

## Chapter 2

# Interactions in dilute gases

### Learning goals

- Why do we need the pseudo-potential?
- How do we derive the scattering length  $a$  for simple potentials?
- What is a Feshbach resonance?

Dilute gases of neutral atoms interact predominantly via their van der Waals interactions. In this section we learn how to formalize their effect on dilute quantum gases. The inclusion of interactions is important for almost all aspects of cold atoms. Cooling into an equilibrium state would not be possible if the atoms were not able to redistribute their momentum and energy, see Fig. 2.1. Moreover, at ultra-low temperatures where gases tend to condense into the lowest energy single-particle state the kinetic energy is largely quenched and hence interaction effects become dominant. Finally, if it were not for interactions effects, almost all phenomena observed in modern quantum gas experiments would allow for a trivial explanation and barely be worth the effort needed for their investigation.

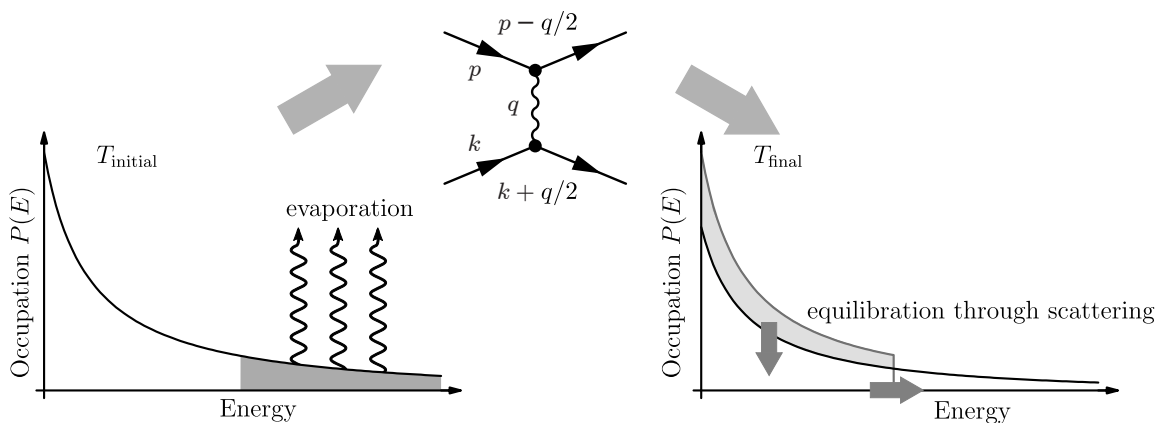


Figure 2.1: **Equilibration due to interactions.** Schematic drawing of the process of equilibration during evaporative cooling. In a first step, hot atoms are removed from the cloud which initially has temperature  $T_{\text{initial}}$ . This process leaves behind a non-equilibrium distribution which is not characterized by a temperature. In a second step particles scatter off each other and redistribute energy and momentum. Eventually, the atomic cloud settles at a new, lower, temperature  $T_{\text{final}}$ . The role of interactions is absolutely central to the redistribution that leads to a thermal cloud again.

## 2.1 Outline

When discussing interactions between ultra-cold atoms we face one major problem. The interaction potential between two neutral atoms is well approximated by the Lennard-Jones potential

$$V(\mathbf{r}) = \frac{A}{r^{12}} - \frac{B}{r^6}, \quad (2.1)$$

where  $r$  is the inter-particle distance. The attractive long-range part describes the van der Waals attraction between neutral atoms while the  $\sim 1/r^{12}$  part models the hard cores of the atoms. Looking at Fig. 2.2 it is evident that the true ground state of *two* neutral atoms is in the form

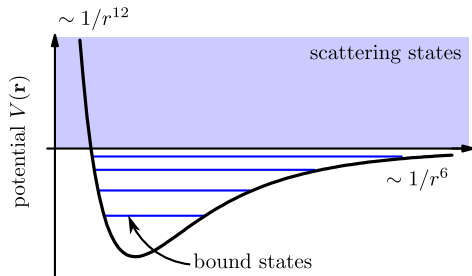


Figure 2.2: **Lennard-Jones potential.** The blue horizontal lines indicate the location of bound states in the potential well at close separations. The shaded area indicates the continuum or “scattering states” that are asymptotically free, i.e., their energy  $E > 0$ .

of a bound state. Moreover, for a collection of *many* atoms we would expect them to crystallize. Rubidium, e.g., has a melting temperature of 39 °C below which it forms a body centered cubic lattice.

We need to find a formulation of the interaction processes that allows us to focus on the “false” equilibrium of a dilute gas rather than a crystal. Moreover, we would like to cast the complicated interaction potential  $V(\mathbf{r})$  into a single number known as the scattering length  $a$ . Our strategy can be summarized as follows:

1. Solve the scattering problem in the full potential  $V(\mathbf{r})$ , focusing on the asymptotically free states at energies  $E > 0$ .
2. Cast this solution into one number, the scattering length  $a$ .
3. Introduce a simplified interaction potential  $V_{\text{pseudo}}(\mathbf{r})$  that does not support any bound states (or crystalline phase). Optimally  $V_{\text{pseudo}}(\mathbf{r})$  is described by one parameter  $g$  alone.
4. Calculate the scattering properties of  $V_{\text{pseudo}}(\mathbf{r})$  to fix  $g$  such that we reproduce the original scattering length  $a$ .

Finally, having  $V_{\text{pseudo}}(\mathbf{r})$  at hand we want to see how we can tweak the interacting parameters in an experiment using a Feshbach resonance.

## 2.2 Scattering theory

We are studying the problem of two interacting particles. Their Hamiltonian is given by

$$H = \frac{\hat{\mathbf{k}}_1^2}{2m} + \frac{\hat{\mathbf{k}}_2^2}{2m} + V(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\hat{\mathbf{k}}_{\text{com}}^2}{4m} + \frac{\hat{\mathbf{k}}_{\text{rel}}^2}{2m_r} + V(\mathbf{r}_{\text{rel}}), \quad (2.2)$$

where  $\hat{\mathbf{k}}_\alpha$  are the momentum operators of the two particles ( $\alpha = 1, 2$ ) or of the center of mass  $\mathbf{r}_{\text{com}} = (\mathbf{r}_1 + \mathbf{r}_2)/2$  and relative ( $\mathbf{r}_{\text{rel}} = \mathbf{r}_1 - \mathbf{r}_2$ ) coordinates ( $\alpha = \text{com}, \text{rel}$ ). The reduced mass

is given by  $m_r = m_1 m_2 / (m_1 + m_2)$ . In the following we concentrate on the relative coordinate and hence write simply  $\mathbf{r}$  and  $\mathbf{k}$ . Hence, we reduced the two-particle problem to a single-particle potential scattering problem.

For our purposes of describing a dilute gas we are interested in asymptotically free, positive-energy solutions. We parameterize these solutions with

$$H\psi_{\mathbf{k}} = E_{\mathbf{k}}\psi_{\mathbf{k}} \quad \text{where} \quad E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}. \quad (2.3)$$

In the standard fashion we make the following Ansatz for our scattering states

$$\left( \begin{array}{c} \text{|||||} \\ \text{|||||} \\ \text{|||||} \\ \text{|||||} \\ \text{|||||} \end{array} \right) \cdot \psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}, \mathbf{r}/r) \frac{e^{ikr}}{r} \quad (2.4)$$

The first part is an incoming plane wave. The second term describes an outgoing spherical wave which is modulated with the scattering amplitude  $f(\mathbf{k}, \mathbf{r}/r)$ . At low energies, i.e.,  $k \ll b$ , where  $1/b$  is the typical distance over which  $V(\mathbf{r})$  varies, we do not resolve the angular properties of the scattering potential. We therefore reduce the scattering amplitude to a single number, the scattering length  $a$

$$e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{k}, \mathbf{r}/r) \frac{e^{ikr}}{r} \xrightarrow{k \rightarrow 0} 1 - \frac{a}{r}. \quad (2.5)$$

More formally, we expand our wave function in spherical harmonics times a radial part

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}(\vartheta, \phi) \frac{u_{kl}(r)}{r} \Rightarrow \left[ \partial_r^2 + k^2 - \frac{l(l-1)}{r^2} - \frac{2m}{\hbar^2} V(r) \right] u_{kl}(r) = 0,$$

in particular for  $l = 0$  (*s*-wave)

$$\left[ \partial_r^2 + k^2 - \frac{2m}{\hbar^2} V(r) \right] u_k(r) = 0. \quad (2.6)$$

In the following we are solving this equation for two one dimensional model potentials to gain further insight into the full problem of the Lennard-Jones potential. The restriction to one dimension is not a real restriction but for spherically symmetric potentials we think of the radial direction as this one dimensional problem. The only restriction is that  $u_k(r)$  has to vanish for  $r \rightarrow 0$ .

### 2.2.1 Square barrier

We start with the square barrier, cf. Fig. 2.3(a),

$$V(r) = \begin{cases} V_0 > 0 & r < b, \\ 0 & r > b. \end{cases} \quad (2.7)$$

We can solve the corresponding equation (2.6) piecewise. For this we write

$$r > b, k \rightarrow 0: \quad \partial_r^2 u(r) = 0 \quad \Rightarrow \quad u(r) = \chi \cdot (r - a) \quad (2.8)$$

$$r < b, k \rightarrow 0: \quad \partial_r^2 u(r) = \kappa^2 u(r) \quad \text{where} \quad \kappa = \sqrt{\frac{2mV_0}{\hbar^2}} \quad \Rightarrow \quad u(r) = \zeta \sinh(\kappa r) \quad (2.9)$$

Note, that in the second line we selected the odd function of  $r$  in order to ensure  $u_k(r) \rightarrow 0$  at the origin. We now need to stitch the two solutions and their derivatives together at  $r = b$

$$\chi(b - a) = \zeta \sinh(\kappa b), \quad (2.10)$$

$$\chi = \zeta \kappa \cosh(\kappa b). \quad (2.11)$$

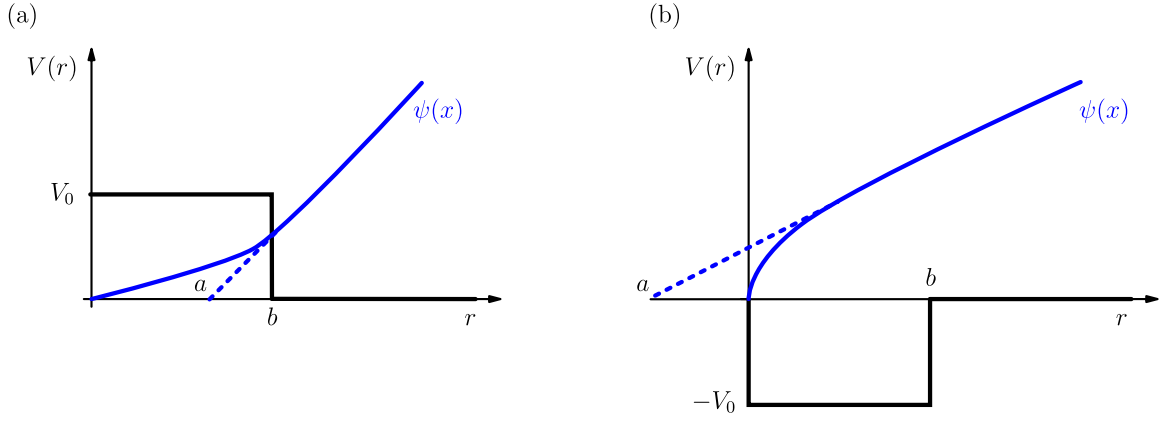


Figure 2.3: **Simple potentials.** (a) Repulsive potential barrier and the resulting scattering wave function. Indicated is the positive value of the scattering length  $a$ . (b) Attractive potential well with the low-energy scattering wave function. The scattering length in this case is smaller than zero  $a < 0$ .

Solving this, we obtain

$$a = b - \frac{\tanh(\kappa b)}{\kappa}. \quad (2.12)$$

Comparing (2.12) with (2.5) we immediately identify  $a$  with the scattering length. In Fig. 2.4(a) we see that for small potential strength  $\kappa$ ,  $a$  tends to zero, i.e., the potential has no effect on the scattering states. For larger  $\kappa$ , on the other hand,  $a$  reaches the actual size of the potential  $b$ . Moreover, in Fig. 2.3 we show the wave function. It is evident that  $a$  is the zero crossing of the extrapolation of the wave function in the outer region. Hence, a positive  $a$  signals that the zero of the wave function is not at the origin (as seen from far away) but pushed further outwards. This allows for the identification of

$$a > 0 \iff \text{“effectively repulsive interactions”}. \quad (2.13)$$

The same holds for a negative  $a$ : the wave function is effectively pulled into the scattering region.

$$a < 0 \iff \text{“effectively attractive interactions”}. \quad (2.14)$$

### 2.2.2 Square well

Let us now consider a potential well, cf. Fig. 2.3(b),

$$V(r) = \begin{cases} -V_0 < 0 & r < b, \\ 0 & r > b. \end{cases} \quad (2.15)$$

We again solve the corresponding equation (??) piecewise

$$r > b, k \rightarrow 0: \quad \partial_r^2 u(r) = 0 \quad \Rightarrow \quad u(r) = \chi(r - a) \quad (2.16)$$

$$r < b, k \rightarrow 0: \quad \partial_r^2 u(r) = -\kappa^2 u(r) \quad \text{where} \quad \kappa = \sqrt{\frac{2mV_0}{\hbar^2}} \quad \Rightarrow \quad u(r) = \zeta \sin(\kappa r) \quad (2.17)$$

The solution for the scattering length yields for this case

$$a = b - \frac{\tan(\kappa b)}{\kappa}. \quad (2.18)$$

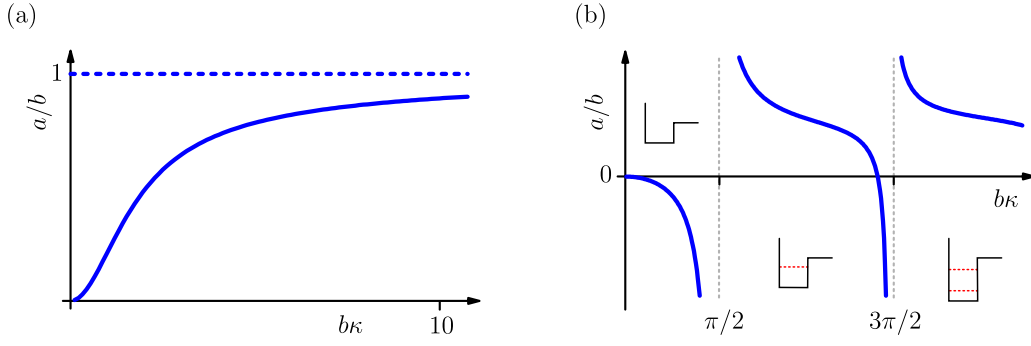


Figure 2.4: **Scattering lengths.** (a) Evolution of the scattering length of a square barrier as a function of its strength  $\kappa$ . For small  $\kappa$  the barrier is essentially inexistent, while for larger  $\kappa$   $a$  tends to the bare barrier size  $b$ . (b) Scattering resonances for an attractive well. Each time a new bound state is entering the well the scattering length is going through a resonance.

In Fig. 2.4(b) we see that the behavior of  $a$  in this case is much more intriguing. As expected, for  $\kappa \rightarrow 0$ ,  $a$  tends to zero and starts to become negative the stronger the potential well becomes. However, at  $b\kappa = \pi/2$  the scattering length goes through a *resonance* and changes sign before it evolves to  $a \rightarrow -\infty$  again at  $b\kappa = 3\pi/2$ . What happens at  $b\kappa = (n + 1/2)\pi$ ? Each time  $b\kappa = (n + 1/2)\pi$ , a new bound state is entering the square well. From this we learn that a nominally attractive well can have both an “attractive” ( $a < 0$ ) or a “repulsive” ( $a > 0$ ) scattering length, depending on the bound-state structure.

### 2.2.3 Intermediate summary

We can now summarize our observations so far.

- a.) Low-energy scattering can be described by a single number, the scattering length  $a$ .
- b.)  $a > 0$ : *effective* repulsion,  $a < 0$ : *effective* attraction.
- c.) Bound states lead to scattering resonances.

## 2.3 Pseudo potential

For a many-body problem we don’t want to deal with the bound states of the Lennard-Jones potential. Moreover, for a metastable Bose Einstein condensate the full  $V(\mathbf{r})$  would necessarily lead to wrong thermodynamic results, i.e., a crystal. Therefore we replace  $V(\mathbf{r})$  with a pseudo potential that yields the same scattering length as the original problem. A good guiding principle to avoid any bound state is to seek a potential which only consists of an “outside” region, i.e., where  $b \rightarrow 0$ .

We know that

$$u = \chi(r - a) \quad \Rightarrow \quad \frac{u(r)}{r} = R(r) = \chi \left( 1 - \frac{a}{r} \right). \quad (2.19)$$

We want  $V(r) \propto q\delta(r)$ . How do we find its exact form? We use the following trick:

$$\partial_r(rR(r)) = \chi. \quad (2.20)$$

We now write the Schrödinger equation and seek to replace  $\chi$  with the above expression

$$\nabla^2 R(r) \stackrel{\nabla^2 \frac{1}{r} = 4\pi\delta(r)}{=} -4\pi a\delta(r)\chi \stackrel{(2.20)}{=} -4\pi a\delta(r)(\partial_r r R(r)). \quad (2.21)$$

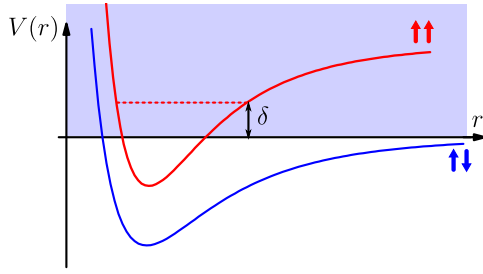


Figure 2.5: **Feshbach resonance.** Illustration of two channels that can be detuned via a magnetic field owing to their different magnetic moment leading to a detuning  $\delta$ . The bound state in the closed channel (red,  $\uparrow\uparrow$ ) leads to a scattering resonance in the open channel (blue,  $\uparrow\downarrow$ ).

Therefore we conclude that a good pseudo potential is given by

$$V_{\text{pseudo}}(\mathbf{r}) = \frac{4\pi a \hbar^2}{m} \delta(\mathbf{r}) \partial_r r. \quad (2.22)$$

Note that here we use the full mass  $m$  again instead of the reduced mass. A form that we often see and use is given by

$$V_{\text{pseudo}}(\mathbf{r}) = \frac{4\pi a \hbar^2}{m} \delta(\mathbf{r}), \quad (2.23)$$

which is okay if we can ensure that there are no (integrable) singularities in the many-body wave function if any two particles approach each other.

## 2.4 Feshbach resonances

Before concluding this section on interactions we discuss the ability to tune the strength of the interactions. Usually we have no easy access to turn either  $b$  or  $\kappa$ . However, we have seen that the essential ingredient to let  $a$  vary largely is a scattering resonance due to a close-by bound-state. We can make use of such a *tunable* bound state by considering two channels as shown in Fig. 2.5.

We consider two “channels” of different spin configurations. Let us assume that we prepared all atoms in the same spin state  $\uparrow$ . The crucial ingredients in a tunable resonance (Feshbach resonance) are listed here:

1. The configurations  $\uparrow\uparrow$  and  $\uparrow\downarrow$  (singlet and triplet) have different magnetic moments. Therefore, an applied magnetic field detunes the two channels with respect to each other.
2. The hyperfine interaction leads to a coupling between the two channels described by their electronic spin  $\hat{\mathbf{S}}$  and their nuclear spin  $\hat{\mathbf{I}}$

$$V_{\text{hf}} = a_{\text{hf}} (\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{I}}_1 + \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{I}}_2) \quad (2.24)$$

$$= \frac{a_{\text{hf}}}{2} \left[ \hat{\mathbf{S}}_{\text{tot}} \cdot (\hat{\mathbf{I}}_1 + \hat{\mathbf{I}}_2) + \underbrace{(\hat{\mathbf{S}}_1 - \hat{\mathbf{S}}_2)}_{\text{changes } \hat{\mathbf{S}}_{\text{tot}}} \cdot (\hat{\mathbf{I}}_1 + \hat{\mathbf{I}}_2) \right]. \quad (2.25)$$

Using this coupling we can imagine that we effectively deal with a single-channel problem where a bound state transitions through the low-energy region and leads to a scattering resonance.

A good introduction to the theory of Feshbach resonance can be found in W. Ketterle and M. W. Zwierlein, [Making, probing and understanding ultracold Fermi Gases](#), on pages 124ff.