condensates where each atom moves in the mean field produced by all other atoms.

Next step: can one change the scattering length?

Atom-Atom Interactions in Ultracold Quantum Gases

Claude Cohen-Tannoudji

Lectures on Quantum Gases
Institut Henri Poincaré, Paris, 27 April 2007

1530
Collège de France

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE

Institut Francilien de Recherche sur les Atomes Froids
IFRAF

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 3ème cycle, Notes de cours rédigées par S.Haroche http://www.phys.ens.fr/cours/notes-de-cours/cct-dea/index.html/

9 – T.Köhler, K.Goral, P.Julienne, Rev.Mod.Phys. 78, 1311-1361 (2006)

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

Feshbach Resonances

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

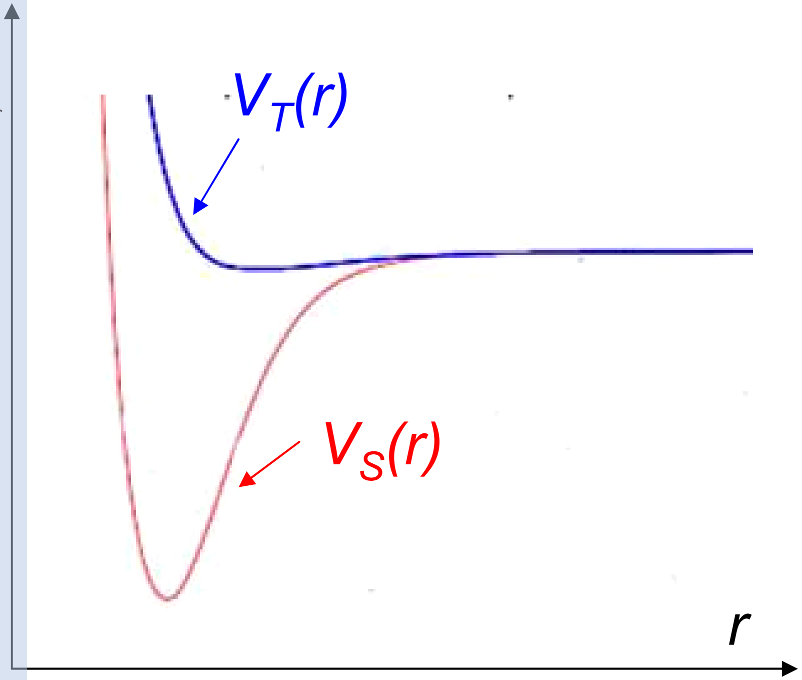
Case of two identical alkali atoms

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

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

$$\boldsymbol{V(r) = V_S(r) P_S + V_T(r) P_T} \quad (2.1)$$

P_S : Projector on $S = 0$ states

P_T : Projector on $S = 1$ states

Microscopic atom-atom interactions (continued)

Electronic interactions

$$\begin{aligned} V_{\text{el}}(\boldsymbol{r}) &= V_S(\boldsymbol{r})P_S + V_T(\boldsymbol{r})P_T \\ &= \frac{1}{4}V_S(\boldsymbol{r}) + \frac{3}{4}V_T(\boldsymbol{r}) + \frac{1}{2\hbar^2}\left[V_T(\boldsymbol{r}) - V_S(\boldsymbol{r})\right]\ \vec{\boldsymbol{S}}_1.\vec{\boldsymbol{S}}_2 \end{aligned} \quad (2.2)$$

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)

Magnetic spin-spin interactions V_{ss}

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

Interaction Hamiltonian

$$V^{\text{int}} = V_{\text{el}} + V_{ss} \quad (2.3)$$

V_{el} is much larger than V_{ss}

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

Channels

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

$$\alpha \quad : \quad \left\{ f_1, m_{f1}, f_2, m_{f2}, \ell = 0 \right\}$$

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

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

where $\psi_\alpha(\mathbf{r})$ is the wave function in channel α 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_α do not evolve independently from each other

Coupled channel equations

The coupled equations of motion of the F_α are of the form:

$$\frac{\partial^2}{\partial r^2} F_\alpha(r, E) + \frac{2\mu}{\hbar^2} \sum_\beta \left[E\, \delta_{\alpha\beta} - V_{\alpha\beta} \right] F_\beta(r, E) = 0 \qquad (2.5)$$

$$V_{\alpha\beta} = \left[E_{f_i, m_{f1}} + E_{f_2, m_{f2}} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] \delta_{\alpha\beta} + V^{\text{int}}_{\alpha\beta}(r) \qquad (2.6)$$

Solving numerically these coupled differential equations gives the asymptotic behavior of F_α for large r from which one can determine the phase shift δ_0 and the scattering length in channel α.

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 $\boldsymbol{B_0}$ is the only external field, the projection M of the total angular momentum along the z-axis of $\boldsymbol{B_0}$ 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 $\boldsymbol{M} = \boldsymbol{m}_{f1} + \boldsymbol{m}_{f2} + \boldsymbol{m}_{\ell}$ with a fixed value of $\boldsymbol{M}$. They can be also classified by the eigenvalues of $\vec{\boldsymbol{F}}^2$, $\boldsymbol{F}_z$, where $\vec{\boldsymbol{F}} = \vec{\boldsymbol{F}}_1 + \vec{\boldsymbol{F}}_2$. This gives the states $\left\{ f_1, f_2, \boldsymbol{F}, \boldsymbol{M}_F, \boldsymbol{m}_{\ell} \right\}$ with $\boldsymbol{M}_F + \boldsymbol{m}_{\ell} = \boldsymbol{M}$

Since $\vec{\boldsymbol{S}}_1 . \vec{\boldsymbol{S}}_2$, and thus $\boldsymbol{V}_{\mathrm{el}}$, commutes with $\vec{\boldsymbol{F}} = \vec{\boldsymbol{S}}_1 + \vec{\boldsymbol{S}}_2 + \vec{\boldsymbol{I}}_1 + \vec{\boldsymbol{I}}_2$ and $\vec{\boldsymbol{L}}$, $\boldsymbol{V}_{\mathrm{el}}$ can couple only states with the same value of $\boldsymbol{F}$ and ℓ

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

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

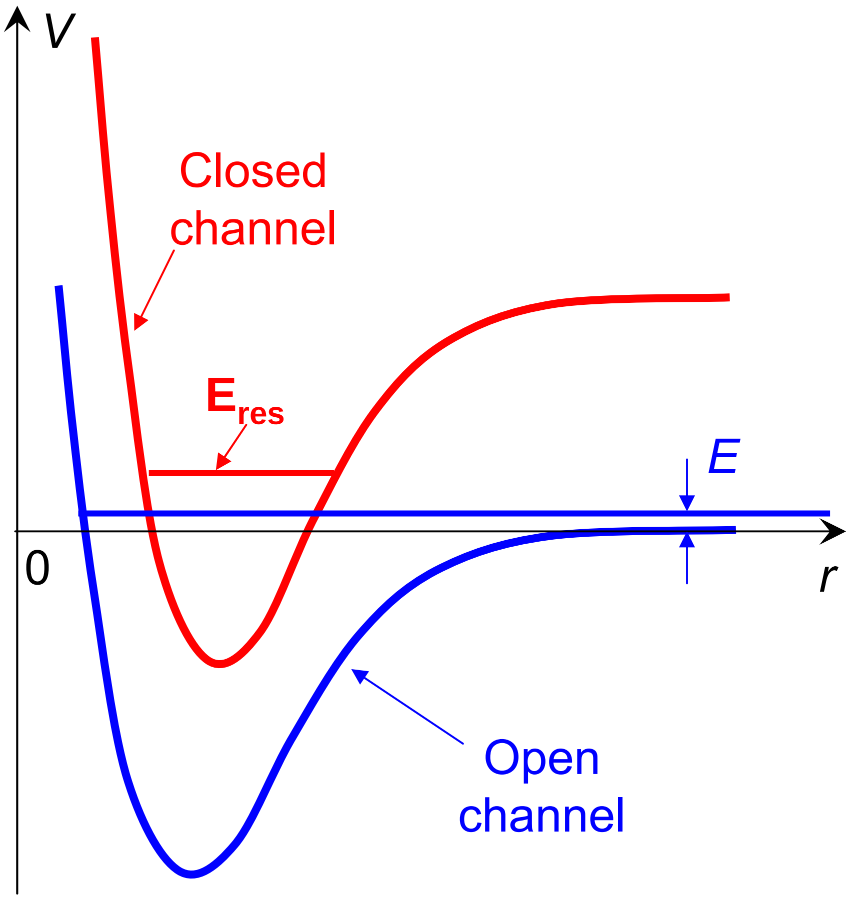
5 - Scattering states of the 2-channel Hamiltonian

- 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

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 φ_{res} in the closed channel.

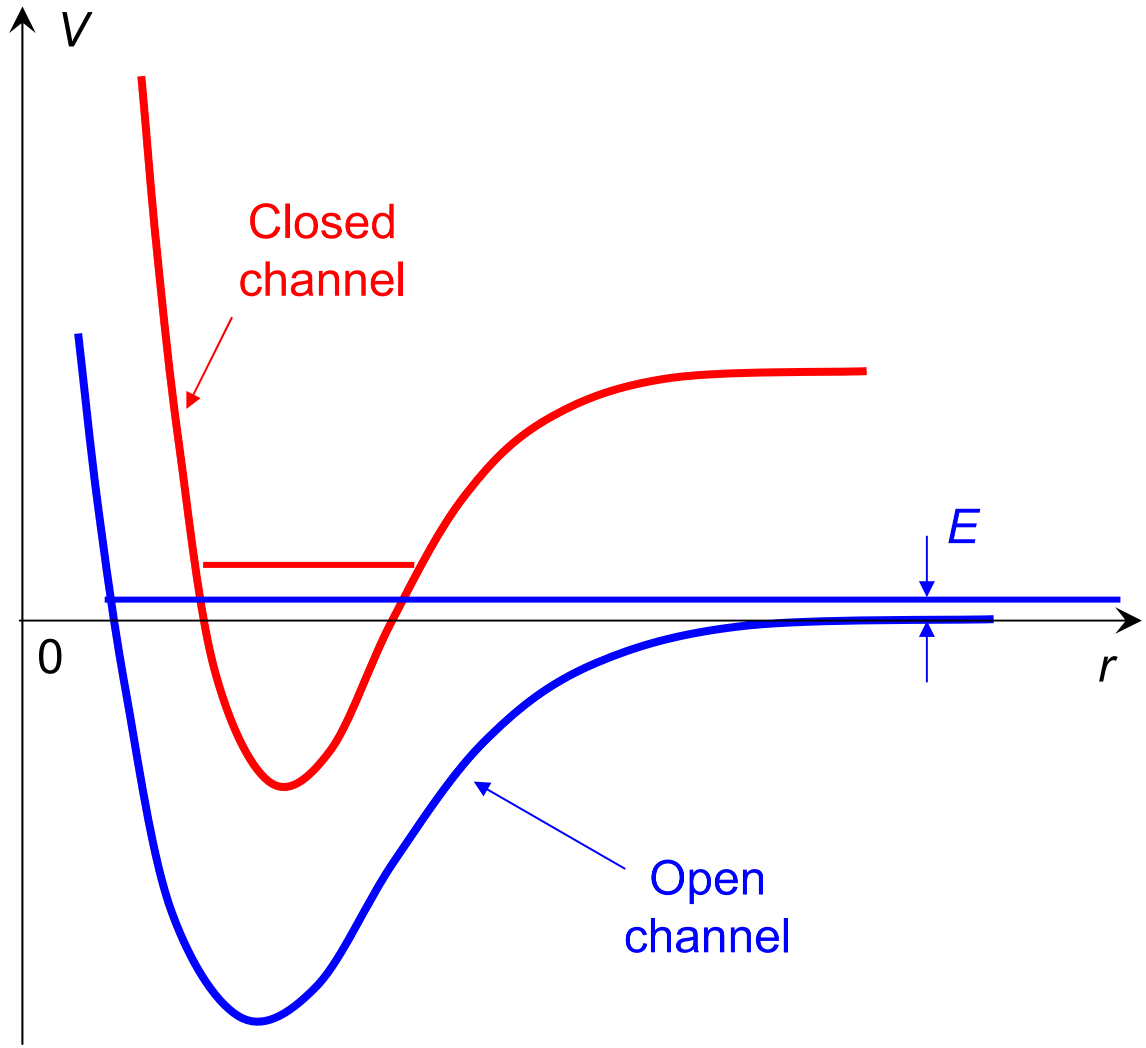
The pair of colliding atoms can make a virtual transition to the bound state and come back to the colliding state. The duration of this virtual transition scales as $\hbar$ / | E_{res}-E |, i.e. as the inverse of the detuning between the collision energy E and the energy E_{res} of the bound state.

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

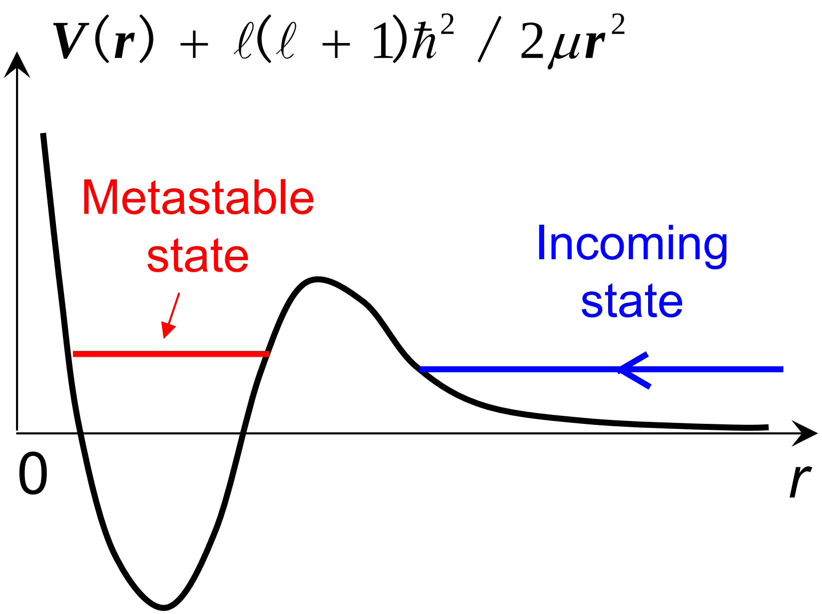
Analogy with resonant light scattering when an impinging photon of energy hν can be absorbed by an atom which is brought to an excited discrete state with an energy $h\nu_0$ above the initial atomic state and then reemitted. There is a resonance in the scattering amplitude when ν is close to ν_0

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

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

Two-channel model

Only two channels are considered, one open and one closed

State of the atomic system

$$|\text{op}\rangle\, \varphi_{\text{op}}(\vec{r}) + |\text{cl}\rangle\, \varphi_{\text{cl}}(\vec{r}) \qquad (2.7)$$

The wave function has two components, one in each channel

Hamiltonian

$$H_{\text{2-channel}} = \begin{pmatrix} H_{\text{op}} & W(r) \\ W(r) & H_{\text{cl}} \end{pmatrix} \qquad (2.8)$$

$$H_{\text{op}} = -\frac{\hbar^2}{2\mu}\Delta + V_{\text{op}}$$
$$H_{\text{cl}} = -\frac{\hbar^2}{2\mu}\Delta + V_{\text{cl}} \qquad (2.9)$$

Resonant bound state in the closed channel

$$H_{\text{cl}}\, \varphi_{\text{res}}(r) = E_{\text{res}}\, \varphi_{\text{res}}(r) \qquad E_{\text{res}} = \hbar\Delta \qquad (2.10)$$

The energy E_{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 $H_{2\text{-channel}}$

$$\begin{pmatrix} H_{op} & W(r) \\ W(r) & H_{cl} \end{pmatrix} \begin{pmatrix} \varphi_{op} \\ \varphi_{cl} \end{pmatrix} = E \begin{pmatrix} \varphi_{op} \\ \varphi_{cl} \end{pmatrix} \qquad (2.11)$$

$$\begin{aligned} H_{op}\ \varphi_{op}(\vec{r}) + W(r)\varphi_{cl}(\vec{r}) &= E\ \varphi_{op}(\vec{r}) \\ W(r)\ \varphi_{op}(\vec{r}) + H_{cl}\ \varphi_{cl}(\vec{r}) &= E\ \varphi_{cl}(\vec{r}) \end{aligned} \qquad (2.12)$$

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 $\varphi_{op}^{\vec{k}}$ and $\varphi_{cl}^{\vec{k}}$

Eigenstates with negative eigenvalues E_b<0

They describe the bound states of the 2 atoms in the presence of W

Their 2 components are denoted φ_{op}^{b} and φ_{cl}^{b}

Single resonance approximation

We will neglect all eigenstates of H_{cl} other than φ_{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

$$H_{\mathrm{cl}} = E_{\mathrm{res}} \left| \varphi_{\mathrm{res}} \right\rangle \left\langle \varphi_{\mathrm{res}} \right| \tag{2.13}$$

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

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

Outline of lecture 2

Scattering states of the two-channel Hamiltonian $H_{2\text{-channel}}$

Open channel component of the scattering state of $H_{2\text{-channel}}$

The first equation (2.12) can be written

$$\left(E - H_{\text{op}} \right) \varphi_{\text{op}}^{\vec{k}}(\vec{r}) = W(r)\, \varphi_{\text{cl}}^{\vec{k}}(\vec{r}) \qquad (2.15)$$

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

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

In (2.16), $G^{+}_{op}(E)$ is a Green function of H_{op}. The term $+i\varepsilon$, where ε 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 $r \to \propto$.

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 $r \to \propto$.

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

Scattering states of the two-channel Hamiltonian $H_{2\text{-channel}}$ (continued)

Closed channel component of the scattering state of $H_{2\text{-channel}}$

The second equation (2.12) can be written:

$$\left(E - H_{\text{cl}}\right)\varphi_{\text{cl}}^{\vec{k}}(\vec{r}) = W(r)\,\varphi_{\text{op}}^{\vec{k}}(\vec{r}) \tag{2.18}$$

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

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

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

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

The closed channel component $\varphi_{\text{cl}}^{\vec{k}}$ is thus proportional to φ_{res}

Dressed states and bare states

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

The eigenstates $\varphi_{\vec{k}}^{+}$ and φ_{res} of H_{op} and H_{cl} are called bare states

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

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

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

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

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

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

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

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. Il we introduce the effective coupling V_{eff} defined by:

$$V_{\text{eff}} = W \frac{|\varphi_{\text{res}}\rangle\langle\varphi_{\text{res}}|}{E - E_{\text{res}} - \langle\varphi_{\text{res}}|W\, G_{\text{op}}^{+}(E)\, W|\varphi_{\text{res}}\rangle} W \qquad (2.24)$$

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

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

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

$$V_{\text{tot}} = V_{\text{op}} + V_{\text{eff}} \qquad (2.26)$$

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)

Asymptotic behavior of the scattering states of $H_{2\text{-channel}}$

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 φ_{res} vanishes for large r.

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

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

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

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

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.

$$a_{op} = a_{bg} \qquad (2.29)$$

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:

$$E = E_{\text{res}} + \langle \varphi_{\text{res}} | W \, G_{\text{op}}^{+}(E) \, W | \varphi_{\text{res}} \rangle \tag{2.30}$$

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

$$\langle \varphi_{\text{res}} | W \, G_{\text{op}}^{+}(0) \, W | \varphi_{\text{res}} \rangle = \sum_{\vec{k}} \frac{\left| \langle \varphi_{\text{res}} | W | \varphi_{\vec{k}}^{+} \rangle \right|^2}{-E_{\vec{k}} + i\,\varepsilon} = \hbar\Delta_0 \tag{2.31}$$

Its interpretation is clear. It gives the shift $\hbar\Delta_0$ of φ_{res} due to the second order coupling induced by *W* between φ_{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 φ_{res}

$$\tilde{E}_{\text{res}} = E_{\text{res}} + \hbar\,\Delta_0 \tag{2.32}$$

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

Remark

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

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

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 φ_{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 φ_{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 $\tilde{E}_{\text{res}}$ 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 ξ 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 ξ.

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

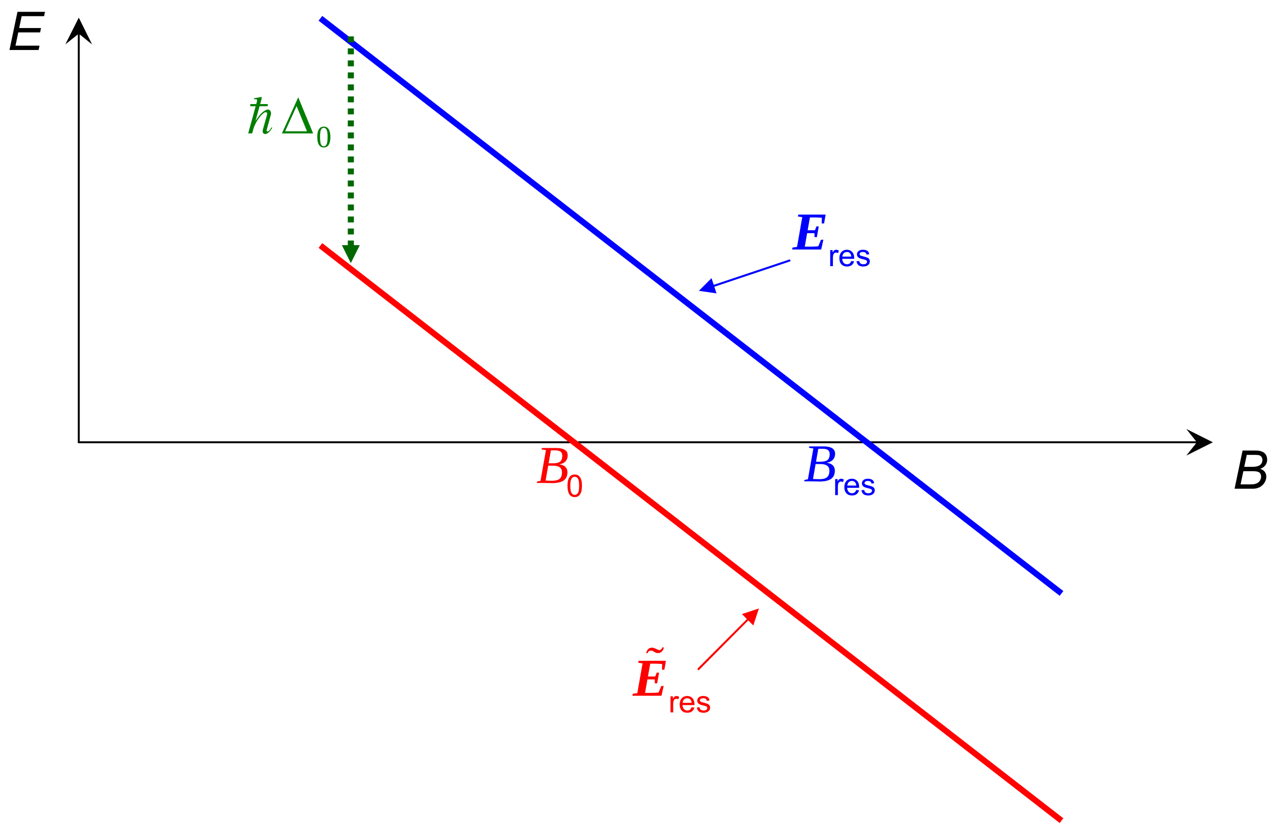
$$\boldsymbol{E}_{\text{res}} = \xi \left(\boldsymbol{B} - \boldsymbol{B}_{\text{res}} \right) \tag{2.34}$$

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

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

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

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



We suppose here $\xi < 0$

Since Δ_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 $\varphi_{\mathrm{op}}^{\vec{k}}$

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

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

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

$$\left\langle \vec{r} \right| G_{\mathrm{op}}^{+}(E) \frac{W \left| \varphi_{\mathrm{res}} \right\rangle \left\langle \varphi_{\mathrm{res}} \right| W}{E - \tilde{E}_{\mathrm{res}}} \left| \varphi_{\vec{k}}^{+} \right\rangle = \int \mathrm{d}^3 r' \left\langle \vec{r} \right| G_{\mathrm{op}}^{+}(E) \left| \vec{r}' \right\rangle \left\langle \vec{r}' \right| \frac{W \left| \varphi_{\mathrm{res}} \right\rangle \left\langle \varphi_{\mathrm{res}} \right| W}{E - \tilde{E}_{\mathrm{res}}} \left| \varphi_{\vec{k}}^{+} \right\rangle \qquad (2.37)$$

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

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

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

One can show (see Appendix) that:

$$G^{+}_{\text{op}}\left(\boldsymbol{E},\vec{\boldsymbol{r}},\vec{\boldsymbol{r}}'\right) \underset{r\to\infty}{\simeq} -\frac{\mathrm{e}^{i\,k\,r}}{\boldsymbol{r}}\,\frac{2\mu}{\hbar^2}\sqrt{\frac{\pi}{2}}\left[\varphi^{-}_{k\,\vec{n}}\left(\vec{\boldsymbol{r}}'\right)\right]^{*} \qquad \vec{\boldsymbol{n}} = \vec{\boldsymbol{r}}\,/\,\boldsymbol{r} \tag{2.39}$$

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

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

In the limit $\boldsymbol{k}\to 0,\quad \boldsymbol{E}\to 0,\ \varphi^{+}_{\vec{k}}\to\varphi^{+}_{\vec{0}}$ and $\varphi^{-}_{k\,\vec{n}}\to\varphi^{-}_{\vec{0}}=\varphi^{+}_{\vec{0}}$ since $\mathrm{e}^{\pm i\,kr}/\boldsymbol{r}\to 1/\boldsymbol{r}$ so that (2.40) can be also written, using (2.35):

$$-\frac{1}{\boldsymbol{r}}\,\frac{2\mu}{\hbar^2}\,2\pi^2\,\frac{\left|\left\langle\varphi^{+}_{\vec{0}}\middle|\boldsymbol{W}\middle|\varphi_{\text{res}}\right\rangle\right|^2}{0-\tilde{\boldsymbol{E}}_{\text{res}}} = +\frac{1}{\boldsymbol{r}}\,\frac{2\mu}{\hbar^2}\,2\pi^2\,\frac{\left|\left\langle\varphi^{+}_{\vec{0}}\middle|\boldsymbol{W}\middle|\varphi_{\text{res}}\right\rangle\right|^2}{\xi\left(\boldsymbol{B}-\boldsymbol{B}_0\right)} \tag{2.41}$$

The coefficient of -1/r in (2.41) gives the contribution of the inter-channel 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:

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

where:

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

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

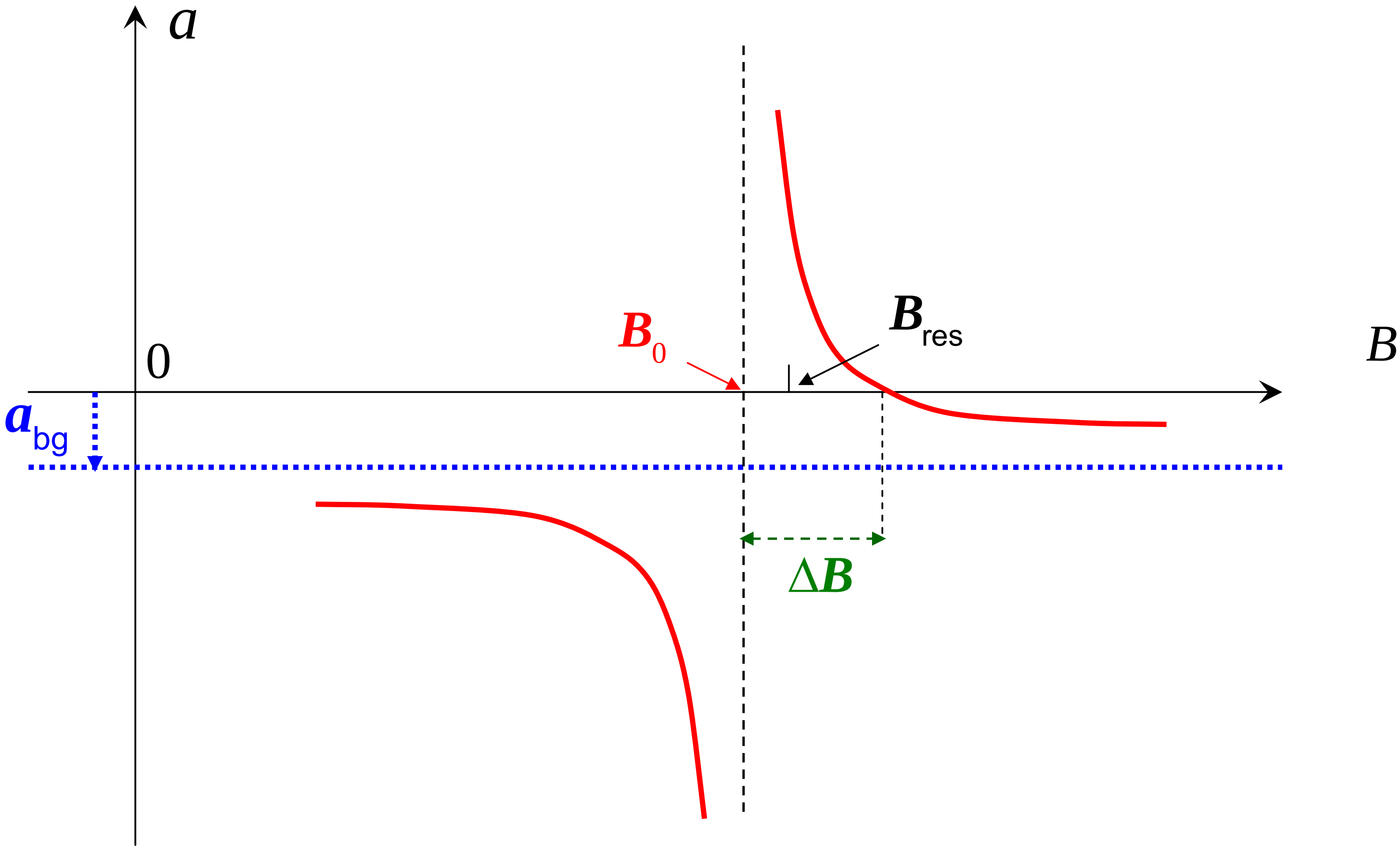
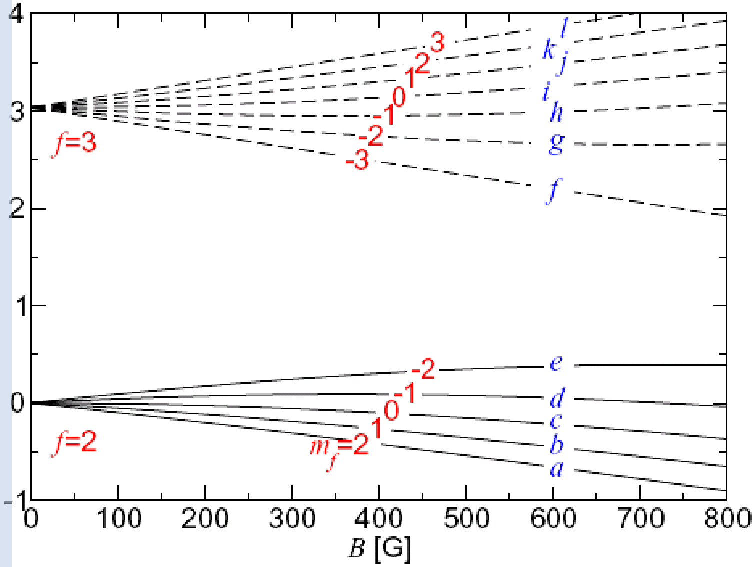


Figure corresponding to two colliding Rb^{85} atoms each in the state $f = 2$, $m_f = -2$ in a s-wave ($\ell = 0$).
In this case, we have $a_{bg} < 0$ and $\xi < 0$

Examples of broad and narrow Feshbach resonances



Zeeman and hyperfine levels of Rb[85]
(Figure taken from Ref.9)

- Entrance channel : ee

$$f_1 = 2, m_{f1} = -2,\ f_2 = 2, m_{f2} = -2,\ \ell = m_\ell = 0$$
$$M = m_{f1} + m_{f2} + m_\ell = -4$$

- Other channels with the same

$M = -4 \quad \ell = m_\ell = 0$

gg, fh   eg,df

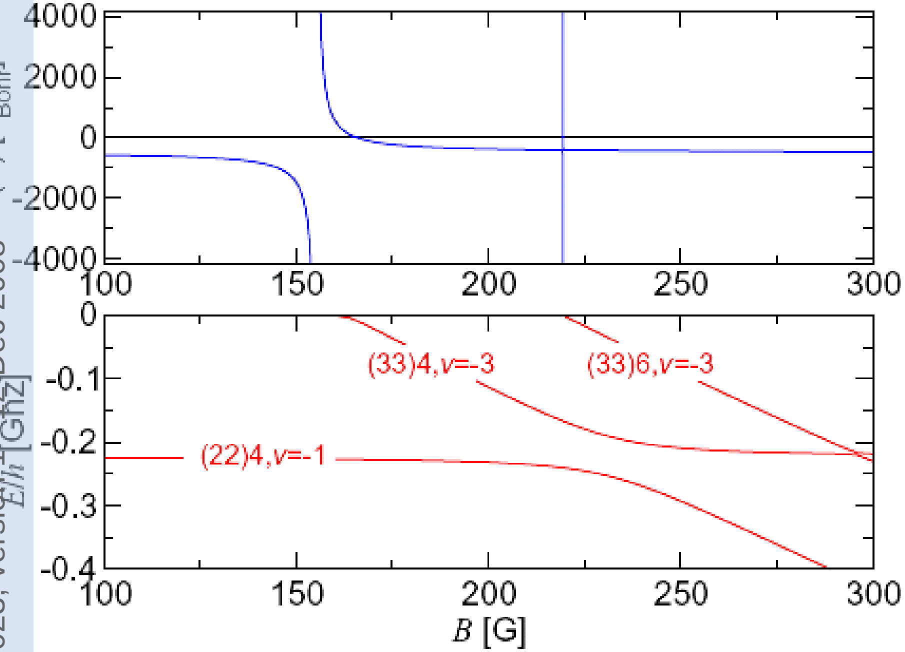
They are open because they are above the entrance channel.
They have the same negative slope ξ with respect to ee when B is varied

Classification by other quantum numbers $(f_1, f_2) F, M, \ell = m_\ell = 0 \quad (\vec{F} = \vec{f}_1 + \vec{f}_2)$

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 $(22), F = 4, M = -4$

If $f_1 = f_2 = 3,\ F = 0, 2, 4, 6$ (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



(Figure taken from Ref.9)

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 = -3

crosses 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 $H_{2\text{-channel}}$

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

We denote such a bound state

$$|\text{op}\rangle\, \varphi^{b}_{\text{op}}(\vec{r}) + |\text{cl}\rangle\, \varphi^{b}_{\text{cl}}(\vec{r}) \qquad (2.44)$$

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

$$\langle \varphi^{b}_{\text{op}} | \varphi^{b}_{\text{op}} \rangle + \langle \varphi^{b}_{\text{cl}} | \varphi^{b}_{\text{cl}} \rangle = 1 \qquad (2.45)$$

Expressing that the state (2.44) is an eigenstate of the Hamiltonian (2.8) with eigenvalue E_b, we get the following 2 equations:

$$\begin{aligned} H_{\text{op}}\, \varphi^{b}_{\text{op}}(\vec{r}) + W(r)\, \varphi^{b}_{\text{cl}}(\vec{r}) &= E_b\, \varphi^{b}_{\text{op}}(\vec{r}) \\ W(r)\, \varphi^{b}_{\text{op}}(\vec{r}) + H_{\text{cl}}\, \varphi^{b}_{\text{cl}}(\vec{r}) &= E_b\, \varphi^{b}_{\text{cl}}(\vec{r}) \end{aligned} \qquad (2.46)$$

Bound states of the two-channel Hamiltonian $H_{2\text{-channel}}$ (continued)

To solve equation (2.46), we can use the Green functions of H_{op} and H_{cl} without the iε term because E_b is negative (below the threshold of V_{op})

$$\left|\varphi_{op}^{b}\right\rangle = G_{op}(E_b)\,W\left|\varphi_{cl}^{b}\right\rangle \qquad \left|\varphi_{cl}^{b}\right\rangle = G_{cl}(E_b)\,W\left|\varphi_{op}^{b}\right\rangle \tag{2.47}$$

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

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

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

$$\begin{pmatrix}\varphi_{op}^{b}\\ \varphi_{cl}^{b}\end{pmatrix} = \frac{1}{N_b}\begin{pmatrix}G_{op}(E_b)\,W\,\varphi_{res}\\ \varphi_{res}\end{pmatrix} \tag{2.49}$$

where N_b is a normalization factor

$$N_b = \sqrt{1 + \left\langle\varphi_{res}\left|W\,G_{op}^{2}(E_b)W\right|\varphi_{res}\right\rangle} \tag{2.50}$$

Implicit equation for the energy E_b

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

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

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

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

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

$$E_b - E_{\rm res} = \left\langle\varphi_{\rm res}\right| W\, G_{\rm op}(E_b)\, W \left|\varphi_{\rm res}\right\rangle \qquad (2.53)$$

Now, using the identity

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

we can rewrite (2.53) as:

$$E_b = E_{\rm res} + \left\langle\varphi_{\rm res}\right| W G_{\rm op}(0) W \left|\varphi_{\rm res}\right\rangle - E_b \left\langle\varphi_{\rm res}\right| W G_{\rm op}(0) G_{\rm op}(E_b) W \left|\varphi_{\rm res})\right\rangle$$

(2.55)

Implicit equation for the energy E_b (continued)

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

$$E_b = \tilde{E}_{res} - E_b \left\langle \varphi_{res} \middle| W\, G_{op}(0)\, G_{op}(E_b)\, W \middle| \varphi_{res} \right\rangle \tag{2.56}$$

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

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

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:

$$E_b = \tilde{E}_{res} - (2\mu)^2 E_b \int d^3k \frac{\left| \left\langle \varphi_{res} \middle| W \middle| \varphi_{\vec{k}}^{+} \right\rangle \right|^2}{\hbar^2 k^2 \left(\hbar^2 k^2 + 2\mu \left| E_b \right| \right)} \tag{2.58}$$

This is an implicit equation for E_b that we will try now to solve

Calculation of the energy E_b

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

$$u = \frac{\hbar\, k}{\sqrt{2\mu \left| E_b \right|}} \qquad (2.59)$$

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

$$\frac{1}{\hbar^3} \frac{4\pi}{\sqrt{2\mu \left| E_b \right|}} \int_0^\infty du \, \frac{\left| \left\langle \varphi_{\text{res}} \left| W \right| \varphi_{\vec{k}}^{+} \right\rangle \right|^2}{\left(u^2 + 1 \right)} \qquad (2.60)$$

Let k_0 be the width of $\left| \left\langle \varphi_{\text{res}} \left| W \right| \varphi_{\vec{k}}^{+} \right\rangle \right|^2$ considered as a function of k.

This defines a value u_0 of u

$$u_0 = \frac{\hbar\, k_0}{\sqrt{2\mu \left| E_b \right|}} \qquad (2.61)$$

characterizing the width in u of the numerator of the integral of (2.60).

Two different limits can be considered: $u_0 \gg 1$ and $u_0 \ll 1$?

Calculation of the energy E_b (continued)

First limit $\quad u_0 \gg 1 \quad \Leftrightarrow \quad |E_b| \ll \hbar^2 k_0^2 / 2\mu$

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:

$$\frac{1}{\hbar^3} \frac{4\pi}{\sqrt{2\mu |E_b|}} \left| \langle \varphi_{\text{res}} | W | \varphi_{\vec{0}}^+ \rangle \right|^2 \underbrace{\int_0^\infty \frac{du}{u^2 + 1}}_{=\pi/2} \tag{2.62}$$

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

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

One can then reexpress $\left| \langle \varphi_{\text{res}} | W | \varphi_{\vec{0}}^+ \rangle \right|^2$ in terms of ΔB 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:

$$E_b = -\frac{\hbar^2}{2\mu a^2} \tag{2.64}$$

Calculation of the energy E_b (continued)

Second limit $u_0 \ll 1 \quad \Leftrightarrow \quad |E_b| \gg \hbar^2 k_0^2 / 2\mu$

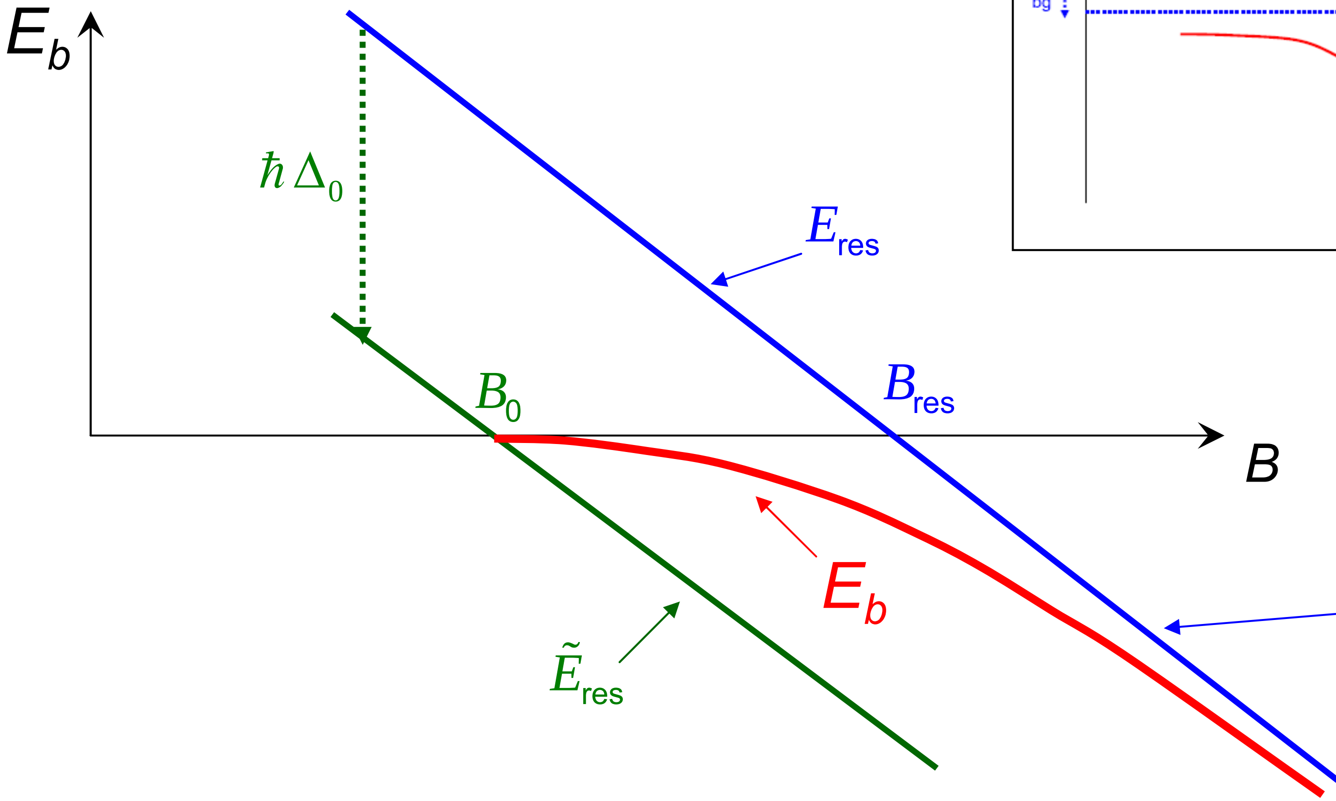
The numerator of the integral of (2.60) varies more rapidly with u than the denominator, so that we can neglect the term u^2 in the denominator.

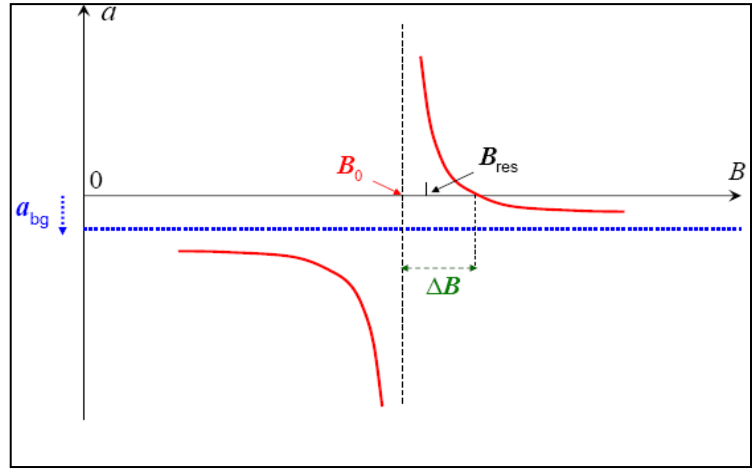
In fact, this approximation amounts to neglecting $\hbar^2 k^2$ compared to $2\mu |E_b|$ in the denominator of the integral of (2.58)

This approximation allows one to transform (2.58) into:

$$\begin{aligned} E_b &= \tilde{E}_{\text{res}} + (2\mu)^2 \int \mathrm{d}^3k \, \frac{\left|\langle \varphi_{\text{res}} | W | \varphi_{\vec{k}}^+ \rangle\right|^2}{2\mu \, \hbar^2 k^2} \\ &= \tilde{E}_{\text{res}} + \int \mathrm{d}^3k \, \frac{\left|\langle \varphi_{\text{res}} | W | \varphi_{\vec{k}}^+ \rangle\right|^2}{\hbar^2 k^2 / 2\mu} \\ &= \tilde{E}_{\text{res}} - \hbar\Delta_0 = E_{\text{res}} = \xi\left(B - B_{\text{res}}\right) \end{aligned} \qquad (2.65)$$

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





- The bound state of $H_{2\text{-channel}}$ appears for $B > B_0$, in the region a>0.
- E_b first decreases quadratically with B-B_0 and then tends to the unperturbed energy E_{res} of the bound state φ_{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 φ_{cl}^{b} in the (normalized) wave function of $H_{\text{2-channel}}$ is given by:

$$\left\langle \varphi_{\text{cl}}^{b} \middle| \varphi_{\text{cl}}^{b} \right\rangle = \frac{1}{N_b^2} \qquad N_b^2 = 1 + \left\langle \varphi_{\text{res}} \middle| W\, G_{\text{op}}^2(E_b) W \middle| \varphi_{\text{res}} \right\rangle \tag{2.66}$$

Using

$$G_{\text{op}}(E_b) = \frac{1}{E_b - H_{\text{op}}} \quad \Rightarrow \quad \frac{\partial}{\partial E_b} G_{\text{op}}(E_b) = -\frac{1}{\left(E_b - H_{\text{op}}\right)^2} = -G_{\text{op}}^2(E_b) \tag{2.67}$$

we can rewrite the second equation (2.66) as:

$$N_b^2 = 1 - \frac{\partial}{\partial E_b} \left\langle \varphi_{\text{res}} \middle| W\, G_{\text{op}}(E_b) W \middle| \varphi_{\text{res}} \right\rangle \tag{2.68}$$

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

$$E_b = \underbrace{E_{\text{res}}}_{=\xi\left(B - B_{\text{res}}\right)} + \left\langle \varphi_{\text{res}} \middle| W\, G_{\text{op}}(E_b) W \middle| \varphi_{\text{res}} \right\rangle \tag{2.69}$$

Wave function of the bound state (continued)

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

$$\frac{\partial E_b}{\partial B} = \xi + \underbrace{\frac{\partial}{\partial E_b}\left\langle \varphi_{\text{res}} \middle| W\, G_{\text{op}}(E_b) W \middle| \varphi_{\text{res}} \right\rangle}_{=1-N_b^2} \frac{\partial E_b}{\partial B} \tag{2.70}$$

This finally gives:

$$\frac{1}{N_b^2} = \frac{\partial E_b / \partial B}{\xi} \tag{2.71}$$

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 ξ 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

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 $V_{op}=0$.

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

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

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

Comparison with quantitative calculations

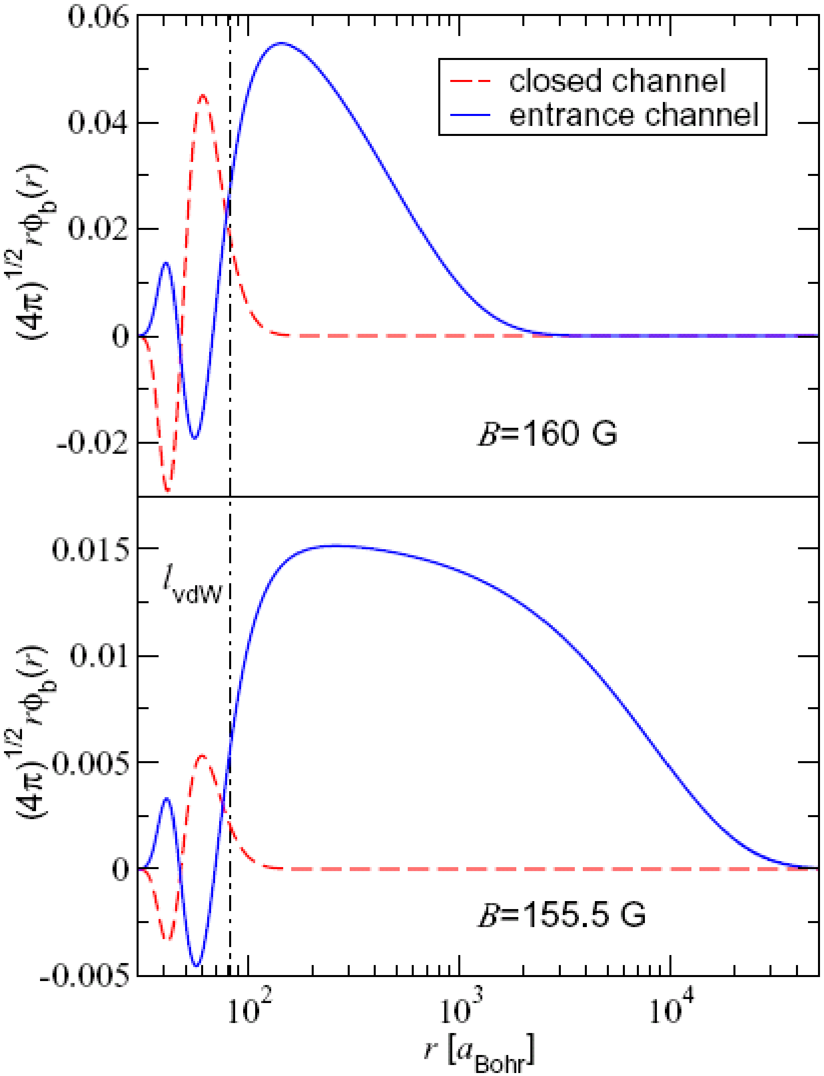


Figure taken from Ref. 9

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

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 $B=B_0$, 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)

APPENDIX

For the 2 lectures of Claude Cohen-Tannoudji on "Atom-Atom Interactions in Ultracold Quantum Gases"

Purpose of this Appendix

1 – Demonstrate the orthonormalization relation

$$\left\langle \varphi_{k'l'm'} \middle| \varphi_{klm} \right\rangle = \delta(k-k')\delta_{ll'}\delta_{mm'} \qquad \text{(A.1)}$$

- The wave function

$$\varphi_{klm}(\vec{r}) = \sqrt{\frac{2}{\pi}} \frac{u_{kl}(r)}{r} Y_{lm}(\theta,\varphi) \qquad \text{(A.2)}$$

describes, in the angular momentum representation, a particle of mass μ, with energy $E=\hbar^2 k^2/2\mu$, in a central potential $V(r)$

- The radial wave function $u_{kl}(r)$ is a regular solution of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2} V_{\text{tot}}(r)\right] u_{kl}(r) = 0 \qquad V_{\text{tot}}(r) = V(r) + \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} \qquad \text{(A.3)}$$

$$u_{kl}(0) = 0 \qquad \text{(A.4)}$$

which behaves, for r→∞, as:

$$u_{kl}(r) \underset{r\to\infty}{\simeq} \sin\left[kr - l\pi/2 + \delta_l(k)\right] \qquad \text{(A.5)}$$

- There are other (non regular) solutions behaving, for r→∞, as:

$$u^{\pm}_{kl}(r) \underset{r\to\infty}{\simeq} \exp\left[\pm i\left(kr - l\pi/2\right)\right] = (\mp i)^l \exp(\pm ikr) \qquad \text{(A.6)}$$

2 – Calculate the Green function of: $H = p^2 / 2\mu + V(r)$

with outgoing and ingoing asymptotic behavior

$$\left(E - H\right) G^{(\pm)}\left(\vec{r}, \vec{r}'\right) = \delta\left(\vec{r} - \vec{r}'\right) \qquad E = \hbar^2 k^2 / 2\mu \qquad \textbf{(A.7)}$$

- Show that:

$$G^{(\pm)}\left(\vec{r}, \vec{r}'\right) = -\frac{2\mu}{\hbar^2}\frac{1}{krr'}\sum_{lm}\exp\left(\pm i\,\delta_l\right) Y_{lm}^*(\theta, \varphi)Y_{lm}(\theta', \varphi')u_{kl}(r_<)u_{kl}^{\pm}(r_>) \qquad \textbf{(A.8)}$$

where $r_>$ ($r_<$) is the largest (smallest) of r and r'

- Introducing the Heaviside function:

$$\theta\left(r - r'\right) = +1 \quad \text{if} \quad r > r' \qquad \textbf{(A.9)}$$
$$= 0 \quad \text{if} \quad r < r'$$

(A.8) can also be written:

$$G^{(\pm)}\left(\vec{r}, \vec{r}'\right) = -\frac{2\mu}{\hbar^2}\frac{1}{krr'}\sum_{lm}\exp\left(\pm i\,\delta_l\right) Y_{lm}^*(\theta, \varphi)Y_{lm}(\theta', \varphi') \times$$
$$\times\left[\theta\left(r - r'\right)u_{kl}(r')u_{kl}^{\pm}(r) + \theta\left(r' - r\right)u_{kl}(r)u_{kl}^{\pm}(r')\right] \qquad \textbf{(A.10)}$$

3 – Calculate the asymptotic behavior of these Green functions

and demonstrate Equation (2.39) of Lecture 2

Wronskian Theorem

The calculations presented in this Appendix use the Wronskian theorem (see demonstration in Ref.2 Chapter III-8)

- Consider the 1D second order differential equation:

$$y''(r) + F(r)y(r) = 0 \qquad \text{(A.11)}$$

Equation (A.4) is of this type with:

$$F(r) = k^2 - \frac{2\mu}{\hbar^2} V_{\text{tot}}(r) \qquad \text{(A.12)}$$

- Let $y_1(r)$ and $y_2(r)$ be 2 solutions of this equation corresponding to 2 different functions $F_1(r)$ and $F_2(r)$, respectively.

The wronskian of y_1 and y_2 is by definition:

$$W(y_1, y_2) = y_1(r)y_2'(r) - y_2(r)y_1'(r) \qquad \text{(A.13)}$$

- One can show that:

$$\begin{aligned} W(y_1, y_2)\Big|_a^b &= \left[W(y_1, y_2)\right]_{r=b} - \left[W(y_1, y_2)\right]_{r=a} \\ &= \int_a^b \left[F_1(r) - F_2(r)\right] y_1(r)\, y_2(r)\, \mathrm{d}r \end{aligned} \qquad \text{(A.14)}$$

Demonstration of (A.1)

We consider 2 different values k_1 and k_2 of k. According to (A.12):

$$F_1(r) - F_2(r) = k_1^2 - k_2^2 \tag{A.15}$$

(A.14) then gives the scalar product of $y_1 = u_{k_1 l}$ and $y_2 = u_{k_2 l}$

$$\int_a^b y_1(r)\, y_2(r)\, \mathrm{d}r = \frac{1}{k_1^2 - k_2^2} W(y_1, y_2)\Big|_a^b \tag{A.16}$$

If we take $a = 0, \left[W(y_1, y_2)\right]_{r=a} = 0$ because of (A.4)

If we take $b = R$ very large compared to the range of $V(r)$, we can use the asymptotic behavior (A.5) of $u_{k_1 l}$ and $u_{k_2 l}$

$$\int_0^R u_{k_1 l}(r)\, u_{k_2 l}(r)\, \mathrm{d}r = \frac{1}{k_1^2 - k_2^2}\left[u_{k_1 l}(r) u'_{k_2 l}(r) - u_{k_2 l}(r) u'_{k_1 l}(r)\right]_{r=R} \tag{A.17}$$

Using (A.15) and putting $\delta_l(k_1) = \delta_1, \delta_l(k_2) = \delta_2$, we get:

$$\int_0^R u_{k_1 l}(r)\, u_{k_2 l}(r)\, \mathrm{d}r = -\frac{1}{2}\frac{\sin\left[\left(k_1 + k_2\right) R - \ell\pi + \delta_1 + \delta_2\right]}{k_1 + k_2} + \frac{1}{2}\frac{\sin\left[\left(k_1 - k_2\right) R + \delta_1 - \delta_2\right]}{k_1 - k_2} \tag{A.18}$$

- When R→∞, the first term of the right side of (A.18) vanishes as a distribution, because it is a rapidly oscillating function of k_1+k_2 (k_1 and k_2 being both positive k_1+k_2 cannot vanish)

- The second term becomes important when k_1-k_2 is close to zero (we have then $\delta_1-\delta_2=0$)

- Using:

$$\lim_{R\to\infty} \frac{1}{\pi} \frac{\sin R\, x}{x} = \delta(x) \qquad \textbf{(A.19)}$$

we get:

$$\int_0^\infty u_{k_1 l}(r)\, u_{k_2 l}(r)\, \mathrm{d}r = \frac{\pi}{2}\,\delta(k_1 - k_2) \qquad \textbf{(A.20)}$$

- We then have, according to (A.2):

$$\int \mathrm{d}^3 r\; \varphi^*_{k'l'm'}(\vec{r})\; \varphi_{klm}(\vec{r}) = \frac{2}{\pi} \underbrace{\int \mathrm{d}\Omega\, Y^*_{l'm'}(\theta,\varphi)\, Y_{lm}(\theta,\varphi)}_{=\delta_{ll'}\delta_{mm'}} \underbrace{\int u_{kl}(r)\, u_{k'l}(r)\,\mathrm{d}r}_{=\frac{\pi}{2}\delta(k-k')}$$

$$= \delta(k - k')\,\delta_{ll'}\delta_{mm'} \qquad \textbf{(A.21)}$$

which demonstrates (A.1).

Demonstration of (A.8)

Let us apply E-H to the right side of (A.8). Using (A.10) and:

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(r) = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2} - \frac{\vec{L}^2}{\hbar^2 r^2} - \frac{2\mu}{\hbar^2}V(r)\right] \quad \textbf{(A.22)}$$

we get, using (A.12):

$$\left(E - H\right)G^{(\pm)}\left(\vec{r},\vec{r}'\right) = -\frac{1}{krr'}\sum_{lm}\exp\left(\pm i\,\delta_l\right)Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi') \times$$
$$\times\left\{\left(F(r) + \frac{\partial^2}{\partial r^2}\right)\left[\theta\left(r - r'\right)u_{kl}(r')u^{\pm}_{kl}(r) + \theta\left(r' - r\right)u_{kl}(r)u^{\pm}_{kl}(r')\right]\right\} \quad \textbf{(A.23)}$$

To calculate the second line of (A.23), we use:

$$\frac{\partial}{\partial r_1}\theta\left(r_1 - r_2\right) = -\frac{\partial}{\partial r_1}\theta\left(r_2 - r_1\right) = \delta\left(r_1 - r_2\right)$$
$$\left[\frac{\partial}{\partial r_1}\delta\left(r_1 - r_2\right)\right]f(r_1) = -f'(r_2)\delta\left(r_1 - r_2\right) + f(r_2)\left[\frac{\partial}{\partial r_1}\delta\left(r_1 - r_2\right)\right] \quad \textbf{(A.24)}$$

The second order derivative of the second line of (A.23) gives 3 types of terms: proportional to $\theta(r - r')$ and $\theta(r' - r)$, to $\delta(r - r')$ and to $\partial\delta(r - r')/\partial r$

- The terms $\propto \theta(\boldsymbol{r} - \boldsymbol{r}')$ are multiplied by $\left[\boldsymbol{F}(\boldsymbol{r}) + \left(\partial^2 / \partial \boldsymbol{r}^2\right)\right] \boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r})$ which vanishes because $\boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r})$ is a solution of (A.3).

The same argument applies for the terms $\propto \theta(\boldsymbol{r}' - \boldsymbol{r})$ which are multiplied by $\left[\boldsymbol{F}(\boldsymbol{r}) + \left(\partial^2 / \partial \boldsymbol{r}^2\right)\right] \boldsymbol{u}_{kl}(\boldsymbol{r}) = 0$

- The terms proportional to $\partial \delta(\boldsymbol{r} - \boldsymbol{r}') / \partial \boldsymbol{r}$ cancel out

- The only terms surviving in the second line of (A.23) are those proportional to $\delta(\boldsymbol{r} - \boldsymbol{r}')$, which gives for this line:

$$\left[\boldsymbol{u}_{kl}(\boldsymbol{r}') \left(\partial \boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r}') / \partial \boldsymbol{r}'\right) - \boldsymbol{u}_{kl}^{\pm}(\boldsymbol{r}') \left(\partial \boldsymbol{u}_{kl}(\boldsymbol{r}') / \partial \boldsymbol{r}'\right)\right] \delta(\boldsymbol{r} - \boldsymbol{r}') \qquad \textbf{(A.25)}$$

- We recognize in the bracket of (A.25) the Wronskian of $\boldsymbol{u}_{kl}$ and $\boldsymbol{u}_{kl}^{\pm}$

We can thus use (A.14) with $\boldsymbol{F}_1 = \boldsymbol{F}_2$ since $\boldsymbol{u}_{kl}$ and $\boldsymbol{u}_{kl}^{\pm}$ correspond to the same value of $\boldsymbol{k}$.

- Equation (A.14) shows that the Wronskian is independant of $\boldsymbol{r}$ when $\boldsymbol{F}_1 = \boldsymbol{F}_2$. We can thus calculate it for very large values of $\boldsymbol{r}$ where we know the asymptotic behavior (A.5) and (A.6) of $\boldsymbol{u}_{kl}$ and $\boldsymbol{u}_{kl}^{\pm}$

- The calculation of the Wronskian appearing in (A.25) is straightforward using (A.5) and (A.6) and gives:

$$W(u_{kl}, u_{kl}^{+}) = -k \exp(\mp i\delta_l) \tag{A.26}$$

- Inserting (A.26) into (A.25) and then in (A.23) gives:

$$(E - H)\, G^{(\pm)}(\vec{r}, \vec{r}') = \frac{1}{r^2}\, \delta(r - r') \sum_{lm} Y_{lm}^{*}(\theta, \varphi) Y_{lm}(\theta', \varphi') \tag{A.27}$$

- We can then use the closure relation for the spherical harmonics (see Ref. 3, Complement AVI):

$$\sum_{lm} Y_{lm}^{*}(\theta, \varphi) Y_{lm}(\theta', \varphi') = \delta(\cos\theta - \cos\theta')\, \delta(\varphi - \varphi') \tag{A.28}$$

to obtain:

$$\begin{aligned} (E - H)\, G^{(\pm)}(\vec{r}, \vec{r}') &= \frac{1}{r^2}\, \delta(r - r')\, \delta(\cos\theta - \cos\theta')\, \delta(\varphi - \varphi') \\ &= \delta(\vec{r} - \vec{r}') \end{aligned} \tag{A.29}$$

which demonstrates (A.8).

Asymptotic behavior of G+

For r very large, only the first term of the bracket of (A.10) is non zero and we get:

$$G^{(+)}(\vec{r},\vec{r}\,') \underset{r\to\infty}{\simeq} -\frac{2\mu}{\hbar^2}\frac{1}{krr'}\sum_{lm} e^{i\delta_l}\, Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi')u_{kl}(r')u^+_{kl}(r) \tag{A.30}$$

According to (A.6), we have

$$G^{(+)}(\vec{r},\vec{r}\,') \underset{r\to\infty}{\simeq} -\frac{2\mu}{\hbar^2}\frac{1}{kr'}\sum_{lm}(-i)^l e^{i\delta_l}\, Y^*_{lm}(\theta,\varphi)Y_{lm}(\theta',\varphi')u_{kl}(r')\frac{e^{ikr}}{r} \tag{A.31}$$

On the other hand, from Eq. (1.46) of lecture 1 and (A.2), we have:

$$\varphi^-_{k\vec{n}}(\vec{r}\,') = \frac{1}{k}\sqrt{\frac{2}{\pi}}\sum_{lm}(i)^l \exp(-i\delta_l)\, Y^*_{lm}(\vec{n})\, Y_{lm}(\vec{n}\,')\,\frac{u_{kl}(r')}{r'} \qquad \vec{n}=\frac{\vec{r}}{r} \quad \vec{n}\,'=\frac{\vec{r}\,'}{r'} \tag{A.32}$$

Using (A.32), we can rewrite (A.31) as:

$$G^{(+)}(\vec{r},\vec{r}\,') \underset{r\to\infty}{\simeq} -\frac{2\mu}{\hbar^2}\sqrt{\frac{\pi}{2}}\left[\varphi^-_{k\vec{n}}(\vec{r}\,')\right]^*\frac{e^{ikr}}{r} \tag{A.33}$$

which demonstrates Eq. (2.39) of lecture 2.