

Atom-Atom Interactions in Ultracold Quantum Gases

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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 3^{ème} 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

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

Change of variables

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

$$M = m_1 + m_2 = 2m \quad \text{Total mass}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \quad \vec{p} = (\vec{p}_1 - \vec{p}_2) / 2 \quad \text{Relative variables}$$

$$\mu = m_1 m_2 / (m_1 + m_2) = m / 2 \quad \text{Reduced mass}$$

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

Hamiltonian of a free particle with mass M

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

Finite range potential

Simple case where $V(\vec{r}) = 0$ 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

$$b_{\text{VdW}} = \left(\frac{2\mu C_6}{\hbar^2} \right)^{1/4} \quad (1.3)$$

See for example Ref. 5

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Scattering by a potential. A brief reminder

Schrödinger equation for the relative particle (with $E > 0$)

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

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

Green function of $\Delta + k^2$

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

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

Integral equation for the solution of Schrödinger equation

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

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

$$\psi(\vec{r}) = \varphi_0(\vec{r}) + \int d^3r' G(\vec{r} - \vec{r}') V(\vec{r}') \psi(\vec{r}') \quad (1.8)$$

Choice of boundary conditions

We choose for φ_0 a plane wave with wave vector \mathbf{k}

$$\varphi_0(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} = e^{i k \vec{\kappa}\cdot\vec{r}} \quad \vec{\kappa} = \vec{k} / k \quad (1.9)$$

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

$$G_+(\vec{r} - \vec{r}') = -\frac{1}{4\pi} \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|} \quad (1.10)$$

We thus get the following solution for Schrödinger equation

$$\psi_{\vec{k}}^+(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|} V(\vec{r}') \psi_{\vec{k}}^+(\vec{r}') \quad (1.11)$$

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

$$\text{If } r \gg b, \quad |\vec{r} - \vec{r}'| \simeq r - \vec{r}' \cdot \vec{n} \quad \text{with } \vec{n} = \vec{r} / r$$

$$\psi_{\vec{k}}^+(\vec{r}) \simeq e^{i\vec{k}\cdot\vec{r}} - f(k, \vec{\kappa}, \vec{n}) \frac{e^{ikr}}{r} \quad (1.12)$$

$$f(k, \vec{\kappa}, \vec{n}) = -\frac{2\mu}{4\pi\hbar^2} \int d^3r' e^{-ik\vec{n}\cdot\vec{r}'} V(\vec{r}') \psi_{\vec{k}}^+(\vec{r}')$$

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 $\exp(i \vec{k} \cdot \vec{r})$ and of an outgoing spherical wave $f(k, \vec{k}, \vec{n}) \exp(i k r) / r$

Scattering amplitude f

$$f(k, \vec{k}, \vec{n}) = -\frac{2\mu}{4\pi\hbar^2} \int d^3r' e^{-i \vec{k}' \cdot \vec{r}'} V(\vec{r}') \psi_{\vec{k}}^+(\vec{r}') \quad (1.13)$$

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

$f(k, \vec{k}, \vec{n})$ 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 \mathbf{k} and \mathbf{k}' , one gets :

$$d\sigma / d\Omega = |f(k, \vec{k}, \vec{n})|^2 \quad (1.14)$$

Born approximation

In the scattering amplitude, the potential V appears explicitly

$$f(k, \vec{k}, \vec{n}) = -\frac{2\mu}{4\pi\hbar^2} \int d^3r' e^{-i\vec{k}'\cdot\vec{r}'} V(\vec{r}') \psi_{\vec{k}}^+(\vec{r}') \quad (1.15)$$

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

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

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 $V(\mathbf{r}')$ in the scattering amplitude

$$f(k, \vec{\kappa}, \vec{n}) = -\frac{2\mu}{4\pi\hbar^2} \int d^3r' e^{-i\vec{\kappa}'\cdot\vec{r}'} V(\vec{r}') \psi_{\vec{\kappa}}^+(\vec{r}') \quad (1.17)$$

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

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

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

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

$$\text{When } k \rightarrow 0, \quad f(k, \vec{\kappa}, \vec{n}) \rightarrow -a$$
$$\psi_{\vec{\kappa}}^+(\vec{r}) \simeq e^{i\vec{\kappa}\cdot\vec{r}} - a \frac{e^{i\kappa r}}{r} \rightarrow 1 - \frac{a}{r} \quad (1.19)$$

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)

$$\left| \psi_{\vec{k}}^+ \right\rangle = \left| \phi_{\vec{k}} \right\rangle + \text{Lim}_{\varepsilon \rightarrow 0_+} \frac{1}{E - T + i\varepsilon} V \left| \psi_{\vec{k}}^+ \right\rangle \quad T = p^2 / 2\mu \quad (1.20)$$

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 $\left| \phi_{\vec{k}} \right\rangle$ at $t = -\infty$ and by switching on slowly V on a time interval on the order of \hbar / ε

Ingoing scattering state

$$\psi_{\vec{k}}^-(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \int d^3r' \frac{e^{-i k|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi_{\vec{k}}^-(\vec{r}') \quad (1.21)$$
$$\left| \psi_{\vec{k}}^- \right\rangle = \left| \phi_{\vec{k}} \right\rangle + \text{Lim}_{\varepsilon \rightarrow 0_+} \frac{1}{E - T - i\varepsilon} V \left| \psi_{\vec{k}}^- \right\rangle$$

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 / ε , one gets the free state $\left| \phi_{\vec{k}} \right\rangle$ at $t = +\infty$

S - Matrix

Definition

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

\tilde{U} : evolution operator in interaction representation

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

Qualitative interpretation

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

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

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 $t = -\infty$.

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Central potential

V depends only on r

1D radial Schrödinger equation

One looks for solutions of the form

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

If we put

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

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

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

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

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

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

Case of a free particle (V=0)

The solutions of the Schrödinger equation are:

$$\varphi_{klm}^{(0)}(\vec{r}) = \sqrt{\frac{2k^2}{\pi}} j_l(kr) Y_{lm}(\vec{n}) \quad (1.29)$$

where the j_l are the spherical Bessel functions of order l

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

For large r we thus have

$$\begin{aligned} \varphi_{klm}^{(0)}(\vec{r}) &\underset{r \rightarrow \infty}{\approx} \sqrt{\frac{2}{\pi}} Y_{lm}(\vec{n}) \frac{\sin(kr - l\pi/2)}{r} \\ &= \sqrt{\frac{2}{\pi}} Y_{lm}(\vec{n}) \frac{\left[e^{i(kr - l\pi/2)} - e^{-i(kr - l\pi/2)} \right]}{2ir} \\ &= \text{outgoing spherical wave} + \text{ingoing spherical wave} \end{aligned} \quad (1.31)$$

These functions form an orthonormal set (see Appendix)

$$\left\langle \varphi_{k'l'm'}^{(0)} \mid \varphi_{klm}^{(0)} \right\rangle = \delta(\mathbf{k} - \mathbf{k}') \delta_{ll'} \delta_{mm'} \quad (1.32)$$

Expansion of a plane wave in free spherical waves

Plane wave

$$\langle \vec{r} | \vec{k} \rangle = (2\pi)^{-3/2} e^{i \vec{k} \cdot \vec{r}} \quad \langle \vec{k}' | \vec{k} \rangle = \delta(\vec{k} - \vec{k}') \quad (1.33)$$

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

One can show that:

$$\begin{aligned} (2\pi)^{-3/2} e^{i \vec{k} \cdot \vec{r}} &= (2\pi)^{-3/2} 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} (i)^l Y_{lm}(\vec{n}) Y_{lm}^*(\vec{k}) j_l(kr) \\ &= \frac{1}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} (i)^l Y_{lm}^*(\vec{k}) \varphi_{klm}^{(0)}(\vec{r}) \end{aligned} \quad (1.34)$$

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

The transformation from the orthonormal basis $\{ | \vec{k} \rangle \}$ to the orthonormal basis $\{ | \varphi_{klm}^{(0)} \rangle \}$ is given by the matrix

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

Effect of a potential. Phase shifts

We come back to the Schrödinger equation with $V \neq 0$. Consider, for r large, an incoming wave $\exp[-i(kr - l\pi/2)]$. 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:

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

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

$$\langle \varphi_{k'l'm'} | \varphi_{klm} \rangle = \delta(k - k') \delta_{ll'} \delta_{mm'} \quad (1.37)$$

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)

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

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:

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

Using $\exp i(kr - l\pi/2 + 2\delta_l) = \exp i(kr - l\pi/2) \times \left[1 + (e^{2i\delta_l} - 1)\right]$
we get: (1.40)

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

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

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

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

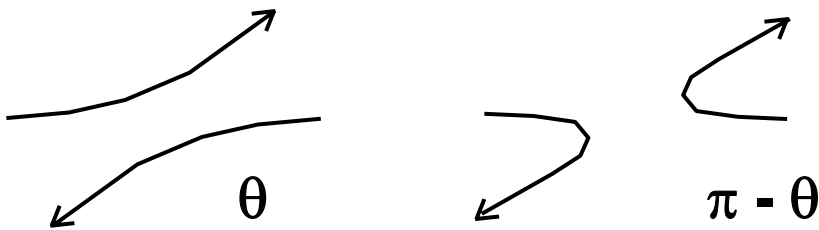
Scattering amplitude in terms of the phase shifts

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

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

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

Scattering of 2 identical particles



Quantum interference between
2 different paths

$$\begin{aligned}
 f_k(\theta) &\rightarrow f_k(\theta) + \varepsilon f_k(\pi - \theta) \\
 \varepsilon &= +1 \text{ } (-1) \text{ for bosons (fermions)}
 \end{aligned}$$

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

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 $\exp(i\delta_l)$.

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

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 $e^{-i\delta_l}$ to 1 which corresponds to acquiring a phase factor $e^{+i\delta_l}$

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 $e^{+i\delta_l} \times e^{+i\delta_l} = e^{+2i\delta_l}$

S – Matrix in the angular momentum representation

$$S_{\vec{k}' \vec{k}} = \langle \vec{k}' | S | \vec{k} \rangle = \langle \psi_{\vec{k}'}^- | \psi_{\vec{k}}^+ \rangle \quad (1.47)$$

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

$$|\psi_{\vec{k}}^+\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \langle \varphi_{klm}^{(0)} | \vec{k} \rangle e^{i\delta_l} |\varphi_{klm}\rangle \quad |\psi_{\vec{k}'}^-\rangle = \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=+l'} \langle \varphi_{k'l'm'}^{(0)} | \vec{k}' \rangle e^{-i\delta_{l'}} |\varphi_{k'l'm'}\rangle \quad (1.48)$$

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

$$S_{\vec{k}' \vec{k}} = \langle \psi_{\vec{k}'}^- | \psi_{\vec{k}}^+ \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=+l'} \langle \vec{k}' | \varphi_{k'l'm'}^{(0)} \rangle e^{+i\delta_l} \underbrace{\langle \varphi_{k'l'm'} | \varphi_{klm} \rangle}_{\delta(\vec{k}-\vec{k}')\delta_{l'l'}\delta_{mm'}} e^{i\delta_{l'}} \langle \varphi_{klm}^{(0)} | \vec{k} \rangle \quad (1.49)$$

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

$$S_{\vec{k}' \vec{k}} = \langle \vec{k}' | S | \vec{k} \rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=+l'} \langle \vec{k}' | \varphi_{k'l'm'}^{(0)} \rangle \langle \varphi_{k'l'm'}^{(0)} | S | \varphi_{klm}^{(0)} \rangle \langle \varphi_{klm}^{(0)} | \vec{k} \rangle \quad (1.50)$$

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

$$\langle \varphi_{k'l'm'}^{(0)} | S | \varphi_{klm}^{(0)} \rangle = e^{+2i\delta_l} \delta(\vec{k} - \vec{k}') \delta_{l'l'} \delta_{mm'} \quad (1.51)$$

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

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- S-Matrix in the angular momentum representation

4 - Low energy limit

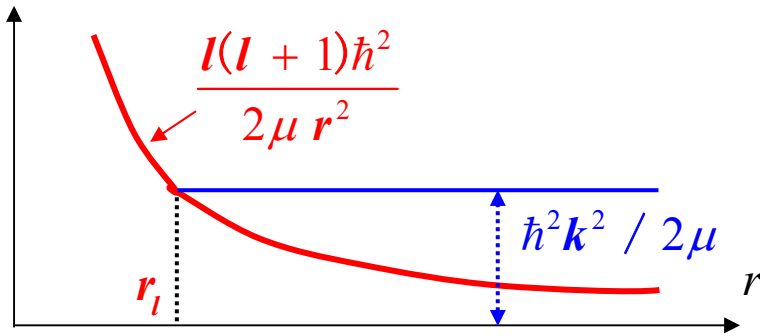
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Central potential. Low energy limit

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



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

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

$$r_l = \sqrt{l(l+1)} \hat{\lambda}_{dB}$$

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

$$b \ll \hat{\lambda}_{dB} \tag{1.52}$$

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

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

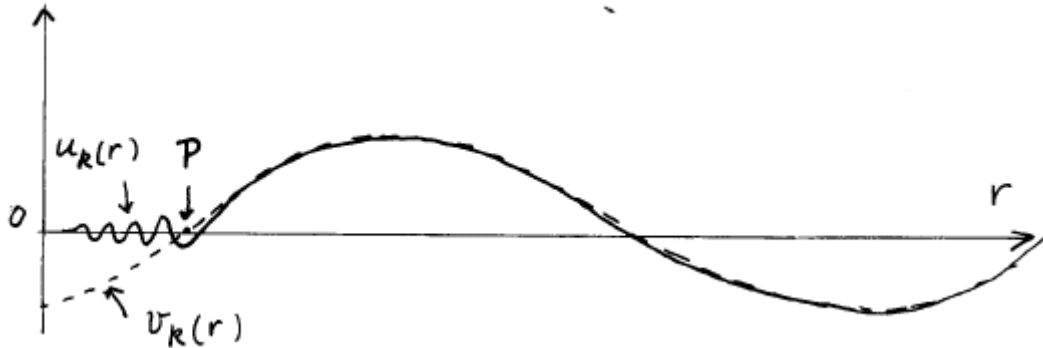
$$\left[\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2} V(r) \right] u_{k0}(r) = 0 \tag{1.53}$$

Scattering length

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

Let v_k be the function $\sin [kr + \delta_0(k)]$ 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 $k \rightarrow 0$ (see figure)



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

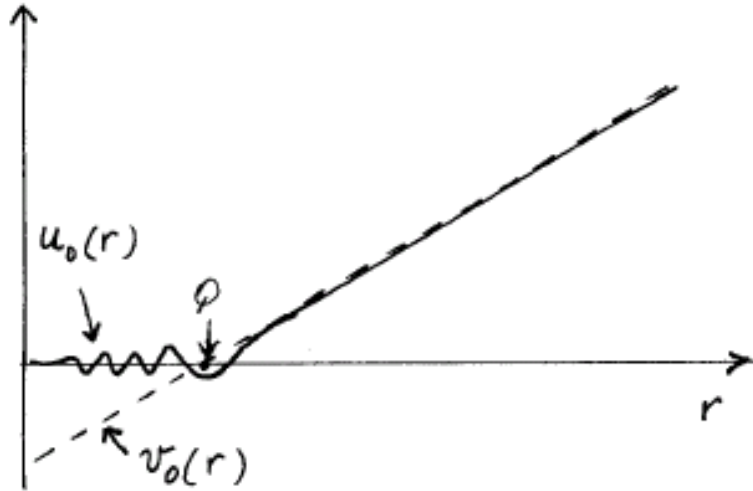
$$v_k(r) = \sin [kr + \delta_0(k)] \xrightarrow{kr \rightarrow 0} \sin \delta_0(k) + kr \cos \delta_0(k) \quad (1.54)$$

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

$$a = \lim_{k \rightarrow 0} \frac{-\tan \delta_0(k)}{k} \quad -\frac{\pi}{2} \leq \delta_0(k) \leq +\frac{\pi}{2} \quad (1.55)$$

Scattering length (continued)

Limit $k=0$



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

Far from $r=0$, the solution of the S.E. is a straight line and

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

The abscissa of Q is equal to a

Scattering cross section

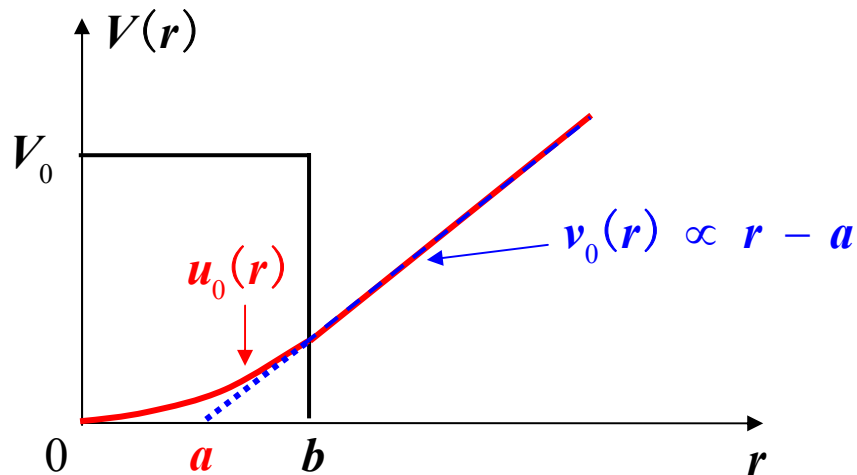
$$\sigma_l(k) = \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l(k) \Rightarrow \sigma_{l=0}(k) = 4\pi \frac{\sin^2 \delta_0(k)}{k^2} \quad (1.58)$$

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

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

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

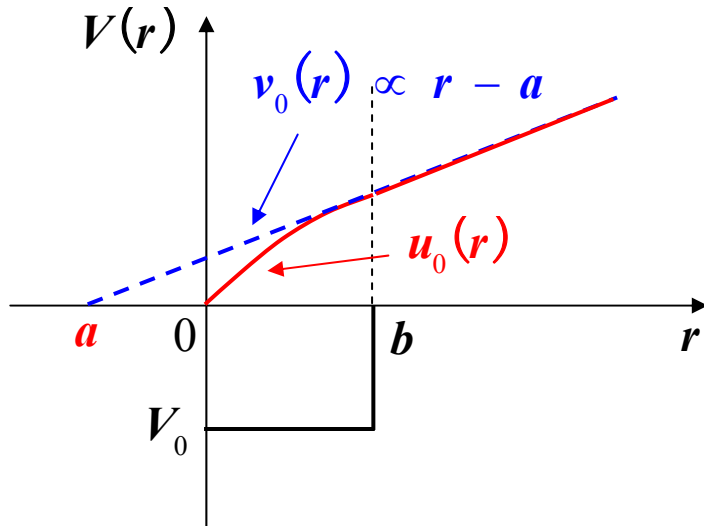
$$0 \leq a \leq b$$

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

$$a \rightarrow b$$

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 $k = 0$

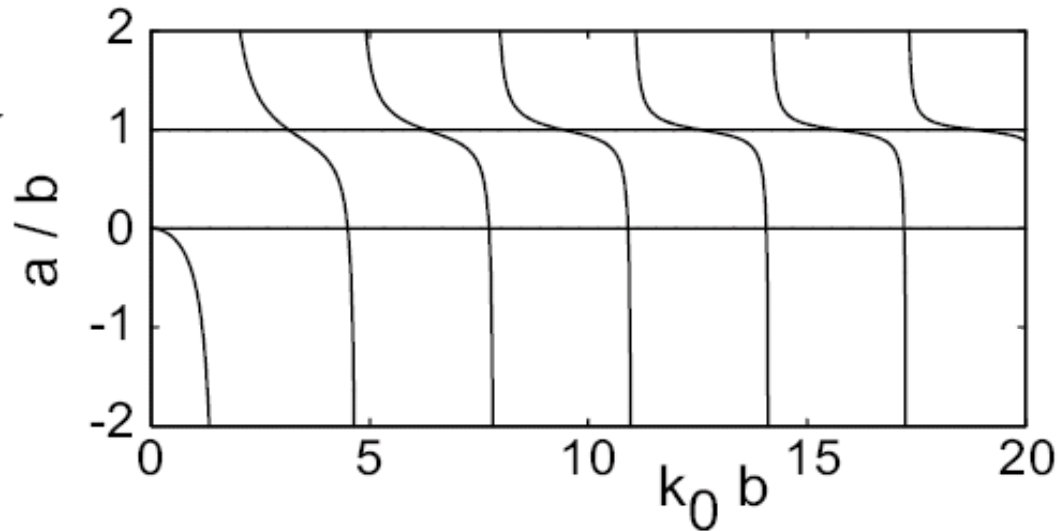
$$u_0''(r) = -k_0^2 u_0(r)$$

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 $a \rightarrow -\infty$. 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

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

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:

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

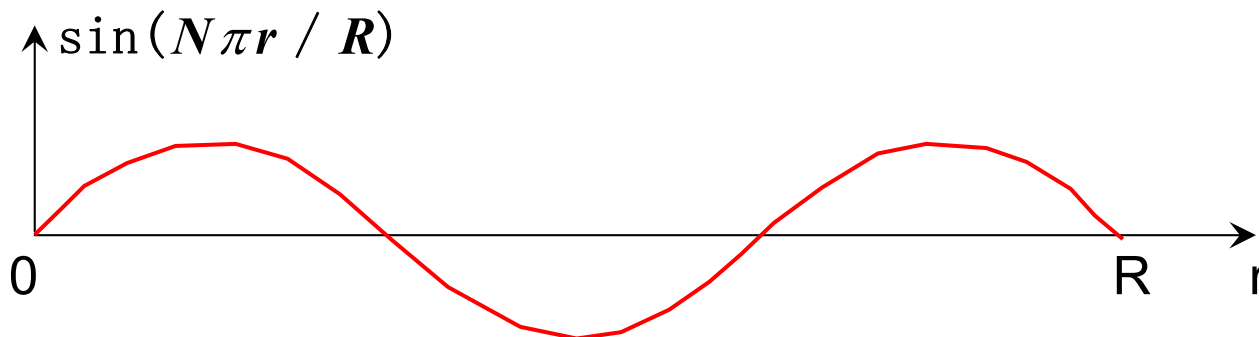
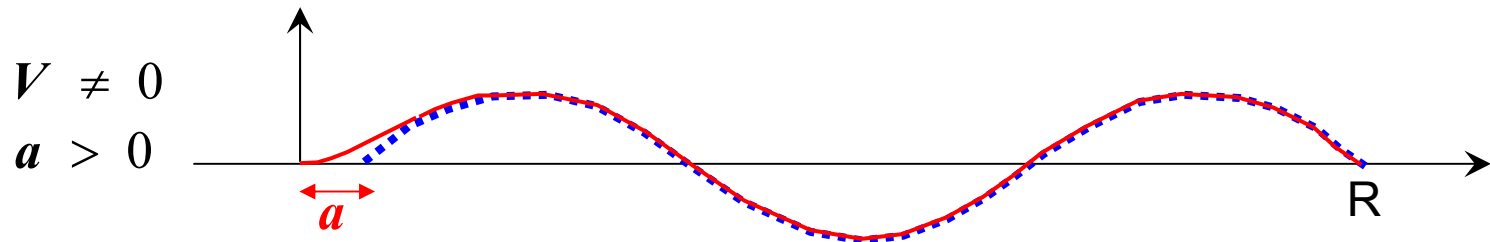
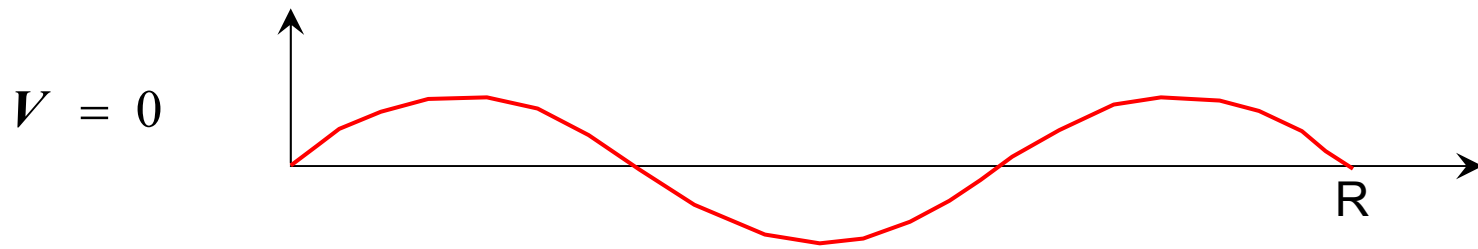
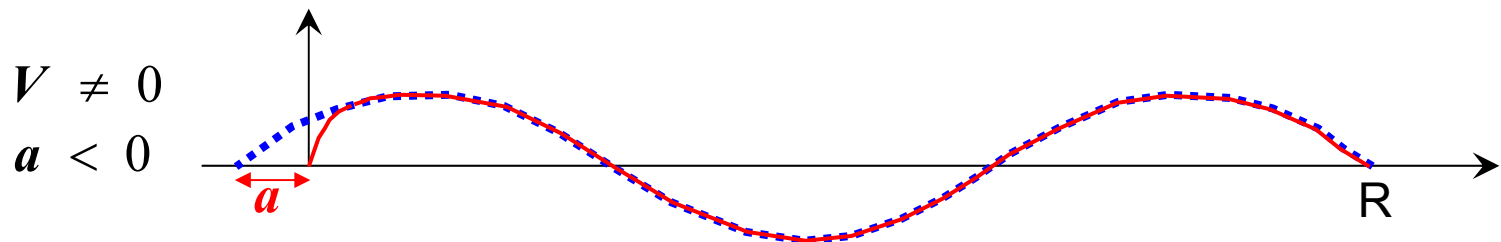


Figure corresponding to $N=3$

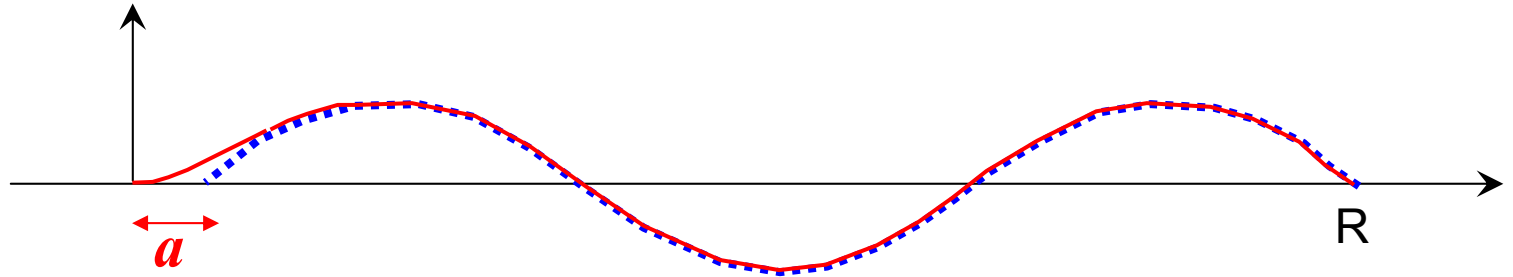


The dotted line is the sinusoid outside the range of the potential
It has a shorter wavelength than for $V=0$, and thus a larger wave number k .
The kinetic energy in this region, which is also the total energy, is larger



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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

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

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

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

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

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

- attractive if $a < 0$

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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

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

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 $\sin [kr + \delta_0(k)] / r$ of the true wave function $u_0(r) / r$

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

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

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)

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

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

$$B = \left[\frac{d}{dr} r\psi \right]_{r=0} \quad (1.67)$$

Equation (1) can be rewritten as:

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

$$\text{where} \quad V_{\text{pseudo}} \psi(\vec{r}) = g \delta(\vec{r}) \frac{d}{dr} [r\psi(\vec{r})] \quad (1.69)$$

V_{pseudo} is called the pseudo-potential. The term $[(d / dr) r]$ 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 $g \delta(\vec{r})$:

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

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 $\neq 0$.

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

The Schrödinger equation for u_0 becomes:

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

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

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

Scattering states of the pseudo-potential (continued)

The solution of the second equation can be written:

$$u_0(\mathbf{r}) = \sin(\mathbf{k} \cdot \mathbf{r} + \delta_0) \quad (1.74)$$

Inserting this solution into the first equation gives:

$$\tan \delta_0 = -k a \quad (1.75)$$

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

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

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

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

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

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

which is valid for all k .

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

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

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

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

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:

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

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

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

which inserted into the first equation gives:

$$\kappa = 1 / a \qquad (1.83)$$

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

$$E = -\frac{\hbar^2}{2\mu a^2} \qquad (1.84)$$

and a wave function:

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

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:

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

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:

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

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 ($V=\infty$ 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:

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

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

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

so that

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

We deduce that

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

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?