

Interactions in cold gases (III)

The three-body problem and the Efimov effect

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Introduction

One of the very first mathematical descriptions of the three-body problem can be found in Newton's *Principia*, published in 1687. We know of Newton's resounding success in solving the problem of two bodies of masses m_1 and m_2 interacting gravitationally:

$$V(\mathbf{r}_1, \mathbf{r}_2) = -\frac{G m_1 m_2}{r_{12}}, \quad r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|. \quad (1)$$

Once the solution to the two-body problem was well established, Newton turned his attention to a three-body system of the Sun–Earth–Moon type shown in figure 1. This problem, called “lunar theory”, corresponds to a potential energy of the system

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = -G \left(\frac{m_1 m_2}{r_{12}} + \frac{m_2 m_3}{r_{23}} + \frac{m_3 m_1}{r_{31}} \right). \quad (2)$$

One of the questions Newton raised was that of the stability of such a system. He tackled it by implementing complex calculations based on perturbation theory. Much to his chagrin—he lost his appetite and his sleep—Newton was unable to come up with a convincing general answer. In fact, he wrote to one of his friends, John Machin, that he never had a headache, except when working on the lunar theory... (Westfall 1980).

This question then occupied the most brilliant mathematicians and physicists during the 18th and 19th centuries: Euler, d'Alembert, Clairaut, Lagrange, Laplace, Poisson, Jacobi, Cauchy... made notable contributions to it without really solving it. At the turn of the 20th century, Poincaré identified a significant dependence on initial conditions for this problem and developed the mathematical tools that are now central to chaos theory, a very active branch of physics and mathematics (Gutzwiller 1998; Chenciner 2014).

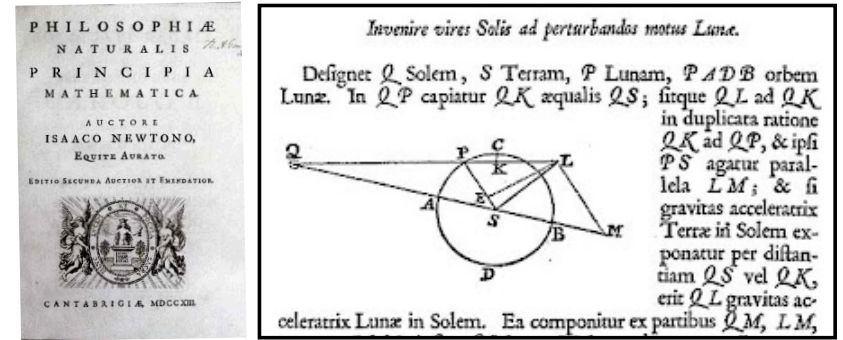


Figure 1. The Sun–Earth–Moon system described by Newton in his *Principia*.

In this lecture series, we will look at the transposition of the three-body problem to the quantum domain. As with the lunar problem, we will focus on a system in which the interaction energy can be written as a sum of binary terms:

$$V = V_{12} + V_{23} + V_{31}. \quad (3)$$

However, the binary interaction will be very different from that of astronomers. The $1/r$ law of gravitational attraction (1) will be replaced by a short-range interaction. More precisely, the range b of the binary interatomic potentials will be assumed to be much smaller than the average distance between the three-body edifices that will be formed (figure 2).

For the moment, we will write this interaction in the form

$$V_{ij} = g \delta(\mathbf{r}_i - \mathbf{r}_j), \quad (4)$$

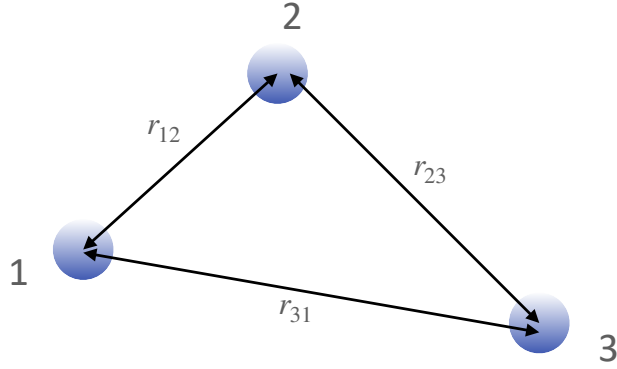


Figure 2. Three interacting bodies. The size of the balls represents the range of the two-body potential, denoted b . We are mainly interested in situations where the distance between particles r_{ij} is larger than b .

where the symbol $\delta(r)$ represents “almost” a Dirac distribution. The focus of this course will be on the resonant case, i.e. a combination of atomic masses and the strength g of the potential such that a two-body bound state is just at the threshold for the Hamiltonian (see figure 3)

$$\hat{H} = \frac{\hat{\mathbf{p}}_1^2}{2m} + \frac{\hat{\mathbf{p}}_2^2}{2m} + \hat{V}_{12}. \quad (5)$$

Note that in the equation above we have given the same mass to both particles, but we will also encounter interesting situations where these masses are different.

A very important notion of the course will be the emergence for the three-body problem of a potential varying as the inverse of the square of a characteristic distance R :

$$V(R) = -\frac{\gamma}{R^2}. \quad (6)$$

The distance R involved here could be, for example, the hyperradius for the three-body system

$$R \propto \sqrt{r_{12}^2 + r_{23}^2 + r_{31}^2}. \quad (7)$$

This emergence of an attractive potential varying as $1/R^2$ was discovered by Vitaly Efimov in a series of remarkable articles (Efimov 1970; Efimov 1971;

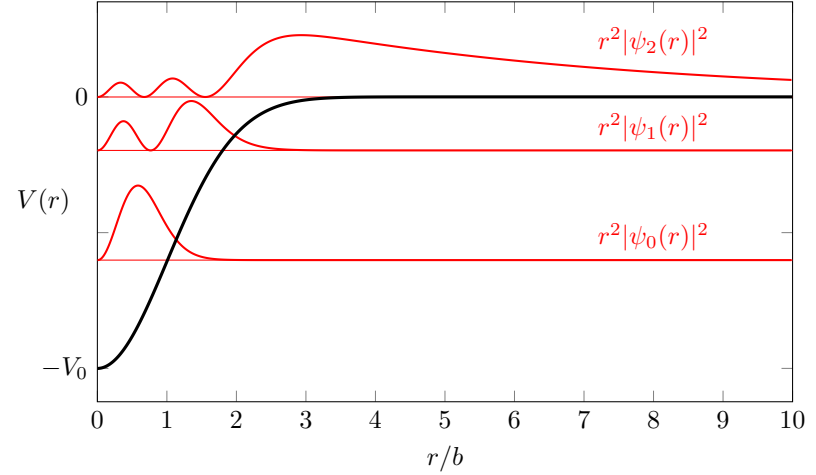


Figure 3. An example of scattering resonance for a Gaussian potential $V(r) = -V_0 \exp(-r^2/2b^2)$, highlighted on the radial probability density $r^2|\psi_n(r)|^2$ of bound states for zero angular momentum ($\ell = 0$). The pair (V_0, b) was chosen so that the last bound state $\psi_2(r)$ is very close to the dissociation limit ($2mb^2V_0/\hbar^2 = 23.5$). The extension of this weakly bound state is then much larger than the range b . The ground state $\psi_0(r)$ and the first excited state $\psi_1(r)$, on the other hand, are strongly bound and have an extension $\sim b$. It is the physics associated with the weakly bound state that will mainly interest us in this course.

Efimov 1972; Efimov 1973). Let us stress that this long-range potential is absent from two-body physics which, as we have written, is short-range, or even zero-range. This is why we call it an “emergent” property, one that materializes only when all three bodies are simultaneously present.

The particularity of the $1/R^2$ potential is its scale invariance, which will occupy us intensively in the first chapters of this course. This invariance can be illustrated in a simple way for the one-particle Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dR^2} + \frac{\gamma}{R^2}. \quad (8)$$

If a wave function $\psi(R)$ is an eigenstate of this Hamiltonian for energy E , then we can verify that the infinite family of functions $\psi(\lambda R)$ for any real



Figure 4. Borromean rings named after the Italian Borromeo family, whose coat of arms has featured the rings since the 15th century. Photo from Wikimedia Commons, taken in the church of San Pancrazio in Florence.

λ is also an eigenstate of $\hat{H}$ for eigenvalue $\lambda^2 E$. This property of the $1/R^2$ potential is unique in the family of power law interactions!

The physics discovered by Efimov (and previously sensed by other physicists such as Thomas (1935)) leads to the existence of Borromean states. Even if the potential $V(r_{12})$ is slightly too weak to admit a two-body bound state, the three-body problem can possess a certain number of bound states. These states only “hold together” because all three bodies are simultaneously present. This situation is reminiscent of the three intertwined and inseparable rings shown in figure 4: if we cut one of them, the other two are freed.

When Efimov published his predictions in the early 1970s, there were very few systems in nature on which one could hope to test them. Efimov was mainly interested in problems of nuclear physics, such as three α particles that could bind to form a ^{12}C carbon nucleus, or the problem of the tritium nucleus formed by two neutrons and a proton. But Efimov’s theory was difficult to apply to these situations because the binary interactions were not sufficiently close to resonance.

Atomic physics, in particular with quantum gases and their adjustable Fano–Feshbach resonances, has considerably enriched the landscape. It

provides systems where the scale invariance found by Efimov and the universality linked to it could be tested quantitatively. Experiments on the He_3 trimer (Schöllkopf & Toennies 1994; Kunitski, Zeller, et al. 2015) and those carried out on a cesium gas (Kraemer, Mark, et al. 2006) have opened up a vast field of research that we will describe in the lectures that follow. Given the limited time available, this description will of course be only partial, and we refer readers wishing to learn more to the review articles published on the subject over the last twenty years, such as Nielsen, Fedorov, et al. (2001), Braaten & Hammer (2006), Braaten & Hammer (2007a), Ferlaino & Grimm (2010), Efimov (2011), Petrov (2012), Wang, Julienne & Greene (2015), Greene, Giannakeas, et al. (2017), Naidon & Endo (2017), and D’Incao (2018).

This year’s lecture series will consist of three main parts, each made up of two chapters.

- In the first two chapters, we will focus on the two-body problem and show why the $1/r^2$ potential is singular among all power-law ($1/r^\beta$) potentials. We will show that this peculiarity of the potential is linked to its scale invariance, and more generally to its conformal invariance, which manifests itself in the dynamics of the problem. We will illustrate these properties on several examples, such as the charge–wire interaction and the charge–dipole interaction. We will also describe some remarkable theoretical results for the one-dimensional (Calogero–Sutherland–Moser) problem.
- In Chapters 3 and 4, we will tackle the three-body problem in a relatively simple version, in which two heavy particles of mass M get bound by a light particle of mass m . We will use a Born–Oppenheimer approach: first, we will assume that the heavy particles are held fixed at a distance R from each other, and we will determine the energy $E(R)$ of the ground state of the light particle. We will then see how a law $E(R) \propto -1/R^2$ can emerge. We then move on to the motion of heavy particles, with $E(R)$ playing the role of the effective interaction potential between them. We will show that a theoretically infinite series of bound states emerges for the mMM system, with geometrically increasing energies. We will describe experiments carried out on gases of cold atoms that have revealed the first states in this sequence.

- Chapters 5 and 6 will be devoted to the three-body problem for identical bosons, which corresponds to the case initially considered by Efimov. The complete theoretical treatment is then considerably more complex than in the mMM case. We will describe the broad lines of the theory using the hyperspherical potential formalism. We will describe a number of experiments carried out recently on a helium beam or on gases of cold atoms. We will also discuss an unexpected universality, that of the *three-body parameter*. The introduction of this parameter is necessary to prevent the three-body system from *falling to the center*, and corresponds to the introduction of a short-range cutoff R_0 . For many atomic species, it appears that R_0 is determined solely by the mass of the atoms and their van der Waals coefficient C_6 . We conclude with a brief discussion of small-body physics beyond the three-boson case considered by Efimov. We will see that Efimovian universality does not hold in general, except in two specific cases that we will discuss.

Note. This course is the third in a series devoted to the interactions between atoms in quantum gases. It is not necessary to have followed or read the previous two years' lecture series to understand this one. All the concepts used will be recalled (without proof) when necessary, and precise references to the previous lecture series will be given.

Acknowledgements. I am very grateful to Jérôme Beugnon, Raphaël Lopes and Sylvain Nascimbène for their comments on a draft version of these lecture notes.

These notes were translated from French using as a first step an automatic translator. This procedure may have introduced some typos or mistakes in the equations. In case of doubt please consult the French version. Thanks in advance for signaling these typos.

Chapter I

The potential in $1/r^2$ and its scale invariance

As announced in the general introduction to this course, the Efimov effect for the three-body problem originates from the emergence of a long-range attractive potential, varying as $1/r^2$ where r is a relevant spatial coordinate, the hyperradius in the case of three interacting particles.

The simple problem of a single particle moving in a g/r^2 potential is in fact very rich and very subtle. The intuition gained from studying the Coulomb potential in $-e^2/r$, for example, is often challenged. For instance, there is no ground state in the potential g/r^2 , when g is negative and sufficiently large in absolute value. Starting from a given bound state, we can produce states of arbitrarily large negative energy. This is the problem of a “particle falling to the center” [Landau & Lifshitz (1975), §35].

The motion of a particle of mass m in the $1/r^2$ potential is a good example of a scale-invariant problem, for which the physical constants needed to describe it provide no length scale. In contrast, the Coulomb problem leads naturally to the length scale given by the Bohr radius $a_0 = \hbar^2/me^2$. The remedy for the “fall to the center” problem imposes an *ad hoc* minimum size on physically acceptable states, which breaks—at least partially—the scale invariance.

The $1/r^2$ potential is dealt with explicitly in several books and articles. In addition to Landau & Lifshitz (1975) already mentioned, let us quote in particular Mott & Massey (1949), chapter II, §7, Case (1950), Coon & Holstein (2002), Essin & Griffiths (2006), Dereziński & Richard (2017) and Paik (2018). Nevertheless, this problem remains relatively unknown and

Essin & Griffiths (2006) suggest a “good” reason for this: “*It violates every rule in the book, and discredits all the intuition we are trying to instill in our students.*” Since this problem plays a central role in Efimovian physics, we think it worth devoting this chapter and the next to it.

In this first chapter, we will begin by recalling the basics of the quantum treatment of the motion of a particle in a central potential, in particular the search for bound states. After establishing some general results for a g/r^β potential, we will concentrate on the $\beta = 2$ case to explore the scale invariance mentioned above. We will also look at a first illustration, involving the interaction between a polarizable atom and a uniformly charged wire.

1 The two-body problem

1-1 Separation of variables

Consider two particles of mass m_j , $j = 1, 2$ interacting via the potential $V(\mathbf{r}_1 - \mathbf{r}_2)$. The total Hamiltonian

$$H_{\text{tot}} = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + V(\mathbf{r}_1 - \mathbf{r}_2) \quad (1)$$

is rewritten in terms of the variables of the center of mass

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad (2)$$

and the relative variable

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{p} = \frac{m_2 \mathbf{p}_1 - m_1 \mathbf{p}_2}{m_1 + m_2}, \quad (3)$$

in the form

$$H_{\text{tot}} = H_{\text{cm}} + H_{\text{rel}} \quad \text{with} \quad H_{\text{cm}} = \frac{\mathbf{P}^2}{2M}, \quad H_{\text{rel}} = \frac{\mathbf{p}^2}{2m_r} + V(\mathbf{r}) \quad (4)$$

where we have introduced the total mass $M = m_1 + m_2$ and the relative mass $m_r = m_1 m_2 / (m_1 + m_2)$.

One can simply check that the variables of the center of mass commute with the relative variables, so that we can look for a basis of eigenfunctions common to H_{cm} and H_{rel} . A basis of eigenfunctions of H_{cm} is given by the states of well-defined momentum (plane waves $e^{i\mathbf{K} \cdot \mathbf{R}}$), which call for no particular comment. In what follows, we will assume that we work in the reference frame of the center of mass, i.e. that we have chosen the state $\mathbf{K} = 0$, and we will concentrate on the eigenstates of H_{rel} .

We have therefore gone from a problem with six degrees of freedom $(\mathbf{r}_1, \mathbf{r}_2)$ to a problem with only three degrees of freedom $(\mathbf{r})$ by exploiting the translation invariance of the Hamiltonian (1).

1-2 Rotational invariance

We now turn to the frequently encountered case of a centrally symmetric potential V : $V(\mathbf{r}) = V(r)$. The relative Hamiltonian H_{rel} then commutes with the three components of the angular momentum operator $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, so we can look for a basis of eigenfunctions common to H_{rel} , $\mathbf{L}^2$, and one of the three components of $\mathbf{L}$, for example L_z .

We therefore write the eigenfunctions $\Psi(\mathbf{r})$ in spherical coordinates as

$$\Psi(\mathbf{r}) = \psi(r) Y_{\ell, m}(\theta, \varphi) \quad (5)$$

where the angular dependence $Y_{\ell, m}(\theta, \varphi)$ is entirely fixed by imposing Ψ to be an eigenstate of $\mathbf{L}^2$ and L_z . Recall that the quantum number ℓ is a non-negative integer, and that it characterizes the eigenvalue of $\mathbf{L}^2$. The

quantum number m , which belongs to the set $\{-\ell, -\ell + 1, \dots, \ell\}$, characterizes the eigenvalue of L_z :

$$\mathbf{L}^2 Y_{\ell, m} = \hbar^2 \ell(\ell + 1) Y_{\ell, m} \quad L_z Y_{\ell, m} = \hbar m Y_{\ell, m}. \quad (6)$$

All that remains is to determine the radial dependence $\psi(r)$ of the wave function Ψ . In practice, it is convenient to introduce the reduced radial wave function $u(r) = r \psi(r)$ which satisfies the one-dimensional equation:

$$-\frac{\hbar^2}{2m_r} u''(r) + \left[V(r) + \frac{\hbar^2 \ell(\ell + 1)}{2m_r r^2} \right] u(r) = E u(r) \quad (7)$$

Each value of ℓ defines an interaction channel, for which we obtain an eigenvalue equation which has the structure of a Schrödinger equation with a total potential:

$$V_{\text{tot}}(r) = V(r) + \frac{\hbar^2 \ell(\ell + 1)}{2m_r r^2} \quad (8)$$

i.e. the sum of the true potential and the centrifugal potential. This equation is defined on the half-line $r \geq 0$. If we assume that $\Psi(\mathbf{r})$ is regular at $r = 0$, this imposes

$$u(0) = 0. \quad (9)$$

Let us further assume that $V(r) \rightarrow 0$ when $r \rightarrow +\infty$. The equation (7) generally admits solutions of negative energy E , corresponding to bound states of the two-body system, and solutions of positive energy, describing an (elastic) collision between the two asymptotically free particles. Given the definition of spherical harmonics, the normalization condition for the wave function of bound states reads

$$\begin{aligned} 1 &= \int |\Psi(\mathbf{r})|^2 d^3r = \int |\psi(r)|^2 |Y_{\ell, m}(\theta, \varphi)|^2 r^2 \sin \theta dr d\theta d\varphi \\ &= \int_0^\infty |u(r)|^2 dr. \end{aligned} \quad (10)$$

By exploiting first the translational invariance of the Hamiltonian (1) and then the rotational invariance of the interaction potential, we have moved from a problem with six degrees of freedom $(\mathbf{r}_1, \mathbf{r}_2)$ to a problem with only one degree of freedom (r) .

1-3 Search for bound states

An important part of this year's course will be devoted to the search for few-body bound states. Let us now show how this search can be carried out for the two-body problem.

We will first look at states with zero angular momentum and then move on to the general case. Let us start by establishing a lower bound on the energy of any bound state. If the potential $V(r)$ is itself bounded from below by a value $-|V_0|$, like the square or Gaussian potentials shown in figures I.1ab, we can simply show that the energy of each bound state, when it exists, is always greater than $-|V_0|$. Simply multiply (7) by $u^*(r)$ and integrate the result between 0 and $+\infty$ to find, using (10):

$$\frac{\hbar^2}{2m_r} \int |u'(r)|^2 dr + \int \left[V(r) + \frac{\hbar^2 \ell(\ell+1)}{2m_r r^2} \right] |u(r)|^2 dr = E. \quad (11)$$

The first term on the left-hand side is always positive (kinetic energy), and the second is greater than or equal to $-|V_0|$, since

$$\int \left[V(r) + \frac{\hbar^2 \ell(\ell+1)}{2m_r r^2} \right] |u(r)|^2 dr \geq \int V(r) |u(r)|^2 dr \geq -|V_0| \int |u(r)|^2 dr \quad (12)$$

hence the result announced using (10).

Existence of bound states. Recall that the existence of bound states is not guaranteed, even if $V(r)$ is negative at every point. Taking the example of the square potential shown in figure I.1a, which we studied in detail in the 2021 lecture series (Chapter 3, §3), let us look at the angular momentum channel $\ell = 0$ and set $V_0 = \hbar^2 k_0^2 / 2m_r$. One can show that the well contains no bound state if $k_0 b / \pi \leq 1/2$, contains a single bound state for $1/2 < k_0 b / \pi < 3/2$, and more generally n bound states for $n - 1/2 < k_0 b / \pi < n + 1/2$.

Number of bound states. In the example of the square well just given, the number of bound states is always finite, whatever the values of the depth V_0 and the range b . The same is true for any potential that tends to 0 sufficiently fast when $r \rightarrow \infty$, but not for the Coulomb potential, which we will examine later.

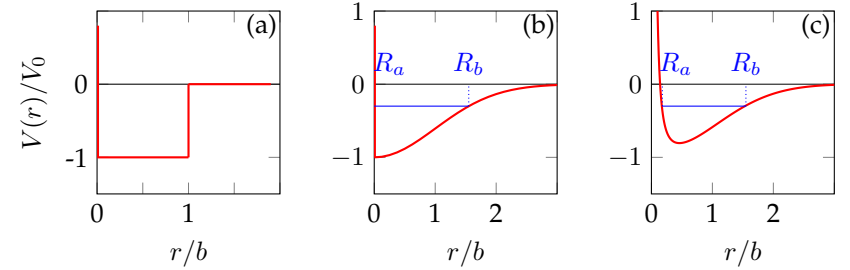


Figure I.1. Some simple two-body potentials. (a) Square well of depth V_0 and range b . (b) Gaussian potential. (c) Gaussian potential superimposed on the centrifugal potential for $\ell \neq 0$. We have indicated in (b) and (c) the turning points used to calculate the energy of a bound state by the WKB method.

A simple method for estimating the number of bound states is to use the semi-classical method, also known as the WKB (Wentzel–Kramers–Brillouin) method. We simply state here the result that is useful for our study, and refer the interested reader to Schiff (1968) and to the 2021 lecture series (Chapter 4, §1), where this method was presented in detail.

The main result of the WKB method for bound states can be written as a condition for quantizing the energy E of the n -th bound state¹:

$$\int_{R_a}^{R_b} k_E(r) dr \approx n\pi \quad (13)$$

where k_E is the local wave number associated with energy E :

$$\frac{\hbar^2 k_E^2(r)}{2m_r} + V_{\text{tot}}(r) = E \quad \text{with} \quad V_{\text{tot}}(r) = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2m_r r^2}. \quad (14)$$

The points R_a and R_b are the left and right turning points of the classical motion: $V_{\text{tot}}(R_a) = V_{\text{tot}}(R_b) = E$.

¹Strictly speaking, the term on the right-hand side of (13) is not $n\pi$, but rather $(n - 1/2)\pi$ or $(n - 1/4)\pi$, depending on whether the variations of the potential at the two classical turning points R_a and R_b are “soft” (figure I.1c) or whether one of the two edges is “hard” (figure I.1b). But this detail is unimportant if we are interested in relatively large values of n .

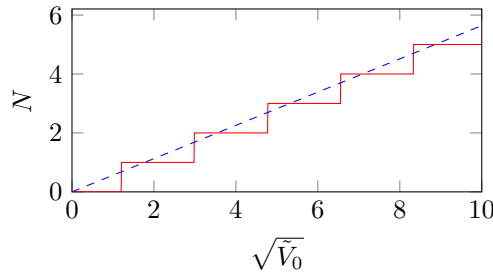


Figure I.2. Solid red line: number of bound states in the Gaussian potential $V(r) = -V_0 e^{-r^2/2b^2}$, with $\tilde{V}_0 = 2m_r V_0 b^2 / \hbar^2$. Dashed blue line: approximate value given by the argument of the function $I(x)$ in (15).

To estimate the position of bound states, we can scan the value of E from $E = -|V_0|$ to $E = 0$. For each value of E , we calculate the integral (13) and we obtain an approximate value of the energy of a bound state when this integral is equal to an integer times π . In particular, the value of the integral at $E = 0$ gives a generally fairly reliable estimate of the number of bound states:

$$N_{\text{bound}} \approx I \left[\frac{1}{\pi} \int_{R_a}^{R_b} k_{E=0}(r) dr \right] \quad (15)$$

where $I(x)$ denotes the nearest integer to x and where R_a and R_b are the turning points of the classical zero-energy motion, for example $R_a = 0$, $R_b = +\infty$ in the case of figure I.1b. The existence of an infinite number of bound states is then revealed by the divergence of this integral at $R_b = \infty$.

The criterion for the validity of the semi-classical approximation is linked to the fact that the wave number $k_E(r)$ must vary fairly slowly with r . More precisely, if we introduce the de Broglie wavelength $\lambda = 2\pi/k$, this criterion reads

$$\frac{1}{2\pi} \frac{d\lambda}{dx} \ll 1. \quad (16)$$

We will see later how this criterion applies to power-law potentials.

Example. For a Gaussian potential $V(r) = -V_0 e^{-r^2/2b^2}$, we find for the argument x of the function $I(x)$ the value $\sqrt{\tilde{V}_0/\pi}$, with $\tilde{V}_0 = 2m_r V_0 b^2 / \hbar^2$. The comparison between the approximate number of bound states $\sqrt{\tilde{V}_0/\pi}$ and the number found by a numerical solution of the Schrödinger equation is shown in figure I.2.

1-4 Zero-energy solution and scattering length

To conclude this brief review of the description of two-body interactions, let us look at the $\ell = 0$ collision channel and its zero-energy solution, which satisfies

$$E = 0 : \quad -u''(r) + \frac{2m_r V(r)}{\hbar^2} u(r) = 0 \quad (17)$$

Consider the solution to this equation which satisfies the boundary condition $u(0) = 0$ [or the condition $u(R_a) = 0$ if we impose a hard core at R_a to regularize the potential $V(r)$]. By examining its number of nodes, we can immediately deduce the number of bound states in the potential $V(r)$ for the channel under consideration (here $\ell = 0$). This point follows directly from the Sturm–Liouville theorem, which allows one to classify the eigenstates of the Hamiltonian by increasing energy by counting the number of nodes in their wave function. The ground state has no node², the first excited state has one node, and so on. If the zero-energy state has n nodes, we can therefore deduce that there are n states of energy $E < 0$.

Scattering length. Suppose that the potential $V(r)$ decreases “sufficiently fast” at infinity [in practice, this means faster than $1/r^3$ (Landau & Lifshitz 1975)]. Let us recall the form of the zero-energy solution of the radial equation (7) in this case: in a region far from the origin, such that the potential $V(r)$ is negligible, i.e. for r large compared with the range b of the potential, this equation simply becomes $u''(r) = 0$, whose solutions are of the form $u(r) = c_0 + c_1 r$, which we write as

$$E = 0, r \gg b : \quad u(r) \propto r - a \quad \Leftrightarrow \quad \psi(r) \propto \frac{1}{a} - \frac{1}{r} \quad (18)$$

²The vanishing of u at $r = 0$, or at the hard core R_a , does not count as a node.

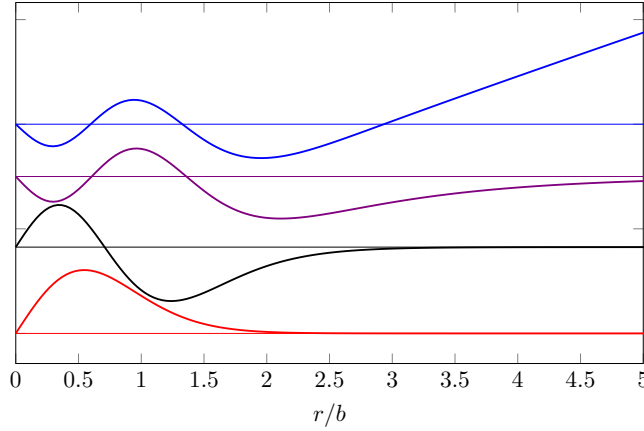


Figure I.3. From bottom to top: reduced wave function $u(r)$ for the three bound states and the zero-energy state in the Gaussian potential $V(r) = -V_0 e^{-r^2/2b^2}$ with $\tilde{V}_0 = 2m_r V_0 b^2 / \hbar^2 = 29$. The states are not normalized.

The quantity a is called the scattering length. It can be positive, zero or negative, or even infinite, and it is the main characteristic of the scattering process at very low energy.

An example is given for the Gaussian potential in figure I.3. We can check the linear behavior $u(r) \propto r - a$ with here $a \approx 3b$. We have also plotted the bound states in this trap (there are three bound states for the value chosen for $\tilde{V}_0 = 2m_r V_0 b^2 / \hbar^2$). As expected, the ground state has no node, and the two excited states have one and two nodes. The zero-energy state has three nodes, the first two being very close to those of the last bound state, and the third is close to the scattering length a .

We refer the reader to Chapter 3 of the 2021 lecture series for a detailed presentation of the treatment of the collision of two particles at low energy and for examples of scattering length calculations.

2 Attractive power-law potentials $1/r^\beta$

2-1 Qualitative approach in terms of wave packets

In the previous section, we did not explicitly consider the case where the potential $V(r)$ could be both attractive and singular at the origin, i.e. $V(r) \rightarrow -\infty$ when $r \rightarrow 0$. The potentials represented in figure I.1 are all bounded below, which immediately puts a lower limit on the energy of the ground state [cf. §1-3].

We now look at power-law potentials

$$V(r) = \frac{g}{r^\beta}, \quad (19)$$

where the exponent β is at this stage arbitrary and where we essentially consider the attractive case, i.e. $g < 0$. At least for the $\ell = 0$ angular momentum channel, the existence of a lower bound for the ground state is therefore not guaranteed.

Let us begin our study with a remark based on dimensional analysis. For a particle of mass m_r placed in a potential g/r^β with $\beta \neq 2$, we can construct a natural length scale for the quantum problem

$$r_* = \left(\frac{m_r |g|}{\hbar^2} \right)^{1/(\beta-2)} \quad (20)$$

For the Coulomb potential, we recover in this way the value of the Bohr radius, up to a multiplicative factor. The length scale r_* is associated with the momentum scale $\hbar/r_*$ and with the energy scale $\hbar^2/m_r r_*^2$. This dimensional argument disappears when we take $\beta = 2$, since (20) no longer makes sense. It is thus clear that the case of $\beta = 2$ will play a special role in the study of power-law potentials.

To get an idea of the different possible scenarios, let us consider a wave packet centered³ at r_0 and of extent also $\sim r_0$ (figure I.4). We know that the average energy of this wave packet is necessarily larger than the energy of the ground state, a consequence of the theorem underlying the variational

³To be more precise, one can take a shell of radius r_0 and thickness Δr equal to a fraction of r_0 . We will not do this here, in order to avoid multiplying the mathematical symbols.

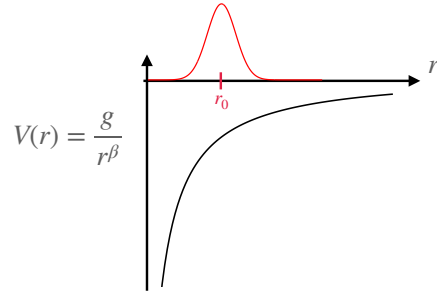


Figure I.4. Wave packet centered at r_0 and of extent $\sim r_0$ in an attractive power-law potential.

method. The kinetic energy of the relative motion $E_k \sim (\Delta p)^2/2m_r$ is related to the confinement over a size r_0 , and hence to a momentum spread Δp of at least $\sim \hbar/r_0$. The kinetic energy and the potential energy E_p are of the order of

$$E_k \sim \frac{\hbar^2}{2m_r r_0^2}, \quad E_p \sim -\frac{|g|}{r_0^\beta}, \quad (21)$$

so that two situations emerge for the variation of the total energy $E = E_k + E_p$ with the size r_0 , depending on whether the exponent β is less than or greater than 2 (see figure I.5). We will now review these two situations.

2-2 The $\beta < 2$ case

In this case, the kinetic energy (positive) is dominant for small values of r_0 and the potential energy (negative) is dominant for large values of r_0 . The total energy therefore passes through a minimum for a value of r_0 of the order of r_* (figure I.5a). This indicates that a ground state may exist, which a quantitative analysis confirms.

The Coulomb potential provides an example of this case, with $\beta = 1$ and $g = -e^2$. Minimizing the total energy

$$E \sim \frac{\hbar^2}{2m_r r_0^2} - \frac{e^2}{r_0} \quad (22)$$

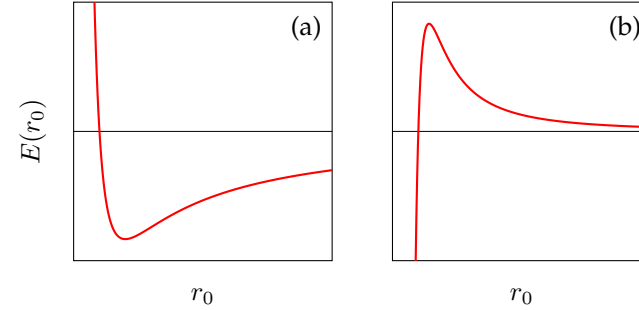


Figure I.5. Total energy of a wave packet of size r_0 in a power-law potential, $V(r) = g/r^\beta$ with $g < 0$. (a) Case $\beta < 2$: the (positive) kinetic energy dominates at short distances. (b) Case $\beta > 2$: the (negative) potential energy dominates at short distances, which makes it possible to generate wave packets of arbitrarily negative energy.

gives the characteristic size $r_0 = \hbar^2/m_r e^2$, equal to the Bohr radius, and the energy $-m_r e^4/2\hbar^2$, the energy of the 1s state of the hydrogen atom⁴.

2-3 The $\beta > 2$ case

The situation is then reversed: the kinetic energy dominates at large values of r_0 , whereas the potential energy dominates at small values of r_0 (figure I.5b). It follows that wave packets can be made with negative energy that is arbitrarily large in absolute value, indicating that the system does not have a well-defined ground state. The spectrum of the Hamiltonian extends to $E = -\infty$, and this situation is referred to as a “fall to the center”.

This case is encountered for van der Waals interactions ($\beta = 6, g = -C_6$) as well as for dipole-dipole interactions ($\beta = 3$) although the latter case is a little more complicated to deal with because of the anisotropic nature of the potential $V(r)$. The solution to this problem is well known, and physically quite relevant. Van der Waals interactions, for example, represent only the

⁴The fact that we find the exact result for the size of the ground state is somewhat fortuitous. Our estimates of the kinetic energy and of the potential energy of the wave packet were only approximate...

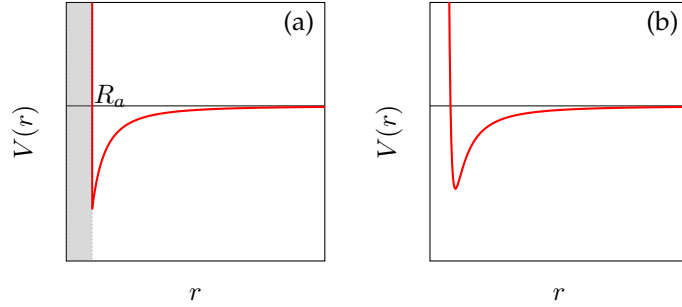


Figure I.6. Addition of a short-range repulsive potential to prevent the fall to the center in an algebraic potential varying as $r^{-\beta}$ with $\beta > 2$. (a): hard core in $r = R_a$, (b): addition of a repulsive potential with a higher power law.

long-distance component of interactions between two neutral atoms. At short distances, when the atoms' electron clouds begin to overlap, repulsive forces become dominant and prevent the collapse that would bring the two atoms together.

A simple phenomenological way of describing this short-range repulsion and avoiding the fall towards the center is to impose a hard core at a distance $R_a > 0$, i.e. $u(R_a) = 0$ (figure I.6a). An alternative is to add a further power-law repulsive potential, for example the Lennard–Jones potential:

$$V_{\text{LJ}}(r) = -\frac{C_6}{r^6} + \frac{C_{12}}{r^{12}} \quad (23)$$

to prevent collapse at $r = 0$ (figure I.6b). In what follows, we will adopt the first strategy, which is simpler to deal with mathematically.

Borderline case $\beta = 2$. This case, which will play a central role in the rest of the course, will be discussed in detail later. Let us simply point out that the fact that the kinetic energy and the potential energy have the same dependence on the size r_0 of the wave packet is a signature of the scale invariance of the potential in r^{-2} .

Exponent β	Behavior at the origin	Number of bound states	Example
$\beta < 2$	regular	infinite	Coulomb
$\beta > 2$	non-regular	finite	van der Waals

Table I.1. Behavior of the bound states of a particle moving in a potential $V(r) = -|g|/r^\beta$. Non-regular behavior at the origin indicates that the potential $V(r)$ needs to be regularized at short distances, for example by adding a hard-core potential, in order to ensure the existence of a finite-energy ground state.

2-4 How many bound states are there?

Having settled the problem of determining the wave functions at $r = 0$, we now turn to the question of the number of bound states.

For the Coulomb potential, the answer is well known. The bound states are labeled by the principal quantum number n and have the energy $E_n = -E_I/n^2$, where $-E_I$ is the energy of the ground state (-13.6 eV for the hydrogen atom). The number n can be written as $n = n' + \ell + 1$, where n' is the radial quantum number, i.e. the number of nodes in the radial wave function $\psi(r)$. Since n can be equal to any positive integer, we deduce that the number of bound states is infinite, whatever the value ℓ of the angular momentum.

This result can be recovered simply from the estimate given in (15). Let us consider states with zero angular momentum for simplicity, i.e. $V_{\text{tot}}(r) = -e^2/r$. The result (15) becomes:

$$N_{\text{bound}} \approx \frac{\sqrt{2m_e e^2}}{\pi \hbar} \int_0^{+\infty} \frac{dr}{\sqrt{r}}. \quad (24)$$

This integral diverges at its upper bound $r = +\infty$, indicating that an infinitely large number of bound states can be formed with energies arbitrarily close to zero.

The divergence of this integral will persist for all power-law potentials $V(r) = -|g|/r^\beta$ up to and including the value $\beta = 2$. We therefore expect an infinite number of bound states for this entire class of exponents.

For $\beta > 2$, we have seen that it is necessary to regularize the potential

$V(r)$ in the vicinity of the origin to ensure the existence of a ground state of well-defined energy. For the regularization obtained by imposing a hard core at $r = R_a$ (figure I.6), we obtain from (15):

$$N_{\text{bound}} \approx I \left[\frac{\sqrt{2m_r|g|}}{\pi\hbar} \int_{R_a}^{+\infty} \frac{dr}{r^{\beta/2}} \right]. \quad (25)$$

The integral is convergent and there is a finite number of bound states.

For the van der Waals potential, $V(r) = -C_6/r^6$, we find

$$N_{\text{bound}} \approx I \left[\frac{2}{\pi} \frac{R_{\text{vdW}}^2}{R_a^2} \right] \quad \text{with} \quad R_{\text{vdW}} = \frac{1}{2} \left(\frac{2m_r C_6}{\hbar^2} \right)^{1/4}, \quad (26)$$

a result already mentioned in the 2021 lecture series (Chapter 4, §2.1). The results presented in this section are collected in table I.1.

Validity of the semi-classical approach. For a power-law potential, the validity criterion written in (16) gives, for the zero-energy solution,

$$\frac{d(1/k)}{dr} = \frac{\hbar\beta}{\sqrt{8m_r|g|}} r^{\frac{\beta}{2}-1} \ll 1. \quad (27)$$

Here again, it is essential to separate the cases $\beta < 2$ and $\beta > 2$:

- If $\beta < 2$, i.e. $\frac{\beta}{2} - 1 < 0$, this validity criterion is satisfied at sufficiently large distances r . Even if the semi-classical approximation does not correctly describe the behavior at small r , the conclusion concerning the existence of an infinite number of bound states, which are essentially located far from the origin, remains valid.
- If $\beta > 2$, i.e. $\frac{\beta}{2} - 1 > 0$, this validity criterion is, by contrast, fulfilled for small values of r . A more detailed study of the case of the van der Waals potential, $\beta = 6$, shows that almost all the bound states are correctly described by the semi-classical approach (cf. the 2021 lecture series, Chapter 4, §4): only the position of the last bound state is poorly estimated by this approach. In particular, the estimate of the total number of bound states given in (26) is quite relevant.

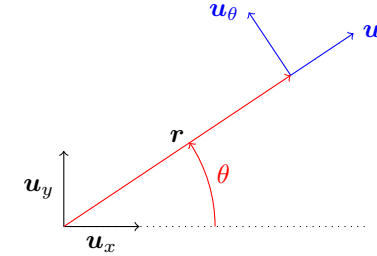


Figure I.7. Definition of polar coordinates to describe the classical motion of a particle in a central potential.

- For $\beta = 2$, we note that the validity criterion (27) does not constrain the position r , but only the amplitude $|g|$ of the potential, which must be significantly larger than $\hbar^2/m_r$. Note that here again the case $\beta = 2$ acts as a boundary separating two radically different situations.

3 The $1/r^2$ potential in classical mechanics

Most of this course will be devoted to the quantum properties of particles moving in a $1/r^2$ potential. However, it is interesting to begin our study with the *classical* version of the problem, which contains several precursors of the specific features we will be dealing with in the following.

3-1 Classical motion and fall to the center

Let us briefly recall the nature of the classical motion of a particle of mass m_r in any central potential. Starting from the position $\mathbf{r} = r\mathbf{u}_r$ of the particle (see figure I.7), we find its velocity in polar coordinates:

$$\frac{d\mathbf{r}}{dt} = \dot{r}\mathbf{u}_r + r\dot{\mathbf{u}}_r = \dot{r}\mathbf{u}_r + r\dot{\theta}\mathbf{u}_\theta. \quad (28)$$

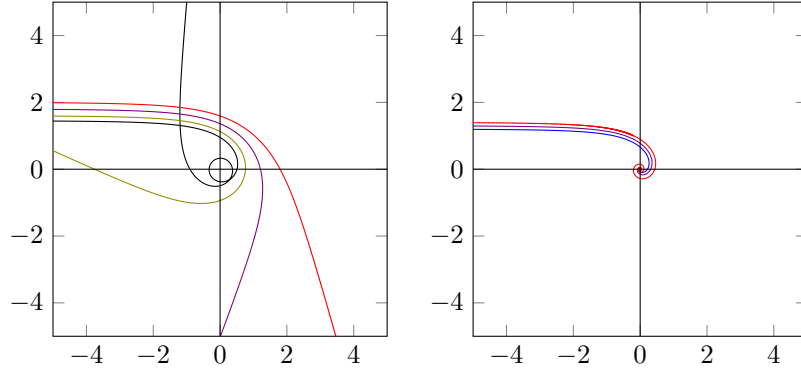


Figure I.8. Classical trajectories in the potential g/r^2 with $g < 0$. Left, angular momentum $L > L_c$: $L/L_c = 1.025, 1.13, 1.27, 1.41$. Right, fall to the center for $L < L_c$: $L/L_c = 0.85, 0.92, 0.99$.

This gives the acceleration

$$\frac{d^2 \mathbf{r}}{dt^2} = (\ddot{r} - r\dot{\theta}^2) \mathbf{u}_r + (2\dot{r}\dot{\theta} + r\ddot{\theta}) \mathbf{u}_\theta. \quad (29)$$

Projecting the equation of motion onto the radial and orthoradial axes leads to

$$m_r (\ddot{r} - r\dot{\theta}^2) = -\frac{dV}{dr} \quad 2\dot{r}\dot{\theta} + r\ddot{\theta} = 0, \quad (30)$$

where, for the case of interest here, $V(r) = g/r^2$.

The second equation of (30) expresses the conservation of angular momentum

$$\mathbf{L} = m_r \mathbf{r} \times \mathbf{v} = m_r r^2 \dot{\theta} \mathbf{u}_z, \quad (31)$$

which means that the motion is planar, this plane being defined by the two vectors $\mathbf{r}_i$ and $\mathbf{v}_i$ (initial position and initial velocity).

The first equation can be interpreted as a one-dimensional equation of motion:

$$m_r \ddot{r} = -\frac{dV_{\text{tot}}}{dr} \quad \text{with} \quad V_{\text{tot}}(r) = V(r) + \frac{L^2}{2m_r r^2} \quad (32)$$

This equation must of course be seen as the classical equivalent of the radial Schrödinger equation given in (7).

For the potential $V(r) = g/r^2$ with $g < 0$, we can see that two cases are possible (figure I.8):

- If $L > L_c$, where L_c is the critical value defined by

$$L_c = \sqrt{2m_r |g|} \quad (33)$$

a particle arriving from infinity cannot approach arbitrarily close to the center, since $V_{\text{tot}}(r) \rightarrow +\infty$ when $r \rightarrow 0$. It may make one or more turns before heading back to infinity.

- If $L < L_c$, the particle falls to the center. This situation is the classical equivalent of a quantum Hamiltonian whose spectrum extends to $-\infty$.

If we introduce the impact parameter b and the velocity v of the atom arriving from infinity, we have $L = m_r v b$, so that the condition for falling to the center can be written

$$L < L_c \quad \Leftrightarrow \quad b < \sqrt{\frac{2|g|}{m_r v^2}}. \quad (34)$$

The fact that the criterion for falling to the center can be written so simply in terms of angular momentum alone is specific to the r^{-2} potential, which has the same spatial dependence as the centrifugal energy term. We will recover the condition (34)—with a slight modification—in the quantum case.

3-2 The atom–charged-wire interaction

We now describe a first experimental implementation of the motion of an atomic particle in a $1/r^2$ potential, realized by Denschlag, Umshaus, et al. (1998). Although we are dealing here with microscopic particles, it is not necessary to use the quantum formalism to treat this problem, which is well described by a classical approach.

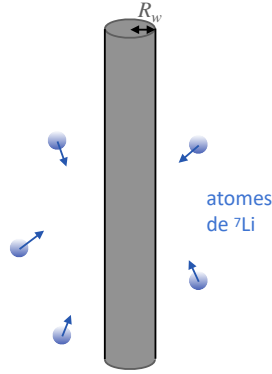


Figure I.9. Principle of the experiment by Denschlag, Umshaus, et al. (1998), studying the motion of polarizable neutral atoms (^7Li) in the electrostatic field created by a uniformly charged wire.

The geometry is two-dimensional, and uses the electrostatic potential created by a uniformly charged rectilinear wire, with a linear charge density that we will denote Λ (figure I.9). The wire is oriented along the z axis and we are interested in the motion of the particles in the xy plane. We denote by $\mathbf{u}_r$ and $\mathbf{u}_\theta$ the two unit vectors, radial and orthoradial respectively, in this plane.

The wire creates at any point in space (apart from the wire itself) the electric field

$$\mathcal{E} = \frac{\Lambda}{2\pi\epsilon_0 r} \mathbf{u}_r. \quad (35)$$

Consider a neutral atom of polarizability $\alpha_a > 0$ placed in this electrostatic field. An electric dipole $\mathbf{d} = \alpha_a \mathcal{E}$ is induced within the atom, and the interaction energy between the atom and the field is:

$$E = -\frac{\alpha_a}{2} \mathcal{E}^2 \equiv \frac{g}{r^2} \quad \text{with} \quad g \equiv -\frac{\alpha_a}{2} \left(\frac{\Lambda}{2\pi\epsilon_0} \right)^2 < 0. \quad (36)$$

We therefore generate the desired attractive potential in $1/r^2$.

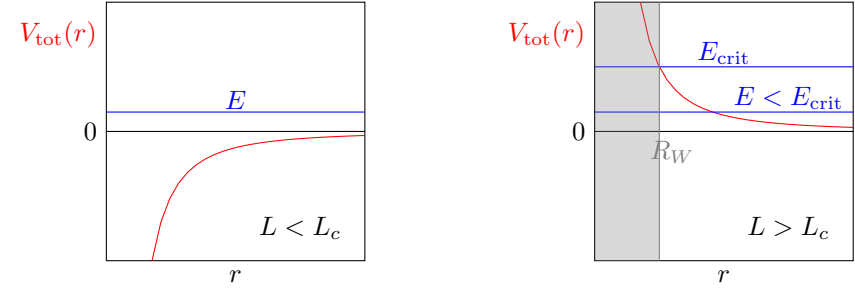


Figure I.10. The two possible cases in the Denschlag, Umshaus, et al. (1998) experiment. If $L < L_c$ (left figure), the fall to the center occurs with certainty, whatever the incident energy. If $L > L_c$ (right figure), the atom can hit the wire of radius R_w if its energy exceeds the critical value $E_{\text{crit}} = V_{\text{tot}}(R_w)$, which corresponds to the condition (37).

3-3 The results of Denschlag et al.

Denschlag, Umshaus, et al. (1998) carried out their experiment with lithium atoms of mass m captured in a magneto-optical trap. The electrically charged wire can be placed in the center of the magneto-optical trap or outside it (inset of figure I.11, left). The rate of atomic loss is measured in both cases, by varying the linear charge of the wire and using the fact that atoms coming into contact with the wire stick to it. The fall to the center therefore results in an increased loss of atoms, in addition to the inevitable losses due to collisions with the molecules of the residual gas in the experimental chamber.

Since the wire has a non-zero radius R_w , it can be shown that the condition (34) for losing an incident atom with impact parameter b and velocity v becomes (see figure I.10)

$$b < \sqrt{R_w^2 + \frac{2|g|}{mv^2}}. \quad (37)$$

This condition must then be averaged over the positions and velocities of the trapped atoms to deduce the rate of atom loss induced by the presence of the charged wire.

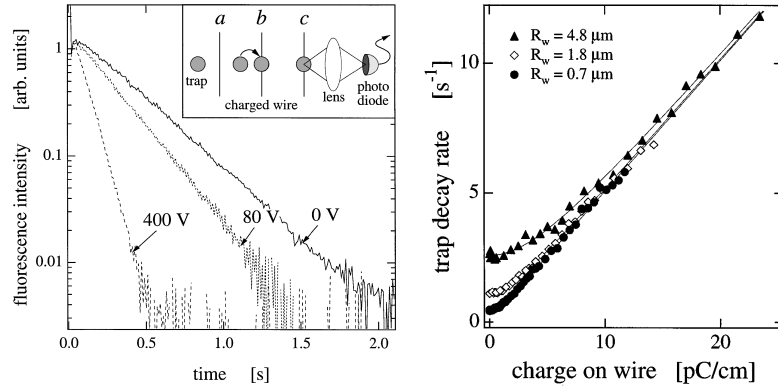


Figure I.11. Losses induced within a magneto-optical trap of lithium atoms by a uniformly charged metal wire. Figure taken from Denschlag, Umshaus, et al. (1998).

A typical result showing the decay of the number of trapped atoms is shown in figure I.11, left. The presence of the charged wire inside the cloud of atoms leads to a spectacular increase of the decay rate. For a wire of given radius R_w , this decay rate increases almost linearly with the linear charge Λ , as expected from (37) when the contribution of R_w becomes negligible (figure I.11, right). The experimental results are in excellent agreement with a model of the process that takes into account the polarizability of the lithium atom.

4 The $1/r^2$ potential in quantum mechanics

We are now interested in the quantum version of the critical case $\beta = 2$, which will play a crucial role in three-body physics. The analysis in terms of wave packets has shown that the two competing contributions, kinetic energy and potential energy, obey the same scaling law with respect to the size r_0 of the wave packet. We can therefore expect the amplitude g of the potential to be the sole parameter controlling the dynamics of the particle.

4-1 Scale invariance

The $1/r^2$ potential has a property that is unique among power-law potentials: it is scale invariant, which means that a given solution of the Schrödinger equation (time-independent or time-dependent) can generate an infinite family of solutions of the same equation. This result is independent of the dimension of space.

Let us start with the time-independent case and consider an eigenfunction $\Psi(\mathbf{r})$ of the Hamiltonian:

$$-\frac{\hbar^2}{2m_r} \nabla^2 \Psi + \frac{g}{r^2} \Psi = E \Psi. \quad (38)$$

Let us introduce the function $\Phi(\mathbf{r})$ defined by

$$\Phi(\mathbf{r}) = \Psi(\lambda \mathbf{r}), \quad (39)$$

where λ is a positive real number, which can be taken to be any value at this stage⁵. It is easy to check that Φ satisfies the equation

$$-\frac{\hbar^2}{2m_r} \nabla^2 \Phi + \frac{g}{r^2} \Phi = (\lambda^2 E) \Phi. \quad (40)$$

The function Φ is therefore also an eigenstate of the Hamiltonian, with energy $\lambda^2 E$. This corresponds to the announced result: starting from the eigenenergy E and its associated eigenfunction, any energy E' with the same sign as E can be written as $E' = \lambda^2 E$ and is therefore also an eigenvalue of the Hamiltonian. This simply follows from the fact that the operator ∇^2 coming from the kinetic energy and the term $1/r^2$ coming from the potential energy have the same behavior in the change of length scale $\mathbf{r} \rightarrow \lambda \mathbf{r}$.

The scale invariance we have just found for the eigenstates of the Hamiltonian can be generalized to time-dependent problems. Consider a wave function $\Psi(\mathbf{r}, t)$ solution of

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m_r} \nabla^2 \Psi + \frac{g}{r^2} \Psi. \quad (41)$$

⁵A value $\lambda > 1$ corresponds to a function Φ which is more concentrated at the origin than the initial function Ψ . Its kinetic energy is therefore increased (it varies on a shorter scale) as is its potential energy in absolute value.

We can then check that the function

$$\Phi(\mathbf{r}, t) = \Psi(\lambda\mathbf{r}, \lambda^2 t) \quad (42)$$

is also a solution of (41). This change of scale on the time is linked to the change of scale on the energy, $E \rightarrow \lambda^2 E$, appearing on (40). Indeed, if $\Psi_E(\mathbf{r})$ is the eigenstate of the Hamiltonian of energy E , the substitution

$$\Psi(\mathbf{r}, t) = \Psi_E(\mathbf{r}) e^{-iEt/\hbar} \longrightarrow \Phi(\mathbf{r}, t) = \Psi_E(\lambda\mathbf{r}) e^{-iE\lambda^2 t/\hbar} \quad (43)$$

shows that we have found a function $\Psi_E(\lambda\mathbf{r})$ of energy $\lambda^2 E$.

Scale invariance in classical mechanics. The scale invariance of the $1/r^2$ potential is also present in classical mechanics. Let us first note that in the change of scale $\mathbf{r} \rightarrow \lambda\mathbf{r}$, $t \rightarrow \lambda^2 t$, the velocities are modified according to the law:

$$\mathbf{v} = \frac{d\mathbf{r}}{dt} \longrightarrow \frac{\mathbf{v}}{\lambda}. \quad (44)$$

We can then check that, starting from a trajectory with initial condition $(\mathbf{r}_i, \mathbf{v}_i)$ and satisfying the equations of motion

$$m \frac{d\mathbf{v}}{dt} = -\nabla \left(\frac{g}{r^2} \right) = \frac{2g}{r^3} \mathbf{u}_r, \quad (45)$$

we obtain a family of trajectories $\mathbf{r}'(t')$, $\mathbf{v}'(t')$ that are also solutions of the equation of motion, by setting $t' = \lambda^2 t$, $\mathbf{r}' = \lambda\mathbf{r}$ and $\mathbf{v}' = \mathbf{v}/\lambda$. All these trajectories can therefore be deduced from each other by a homothety of ratio λ . Note also that the angular momentum $\mathbf{L} = m\mathbf{r} \times \mathbf{v}$ is not modified by this change of scale, which ensures that the condition of falling to the center (34) remains the same for all members of the same family. This was, of course, essential if we were to be able to go from one member of the family to another using a homothety.

4-2 Breaking scale invariance

For positive energies E , describing the scattering states, this result concerning scale invariance calls for no particular comment. It can be very convenient in practice, since it ensures that knowledge of a scattering state at a

given energy generates an infinite family of other scattering states, of arbitrary energy.

For negative energies E , describing bound states, this result is problematic. It indicates that if a bound state of energy E exists, we can generate states of energy $E' = \lambda^2 E$ arbitrarily negative: the spectrum of the Hamiltonian is therefore not bounded below, which is not physically acceptable. Mathematically, this indicates that the Hamiltonian is not self-adjoint (see note below).

The remedy for this difficulty has already been mentioned above for potentials in $1/r^\beta$ with $\beta > 2$: to prevent the particle from falling to the center, the potential in the vicinity of the origin must be regularized, for example by imposing a hard core at $r = R_a > 0$. Note that this remedy breaks the continuous scale invariance we have just described. Given any $\lambda > 0$ and an eigenstate $\Psi(r)$ of energy $E < 0$ satisfying $\Psi(r) = 0$ at $r = R_a$, there is no reason why the transformed state $\Phi(r) = \Psi(\lambda r)$ should also satisfy $\Phi(r) = 0$ at R_a . In other words, once the hard core is imposed at R_a , starting from $\Psi(r)$ with energy $E < 0$, we will not be able to construct eigenstates of energy $E' < 0$ with $|E'|$ arbitrarily large, which would lead to a spectrum unbounded from below.

Note: Hermitian operators and self-adjoint operators. In mathematics, one defines the adjoint $\hat{A}^\dagger$ of an operator $\hat{A}$ in the following way (see for example the discussions of Bonneau, Faraut, et al. (2001) and Araujo, Coutinho, et al. (2004), who consider simple examples based on the one-dimensional Schrödinger equation):

- We start with an operator $\hat{A}$ defined by its action on wave functions $|\phi\rangle$ and by its domain $\mathcal{D}(\hat{A})$, i.e. the space of physically relevant wave functions on which $\hat{A}$ will act. The definition of the domain takes into account boundary conditions, such as the constraint $u(0) = 0$ for the reduced radial wave function.
- We define the domain of the adjoint $\mathcal{D}(\hat{A}^\dagger)$ as the set of functions $|\psi\rangle$ such that the linear form

$$|\phi\rangle \in \mathcal{D}(\hat{A}) \longrightarrow \langle\psi|\hat{A}\phi\rangle \quad (46)$$

is continuous. We then know that for each $|\psi\rangle \in \mathcal{D}(\hat{A}^\dagger)$, there exists a state $|\psi'\rangle$ of the Hilbert space such that $\langle\psi|\hat{A}\phi\rangle = \langle\psi'|\phi\rangle$ for all $|\phi\rangle \in \mathcal{D}(\hat{A})$. We set $|\hat{A}^\dagger\psi\rangle = |\psi'\rangle$, i.e.

$$\langle\psi|\hat{A}\phi\rangle = \langle\hat{A}^\dagger\psi|\phi\rangle. \quad (47)$$

- The operator $\hat{A}$ is said to be symmetric (or Hermitian) if $\hat{A}$ and $\hat{A}^\dagger$ have the same mathematical expression, in terms of derivatives with respect to the variable r or of multiplication by functions of r , for example.
- The operator $\hat{A}$ is said to be self-adjoint if it is symmetric and if the domains $\mathcal{D}(\hat{A})$ and $\mathcal{D}(\hat{A}^\dagger)$ coincide.

It can be shown that the existence of a lower bound on the energy spectrum, and therefore of a ground state, is guaranteed only for self-adjoint operators. In finite dimension, the operator $\hat{A}$ can be represented by a square matrix and the two notions “Hermitian” and “self-adjoint” coincide. In infinite dimension, this is not always the case, a simple example being provided by the infinite square potential well (Bonneau, Faraut, et al. 2001). A discussion of this problem for the specific case of the potential in $1/r^2$ can be found in Essin & Griffiths (2006).

4-3 Zero-energy solution

Let us now return to the specific case of three-dimensional motion. Recall that since the potential g/r^2 is isotropic, we can look for the eigenstates of the Hamiltonian in the form $\psi(r) Y_{\ell,m}(\theta, \varphi)$. The eigenvalue equation for the reduced radial wave function $u(r) = r\psi(r)$ reads

$$-\frac{\hbar^2}{2m_r} \frac{d^2u}{dr^2} + \left[\frac{g}{r^2} + \frac{\hbar^2 \ell(\ell+1)}{2m_r r^2} \right] u(r) = E u(r) \quad (48)$$

with $E < 0$ for a bound state, which can be written

$$-u'' + \frac{\alpha}{r^2} u = \epsilon u \quad (49)$$

where we have set

$$\alpha = \frac{2m_r g}{\hbar^2} + \ell(\ell+1) \quad \epsilon = \frac{2m_r E}{\hbar^2} \quad (50)$$

For the angular momentum channel $\ell = 0$, the coefficient α is simply the scaled version of g : $\alpha = 2m_r g/\hbar^2$. If the angular momentum is non-zero, we first add the centrifugal potential $\hbar^2 \ell(\ell+1)/2m_r r^2$ to the potential g/r^2 since they both have the same variation with respect to r , before proceeding with the scaling.

Note that even if the coefficient g is chosen here to be negative (attractive potential), the coefficient α can be positive or negative, depending on the value of the angular momentum. In what follows, we will mainly be interested in the case where α remains negative, i.e. an angular momentum low enough for the attraction due to $V(r)$ to dominate the centrifugal repulsion. For $\alpha > 0$, the equation (49) obviously has no bound states.

In this section, we will only be interested in the zero-energy solution and we will postpone the explicit search for the bound states to the next chapter. As we saw in § 1-4, the number of nodes of this zero-energy solution gives an immediate indication of the number of bound states. It should also be recalled that the $1/r^2$ potential decreases too slowly when $r \rightarrow +\infty$ for the notion of scattering length to be applicable.

We therefore consider the equation

$$-u'' + \frac{\alpha}{r^2} u = 0, \quad u(R_a) = 0. \quad (51)$$

The solutions can be found in a simple form for the $1/r^2$ potential:

$$u(r) = r\psi(r) = r^{s+1} \quad (52)$$

with $[-s(s+1) + \alpha] r^{s-1} = 0$. The exponent s is therefore a solution of the second-degree equation

$$s^2 + s - \alpha = 0 \quad (53)$$

whose roots can be written as

$$s_1 = -\frac{1}{2} + \sqrt{\alpha + \frac{1}{4}} \quad s_2 = -\frac{1}{2} - \sqrt{\alpha + \frac{1}{4}} \quad (54)$$

These two roots, real or complex depending on the sign of $\alpha + \frac{1}{4}$, correspond to two independent solutions of the equation (51), as expected for a second-order equation.

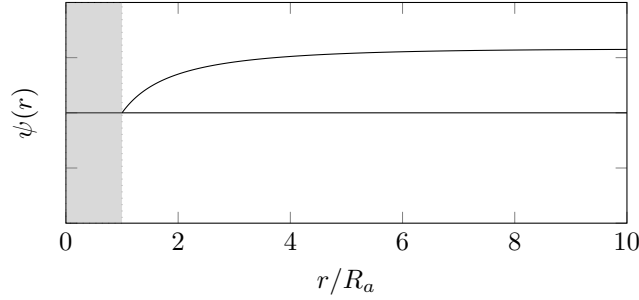


Figure I.12. Case $\alpha > -1/4$. Zero-energy eigenfunction for the potential α/r^2 , plotted for $\alpha = -1/8$.

Taking into account the boundary condition for a hard core at R_a gives the desired solution:

$$\psi(r) = \left(\frac{r}{R_a}\right)^{s_1} - \left(\frac{r}{R_a}\right)^{s_2} \quad (55)$$

up to a multiplicative constant.

There are two cases to discuss, depending on the sign of the argument of the square root in (54).

Case: $\alpha > -1/4$. This case, which occurs if $|g|$ is chosen to be small from the beginning or when we take ℓ to be large enough, leads to real values for s_1 and s_2 , with $s_2 < -\frac{1}{2} < s_1$. The function $\psi(r)$ then has no nodes (figure I.12), which means that there are no negative energy eigenstates, and therefore no bound states.

This very strong result comes from the radical way in which the potential is regularized at the origin, by imposing a hard core at R_a . A milder regularization could lead to the presence of one or more bound states but, in any case, we do not find here an infinite number of bound states, as was the case for the Coulomb potential, or as we will see below for a larger value of $|\alpha|$.

Note that regularization by a hard core at R_a is not essential in the case

$\alpha > -1/4$. Letting R_a tend to 0 in the expression (55), we find, up to a multiplicative factor,

$$\psi(r) \propto r^{s_1} - R_a^{\sqrt{4\alpha+1}} r^{s_2} \quad (56)$$

which means that the weight of r^{s_2} in this solution tends to 0 when $R_a \rightarrow 0$. This result can also be obtained by requiring the integral giving the mean value of the potential energy, which is proportional to

$$\int \frac{g}{r^2} |\psi(r)|^2 d^3r = 4\pi g \int_0^\infty |\psi(r)|^2 dr, \quad (57)$$

to be convergent at $r = 0$. This means that $\psi(r)$ must diverge less rapidly than $r^{-1/2}$ in the vicinity of the origin. This is the case for the root s_1 , but not for the root s_2 .

Case: $\alpha < -1/4$. This is the situation in which we will be mostly interested in the next chapters. In this case, the two roots (54) are complex conjugates of each other and are written as

$$\alpha < -1/4 : \quad s_1 = -\frac{1}{2} + i|s_0|, \quad s_2 = -\frac{1}{2} - i|s_0|, \quad (58)$$

with

$$\alpha < -1/4 : \quad s_0 \equiv \sqrt{\alpha + \frac{1}{4}} = i \left[\frac{2m_r|g|}{\hbar^2} - \left(\ell + \frac{1}{2} \right)^2 \right]^{1/2} \in i\mathbb{R} \quad (59)$$

The function $\psi(r)$ then reads

$$\psi(r) = \sqrt{\frac{R_a}{r}} \left[e^{i|s_0| \ln(r/R_a)} - e^{-i|s_0| \ln(r/R_a)} \right] \quad (60)$$

or, up to a multiplicative constant

$$\psi(r) = \frac{1}{\sqrt{r}} \sin[|s_0| \ln(r/R_a)] \quad (61)$$

This “log-periodic” function is plotted in figure I.13 for $|s_0| = 10$.

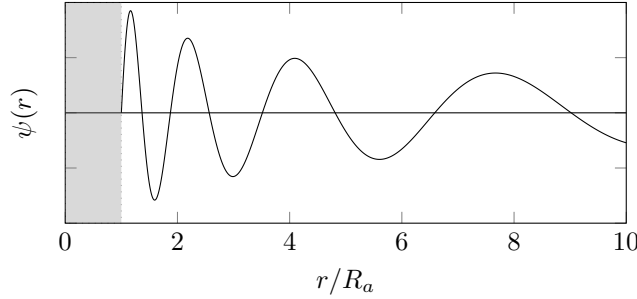


Figure I.13. Case $\alpha < -1/4$. Zero-energy eigenfunction for the potential α/r^2 , plotted for $s_0 \equiv (\alpha + 1/4)^{1/2} = 10i$.

This function has an infinite number of nodes, located at points r_n such that

$$|s_0| \ln(r_n/R_a) = n\pi \quad \Rightarrow \quad r_n = R_a e^{n\pi/|s_0|}. \quad (62)$$

where n is a strictly positive integer. These nodes form a geometric sequence of common ratio $e^{\pi/|s_0|} > 1$. We deduce that there are infinitely many bound states in this potential, despite the regularization by the hard core at R_a . The situation is therefore radically different from that found for potentials decreasing more rapidly at infinity ($\beta > 2$).

To summarize, the potential α/r^2 for $\alpha < -1/4$ combines the two types of “pathology” described in §2 (cf. table I.2):

- This potential diverges rapidly in the vicinity of the origin and requires regularization, for example with a hard core at R_a , just like the potentials $1/r^\beta$ with $\beta > 2$. This regularization is not necessary, on the other hand, for the Coulomb potential $1/r$. As mentioned above (see figure I.6), we can choose a milder regularization to prevent the fall to the center, or even invoke effects linked to mean-field interactions in N -body systems [see for example Sakaguchi & Malomed (2011), Astrakharchik & Malomed (2015), and Malomed (2018)].
- This potential tends slowly to 0 at infinity and leads to an infinite number of weakly bound states, just like the Coulomb potential.

Exponent β	Behavior at the origin	Number of bound states	Example
$\beta < 2$	regular	infinite	Coulomb
$\beta > 2$	non-regular	finite	van der Waals
$\beta = 2$ and $\alpha < -1/4$	non-regular	infinite	Efimovian

Table I.2. Completed version of table I.1, including the case of the g/r^2 potential.

The case of the Coulomb potential. In this case, the zero-energy solution of $\psi'' + \frac{2}{r}\psi' + \frac{1}{r}\psi = 0$ (state $\ell = 0$) reads $\psi(r) = J_1(2\sqrt{r})/\sqrt{r}$, where J_1 is the Bessel function of order 1. The function $\psi(r)$ therefore has infinitely many zeros, but no singularity at $r = 0$.

4-4 Critical point $\alpha = -1/4$ and quantum anomaly

The study of the quantum problem revealed the existence of the critical point $\alpha = -1/4$, i.e.

$$\frac{2m_r g}{\hbar^2} + \ell(\ell + 1) = -\frac{1}{4} \quad (63)$$

or

$$\left(\ell + \frac{1}{2}\right) \hbar = \sqrt{2m_r |g|}. \quad (64)$$

It is interesting to relate this critical point to the one found in classical mechanics, $L_c = \sqrt{2m_r |g|}$, by identifying the characteristic value of the angular momentum of the channel associated with the quantum number ℓ : $L \sim (\ell + \frac{1}{2}) \hbar$. We therefore find the same critical point in both classical and quantum problems.

When α is greater than the critical value $-1/4$ (quantum case) or when $L > L_c$ (classical case), the classical and quantum approaches both reveal scale invariance without any notable singularity:

- at the classical level, an infinite family of trajectories $\mathbf{r}_\lambda(t)$ with $r \rightarrow +\infty$ when $t \rightarrow \pm\infty$, these trajectories being deduced from one another by a homothety of ratio λ .
- at the quantum level, an infinite family of eigenstates, all of positive energy, deduced from one another by $\Phi_\lambda(\mathbf{r}) = \Psi(\lambda\mathbf{r})$.

When α is less than the critical value $-1/4$, scale invariance remains intact at the classical level, with families of trajectories all “falling to the center”. We have seen, on the other hand, that this scale invariance is broken at the quantum level, owing to the unavoidable introduction of the regularization scale R_a needed to ensure that the Hamiltonian remains self-adjoint.

This breaking of the scale invariance is an example of a quantum anomaly (Coon & Holstein 2002; Moroz 2011; Sundaram, Burgess, et al. 2021). Starting from a problem that possesses a certain symmetry at the classical level, in this case scale invariance, we find that this symmetry cannot be maintained when the problem is quantized. Here, as we shall see later, part of this symmetry does survive, in that a scale invariance remains once the quantum version of the problem has been set up. The link between this critical point and the usual notion of phase transition is discussed by Ovdad & Akkermans (2021).

Chapter II

Stationary states and dynamics in a $1/r^2$ potential

In the previous chapter, we explained the importance of a good understanding of the motion of a particle in an attractive potential varying as $-1/r^2$ in order to tackle three-body physics in the Efimov regime. This type of potential emerges when the binary interactions are resonant, i.e. described by an infinite scattering length, or at least one that is larger than the size of the atomic edifices under consideration.

Here we continue our study of the one-body problem described by the eigenvalue equation

$$-\frac{\hbar^2}{2m_r} \nabla^2 \Psi + \frac{g}{r^2} \Psi = E \Psi, \quad g < 0, \quad (1)$$

for which we presented the zero-energy solution in the previous chapter. We will continue this study and determine the possible bound states ($E < 0$) for this problem. We will illustrate our results with a concrete problem: Can an electric charge and an electric dipole form a bound state? We will end our study with a generalization of the scale invariance already discussed. We will introduce the notion of conformal invariance and explain why this leads to remarkable properties for the dynamics of the system.

Let us begin by recalling the main results obtained in the previous chapter. To take advantage of the rotational invariance of the problem, we can work in a channel of given angular momentum ℓ and look for $\Psi(\mathbf{r})$ in the form $\Psi(\mathbf{r}) = \psi(r) Y_{\ell,m}(\theta, \varphi)$ where $Y_{\ell,m}$ is a spherical harmonic. We introduce the reduced radial wave function $u(r) = r \psi(r)$ which satisfies the

one-dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m_r} \frac{d^2 u}{dr^2} + \left[\frac{g}{r^2} + \frac{\hbar^2 \ell(\ell+1)}{2m_r r^2} \right] u(r) = E u(r). \quad (2)$$

This equation can be written in the compact form

$$\boxed{-u'' + \frac{\alpha}{r^2} u = \epsilon u} \quad (3)$$

with

$$\boxed{\alpha = \frac{2m_r g}{\hbar^2} + \ell(\ell+1) \quad \epsilon = \frac{2m_r E}{\hbar^2}} \quad (4)$$

For zero energy $\epsilon = 0$, the solutions to this equation can be found in the form of a power law

$$u(r) = r \psi(r) = r^{s+1} \quad \text{with} \quad s^2 + s - \alpha = 0. \quad (5)$$

The two roots of this second-degree equation each give a possible exponent for the power law

$$s_1 = -\frac{1}{2} + \sqrt{\alpha + \frac{1}{4}}, \quad s_2 = -\frac{1}{2} - \sqrt{\alpha + \frac{1}{4}}. \quad (6)$$

The case of interest for the rest of this course, leading to the existence of bound states, corresponds to the situation $\alpha + \frac{1}{4} < 0$ for which the two

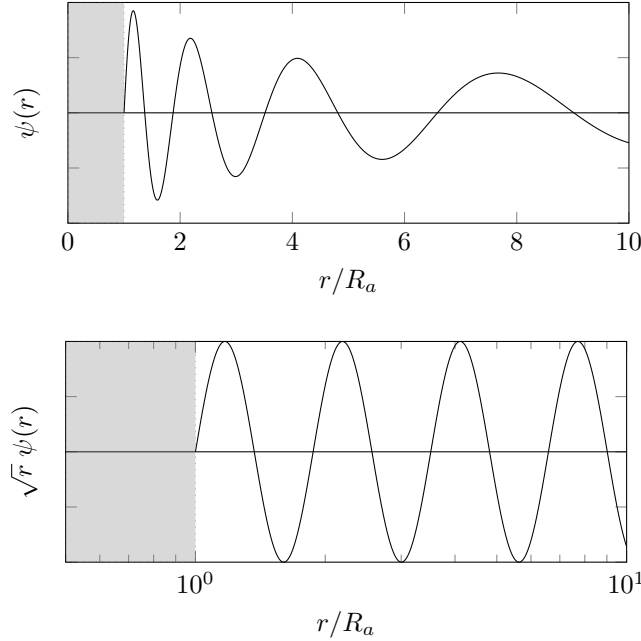


Figure II.1. Zero-energy wave function in a $1/r^2$ potential in the case $\alpha < -1/4$. Top: linear coordinates, bottom: semi-logarithmic coordinates.

roots are complex conjugates of each other

$$s_1 = -\frac{1}{2} + i|s_0|, \quad s_2 = -\frac{1}{2} - i|s_0|, \quad (7)$$

with the imaginary number s_0 defined by

$$s_0 \equiv \sqrt{\alpha + \frac{1}{4}} \in i\mathbb{R} \quad (8)$$

To solve the problem of the “fall to the center”, i.e. the absence of a lower bound for the spectrum of the Hamiltonian appearing in (1) or in (3), we assume the presence of a hard core at $r = R_a > 0$, which amounts

to imposing $\psi(R_a) = u(R_a) = 0$. The zero-energy solution then reads

$$E = 0 : \quad \psi(r) = \frac{1}{\sqrt{r}} \sin[|s_0| \ln(r/R_a)] \quad (9)$$

and it has an infinite number of nodes, located at points r_n such that (cf. figure II.1)

$$|s_0| \ln(r_n/R_a) = n\pi \quad \Rightarrow \quad r_n = R_a e^{n\pi/|s_0|}. \quad (10)$$

We will now use these results to construct the negative energy states.

1 The bound states of the α/r^2 potential

1-1 Absence of bound states for $\alpha > -1/4$

By examining the form of the wave function at zero energy in the presence of a hard core at R_a , we showed in the previous chapter that there can be no bound state when α is greater than the critical value $-1/4$. This wave function reads

$$\psi(r) = \left(\frac{r}{R_a}\right)^{s_1} - \left(\frac{r}{R_a}\right)^{s_2} \quad (11)$$

where s_1 and s_2 are the solutions of the second-degree equation (5): $s^2 + s - \alpha = 0$. As these roots s_1 and s_2 are real if $\alpha > -1/4$, this means that $\psi(r)$ has no node in the interval $]R_a, +\infty[$: this is the ground state of the system and there can be no eigenstate with energy less than 0.

Let us show how to recover this result directly, in the absence of any regularization procedure for the potential in $1/r^2$. To do this, we will follow a method proposed by Essin & Griffiths (2006). We begin by noting that the Schrödinger equation (3) satisfied by the reduced radial function can be put into the form

$$\epsilon u = \left(-\frac{d^2}{dr^2} + \frac{\alpha}{r^2}\right) u = \left(\frac{d}{dr} + \frac{s+1}{r}\right) \left(-\frac{d}{dr} + \frac{s+1}{r}\right) u \quad (12)$$

where s is a solution of $s^2 + s - \alpha = 0$. Note that if s is real, we find, for any pair of functions $u_1(r), u_2(r)$ that are regular on the interval $[0, +\infty[$, tend

to 0 at $+\infty$ and satisfy the boundary condition $u_j(0) = 0$,

$$\int_0^\infty u_2^*(r) \left[\left(\frac{d}{dr} + \frac{s+1}{r} \right) u_1(r) \right] dr = \int_0^\infty \left[\left(-\frac{d}{dr} + \frac{s+1}{r} \right) u_2(r) \right]^* u_1(r) dr \quad (13)$$

Suppose that a bound state of energy $E < 0$ and reduced radial wave function $u(r)$ (normalized) exists. Multiply the eigenvalue equation (12) by $u(r)$, integrate over the interval $[0, +\infty[$ and use the result (13). We find

$$\frac{2m_r E}{\hbar^2} = \int \left| \left(-\frac{d}{dr} + \frac{s+1}{r} \right) u(r) \right|^2 dr \quad (14)$$

which is clearly impossible for an energy $E < 0$, since the right-hand side is always non-negative. There can therefore be no bound state regular on $[0, +\infty[$.

1-2 Scale invariance partially recovered

The search for bound states involves solving the differential equation (3). This can of course be done numerically, or by using special functions, in this case the modified Bessel functions of the first and second kind, $I_\nu(x)$ and $K_\nu(x)$, solutions of

$$x^2 y''(x) + x y'(x) - (x^2 + \nu^2) y(x) = 0 \quad (15)$$

For $\alpha < -1/4$, we can in fact rewrite the eigenvalue equation in this form by setting, for $E < 0$,

$$x = \kappa r \quad y(x) = \frac{u(r)}{\sqrt{r}} = \sqrt{r} \psi(r) \quad \text{with} \quad \nu = s_0, \quad \kappa = \frac{\sqrt{2m_r |E|}}{\hbar}, \quad (16)$$

and as before $s_0 = (\alpha + 1/4)^{1/2} \in i\mathbb{R}$. To obtain a normalizable function, tending to 0 at infinity, we must in fact restrict ourselves to the function $K_{|s_0|}$ (Essin & Griffiths 2006) and the values of κ corresponding to the bound states are obtained by requiring $\psi(r)$ to vanish at R_a .

The wave functions $\psi_n(r)$ of the first bound states are plotted in figures II.2 and II.3, together with the zero-energy wave function (9). To bring

out the important features of these wave functions, we have in fact plotted $\sqrt{r} \psi(r)$ and chosen logarithmic coordinates for the x axis, so that the wave function (9) for $E = 0$ is a simple sinusoid.

This plot calls for a number of comments which will play an important role throughout the rest of this course:

1. A significant part of the plot of the excited bound states (and to a lesser extent of the ground state $n = 0$) is virtually identical to the zero-energy state. This is easy to understand: as soon as r is significantly smaller than the turning point of the classical motion R_b , defined by $|\alpha|/R_b^2 = \kappa^2$, the differential equation defining the bound state

$$-u'' + \frac{\alpha}{r^2} u = -\kappa^2 u \quad (17)$$

is practically identical to the equation for zero energy

$$-u'' + \frac{\alpha}{r^2} u = 0 \quad (18)$$

since the contribution of $\kappa^2 u$ is then negligible compared with that of $\alpha u/r^2$. For example, in figure II.3, the excited state $\psi_{n=4}(r)$ ($\kappa R_a \approx 6.4 \times 10^{-4}$) is very close to the zero-energy state over the whole range $r/r_0 \in [1, 1000]$, i.e. up to $\kappa r \sim 0.6$.

2. The fact that the bound states are over most of their range (*grossa modo* before their last arch) well described by the zero-energy solution, $\sqrt{r} \psi(r) \propto \sin[|s_0| \ln(r/R_a)]$ restores a scale invariance, discrete this time. For example, consider the wave function of the fourth excited state, $\psi_4(r)$, and perform the scale transformation

$$\phi(r) = \psi_4(\lambda r) \quad (19)$$

with

$$|s_0| \ln(\lambda) = \pi. \quad (20)$$

In logarithmic coordinates, this homothety on r is equivalent to a translation to the left by a length $\ln(\lambda)$, discarding the part of the function that ends up below the hard core at R_a . The choice proposed for λ ensures, however, that for a state of the form $\sin[|s_0| \ln(r/R_a)]$ we again find a zero at $r = R_a$. We thus generate another possible eigenstate of the Hamiltonian, with one node fewer than the starting state ψ_4 . The state ψ_3 is thus obtained to a very good approximation, and so on.

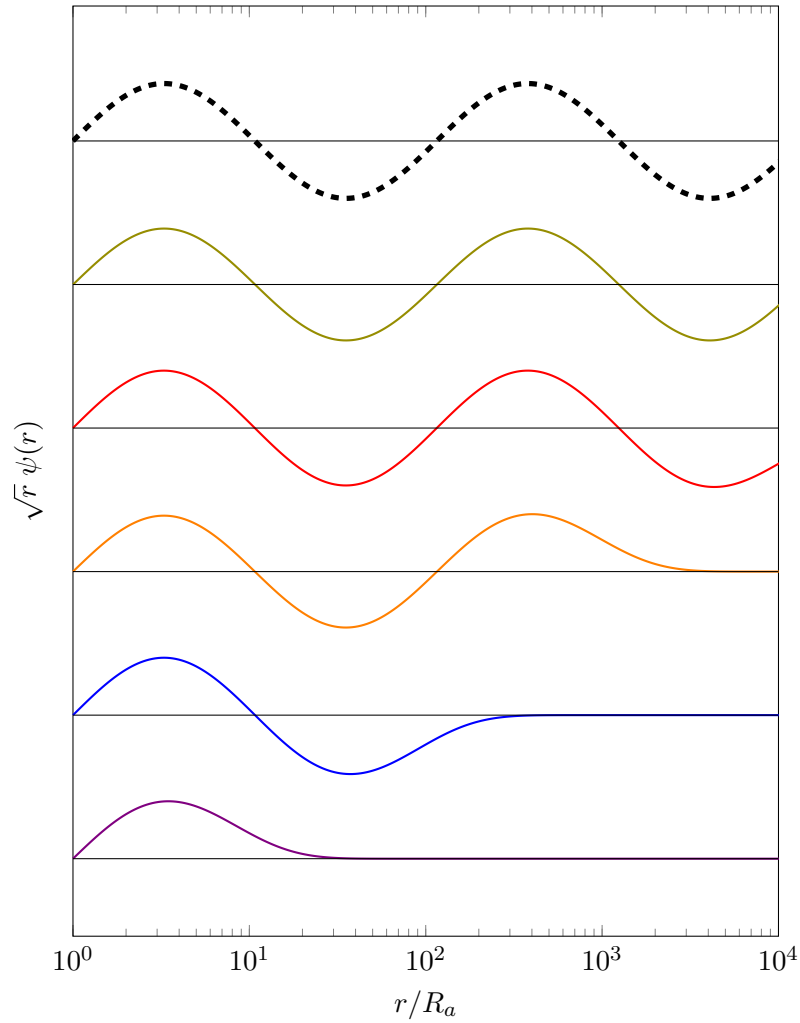


Figure II.2. Solid lines: radial wave functions $\sqrt{r} \psi_n(r)$ (unnormalized) of the first five bound states in the potential $-|g|/r^2$ truncated by a hard core at R_a . The black dotted curve represents the zero-energy state given in (9). These curves are drawn for $\alpha = -2$ (and therefore $|s_0| \sim 1.32$). The scaling law $\psi_{n+1}(\mathbf{r}) \propto \psi_n(\mathbf{r}/\lambda)$ shows up here as a simple invariance under a discrete translation, because the x axis is logarithmic.

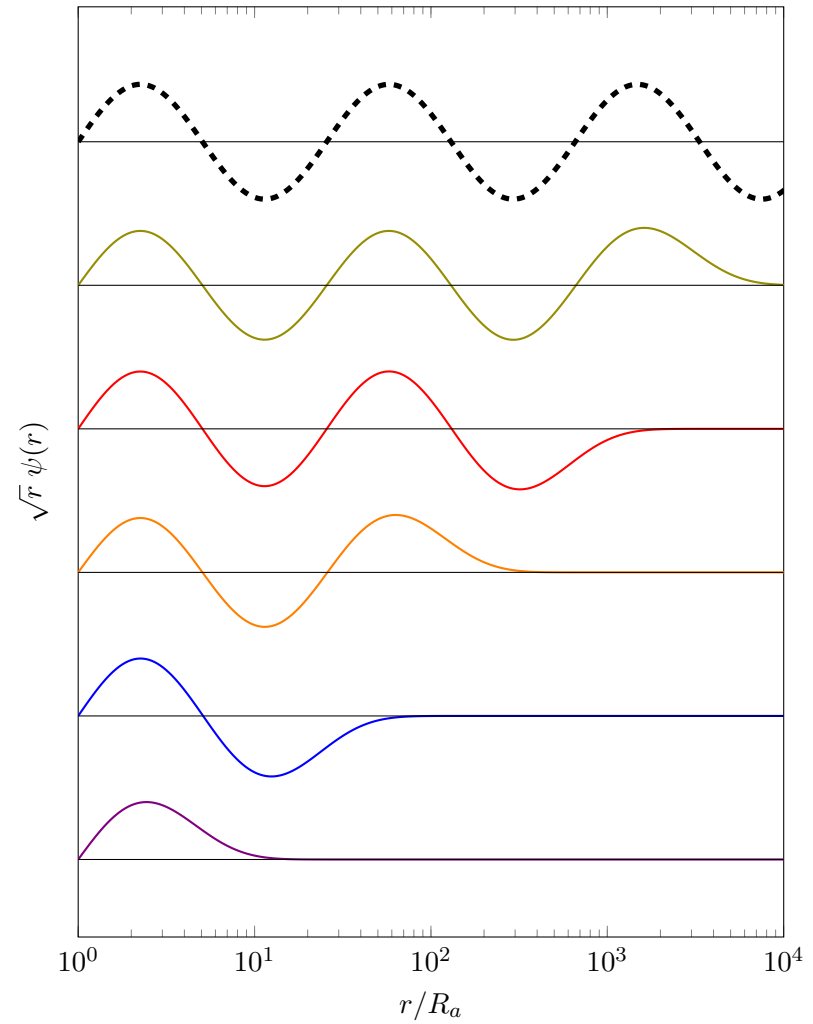


Figure II.3. Same as figure II.2, for $\alpha = -4$ (and therefore $|s_0| \sim 1.94$).

3. The fact that the bound state $\psi_{n-1}(r)$ is deduced from the bound state $\psi_n(r)$ by a scaling transformation of parameter λ given in (19) means that their energies are related by

$$E_n = \frac{1}{\lambda^2} E_{n-1} \quad \Leftrightarrow \quad \frac{E_n}{E_{n-1}} = e^{-2\pi/|s_0|} \quad (21)$$

We thus obtain the energies of the infinite series of bound states, increasingly close to the dissociation limit $E = 0$, these energies forming a geometric sequence of common ratio $e^{-2\pi/|s_0|}$. The numerically calculated energies are plotted in figure II.4 for two different values of α (and hence of $|s_0|$), and it can be seen that this scaling law is very well satisfied. This discrete scale invariance will play a central role in Efimov physics. Figure II.5 shows another way of plotting this set of data, demonstrating that the ratio E_{n+1}/E_n is indeed quasi-independent of n , for a given value of α .

In summary, the introduction of a hard core at R_a has broken the continuous scale invariance of the original problem, but has not destroyed it completely. A discrete scale invariance remains, with the scale factor $e^{\pi/|s_0|}$ for distances and $e^{2\pi/|s_0|}$ for energy, these scale factors being (fortunately!) independent of the value chosen for R_a .

What values should be taken for α (or s_0)? In the above, the amplitude g of the potential $V(r)$, and hence the dimensionless coefficients α and s_0 defined in (4) and (8), are arbitrary. In the standard Efimov effect, which occurs between three identical bosonic particles with a resonant binary interaction, we shall see in Chapters 5 and 6 that we arrive at $\alpha \approx -1.263$, which in absolute value is well above the $-1/4$ threshold that we have identified. The parameter s_0 is then $s_0 \approx i \times 1.00624$ and the associated scale parameter is $\lambda = e^{\pi/|s_0|} \approx 22.7$. This number is relatively large and makes it difficult to observe several bound states since there is a factor $\lambda^2 \approx 515$ between the energies of two consecutive states.

In the case where two particles of mass M are in resonant interaction with a third of mass m , we will see in Chapters 3 and 4 that an effective interaction in $-1/r^2$ can also occur. In this case, the parameter $|s_0|$ can become arbitrarily large as M/m tends to infinity. This facilitates the obser-

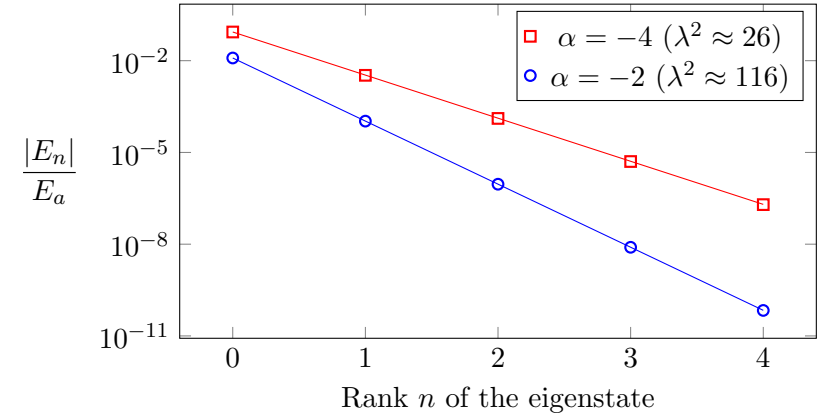


Figure II.4. Binding energies E_n of the first bound states in a $-1/r^2$ potential truncated by a hard core at R_a , for two values of the dimensionless parameter α . The index $n = 0$ corresponds to the ground state. The unit of energy is $E_a \equiv \hbar^2/m_\tau R_a^2$. The solid lines represent the scaling law $E_n = E_0/\lambda^{2n}$.

vation of several consecutive bound states since the scaling parameter λ is then significantly reduced.

1-3 The energy of the ground state

Once the relation (21) between the energies of the different bound states has been established, all that remains is to determine the energy of one bound state, for example the ground state, in order to deduce the energies of the others. In what follows, we will use the natural energy scale of the problem, $E_a \equiv \hbar^2/m_\tau R_a^2$, and we will consider only the angular momentum channel $\ell = 0$, in order to simplify the notation.

Several approaches can be developed for this. The first is numerical, and leads to the results plotted in figure II.6 as a black solid line. Another approach is to use the asymptotic expression for the zeros of the modified Bessel function of the second kind, $K_{i|s_0|}(x)$, which is the physically relevant solution of the Schrödinger equation for a bound state [cf. (15)]. This

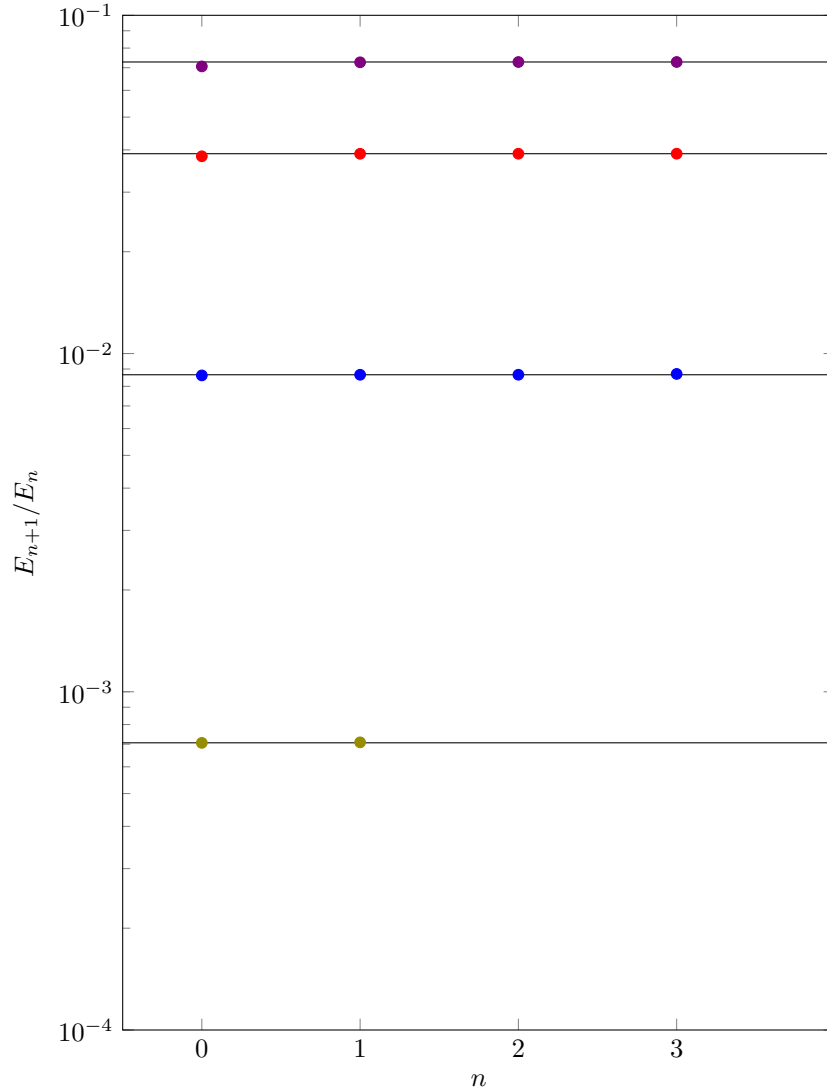


Figure II.5. Ratio E_{n+1}/E_n for different values of α . From bottom to top: $\alpha = -1, -2, -4, -6$. The solid lines indicate the prediction $e^{-2\pi/|s_0|}$ with $s_0 \equiv \sqrt{\alpha + 1/4}$. For $\alpha = -1$, only the first three bound states could be determined with reasonable accuracy. The index $n = 0$ corresponds to the ground state.

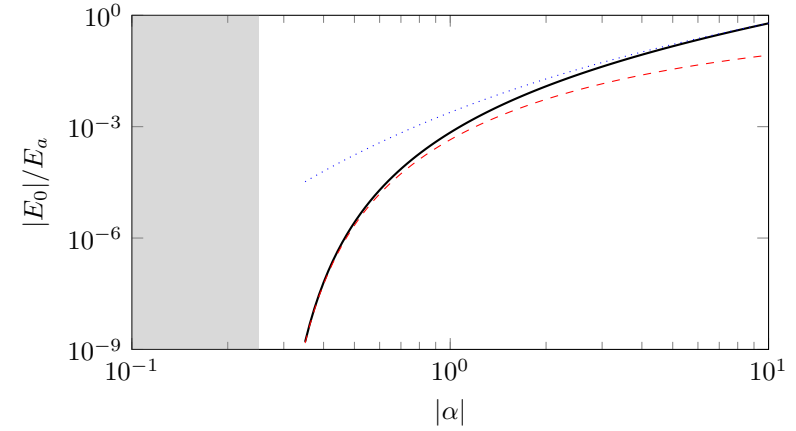


Figure II.6. Absolute value of the ground state energy in an attractive g/r^2 potential, with $g = \hbar^2\alpha/2m_r$ and $\alpha < 0$, in the presence of a hard core at R_a . The unit of energy is $E_a \equiv \hbar^2/m_r R_a^2$. Bound states exist only for $|\alpha| > 1/4$. The red dashed curve gives the approximate result (22) of Essin & Griffiths (2006), valid for $|\alpha|$ close to $1/4$. The dotted curve shows the result (26) of the WKB approach presented in the text.

approach has been developed in particular by Essin & Griffiths (2006). We will not reproduce it here, and simply give its result in the limit $\alpha \approx -1/4$:

$$|\alpha| \rightarrow 1/4_+ : \quad \frac{E_0}{E_a} \approx -\frac{2}{\gamma^2} \exp\left(-\frac{2\pi}{|s_0|}\right) \quad (22)$$

where $\gamma = e^C$, $C = 0.577 \dots$ being the Euler constant. This prediction is shown as a red dashed line in figure II.6. It is particularly useful for the study of the neighborhood of the critical point $\alpha = -1/4$ using a “renormalization group” approach. We will not go into detail about this approach here, since it will not be needed in the following chapters. The interested reader is referred to Gupta & Rajeev (1993), Camblong, Epele, et al. (2000), Camblong, Epele, et al. (2001a), Camblong, Epele, et al. (2001c), Burgess, Hayman, et al. (2017), and Paik (2018).

We can also use the WKB approximation to estimate the energy of the

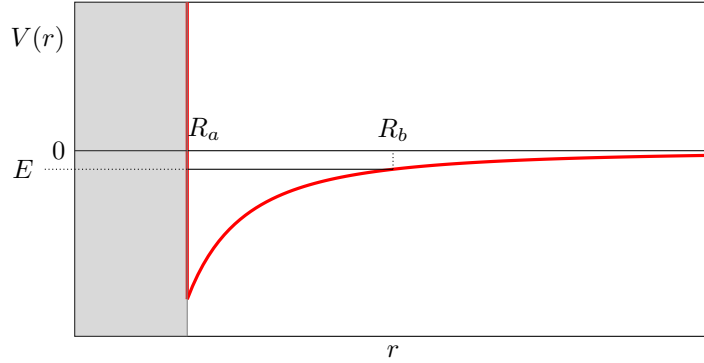


Figure II.7. Turning points R_a and R_b associated with energy $E < 0$, entering the calculation of the WKB integral (23).

ground state, although we know that this approximation is better suited to the quasi-classical regime, i.e. to excited states. We saw in Chapter 1 (§2.4) that, for a $1/r^2$ potential, this approximation is valid for $|\alpha|$ significantly greater than 1, i.e. in the opposite regime to that of the result (22). With a hard core at R_a , the semi-classical quantization condition reads

$$\int_{R_a}^{R_b} k(r, E_n) dr = \left(n + \frac{3}{4}\right) \pi \quad (23)$$

with $n = 0$ for the ground state. The outer turning point R_b is related to the energy E_0 by (cf. figure II.7)

$$E_0 = \frac{\hbar^2 \alpha}{2m_r R_b^2} < 0 \quad (24)$$

and a relatively simple calculation of the integral in (23) leads to

$$\ln [\tan(u/2)] + \cos(u) = -\frac{3\pi}{4\sqrt{|\alpha|}} \quad \text{with} \quad \sin u = \frac{R_a}{R_b}. \quad (25)$$

To simplify, let us restrict ourselves to the case where α is not extremely large compared with 1, which means that R_b is significantly larger than R_a . In practice, this simplification is still valid for $\alpha \sim 10$ and allows u

to be treated as a small parameter in (25). We then find $u \approx 2 \exp[-1 - 3\pi/(4\sqrt{|\alpha|})]$, which leads to

$$\text{WKB approach:} \quad \frac{E_0}{E_a} \approx -\frac{2|\alpha|}{e^2} \exp\left(-\frac{3\pi}{2\sqrt{|\alpha|}}\right) \quad (26)$$

The result is plotted as a dotted line in figure II.6. For even larger values of α (not relevant in practice for the problems that will interest us in this course), R_b and R_a are comparable and the approximation leading to (26) is no longer valid. The ground state is then concentrated at the very bottom of the potential well and we expect $E_0 \approx -\frac{|\alpha|}{2} E_a$.

Approximate scaling law. Assuming $R_a/R_b \ll 1$, the WKB approach provides an approximate value for the energy of each bound state:

$$\text{WKB approach:} \quad \frac{E_n}{E_a} \approx -\frac{2|\alpha|}{e^2} \exp\left[-\frac{2\pi}{\sqrt{|\alpha|}} \left(n + \frac{3}{4}\right)\right] \quad (27)$$

which corresponds to the scaling law $E_{n+1}/E_n = \exp(-2\pi/\sqrt{|\alpha|})$. We recover the law (21) provided we make the substitution

$$|s_0| = \sqrt{\left|\alpha + \frac{1}{4}\right|} \approx \sqrt{|\alpha|}, \quad (28)$$

valid under the assumption that $|\alpha|$ is significantly greater than 1, which is a necessary condition for the validity of the WKB approach, as mentioned above.

2 Electrostatic interaction and potential in $1/r^2$

2-1 The charge-dipole interaction

In the following chapters we will study the emergence of a $1/r^2$ potential from a short-range (but resonant) interaction between different constituents. Here, we look at a physical situation where the potential in $1/r^2$

is naturally present: the interaction between an electric charge q and an electric dipole $\mathbf{D}$, assumed to be point-like. The electrostatic interaction energy between these two objects reads

$$V = \frac{q \mathbf{D} \cdot \mathbf{r}}{4\pi\epsilon_0 r^3} = \frac{qD}{4\pi\epsilon_0 r^2} \cos \theta \quad (29)$$

where θ denotes the angle between the orientation of the dipole and the radius vector $\mathbf{r}$ joining the dipole and the charge (figure II.8). We thus recover the radial dependence in $1/r^2$, superimposed on an angular dependence in $\cos \theta$, which is a new ingredient compared with what we studied previously.

The orientation of the dipole is assumed to be fixed and we will take it to be aligned with the z axis by convention. We are interested here in the eigenstates $\Psi(\mathbf{r})$ of the Hamiltonian of the relative motion

$$\left(\frac{-\hbar^2}{2m_r} \nabla^2 + \frac{qD}{4\pi\epsilon_0 r^2} \cos \theta \right) \Psi(\mathbf{r}) = E \Psi(\mathbf{r}). \quad (30)$$

Since the system is invariant under rotation about the z axis, we look for these eigenstates in spherical coordinates in the form

$$\Psi(\mathbf{r}) = \frac{1}{r} \Phi(r, \theta) e^{im\varphi}, \quad (31)$$

where φ denotes the azimuthal angle and θ the polar angle with respect to the z axis. We are therefore looking for eigenfunctions common to the Hamiltonian and to the projection $\hat{L}_z$ of the angular momentum operator on the z axis (with eigenvalue $\hbar m$).

In what follows, we will use the expression for the Laplacian operator ∇^2 in these coordinates:

$$\nabla^2 = \nabla_r^2 + \frac{1}{r^2} (\nabla_\theta^2 + \nabla_\varphi^2) \quad (32)$$

where we have set

$$\nabla_r^2 \Psi \equiv \frac{1}{r} \frac{\partial^2}{\partial r^2} (r\Psi) \quad \nabla_\theta^2 \Psi \equiv \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Psi}{\partial \theta} \right) \quad \nabla_\varphi^2 \Psi \equiv \frac{1}{\sin^2 \theta} \frac{\partial^2 \Psi}{\partial \varphi^2} \quad (33)$$

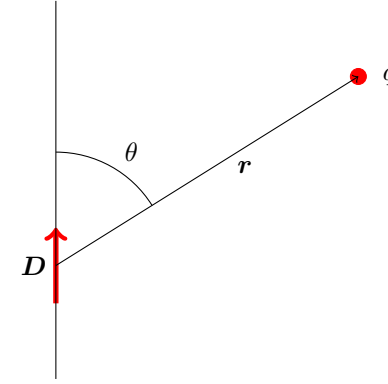


Figure II.8. Electrostatic interaction between a charge q and a dipole $\mathbf{D}$.

We are therefore looking for the functions $\Phi(r, \theta)$ as solutions of the eigenvalue equation:

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \nabla_\theta^2 + \frac{1}{r^2} \left(\frac{m^2}{\sin^2 \theta} + \tilde{D} \cos \theta \right) \right] \Phi = \epsilon \Phi \quad (34)$$

where we have introduced the reduced dipole (a dimensionless quantity)

$$\tilde{D} = \frac{2m_r q D}{4\pi\epsilon_0 \hbar^2} \quad (35)$$

This problem was the subject of several theoretical studies (essentially in agreement with one another) in the mid-1960s by Turner & Fox (1966), Mittleman & Myerscough (1966), Brown & Roberts (1967), Levy-Leblond (1967), and Coulson & Walmsley (1967). It was also investigated experimentally by Desfr  ois, Abdoul-Carime, et al. (1994), before being taken up theoretically again—in particular with tools from the renormalization group approach—by Camblong, Epele, et al. (2001b), Alhaidari (2008), Connolly & Griffiths (2007), and Alhaidari & Bahlouli (2008).

2-2 Can a charge bind a dipole?

To find the bound states solving (30), we look for the solutions Φ in factorized form

$$\Phi(r, \theta) = u(r) f(\theta), \quad (36)$$

using the separation-of-variables method. We will use a similar method in Chapters 5 and 6 when we tackle the three-body problem using the hyper-spherical potentials technique.

The eigenvalue equation (34) now reads

$$-u''f + \frac{u}{r^2} \left\{ \left[-\nabla_\theta^2 + \frac{m^2}{\sin^2 \theta} + \tilde{D} \cos \theta \right] f \right\} = \epsilon u f. \quad (37)$$

The strategy is then simple: we start by looking for eigenfunctions $f(\theta)$ of the operator appearing between braces $\{\dots\}$ in (37) in the form:

$$\boxed{\left[-\nabla_\theta^2 + \frac{m^2}{\sin^2 \theta} + \tilde{D} \cos \theta \right] f(\theta) = \alpha f(\theta)} \quad (38)$$

The eigenvalue α plays the role of *separation constant* here. Once the possible eigenvalues have been determined, we insert the result into (37) to obtain the eigenvalue equation for the radial function $u(r)$:

$$-u''(r) + \frac{\alpha}{r^2} u(r) = \epsilon u(r) \quad (39)$$

This brings us back to our now familiar radial equation in an α/r^2 potential.

We know from our previous study that the question of the existence of bound states boils down to the condition:

$$\text{bound states if and only if } \alpha < -\frac{1}{4} \quad (40)$$

and the whole question is therefore transferred to the eigenvalue equation (38) for the function $f(\theta)$. For a given dipole $\tilde{D}$, we look for the smallest possible eigenvalue α , in order to determine whether it reaches the critical threshold $-1/4$. To reach this threshold, it is clearly advantageous to minimize the (positive) potential $m^2/\sin^2 \theta$ by taking $m = 0$. This brings us back to the simpler problem:

$$\boxed{\left(-\nabla_\theta^2 + \tilde{D} \cos \theta \right) f(\theta) = \alpha f(\theta)} \quad (41)$$

This equation can be solved by expanding $f(\theta)$ on the basis of the Legendre polynomials $P_n(\cos \theta)$:

$$f(\theta) = \sum_{n=0}^{\infty} c_n P_n(\cos \theta), \quad (42)$$

these polynomials being solutions of the equation

$$-\nabla_\theta^2 P_n(\cos \theta) = n(n+1) P_n(\cos \theta). \quad (43)$$

Legendre polynomials also satisfy the relation

$$x P_n(x) = \frac{n}{2n+1} P_{n-1}(x) + \frac{n+1}{2n+1} P_{n+1}(x). \quad (44)$$

This gives a tridiagonal system for determining the coefficients c_n :

$$\tilde{D} \frac{n}{2n-1} c_{n-1} + [n(n+1) - \alpha] c_n + \tilde{D} \frac{n+1}{2n+3} c_{n+1} = 0. \quad (45)$$

In practice, we can truncate this system at a value $n_{\max}$ and then write the condition for the existence of a solution $\{c_n\} \neq 0$: the determinant of this system must vanish. If we take $n_{\max} = 1$, we arrive at

$$\begin{vmatrix} -\alpha & \tilde{D}/3 \\ \tilde{D} & 2 - \alpha \end{vmatrix} = \alpha^2 - 2\alpha - \frac{\tilde{D}^2}{3} = 0, \quad (46)$$

in which case the critical value $\alpha_c = -1/4$ is reached for $\tilde{D}_c = 3\sqrt{3}/4 \approx 1.299$. This result can be refined by taking a larger $n_{\max}$ and we find $\tilde{D}_c \approx 1.279$ (figure II.9).

Let us consider the case of an electron in the presence of a much heavier electric dipole, i.e. $m_r \approx m_{\text{electron}}$. We then obtain:

$$\boxed{D_c = 5.5 \times 10^{-30} \text{ C m} = 1.6 \text{ Debye}} \quad (47)$$

with 1 Debye = 3.336×10^{-30} C m. For a dipole below this value, there is no charge-dipole bound state. For a dipole larger than this value, our model predicts instead an infinite number of bound states in the $m = 0$ channel.

As we saw earlier, to ensure that the system has a ground state, we have to take into account the fact that the potential α/r^2 does not apply up to

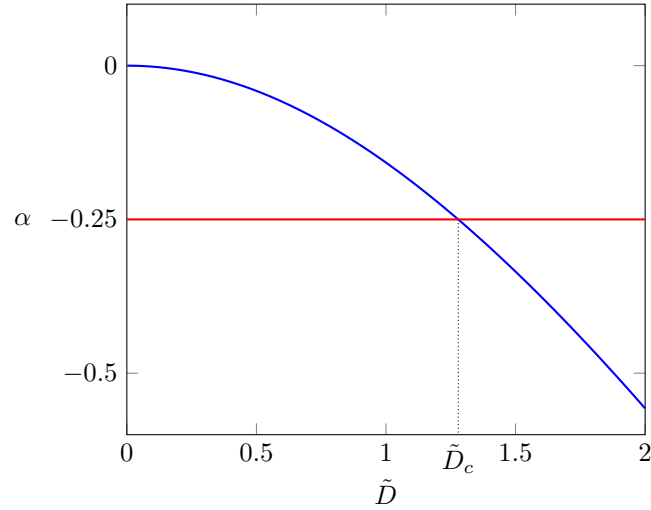


Figure II.9. Minimum eigenvalue α for the angular eigenvalue problem (41), as a function of the reduced dipole $\tilde{D}$. The critical value $\alpha = -1/4$ is obtained for $\tilde{D}_c \approx 1.279$.

arbitrarily small distances. In this case, the notion of an electric dipole is not valid at very short distances: it is an idealization of a system of two charges $\pm Q$ separated by a distance d , with $D = Qd$. When the variable r becomes $\lesssim d$, the three-body problem $+Q, -Q, q$ must be solved explicitly [see for example Wallis, Herman, et al. (1960), Mittleman & Myerscough (1966), Levy-Leblond (1967), and Crawford (1967)]. We then recover the discrete scale invariance presented in the previous section.

2-3 The experiment by Desfrancois *et al.*

The experiment by Desfrancois, Abdoul-Carime, et al. (1994) starts with the selection of a series of molecular species with (i) a non-zero electric dipole moment, already measured elsewhere, and (ii) a closed-shell electronic structure, so that the electron affinity of the molecule M is, with high probability, negative.

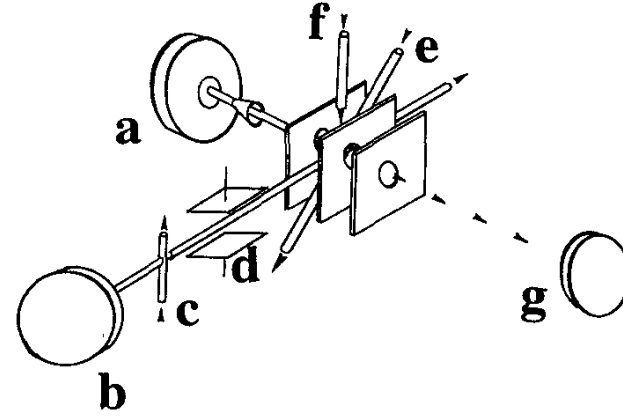
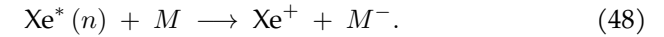


Figure II.10. Experimental diagram used to study the capture of an electron by a dipolar molecule. (a): valve for the molecular jet, (b): valve for the xenon atoms, (c): excitation of the xenon by an electron beam, (d): filtering region for the different Rydberg levels, (g): multichannel plate for ion detection. Figure taken from Desfrancois, Khelifa, et al. (1992).

To measure whether an electron can bind to the molecule under the effect of the dipolar potential alone, a collision is carried out between a beam of these molecules¹ and xenon atoms prepared in a Rydberg state (high principal quantum number n , figure II.10). This quantum number is varied from $n = 7$ to $n = 70$: the energy required to detach the outer electron from the xenon atom is thus varied over a wide range, this electron then being captured by the dipolar molecule:



The M^- ions are then accelerated and detected behind a mass spectrometer. Figure II.11 shows the creation rate of M^- as a function of the quantum number n of the Rydberg state of xenon. The fairly pronounced peak in this rate is consistent with the idea that the electron can be resonantly captured

¹The molecules are seeded in a beam of helium atoms and they have a rotational temperature of 5 to 10 K.

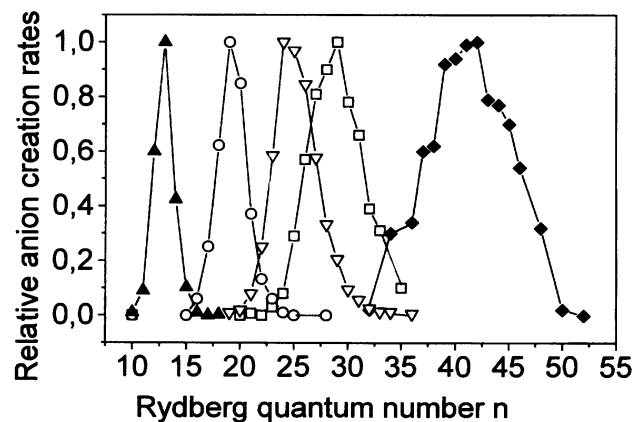


Figure II.11. The formation rate of M^- as a function of the principal quantum number of the Rydberg state of Xe supplying the electron to the neutral molecule M . In order of decreasing dipole moment: filled triangles: acetonitrile; open circles: cyclohexanone; open triangles: acetone; open squares: cyclobutanone; diamonds: acetaldehyde. Figure taken from Desfr  ois, Abdoul-Carime, et al. (1994).

by the molecule to form a bound state. The energy at which this resonance occurs depends on the molecule.

To determine the precise binding energy of M^- , one measures the electric field required to detach the electron captured during the reaction (48). The results are plotted in figure II.12 as a function of the dipole moment of the molecule. For molecules with a dipole moment smaller than 2.6 Debye, no signal was measured. For larger dipole moments, a bound state is indeed detected with an energy in good agreement with the theoretical modeling proposed by the authors. This model consists in truncating the α/r^2 potential at short distance by another potential involving known molecular parameters (polarizability, for example).

It should be noted that in this experiment, only one bound state of the electron around the molecular dipole was detected, whereas the theory we have developed so far predicts an infinite number of them, forming a geometric sequence. Desfr  ois, Abdoul-Carime, et al. (1994) related their finding to the prediction of Garrett (1980), according to which the motion

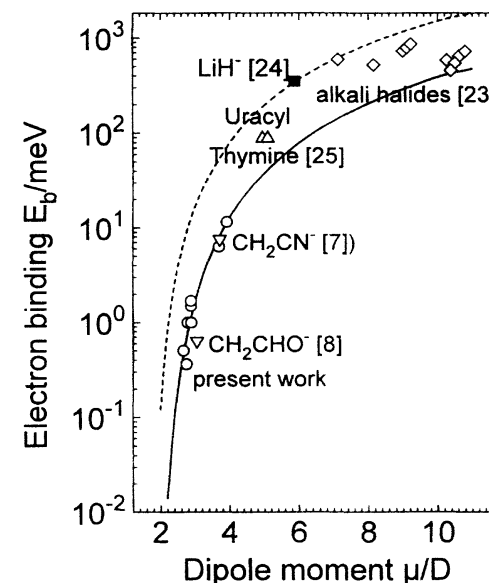


Figure II.12. Binding energy of the M^- structure as a function of the electric dipole moment (denoted μ here and measured in Debye) of the parent molecule M . The solid and dashed lines correspond to two theoretical predictions based on different models of the short-range physics, when the charge–dipole distance becomes comparable to the extent of the dipole itself. Figure taken from Desfr  ois, Abdoul-Carime, et al. (1994).

of the atoms making up the dipolar molecule strongly restricts the number of possible M^- states.

It should also be noted that the threshold value found experimentally, 2.6 Debye, is significantly higher than the limit found in (47). This is due (at least in part) to the fact that the authors only had relatively complex molecules at their disposal, and the detection of weakly bound states was then complicated by the rotational motion of these molecules at the temperatures available. Recent progress in the preparation of ultracold diatomic molecules could make it possible to repeat these experiments with dipole moments close to the critical value expected theoretically (table II.1).

molecule	dipole (Debye)
RbYb	0.21
KRb	0.57
RbCs	1.2
RbSr	1.5
NaK	2.7
NaRb	3.3
LiRb	4.1
LiCs	5.5

Table II.1. Dipole moment of some diatomic molecules used in ultracold gas experiments. Values taken from Gadway & Yan (2016).

3 $1/r^2$ potential and conformal invariance

3-1 The symmetries of the Schrödinger equation

The scale invariance of the potential in $1/r^2$ that we mentioned in the previous chapter is part of a larger set of symmetries of the Schrödinger equation, called the conformal invariance group. These symmetries come in addition to geometric invariance properties such as translation symmetry and rotation symmetry.

For a free particle described by the Schrödinger equation, this conformal invariance was discovered by Hagen (1972) and Niederer (1972). It was extended to the case of a particle in a harmonic trap by Niederer (1973), then to the case of the potential we are interested in here, $1/r^2$, by Alfaro, Fubini, et al. (1976).

This invariance can be generalized to a set of interacting particles, provided that the corresponding potential satisfies the scale invariance property (Pitaevskii & Rosch 1997)

$$V(\lambda \mathbf{r}_1, \dots, \lambda \mathbf{r}_N) = \frac{1}{\lambda^2} V(\mathbf{r}_1, \dots, \mathbf{r}_N). \quad (49)$$

It is also present in a gas of spin-1/2 fermions at the unitary limit with $m_\uparrow = m_\downarrow$ (Werner & Castin 2006). In this case, the scattering length is infinite and therefore provides no length scale. Furthermore, the fermionic nature of

the particles prevents the formation of three-body structures, which would otherwise provide a length scale that would destroy the scale invariance.

This conformal invariance also occurs for the two-dimensional Gross-Pitaevskii equation, which uses a classical field approach to describe the dynamics of particles interacting via a contact potential $g\delta(\mathbf{r}_i - \mathbf{r}_j)$ (Pitaevskii & Rosch 1997; Saint-Jalm, Castilho, et al. 2019). In this case, scale invariance results from the fact that we have in two dimensions

$$\delta(\lambda \mathbf{r}) = \frac{1}{\lambda^2} \delta(\mathbf{r}). \quad (50)$$

The invariance properties of the Schrödinger equation are investigated as follows. Starting from a solution $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)$ of this equation in an external potential $U(\mathbf{r})$:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi \quad \text{with} \quad \hat{H} = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U(\mathbf{r}_i) \right] + V(\mathbf{r}_1, \dots, \mathbf{r}_N), \quad (51)$$

we look for transformations of positions and time

$$\boxed{\mathbf{r}'_i = g(\mathbf{r}_i, t) \quad t' = h(t)} \quad (52)$$

accompanied by a gauge change of the wave function

$$\boxed{\psi'(\mathbf{r}'_1, \dots, \mathbf{r}'_N, t') = f(\mathbf{r}_1, \dots, \mathbf{r}_N, t) \psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)} \quad (53)$$

so that ψ' is also a solution of the Schrödinger equation (51).

3-2 Single particle in an external potential

To simplify this presentation, we will consider here the case of a single particle, but the results can be extended without difficulty to the case of N particles, see for example Werner & Castin (2006). We will not deal here with the well-known translation or rotation symmetries, and will concentrate on the “hidden” symmetry (or dynamical symmetry) related to conformal invariance.

We first consider the case where the particle is free or moving in the potential $U(r) = g/r^2$. The Schrödinger equation thus reads

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{g}{r^2} \psi. \quad (54)$$

We choose a real 2×2 matrix with determinant 1:

$$[M] = \begin{pmatrix} \gamma_1 & \gamma_2 \\ \gamma_3 & \gamma_4 \end{pmatrix} \quad \text{with} \quad \gamma_1 \gamma_4 - \gamma_2 \gamma_3 = 1, \quad (55)$$

i.e. an element of $\text{SL}_2(\mathbb{R})$, and we consider the transformations:

$$\boxed{\mathbf{r}' = g(\mathbf{r}, t) = \frac{\mathbf{r}}{\gamma_3 t + \gamma_4}, \quad t' = h(t) = \frac{\gamma_1 t + \gamma_2}{\gamma_3 t + \gamma_4}} \quad (56)$$

One can check (the calculation is tedious, but presents no particular difficulty) that this transformation, together with the gauge change

$$\boxed{f(\mathbf{r}, t) = (\gamma_3 t + \gamma_4)^{D/2} \exp\left(-i \frac{m \gamma_3 r^2 / 2}{\gamma_3 t + \gamma_4}\right)} \quad (57)$$

where D is the dimension of the space ($D = 3$ in this course), meets our requirements: the function $\psi'(\mathbf{r}', t')$ is also a solution of (54) (Niederer 1972; Alfaro, Fubini, et al. 1976).

To gain a physical intuition for the transformations described by (56), note that four real parameters are needed to describe the 2×2 matrix $[M]$. Taking into account the constraint on its determinant, this leaves three independent parameters. We can thus identify three types of transformation, corresponding to three important special cases for this matrix:

- Translations in time:

$$[M] = \begin{pmatrix} 1 & t_0 \\ 0 & 1 \end{pmatrix} : \quad \mathbf{r}' = \mathbf{r}, \quad t' = t + t_0. \quad (58)$$

This invariance is simply due to the fact that the Hamiltonian is stationary.

- Dilations:

$$[M] = \begin{pmatrix} \lambda & 0 \\ 0 & 1/\lambda \end{pmatrix} : \quad \mathbf{r}' = \lambda \mathbf{r}, \quad t' = \lambda^2 t \quad (59)$$

which we have already introduced above. The invariance of the Schrödinger equation is ensured by the scale invariance of the $1/r^2$ potential.

- Expansions:

$$[M] = \begin{pmatrix} 1 & 0 \\ \gamma_3 & 1 \end{pmatrix} : \quad \mathbf{r}' = \frac{\mathbf{r}}{\gamma_3 t + 1}, \quad t' = \frac{t}{\gamma_3 t + 1}, \quad (60)$$

which can be seen as dilations with a time-dependent scale factor.

Note that the gauge transformation (57) is trivial in the first two cases since we then have $\gamma_3 = 0$.

We have thus found a continuous group of transformations, with three independent parameters. The operation associated with the successive application of two transformations $[M]$ and $[M']$ is characterized by the matrix $[M'']$ obtained from the matrix product $[M'] \times [M]$, which makes this matrix formulation all the more natural. Note also that the identity matrix, $\gamma_1 = \gamma_4 = 1, \gamma_2 = \gamma_3 = 0$, corresponds to no modification of the wave functions: $\mathbf{r}' = \mathbf{r}, t' = t, \psi' = \psi$. The transformations (52-53) and (56-57) therefore provide a linear representation of the group of real 2×2 matrices of determinant 1, $\text{SL}_2(\mathbb{R})$.

Once this structure has been identified, the next step is in principle to determine its infinitesimal generators. However, before doing this, it is useful to generalize the above results to the case of a particle in a harmonic trap (Niederer 1973).

In what follows, we therefore consider the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + U(r) \quad (61)$$

where $U(r)$ is the isotropic potential

$$U(\mathbf{r}) = \frac{g}{r^2} + U_{\text{ho}}(r) \quad \text{with} \quad U_{\text{ho}}(r) = \frac{1}{2} m \omega^2 r^2. \quad (62)$$

The $m\omega^2 r^2/2$ part breaks the scale invariance found for g/r^2 , but we can simply modify the transformations (56)-(57) to recover the conformal invariance of the Schrödinger equation. Still starting with a 2×2 matrix with real coefficients and determinant 1, let us take

$$\mathbf{r}' = \frac{\mathbf{r}}{\lambda(t)}, \quad \tan(\omega t') = \frac{\gamma_1 \tan(\omega t) + \gamma_2}{\gamma_3 \tan(\omega t) + \gamma_4} \quad (63)$$

with

$$\lambda(t) = [(\gamma_1 S + \gamma_2 C)^2 + (\gamma_3 S + \gamma_4 C)^2]^{1/2}, \quad S = \sin(\omega t), \quad C = \cos(\omega t). \quad (64)$$

Here again, a calculation (also tedious) shows that the function ψ' , constructed from ψ and the gauge transformation

$$f(\mathbf{r}, t) = \lambda^{D/2}(t) \exp\left(-i \frac{m \dot{\lambda} r^2}{2\lambda}\right) \quad (65)$$

is also a solution of the Schrödinger equation [see Werner & Castin (2006) for the N -particle version of the same problem].

3-3 The generators associated with conformal invariance

Since we now have a group of continuous transformations that leave the Schrödinger equation invariant

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + \left(\frac{g}{r^2} + \frac{1}{2} m \omega^2 r^2 \right) \psi, \quad (66)$$

it is interesting to find the generators associated with these transformations.

To begin with, let us recall what these generators are for the usual geometric transformations, translations or rotations. For translation along x , for example,

$$\psi(x, y, z) \longrightarrow \psi'(x, y, z) = \psi(x - x_0, y, z) \quad (67)$$

we take x_0 to be infinitesimally small, so that

$$\psi'(x, y, z) \approx \psi(x, y, z) - x_0 \frac{\partial \psi}{\partial x} \quad (68)$$

which we write as

$$\psi' \approx \left(1 - i \frac{x_0 \hat{p}_x}{\hbar} \right) \psi \quad \text{with} \quad \hat{p}_x = -i\hbar \frac{\partial}{\partial x}. \quad (69)$$

The operator $\hat{p}_x$ introduced here coincides with the usual expression for the x component of the momentum operator. The infinitesimal generators of the translations are therefore the three components of the momentum operator $\hat{\mathbf{p}}$, for which we recall the commutation relations:

$$[\hat{p}_i, \hat{p}_j] = 0. \quad (70)$$

For a rotation of angle φ_0 about axis z , we have in spherical coordinates:

$$\psi(r, \theta, \varphi) \longrightarrow \psi'(r, \theta, \varphi) = \psi(r, \theta, \varphi - \varphi_0), \quad (71)$$

which gives, for an infinitesimally small φ_0 ,

$$\psi' \approx \left(1 - i \frac{\varphi_0 \hat{L}_z}{\hbar} \right) \psi \quad \text{with} \quad \hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}. \quad (72)$$

The infinitesimal generators of rotations are therefore the three components of the angular momentum operator $\hat{\mathbf{L}}$, for which we recall the commutation relations:

$$[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k. \quad (73)$$

We can proceed in the same way for the transformations related to conformal invariance identified above. The detailed calculations are presented, for example, in the appendix of the article by Saint-Jalm, Castilho, et al. (2019); here we simply give the result at time $t = 0$ for the transformation (63-65). A possible choice for the three generators is (Pitaevskii & Rosch 1997)

$$\hat{\mathcal{L}}_1 = \frac{1}{2\hbar\omega} (\hat{H} - 2U_{\text{ho}}) \quad \hat{\mathcal{L}}_2 = \frac{1}{4\hbar} (\mathbf{p} \cdot \mathbf{r} + \mathbf{r} \cdot \mathbf{p}) \quad \hat{\mathcal{L}}_3 = \frac{1}{2\hbar\omega} \hat{H} \quad (74)$$

The group associated with this conformal symmetry is characterized by the commutation relations between the generators

$$[\hat{\mathcal{L}}_1, \hat{\mathcal{L}}_2] = -i\hat{\mathcal{L}}_3 \quad [\hat{\mathcal{L}}_2, \hat{\mathcal{L}}_3] = i\hat{\mathcal{L}}_1 \quad [\hat{\mathcal{L}}_3, \hat{\mathcal{L}}_1] = i\hat{\mathcal{L}}_2 \quad (75)$$

These relations seem close to those for angular momentum (73), but the presence of the $-$ sign in the former significantly changes the algebra. These relations are in fact characteristic of the $\text{SO}(2,1)$ algebra, the Lorentz group with two space dimensions and one time dimension, whereas the angular momentum algebra corresponds to $\text{SO}(3)$. These relations can be generalized to the N -particle case (Werner & Castin 2006).

Example: operator associated with an infinitesimal dilation. Consider the dilation with parameter λ very close to 1 and let $\gamma_4 = 1/\gamma_1 = 1 + \epsilon$, $\gamma_2 = \gamma_3 = 0$ in (56,57,59) with $\epsilon \ll 1$. To first order in ϵ , we find in dimension D :

$$\psi'(\mathbf{r}) = \gamma_4^{D/2} \psi(\gamma_4 \mathbf{r}) = (1 + \epsilon)^{D/2} \psi[(1 + \epsilon) \mathbf{r}] \quad (76)$$

$$\approx \psi(\mathbf{r}) + \epsilon \left(\frac{D}{2} + \mathbf{r} \cdot \nabla \right) \psi(\mathbf{r}) \quad (77)$$

$$= \psi(\mathbf{r}) + \frac{\epsilon}{2} [\nabla \cdot (\mathbf{r} \psi) + \mathbf{r} \cdot \nabla \psi] \quad (78)$$

which can also be written as $(1 + 2i\epsilon \hat{\mathcal{L}}_2) \psi$. This shows that the operator $\hat{\mathcal{L}}_2$ is the generator associated with the spatial scale transformation introduced earlier.

3-4 The tower of eigenstates

The commutation relations between the operators $\hat{\mathcal{L}}_i$ allow us to identify a series of important properties of the system, both statically and dynamically (Pitaevskii & Rosch 1997).

We will concentrate here on the search for stationary states and to do this we introduce the two operators

$$\hat{\mathcal{L}}_{\pm} = \hat{\mathcal{L}}_1 \pm i\hat{\mathcal{L}}_2. \quad (79)$$

Using the fact that $\hat{\mathcal{L}}_3$ is proportional to $\hat{H}$, it is immediate to verify that

$$[\hat{H}, \hat{\mathcal{L}}_{\pm}] = \pm 2\hbar\omega \hat{\mathcal{L}}_{\pm}. \quad (80)$$

Starting from an eigenstate $|\psi\rangle$ of $\hat{H}$ of energy E , we deduce from this relation that

$$\hat{H} (\hat{\mathcal{L}}_+ |\psi\rangle) = (E + 2\hbar\omega) (\hat{\mathcal{L}}_+ |\psi\rangle) \quad \hat{H} (\hat{\mathcal{L}}_- |\psi\rangle) = (E - 2\hbar\omega) (\hat{\mathcal{L}}_- |\psi\rangle) \quad (81)$$

By repeated application of $\hat{\mathcal{L}}_{\pm}$, we generate a tower of eigenenergies $E + 2n\hbar\omega$, $n \in \mathbb{Z}$.

If we restrict ourselves to the case of a coefficient g sufficiently large to avoid the fall to the center ($\alpha > -1/4$), we know that there is a well-defined ground state and that the energies are bounded below. The tower is therefore semi-infinite, and its bottom must correspond to a state such that $\hat{\mathcal{L}}_- |\psi_{\text{bottom}}\rangle = 0$. Here again, the result carries over as it stands to the case of N interacting particles exhibiting scale invariance (Werner & Castin 2006).

The existence of this tower of states can be verified explicitly for the case of the one-particle Hamiltonian (61-62), for example by considering isotropic solutions. Let us introduce the reduced radial wave function $u(r) = r \psi(r)$, which satisfies the eigenvalue equation

$$-u''(r) + \left(\frac{\alpha}{r^2} + r^2 \right) u(r) = \frac{2E}{\hbar\omega} u(r), \quad (82)$$

where distances are expressed in units of $a_{\text{ho}} = (\hbar/m\omega)^{1/2}$.

Let us look for a solution of this equation in the form

$$u_0(r) = r^{s+1} e^{-r^2/2} \quad (83)$$

where the Gaussian envelope is characteristic of the eigenstates of the harmonic oscillator. We find that u is a solution of (82) if and only if

$$E_0 = \hbar\omega \left(s + \frac{3}{2} \right) \quad \text{and} \quad s^2 + s - \alpha = 0 \quad (84)$$

We have already encountered this second-degree equation in our search for the zero-energy solution in the $1/r^2$ potential. Here we will concentrate on the case $\alpha > -1/4$, so that the roots of this equation are real. The case $\alpha < -1/4$, leading to complex roots, requires regularization of the potential in $1/r^2$ as we saw above.

We must choose the larger of the two possible roots for s :

$$s = -\frac{1}{2} + \sqrt{\alpha + \frac{1}{4}}, \quad (85)$$

this root always being larger than $-1/2$. The other root is always less than $-1/2$ and would lead to a divergent integral for the average potential energy. Note that for $g = 0$, we have $s = 0$ and we return to the ground state of the harmonic oscillator $\psi(r) = e^{-r^2/2}$.

The state $u(r)$ obtained in this way has no node other than $r = 0$ and therefore corresponds to the ground state of the problem. When the operator $\hat{\mathcal{L}}_+$ acts on this state, we have seen that it generates a tower of energy states

$$E_n = \hbar\omega \left(2n + s + \frac{3}{2} \right) \quad (86)$$

At each stage, the operator $\hat{\mathcal{L}}_+$ involves $\frac{d^2}{dr^2}$, $r \frac{d}{dr}$, as well as multiplication by r^2 and r^{-2} . One can then show quite easily that the wave function u_n obtained after n applications of $\hat{\mathcal{L}}_+$ has the following structure:

$$u_n(r) = r^{s+1} e^{-r^2/2} P_n(r^2) \quad (87)$$

where P_n is a polynomial of degree n [generalized Laguerre polynomial, Werner & Castin (2006)]. The function u_n has n positive roots, and it is therefore the n th excited state.

The action of $\hat{\mathcal{L}}_+$ therefore makes it possible to generate the entire spectrum of $\hat{H}$ for isotropic states and to obtain the corresponding eigenstates. We can also check directly that a state of the form (87) can be a solution of (82) by establishing the recurrence relation between the different coefficients of the polynomial P_n .

3-5 The breathing mode

Pitaevskii & Rosch (1997) showed that a spectacular manifestation of the dynamical symmetry related to the $SO(2,1)$ group is the existence of an undamped breathing mode (see also Kagan, Surkov, et al. (1996)). They studied the case of a two-dimensional Bose gas described by a classical field approach, but this result extends to other systems exhibiting conformal invariance such as the 3D Fermi gas in the unitary regime (Castin 2004; Werner & Castin 2006), or an assembly of interacting particles with a $1/r_{ij}^2$ potential, whatever the dimension of space (Benjamin, Quiroga, et al. 1996).

We will show that the time evolution of the second moment of the position $\langle r^2 \rangle = \frac{2}{m\omega^2} \langle \hat{U}_{ho} \rangle$ is periodic, whatever the initial conditions. To do this, we use the equations of motion of the generators $\hat{\mathcal{L}}_j$ in the Heisenberg picture:

$$\frac{d\hat{U}_{ho}}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{U}_{ho}] = -i 2\hbar\omega^2 [\hat{\mathcal{L}}_1, \hat{\mathcal{L}}_3] = 2\hbar\omega^2 \hat{\mathcal{L}}_2 \quad (88)$$

and

$$\frac{d\hat{\mathcal{L}}_2}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{\mathcal{L}}_2] = i 2\omega [\hat{\mathcal{L}}_3, \hat{\mathcal{L}}_2] = 2\omega \hat{\mathcal{L}}_1 = \frac{1}{\hbar} (\hat{H} - 2\hat{U}_{ho}). \quad (89)$$

By combining these two equations, we arrive at:

$$\frac{d^2\hat{U}_{ho}}{dt^2} + 4\omega^2\hat{U}_{ho} = 2\omega^2\hat{H}. \quad (90)$$

Let us take the average of this equation over the initial state. Using the fact that $\langle \hat{H} \rangle \equiv E$ is a constant of motion, we deduce that the second moment of the position $\langle r^2 \rangle$ obeys the differential equation:

$$\frac{d^2\langle r^2 \rangle}{dt^2} + 4\omega^2\langle r^2 \rangle = \text{Constant} \quad (91)$$

It therefore evolves periodically in time with the period π/ω .

This mode has been observed in the context of 2D gases described by the classical Gross–Pitaevskii field equation, and small deviations due to the quantum nature of the motion of the atoms have also been measured (see the 2017 lecture series, Chapter 6). However, it has not yet been demonstrated experimentally for particles with an interaction potential varying as $1/r^2$.

4 The one-dimensional case

4-1 The spectrum of the N -body problem

In a famous article, Calogero (1971) derived the spectrum of N bosonic or fermionic particles evolving on an axis, with binary interactions described by the potential $V(x_{ij}) \propto x_{ij}^2 + x_{ij}^{-2}$, with $x_{ij} = x_i - x_j$. By means of a

transformation of the variables, we can map this problem to a 1D assembly of N particles evolving under the effect of the Hamiltonian

$$\hat{H} = \sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2 \right) + \sum_{i < j} \frac{g}{(x_i - x_j)^2} \quad (92)$$

This problem can be extended to the case of particles moving freely on a circle of perimeter L , with an interaction in $\sin^{-2}(\pi(x_i - x_j)/L)$ (Sutherland 1972).

We start by specifying the boundary conditions on the admissible wave functions $\Psi(x_1, \dots, x_N)$. Let us consider the case $N = 2$ for the sake of simplicity. For the average potential energy to be non-divergent, the integral

$$\int \frac{g}{x^2} |\Psi(x, X)|^2 dx dX \quad (93)$$

has to be convergent at $x = 0$, with $x = x_1 - x_2$ and $X = (x_1 + x_2)/2$ denoting the relative variable and the center-of-mass variable respectively. Whatever the non-zero value of g , $\Psi(x, X)$ must therefore vanish faster than $\sqrt{x}$ when $x \rightarrow 0$. This condition is obviously absent when g is strictly zero. This means that we cannot hope to recover the case of particles with no interaction by taking the limit $g \rightarrow 0$ in what follows, unlike the 3D case studied above (cf. §3-4).

Calogero showed that this problem is exactly solvable and that its energy spectrum consists of equidistant values, separated by $\hbar\omega$ whatever the strength of the coupling g provided that $\alpha > -1/4$:

$$E_n = \hbar\omega \left(n + \frac{N(N-1)}{2}s + \frac{N^2}{2} \right) \quad \text{with} \quad s = -\frac{1}{2} + \sqrt{\alpha + \frac{1}{4}} \quad (94)$$

where $\alpha = mg/\hbar^2$ and n is a non-negative integer ($n = 1$ is excluded). He also found the explicit form of the ground state (with $a_{\text{ho}} = (\hbar/m\omega)^{1/2}$):

$$\Psi(x_1, \dots, x_N) = \prod_{i < j} (x_i - x_j)^{s+1} \exp \left(- \sum_i x_i^2 / 2a_{\text{ho}}^2 \right) \quad (95)$$

which is, as expected, a wave function with no node other than at the points $x_i = x_j$. As an exercise, we can check that this wave function is indeed an

eigenstate of (92) with the eigenvalue E_n corresponding to $n = 0$. The degeneracy of each energy level given in (94) is discussed in detail in Calogero (1971).

Case of $N = 2$ particles. In this case, we can separate the motion of the center of mass, which is purely harmonic with a spectrum in $(n_1 + 1/2)\hbar\omega$, $n_1 \in \mathbb{N}$, and the motion of the relative particle, which we have studied in §3-4. The Schrödinger equation governing the relative motion is

$$-\psi'' + \left(\frac{\alpha}{x^2} + x^2 \right) \psi = \frac{2E}{\hbar\omega} \psi \quad (96)$$

where $\alpha = 2m_{\text{r}}g/\hbar^2$ and distances are expressed in units of $\sqrt{\hbar/m_{\text{r}}\omega}$, with $m_{\text{r}} = m/2$ the reduced mass. The transposition of (84-85) gives for relative motion the ground state $\psi(x) = x^{s+1}e^{-x^2/2}$ and the energy $\hbar\omega(s + 3/2)$ with s given in (94), hence the total energy of the ground state for the two motions as a whole² $E_0 = \hbar\omega(s + 2)$. The energy given in (94) is found by inserting $N = 2, n = 0$. The ground state is

$$\begin{aligned} \Psi(x, X) &= x^{s+1} e^{-x^2 m \omega / 4 \hbar} e^{-X^2 m \omega / \hbar} \\ &= (x_1 - x_2)^{s+1} e^{-m \omega (x_1^2 + x_2^2) / 2 \hbar}. \end{aligned} \quad (97)$$

The first excited state, of energy $\hbar\omega(s + 3)$, is obtained by placing the center of mass in its first excited state, while leaving the relative motion in its ground state. The excited states of the relative motion, of energy $\hbar\omega(2n + s + 3/2)$, are obtained by constructing the “tower of states” described in §3-4 (see also Werner (2008), appendix B).

4-2 The dynamics of the system

Since the N -body spectrum consists of equidistant levels separated by the energy $\hbar\omega$, we can deduce that any observable will have a periodic evolution. Indeed any initial state $|\Phi(0)\rangle$ can be decomposed on the basis of the

²When $g \rightarrow 0, s \rightarrow 0$ and this energy tends to $2\hbar\omega$, which corresponds to the first excited state of two independent particles placed in a harmonic potential. We therefore do not find the ground state of the system at g strictly zero, which is a consequence of the condition imposed on the wave functions, cf. discussion after (93).

eigenstates $|\Psi_\nu\rangle$ of the N -body system

$$|\Phi(0)\rangle = \sum_\nu c_\nu |\Psi_\nu\rangle. \quad (98)$$

This gives the state at time t (apart from a global phase, which is unimportant):

$$|\Phi(t)\rangle = \sum_\nu c_\nu e^{-in_\nu \omega t} |\Psi_\nu\rangle \quad (99)$$

so that the mean value of any operator $\hat{O}$ reads

$$\langle \hat{O} \rangle(t) = \sum_{\nu, \nu'} c_\nu^* c_{\nu'} \langle \Psi_\nu | \hat{O} | \Psi_{\nu'} \rangle e^{i(n_\nu - n_{\nu'}) \omega t}. \quad (100)$$

This quantity is periodic, with period $2\pi/\omega$. This result, valid in 1D, is of course much stronger than the periodicity of $\langle r^2 \rangle$ obtained in § 3-5 (but this was valid in any dimension).

4-3 The classical motion

The remarkable simplicity found for the spectrum of the quantum motion also occurs for the classical motion of N particles. For $g > 0$, we can show in particular the following result, illustrated in figure II.13. Let us start from an asymptotic state ($t \rightarrow -\infty$) in which the particles are far from each other (negligible interaction energy), with the ordering $x_1 < x_2 < \dots < x_N$ and initial velocities $v_1 > v_2 > \dots > v_N$. The particles come together under the effect of their initial velocities, and then separate again. For the final velocities v'_i one always finds

$$v'_i = v_{N+1-i}, \quad i = 1, \dots, N \quad (101)$$

i.e. a simple two-by-two exchange of particle velocities, as if the particles had passed through each other without interacting! This result follows from the integrability of the N -body system for a potential in $1/r^2$, for which one can exhibit N constants of motion.

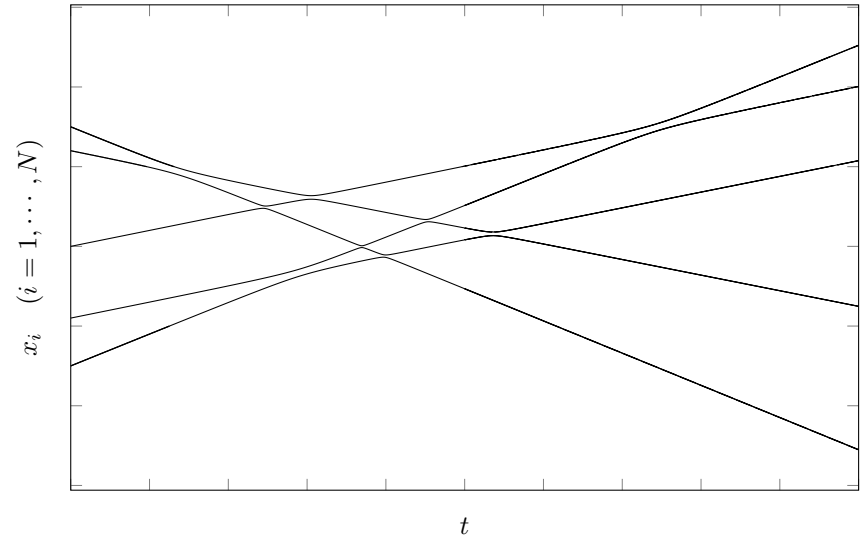


Figure II.13. Collision between $N = 5$ particles interacting through the binary potential $g/(x_i - x_j)^2$, with $g > 0$.

Chapter III

From contact interactions to the $1/r^2$ potential

In this chapter we approach the three-body problem from its simplest angle, that of two heavy particles, of mass M , bound together by a light particle of mass $m \ll M$. This hierarchy of masses will considerably simplify our study, compared with the case of three identical particles, which will be discussed in Chapters 5 and 6. We will use the Born–Oppenheimer approach, originally developed in molecular physics to take advantage of the large difference in mass between the electrons that form the chemical bond and the atoms that make up a molecule.

This Born–Oppenheimer approach consists in working in two stages, taking advantage of the two very different time scales of the problem, that associated with the fast motion of the light particle and that associated with the slow motion of the two heavy particles:

- First, we treat the one-body problem describing the motion of the light particle m in the force field created by the heavy particles M , assumed to be held fixed at a distance R . We find a set of eigenenergies $E_n(R)$ for this light particle, in particular the ground-state energy $E_0(R)$.
- Secondly, we look at the motion of the heavy particles, in particular the variation in time of their separation R . It is assumed that the state of the light particle follows this motion adiabatically, so that the energies $E_n(R)$ act as the effective interaction potentials between the two heavy particles.

This separation of the three-body problem into a one-body problem fol-

lowed by a two-body problem is obviously a considerable simplification. The remarkable point is that it recovers the essential universality of Efimov physics for three identical particles, with a “bonus”: the additional control parameter provided by the ratio M/m .

This mMM situation was proposed by Efimov (1973) for the case of a contact interaction, which we will also consider in what follows. It was then taken up by Fonseca, Redish, et al. (1979) for a separable potential of the type introduced by Yamaguchi (1954).

The questions we wish to address in this course and the next are, for example:

- Can there be a three-body bound state mMM even if the dimer mM is not bound?
- If both the mM dimer and the mMM trimer are bound, which is the more stable? Would the trimer not gain by ejecting an M particle in order to lower its energy further?

We shall begin this chapter with a presentation of the contact interaction in §1. We will take it into account using the Bethe–Peierls boundary condition, which will enable us to clarify the notion of a scattering resonance. We will then begin our study of the three-body problem with this resonant case (infinite scattering length), in order to bring out the emergence of the potential $E_0(R) \propto 1/R^2$ underlying the Efimov effect (§2). §3 will

be devoted to determining the effective interaction $E_0(R)$ on either side of the resonance. Finally, we will briefly explain in §4 how this approach can be generalized to the case where several light particles and several heavy particles are present simultaneously.

The second stage of the Born–Oppenheimer approach, i.e. the motion of the heavy particles under the effect of the effective interaction $E_0(R)$, will be dealt with in the next chapter.

1 Two-body interaction at low energy

1-1 s -wave scattering

In this chapter we restrict ourselves to the case of neutral particles whose velocity is sufficiently low that in the two-body problem, only the interactions in the channel of zero angular momentum (s wave) are significant.

The asymptotic expression for the scattering state describing this interaction is

$$r \gg b : \quad \psi_{\mathbf{k}}(\mathbf{r}) \sim e^{i\mathbf{k} \cdot \mathbf{r}} + f(k) \frac{e^{ikr}}{r}, \quad (1)$$

where $\mathbf{k}$ is the incident relative wave vector. The scattering state is an eigenstate of the Hamiltonian describing the relative motion of the two particles, with eigenvalue $E = \hbar^2 k^2 / 2m_r$, where m_r is the reduced mass. It describes the physical situation of a collision with incident relative momentum $\hbar\mathbf{k}$ and an outgoing spherical wave of amplitude $f(k)$ (figure III.1).

The asymptotic expression (1) is close to the exact expression of $\psi_{\mathbf{k}}(\mathbf{r})$ when r is greater than the range b of the scattering potential. For atom–atom scattering, this range is given by

$$R_{\text{vdW}} = \frac{1}{2} \left(\frac{2m_r C_6}{\hbar^2} \right)^{1/4} \quad (2)$$

for a van der Waals-type interaction potential $-C_6/r^6$.

The interaction between two particles is therefore described by the scattering amplitude $f(k)$, which is given by (cf. the 2021 lecture series, Chapter

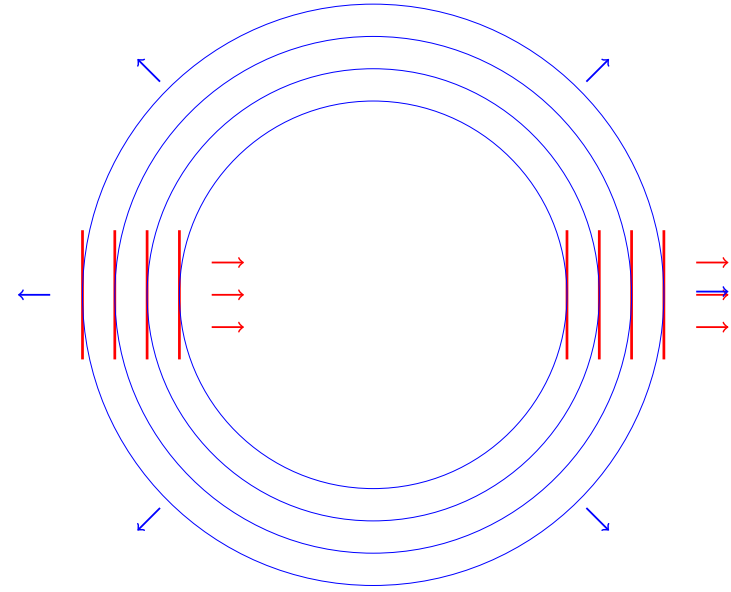


Figure III.1. The physical situation described by the scattering state (1), with the incident plane wave of wave vector $\mathbf{k}$ and the scattered spherical wave e^{ikr}/r , of amplitude $f(k)$.

3)

$$f(k) \approx \frac{-a}{1 + ika + \frac{1}{2}r_e k^2}, \quad (3)$$

where a is the scattering length and r_e is the effective range. At the small values of k that we are interested in here, the effective range term will be negligible and we will keep only $1 + ika$ in the denominator of this fraction. The scattering length a can be positive or negative, or even zero or infinite.

When $kr \ll 1$, the expression (1) can be simplified to give:

$$\begin{aligned} b \ll r \ll k^{-1} : \quad \psi_{\mathbf{k}}(\mathbf{r}) &\sim 1 - \frac{a}{1 + ika} \left(\frac{1 + ikr}{r} \right) + \mathcal{O}(r) \\ &\sim \frac{-a}{1 + ika} \left(\frac{1}{r} - \frac{1}{a} \right) + \mathcal{O}(r) \end{aligned} \quad (4)$$

which we will write more simply in the form (at this stage the state $\psi_{\mathbf{k}}$ is not normalized, and is therefore defined up to a multiplicative factor):

$$b \ll r \ll k^{-1} : \quad \psi_{\mathbf{k}}(\mathbf{r}) \sim \frac{1}{r} - \frac{1}{a} + \mathcal{O}(r) \quad (5)$$

i.e. a term in r^{-1} , a term in r^0 , and correction terms in r^n with $n \geq 1$.

1-2 Scattering resonances

In what follows, we will assume that the interaction potential $V(r)$ between the particles has an attractive component and can give rise to one or more bound states. When the attractive component of $V(r)$ is gradually increased to give rise to a new bound state, we observe the following variation in the scattering length (Levinson's theorem):

- When the attractive component is slightly too small for the bound state to appear, the scattering length is large and negative.
- At the threshold for the appearance of the bound state, the scattering length is infinite. Its sign is unimportant; it is rather the statement $1/a = 0$ that is relevant at this point, as can be seen from the asymptotic expression (5).
- When the attractive component has exceeded the threshold value for the appearance of the bound state, the scattering length is large and positive.

This behavior is illustrated for an attractive square well of depth V_0 and range b (figure III.2, top). The threshold for the appearance of the first bound state is (the 2021 lecture series, Chapter 3, §3)

$$k_0 b = \frac{\pi}{2} \quad \text{with} \quad \frac{\hbar^2 k_0^2}{2m_r} = V_0, \quad (6)$$

and the threshold for the n -th bound state is

$$k_0 b = \left(n - \frac{1}{2}\right) \pi. \quad (7)$$

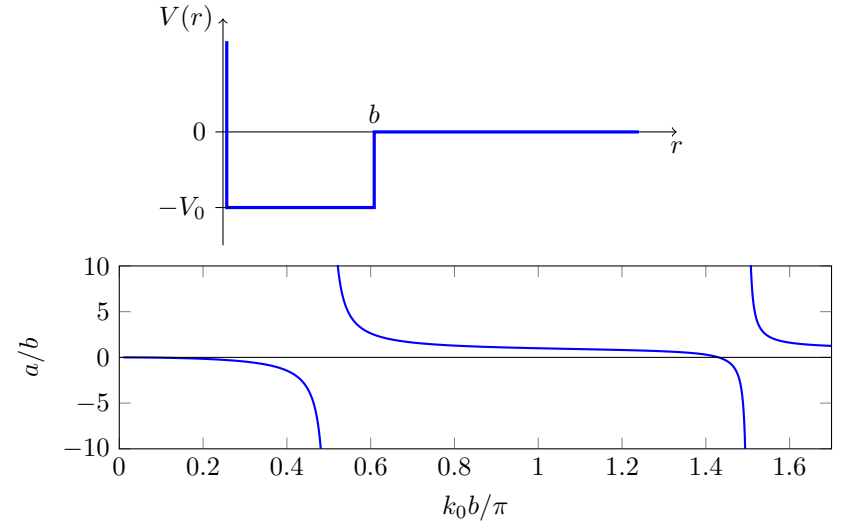


Figure III.2. Top: square potential well of depth V_0 and range b . Bottom: variation of the scattering length of a square well with its depth V_0 .

The scattering length is

$$a = b - \frac{\tan(k_0 b)}{k_0} \quad (8)$$

and it diverges for each value of k_0 that satisfies (7). The variation of a with depth V_0 is plotted in figure III.2, bottom.

In what follows, we are interested in the physical effects that appear when a two-particle system is about to have a bound state, or when this bound state has just appeared. In the context of square-well modeling, this amounts to placing ourselves around the point (6), $k_0 b \approx \pi/2$ (figure III.3).

Note. Strongly bound states, although present in practice, will not play a role for the time being. They will come into play later as ingredients for inelastic processes in a three-body collision: initially free atoms can form a strongly bound dimer after the collision, with conservation of energy and momentum ensured by the presence of the third body.

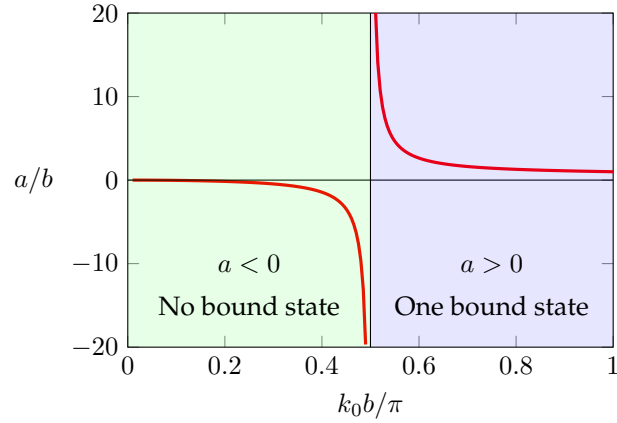


Figure III.3. Zoom of figure III.2 around the threshold for the appearance of the first bound state, at $k_0 b = \pi/2$.

1-3 The pseudo-potential

The pseudo-potential is defined in three dimensions. It can be seen as a potential of zero range b , leading to s -wave scattering only, with an adjustable scattering length a .

The action of the pseudo-potential $\hat{V}_{\text{pp}}$ on a wave function $\psi(\mathbf{r})$ reads

$$\hat{V}_{\text{pp}} \psi(\mathbf{r}) = g \delta(\mathbf{r}) \frac{\partial}{\partial r} [r \psi(\mathbf{r})]. \quad (9)$$

We can analytically determine an eigenstate basis of the relative Hamiltonian describing the interaction between two particles under the effect of this pseudo-potential:

$$\hat{H} = \frac{\hat{p}^2}{2m_r} + \hat{V}_{\text{pp}}. \quad (10)$$

For $g < 0$, only positive-energy eigenstates are found

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} - \frac{a}{1 + ika} \frac{e^{ikr}}{r} \quad E = \frac{\hbar^2 k^2}{2m_r} \quad (11)$$

with

$$g = \frac{2\pi \hbar^2 a}{m_r} \quad (12)$$

For $g > 0$, we must add to this family of eigenstates the (unique) bound state

$$\psi(\mathbf{r}) = \frac{e^{-r/a}}{r} \quad E = -\frac{\hbar^2}{2m_r a^2} \quad (13)$$

to form a basis of Hilbert space.

We studied the properties of this pseudo-potential in detail in the 2021 lecture series (Chapter 3, §4). We simply recall a number of important properties here:

- The expression (11) is reminiscent of the asymptotic form of a scattering state. However, this expression is valid here whatever the value of $r \neq 0$, which corresponds well to the idea of a potential of zero range b .
- The expression (11) gives the exact value of the scattering amplitude of the pseudo-potential:

$$f(k) = \frac{-a}{1 + ika}. \quad (14)$$

It follows that there is no effective-range correction r_e as in (3), nor any higher-order correction in k . The quantity a defined from (12) gives the *exact* value of the scattering length.

- All the eigenfunctions (11) and (13) have the same behavior near the origin for $a \neq 0$:

$$r \ll k^{-1}, a : \quad \psi(\mathbf{r}) \sim \frac{1}{r} - \frac{1}{a} + \mathcal{O}(r). \quad (15)$$

Since the physically acceptable functions must be written as linear combinations of the eigenfunctions of the Hamiltonian, this means that a problem involving the pseudo-potential does not have the same function space as a problem with a regular potential. For a regular potential, we consider only functions that are regular everywhere, in particular at $r = 0$. They must therefore be written as

$$\text{Regular potential:} \quad \psi(\mathbf{r}) = \beta + \mathcal{O}(r) \quad (16)$$

where β is any constant, possibly zero. For the pseudo-potential, these functions must be written as

$$\text{Pseudo-potential: } \psi(\mathbf{r}) = \frac{\alpha}{r} + \beta + \mathcal{O}(r) \quad (17)$$

with the link between the coefficients α and β :

$$\beta = -\frac{\alpha}{a}, \quad (18)$$

so that the physically relevant functions read

$$\text{Pseudo-potential: } \psi(\mathbf{r}) = \alpha \left(\frac{1}{r} - \frac{1}{a} \right) + \mathcal{O}(r) \quad (19)$$

Note that this pseudo-potential can be approximated by returning to the square well of § 1-2 and taking the limit of zero range $b \rightarrow 0$ and infinite depth $k_0 \rightarrow \infty$. More precisely, this limit must be taken with $k_0 b = \frac{\pi}{2} + \frac{1}{k_0 a_s}$, where a_s is the target scattering length, which is equivalent to being in the vicinity of the threshold for the appearance of the first bound state.

1-4 Bethe–Peierls boundary conditions

A convenient way of dealing with problems in which the pseudo-potential comes into play is to impose *a priori* the boundary conditions (19) as the domain of admissible functions. This effectively eliminates the point $r = 0$ from the relevant domain of space, and we can then restrict ourselves to a purely kinetic Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m_\tau}. \quad (20)$$

The situation is very similar to the approach taken to treat the square-well potential in introductory quantum mechanics courses (see figure III.4). If the well is of finite depth, we explicitly treat the action of the potential $V(x)$ in both the allowed and forbidden regions in order to find the eigenstates of the problem. But when we take the limit of the infinitely deep well (the counterpart of our zero-range limit), we drop the potential $V(x)$ and replace it by the boundary condition $\psi(\pm b/2) = 0$ on all the wave functions.

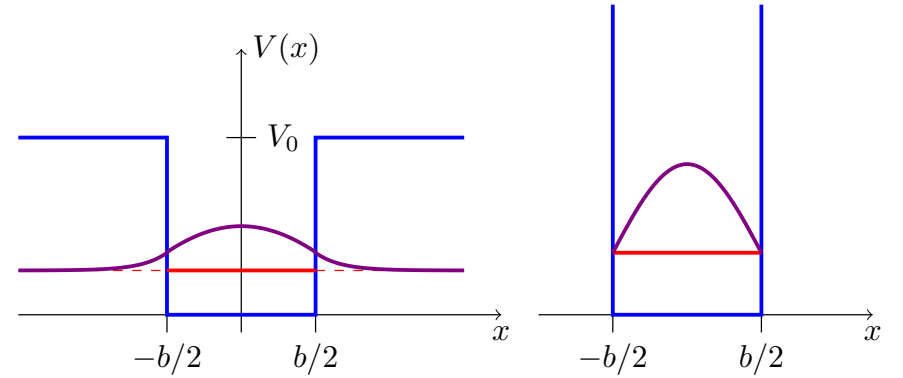


Figure III.4. The two approaches to treating a square well. Left: the allowed and forbidden regions are treated separately, using the explicit form of $V(x)$ in each region, and the solutions are matched. Right: the limit $V_0 \rightarrow \infty$ is taken and the potential is accounted for by the boundary condition $\psi(\pm b/2) = 0$. The energy is then purely kinetic.

There are several equivalent techniques for writing the Bethe–Peierls boundary condition (19) in practice. Note, for example, that

$$\lim_{r \rightarrow 0} [r\psi(\mathbf{r})] = \alpha \quad \lim_{r \rightarrow 0} \left[\frac{\partial [r\psi(\mathbf{r})]}{\partial r} \right] = -\frac{\alpha}{a} \quad (21)$$

so that, whatever the value of the multiplicative coefficient α , we can impose

$$\lim_{r \rightarrow 0} \left[\frac{\partial [r\psi(\mathbf{r})]}{\partial r} \right] = -\frac{1}{a} \lim_{r \rightarrow 0} [r\psi(\mathbf{r})]. \quad (22)$$

This condition can also be written as

$$\lim_{r \rightarrow 0} \frac{\partial \ln [r\psi(\mathbf{r})]}{\partial r} = -\frac{1}{a}. \quad (23)$$

Finally, we can determine “by hand” the coefficients of r^{-1} and r^0 and force these two coefficients to be in the ratio $-a$. This is the method we will use in the following.

2 Long-range force for the mMM problem

2-1 The mMM three-body problem

In the exact approach to the three-body problem, all the particles are treated on the same footing, which involves manipulating wave functions of many variables (nine position coordinates). Before tackling this exact approach in a later chapter, we will deal here with a simpler, but very instructive, case introduced by Efimov (1973) [see also Fonseca, Redish, et al. (1979)]: one of the three particles (of mass m) is much lighter than the other two (of mass M) and it interacts in a quasi-resonant manner with them; the two heavy particles do not interact with each other, except possibly through a hard-core potential that prevents them from approaching closer than R_0 , in order to avoid the fall to the center studied in the previous chapters.

As explained in the introduction to this chapter, this mass hierarchy will allow us to use an approximation identical in every respect to the Born–Oppenheimer approximation of molecular physics (the light particle playing the role of an electron), by separating our treatment into two stages:

- First, we will assume that the two heavy particles are held fixed, separated by a distance R , and we will study the motion of the light particle interacting with them. This is a one-body problem, and we want to determine in particular the energy of the ground state, which from now on we will denote by $E_0(R) \equiv E(R)$.
- In a second stage (see the next chapter), we will treat the energy $E(R)$ as an interaction potential between the two heavy particles and study their motion. This is a two-body problem, for which the solution is well defined.

The main result of this approach is the emergence, in the case where the mM interaction is resonant, of the effective attractive potential $E(R) \propto -1/R^2$, leading to the scale invariance discussed in Chapters 1 and 2.

Note. One may wonder about the special case $R = 0$, when the two heavy particles are superimposed. In fact, this problem is ill defined in the context

of an interaction described by the pseudo-potential, and we need to go back to a non-zero interaction range to give it a precise meaning. We will do so in the next chapter, when we describe the *Thomas collapse*.

2-2 Bound states for the light particle

We tackle the three-body problem mMM , with the particles M assumed for the moment to be infinitely heavy, and therefore fixed. We denote their separation by R and assume that they are placed symmetrically with respect to the origin of coordinates, at the points $\pm \mathbf{R}/2$ (with $\mathbf{R} \neq 0$). We are interested in the bound states of the light particle of mass m by assuming that it interacts in the same way with the two heavy particles, an interaction described by a pseudo-potential associated with the scattering length a .

We will look for the bound state(s) by treating the action of the pseudo-potential through the Bethe–Peierls boundary conditions. Let us denote by

$$E = -\frac{\hbar^2 \kappa^2}{2m_r} \quad (24)$$

the energy of the bound state sought, with $\kappa > 0$. Note that since $M \gg m$, we have $m_r \approx m$. Our aim is to determine the value of κ as a function of the two parameters of the problem, the scattering length a characterizing the mM interaction and the distance R between the two heavy particles.

Away from the points $\pm \mathbf{R}/2$, the wave function of the bound state must be a *regular* solution of the equation

$$-\frac{\hbar^2}{2m_r} \nabla^2 \psi(\mathbf{r}) = E \psi(\mathbf{r}) \quad \Rightarrow \quad \nabla^2 \psi = \kappa^2 \psi \quad (25)$$

and this wave function must obey the boundary conditions (up to a multiplicative coefficient)

$$\mathbf{r} \rightarrow \pm \mathbf{R}/2 : \quad \psi(\mathbf{r}) \propto \frac{1}{|\mathbf{r} \mp \mathbf{R}/2|} - \frac{1}{a} \quad (26)$$

This wave function is therefore of the form:

$$\psi(\mathbf{r}) = A \frac{e^{-\kappa|\mathbf{r}-\mathbf{R}/2|}}{|\mathbf{r}-\mathbf{R}/2|} + B \frac{e^{-\kappa|\mathbf{r}+\mathbf{R}/2|}}{|\mathbf{r}+\mathbf{R}/2|} \quad (27)$$

We now need to find, for a given R , the choice of κ , A and B which ensures that this boundary condition is satisfied.

When we take the limit $\mathbf{r} \rightarrow \mathbf{R}/2$, the terms in $|\mathbf{r} - \mathbf{R}/2|^{-1}$ and in $|\mathbf{r} - \mathbf{R}/2|^0$ read

$$|\mathbf{r} - \mathbf{R}/2|^{-1} : \quad A \quad (28)$$

$$|\mathbf{r} - \mathbf{R}/2|^0 : \quad -A\kappa + B \frac{e^{-\kappa R}}{R}. \quad (29)$$

These two terms must be in the ratio $-1/a$ in order to satisfy the boundary condition (26), which imposes

$$-A\kappa + B \frac{e^{-\kappa R}}{R} = -\frac{A}{a}. \quad (30)$$

Similarly, for $\mathbf{r} \rightarrow -\mathbf{R}/2$ we find

$$A \frac{e^{-\kappa R}}{R} - B\kappa = -\frac{B}{a}. \quad (31)$$

For each value of κ , we therefore obtain a system of two equations in the two unknowns A and B :

$$A \left(\frac{1}{a} - \kappa \right) + B \frac{e^{-\kappa R}}{R} = 0 \quad (32)$$

$$A \frac{e^{-\kappa R}}{R} + B \left(\frac{1}{a} - \kappa \right) = 0. \quad (33)$$

This system admits a solution other than the trivial one $(0, 0)$ if and only if its determinant vanishes, which requires κ to be such that

$$\begin{vmatrix} \frac{1}{a} - \kappa & \frac{e^{-\kappa R}}{R} \\ \frac{e^{-\kappa R}}{R} & \frac{1}{a} - \kappa \end{vmatrix} = 0 \quad \Leftrightarrow \quad \frac{1}{a} - \kappa = \pm \frac{e^{-\kappa R}}{R} \quad (34)$$

which leads to the following two equations:

$$\boxed{\kappa R - \frac{R}{a} = e^{-\kappa R} \quad \text{and therefore} \quad A = B} \quad (35)$$

and

$$\boxed{\kappa R - \frac{R}{a} = -e^{-\kappa R} \quad \text{and therefore} \quad A = -B} \quad (36)$$

The symmetry or antisymmetry of the coefficients A and B could have been anticipated, since the two particles M play identical roles. In other words, the Hamiltonian and the Bethe–Peierls boundary conditions are invariant under the change $\mathbf{r} \rightarrow -\mathbf{r}$, and we can therefore look for the eigenstates of the Hamiltonian in the form of even or odd functions.

These two symmetric and antisymmetric solutions are very similar to the bonding and antibonding orbitals of the chemical bond. It is easy to check that the value of κ solving (35) is always larger than that solving (36), which means that (35) corresponds to the lower energy $-\hbar^2 \kappa^2 / 2m$. The wave function of the light particle (27) then has no node, since $A = B$, as expected for a ground state. By contrast, the solution of (36) leads to $A = -B$, and the wave function (27) vanishes on the median plane of the two heavy particles.

To make progress in solving this problem, it is now useful to separate the three cases $|a| = +\infty$, $a > 0$, and $a < 0$, and we will start with the resonant case, $|a| = +\infty$.

2-3 The resonant case $|a| = +\infty$

A particularly remarkable situation occurs in the resonant case $a = \pm\infty$, for which the two equations (35) and (36) read

$$\boxed{\text{symmetric solution:} \quad \kappa R = e^{-\kappa R}} \quad (37)$$

and

$$\boxed{\text{antisymmetric solution:} \quad \kappa R = -e^{-\kappa R}} \quad (38)$$

Since the quantities κ and R are both positive, only the first of these two equations, which corresponds to the bonding orbital $A = B$ in (27), has a solution.

Recall that we are then just at the threshold for the appearance of a bound state for the mM two-body problem, when only one of the heavy particles is present. On the other hand, when both heavy particles are present, the solution of (37) is a non-zero value of κ , hence a bound state

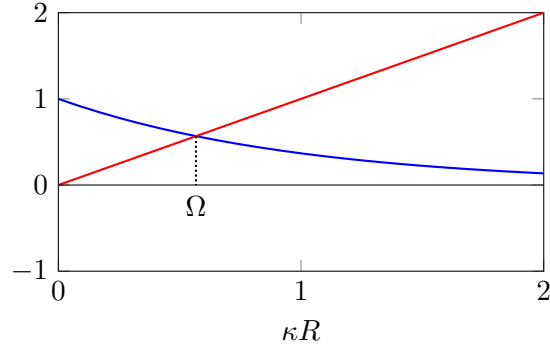


Figure III.5. Graphical solution of equation (35) in the case $|a| = +\infty$, i.e. $\kappa R = \exp(-\kappa R)$. There is one and only one solution, $\kappa R = \Omega$ with $\Omega \approx 0.567143$.

of the light particle around the heavy particles:

$$a = \pm\infty : \quad \kappa = \frac{\Omega}{R} \quad \text{with} \quad \Omega \approx 0.567 \quad (39)$$

where the constant Ω is the unique solution of the transcendental equation $\Omega = e^{-\Omega}$ (figure III.5).

The energy of the light particle interacting with the two heavy particles is then

$$a = \pm\infty : \quad E(R) = -\Omega^2 \frac{\hbar^2}{2mR^2} \quad \text{with} \quad \Omega^2 \approx 0.322 \quad (40)$$

When we later interpret this energy as an interaction potential between the two heavy particles, we will thus have the $1/R^2$ law leading to the scale invariance mentioned in the previous chapters. We can therefore see how a long-range interaction can emerge from a potential of zero range.

Note that simple dimensional analysis already tells us that the ground-state energy of the light particle in the case $a = \infty$ must be proportional to $\hbar^2/mR^2$, since this is the only energy scale in the problem. It cannot, however, give us the sign of this energy, let alone the proportionality coefficient $-\Omega^2/2$.

3 Finite scattering length and mMM problem

3-1 Preliminary: the Lambert function

In what follows, we will use the Lambert function $W(x)$ [cf. figure III.6] defined as the unique solution $W(x)$ for $x \geq -e^{-1}$ of the equation

$$We^W = x. \quad (41)$$

The function $W \rightarrow We^W$ being a bijection from $[-1, +\infty[$ to $[-e^{-1}, +\infty[$, it is invertible, and there is only one solution W of (41) for any value of x in the interval $[-e^{-1}, +\infty[$. The Lambert function is increasing and we find for small values of x :

$$|x| \ll 1 : \quad W(x) \approx x - x^2 + \mathcal{O}(x^3), \quad (42)$$

In the opposite regime of large values of x , we have

$$x \gg 1 : \quad W(x) \approx \ln x, \quad (43)$$

with logarithmic corrections. Finally, let us mention a particular point which we have already encountered in §2-3: $\Omega \equiv W(1) = 0.567 \dots$, i.e. the solution of $\Omega e^\Omega = 1$.

3-2 Case of a positive scattering length

We are interested here in the situation where a two-body bound state mM exists. We find this bound state by taking the limit $R \rightarrow \infty$ in (34), which leads to $\kappa = 1/a$: the light particle binds to one of the two heavy particles to form an mM dimer of energy $-\hbar^2/2ma^2$. The question is now whether we can obtain a lowering of the energy of this bound state, i.e. an increase of κ , when the two heavy particles approach each other.

The bonding orbital. This solution is associated with the wave number κ solving (35), which we reproduce here:

$$\kappa R - \frac{R}{a} = e^{-\kappa R}. \quad (44)$$

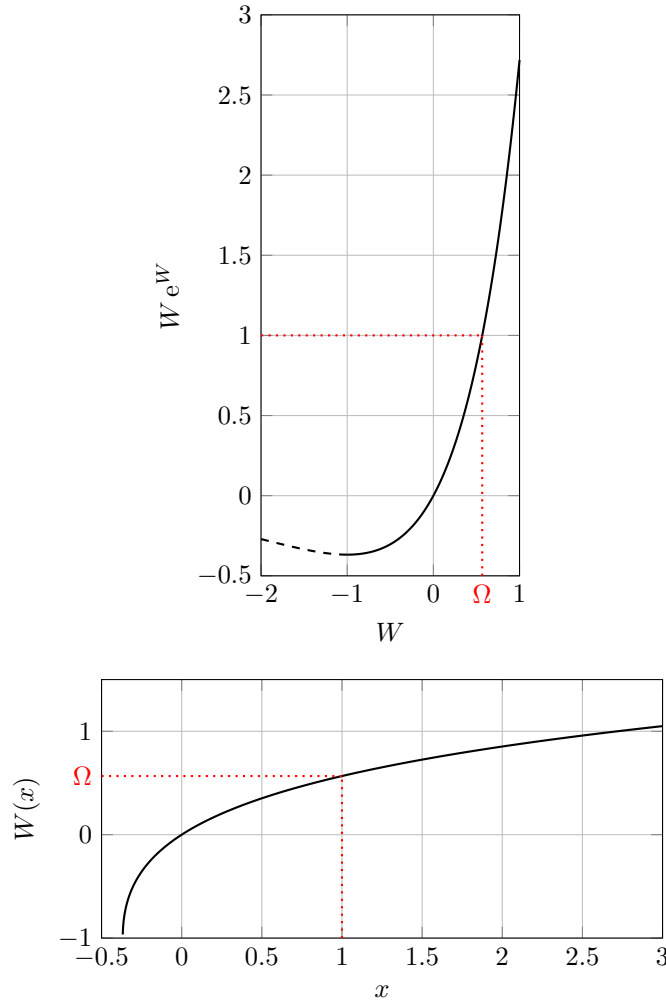


Figure III.6. Top: the function $W \rightarrow W e^W$. Bottom: the Lambert function $W(x)$ is the inverse of the function plotted at the top, defined on the domain $x \geq -e^{-1}$.

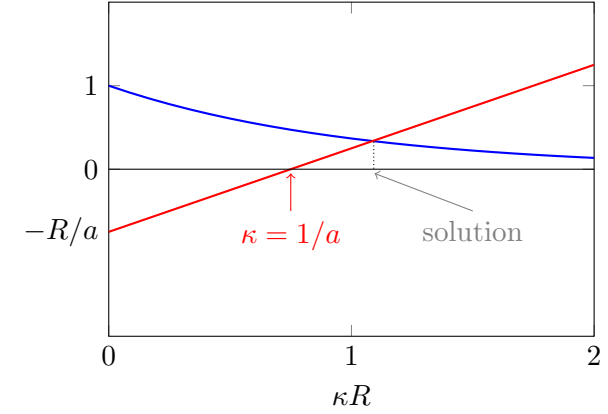


Figure III.7. Graphical solution of equation (44) in the case $a > 0$ for the bonding orbital, i.e. $x - x_0 = e^{-x}$ with $x = \kappa R$ and $x_0 = R/a$. There is one and only one solution with $\kappa > 1/a$ for any value of R .

For a given value of R/a , this transcendental equation in the unknown κR can be solved graphically, and we immediately find that there is always one and only one solution (figure III.7). This choice leads to the symmetric wave function $A = B$ in (27).

This solution can be written formally in terms of the Lambert function introduced in §3-1. To do this, let us write (44) in the form

$$\left(\kappa - \frac{1}{a}\right) R = e^{-\kappa R} = e^{-(\kappa - \frac{1}{a})R} e^{-R/a}, \quad (45)$$

or

$$W e^W = e^{-R/a} \quad \text{with} \quad W = \left(\kappa - \frac{1}{a}\right) R, \quad (46)$$

which leads to:

$$a > 0, \text{ bonding orbital:} \quad \kappa(R) = \frac{1}{a} + \frac{W(e^{-R/a})}{R} \quad (47)$$

The corresponding energy $E(R) = -\hbar^2 \kappa^2(R)/2m$ for the mMM system is plotted as a solid line in figure III.8. It is always lower than the energy

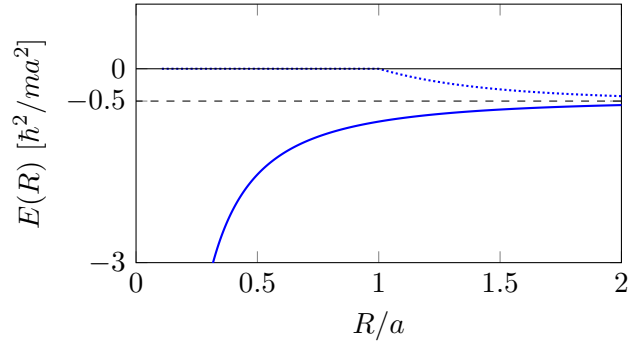


Figure III.8. For $a > 0$, variation of the energy $E(R)$ of the light particle (in units of $\hbar^2/ma^2$) as a function of the distance R (in units of a) between the two heavy particles. For the bonding orbital [$A = B$ in (27) and solution of (44)], the energy represented by the solid line is lower at any point R than the energy of the mM dimer, given by $-\hbar^2/2ma^2$. For the antibonding orbital [$A = -B$ in (27) and solution of (51)], the energy represented by the dashed line is a decreasing function of R for $R > a$ and cannot lead to the formation of a stable three-body structure.

$-\hbar^2/2ma^2$ of the mM dimer. This suggests that the exchange of the light particle between the two heavy particles stabilizes the three-body system, a point we will come back to in more detail later.

At large distances $R \gg a$, we can use the expansion $W(x) \sim x$ for $x \ll 1$, which leads to

$$R \gg a : \quad \kappa \approx \frac{1}{a} + \frac{e^{-R/a}}{R} \quad (48)$$

and therefore the energy

$$R \gg a > 0, \text{ bonding orbital: } E(R) \approx -\frac{\hbar^2}{2ma^2} - \frac{\hbar^2}{ma} \frac{e^{-R/a}}{R} \quad (49)$$

which corresponds to a Yukawa potential of range a .

In the limit $R \ll a$, we can neglect the term in $1/a$ in (44) compared with the term in $1/R$ ($e^{-\kappa R}$ is of order 1 in this case), and we are back to

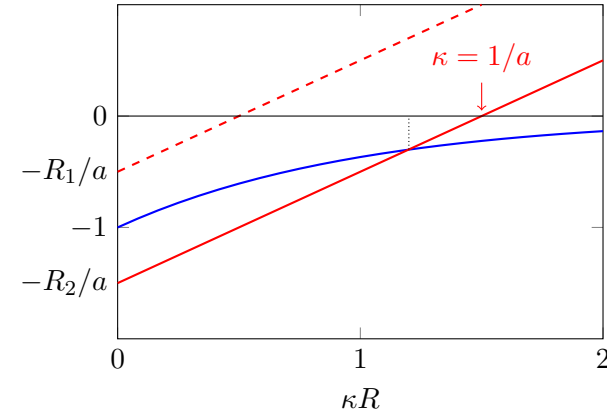


Figure III.9. Graphical solution of equation (51) in the case $a > 0$ for the antibonding orbital, i.e. $x - x_0 = -e^{-x}$ with $x = \kappa R$ and $x_0 = R/a$. We have taken two values of R , $R_1 < a$ and $R_2 > a$. There is a solution for R_2 (solid line), but not for R_1 (dashed line).

the situation (37), which leads to

$$R \ll a : \quad \kappa \approx \frac{\Omega}{R}, \quad E(R) \approx -\Omega^2 \frac{\hbar^2}{2mR^2}, \quad \Omega^2 \approx 0.322. \quad (50)$$

The scale invariance associated with the $-1/R^2$ potential will not be exact, however, since this potential does not extend to infinity.

The antibonding orbital. Let us now consider equation (36), leading to the solution $A = -B$, i.e. an antibonding orbital whose wave function for the light particle vanishes on the median plane of the two heavy atoms.

We must therefore solve

$$\kappa R - \frac{R}{a} = -e^{-\kappa R}. \quad (51)$$

This equation has a solution if and only if $R/a > 1$, and the value of κ obtained is always less than $1/a$ (figure III.9). In other words, the three-body binding energy $-\hbar^2 \kappa^2/2m$ is smaller (in absolute value) than the binding

energy $-\hbar^2/2ma^2$ of the mM dimer alone. The energy of the system is therefore minimized by moving the two heavy particles away from each other ($R \rightarrow \infty$), which is not favorable to the formation of an mMM trimer (figure III.8, dashed curve).

When this solution exists, it can also be expressed in terms of the Lambert function:

$$R > a > 0, \text{ antibonding orbital: } \kappa(R) = \frac{1}{a} + \frac{W(-e^{-R/a})}{R} \quad (52)$$

which is defined when its argument is greater than $-e^{-1}$, i.e. for $R > a$. From this we can deduce the long-range energy:

$$R \gg a > 0, \text{ antibonding orbital: } E(R) \approx -\frac{\hbar^2}{2ma^2} + \frac{\hbar^2}{ma} \frac{e^{-R/a}}{R} \quad (53)$$

3-3 Case of a scattering length $a < 0$

In this case, there is no bound state for the mM dimer: the attraction between M and m is not strong enough to bind the two particles. If, on the other hand, R is small enough, more precisely if $R < |a|$, the graphical solution of figure III.10 shows that there is a solution $\kappa > 0$ of equation (35) for the bonding orbital, which we rewrite here taking into account the fact that a is negative:

$$\kappa R + \frac{R}{|a|} = e^{-\kappa R}. \quad (54)$$

The energy of the light particle is therefore negative in the case $R < |a|$ (figure III.11). It increases with R up to the point $R = |a|$, and vanishes beyond that point. The interaction potential is attractive (with bounded support), and this opens up the possibility that one or more bound states of the mMM three-body system may exist in this case, as we shall see in the next chapter.

The solution of (54) can always be found using the Lambert function:

$$a < 0, R < |a|, \text{ bonding orbital: } \kappa = -\frac{1}{|a|} + \frac{W(e^{R/|a|})}{R} \quad (55)$$

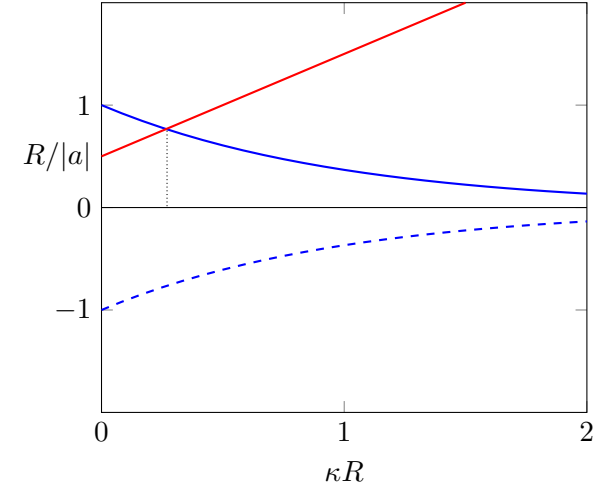


Figure III.10. Graphical solution of equation (54) in the case $a < 0$, i.e. $x + x_0 = e^{-x}$ for the bonding orbital and $x + x_0 = -e^{-x}$ for the antibonding orbital ($x = \kappa R$, $x_0 = R/|a|$). The solution for the bonding orbital exists only if $R/|a| < 1$. There is never a solution for the antibonding orbital.

We are interested in solutions with $\kappa > 0$, so that the wave function (27) tends to 0 at infinity. It is therefore necessary that

$$W(e^{R/|a|}) > \frac{R}{|a|} \quad (56)$$

which gives back the criterion $R < |a|$ (we have $W(e) = 1$).

Finally, let us note that equation (36), which determines the value of κ for the antibonding orbital, has no solution for $a < 0$, since the two terms on the left-hand side are then positive whereas the right-hand side is negative.

4 Generalization to the N -body problem

The modeling of mM binary interactions by the Bethe–Peierls boundary condition is formally very simple and lends itself well to a generalization

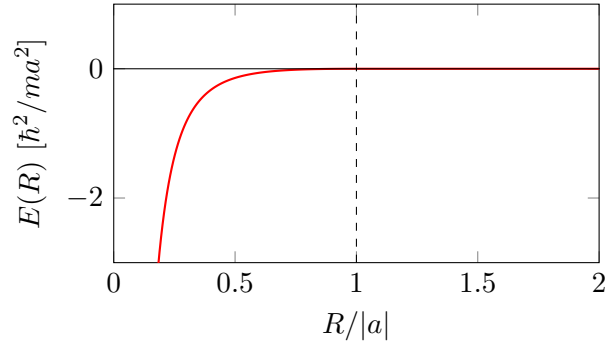


Figure III.11. For $a < 0$, variation of the energy $E(R)$ of the light particle (in units of $\hbar^2/ma^2$) as a function of the distance R (in units of a) between the two heavy particles. Recall that in this case, with $a < 0$, the mM dimer is not bound and the energy of the mM system is always positive. The ground-state energy of the light particle in the mMM system is negative for $R < |a|$, and zero beyond that.

in which the number of light and/or heavy particles is increased. We will give a few examples of this in the following sections.

4-1 Binding of the tetramer $mmMM$?

To begin our study of more than three bodies, let us assume that we have two identical light particles that do not interact with each other. These particles move around the heavy particles, still assumed to be held fixed at $\pm R/2$. The question arises as to the stability of this structure: does its energy decrease when the heavy particles are brought together from $R = \infty$? This question is equivalent, for a pseudo-potential interaction, to that of the formation of the H_2 molecule, in a singlet or triplet state, with the two protons in the role of heavy particles and the two electrons in the role of light particles.

This question is only relevant if the m particles are fermionic. If they are bosons, we can of course accumulate as many as we like in the bonding

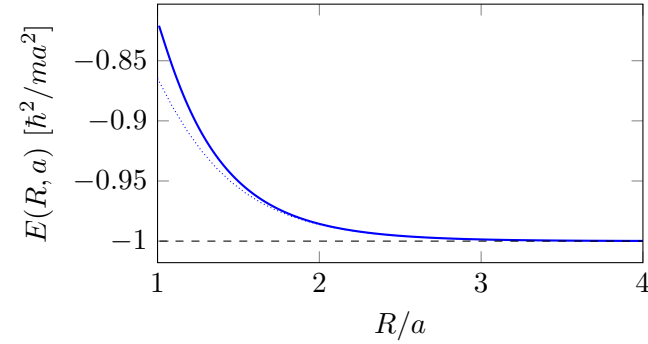


Figure III.12. Energy of the $mmMM$ system when the two light particles are placed on the two bonding and antibonding orbitals. The heavy particles M are assumed to be fixed and separated by a distance R . The calculation is made for $0 < a < R$, a necessary condition for the antibonding orbital to exist.

orbital and obtain a structure whose energy increases with R . We can then hope to form a bound state, at least in the absence of a short-range repulsive potential between the heavy particles.

If the m particles are spin-1/2 fermions, we can place two particles in the bonding orbital provided the total spin state is a singlet, and obtain the energy $2E(R)$, where $E(R) = -\hbar^2\kappa^2/2m$ with κ given in (47) or (55). Here again, we obtain an $mmMM$ state whose energy increases with R , and which will therefore tend to form a bound state.

The case where the light particles are polarized fermions is less obvious. In this case, one light particle must be placed in the bonding orbital and the other in the antibonding orbital, which of course requires the latter to exist. This condition immediately excludes the situation $a < 0$ and $a = \infty$. In the case $a > 0$, we must place ourselves in the situation $R > a$, and the energy obtained reads

$$R > a : \quad E_{\text{tot}}(R) = E_+(R) + E_-(R) = -\frac{\hbar^2}{2m} (\kappa_+^2 + \kappa_-^2) \quad (57)$$

with

$$\kappa_{\pm}(R) = \frac{1}{a} + \frac{W(\pm e^{-R/a})}{R}. \quad (58)$$

This energy is plotted in figure III.12. It is a decreasing function of R , which indicates that the $mmMM$ structure is not bound. It tends to separate into two mM dimers, which are indeed bound, since we have considered the case $a > 0$.

We can find an asymptotic expression for $E_{\text{tot}}(R)$ for $R \gg a$ using the expansion (42) of the Lambert function:

$$\kappa_{\pm}(R) \approx \frac{1}{a} \pm \frac{e^{-R/a}}{R} - \frac{e^{-2R/a}}{R}. \quad (59)$$

This gives, for $E_{\text{tot}}(R)$ as defined in (57),

$$R > a > 0 : \quad E_{\text{tot}}(R) \approx -\frac{\hbar^2}{ma^2} + \frac{2\hbar^2}{maR} \left(1 - \frac{a}{2R}\right) e^{-2R/a} \quad (60)$$

which is indeed a decreasing function of R and leads to dissociation into two dimers. This energy is plotted as a dotted line in figure III.12 and it gives a good approximation to the exact result as soon as $R \gtrsim 1.5a$. This result is a special case of the one derived for N heavy particles and N light particles by Petrov, Astrakharchik, et al. (2007) (see §4-4).

4-2 Two heavy particles and N light particles

In this section, we consider extending the procedure developed previously to the case where the two heavy particles are immersed in a bath of light particles. We assume that these light particles are polarized fermions and that they are prepared at zero temperature. We wish to determine the type of bath-mediated interaction that occurs between the two heavy particles.

In general, a heavy particle placed in a bath of light particles (bosonic or fermionic) forms a polaron (see Scazza, Zaccanti, et al. (2022) for a recent review). The problem that interests us here can therefore be formulated in terms of the polaron-polaron interaction, in the simple case of a bath of fermions with no interaction [see Fujii, Hongo, et al. (2022) and its references for a discussion of a superfluid bath, i.e. one composed of interacting particles].

To solve the problem we are interested in, namely the zero-temperature state of the bath of polarized fermions, it is necessary to determine the N

first energy levels of the light particles due to the presence of the heavy particles in $\pm R/2$. This problem was treated by Nishida (2009), and we follow his approach here, which is directly inspired by the approach of Beth & Uhlenbeck (1937) to the calculation of the second virial coefficient (the 2022 lecture series, Chapter 1).

The states accessible to light particles are of two types:

- Discrete negative energy state(s): we know that there are one or two in the case $a > 0$ (depending on the value of the ratio R/a) and only one for $a < 0$ or $a = \infty$. We already know these states, obtained by solving (35-36).
- Continuum states: these states have positive energy, they extend over the whole space, and their wave function is “distorted” by the presence of the heavy particles.

Since we already know the two discrete states, let us move on to the continuum states. These are solutions of

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi \quad \Leftrightarrow \quad \nabla^2 \psi + k^2 \psi = 0 \quad \text{with} \quad E = \frac{\hbar^2 k^2}{2m}. \quad (61)$$

We are interested in solutions that are regular everywhere except at $\mathbf{r} = \pm \mathbf{R}/2$ and that satisfy the Bethe–Peierls condition at these two points.

Scattering states for a single center. Let us first recall what is expected for a single scattering center described by the Bethe–Peierls condition and placed at $\mathbf{r} = 0$. We know that scattering occurs only in the s wave, and that the other partial waves are not affected by the scattering center. For any incident wave vector $\mathbf{k}$, the scattering state is of the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + f(k) \frac{e^{ikr}}{r}, \quad (62)$$

which, after projection onto the s wave (i.e. averaging over the angles θ, φ of spherical coordinates), gives

$$\bar{\psi}_{\mathbf{k}}(r) = \frac{e^{ikr} - e^{-ikr}}{2ikr} + f(k) \frac{e^{ikr}}{r}, \quad (63)$$

or equivalently

$$\bar{\psi}_{\mathbf{k}}(r) = -\frac{e^{-ikr}}{2ikr} + \frac{e^{ikr}}{2ikr} e^{2i\delta(k)} \quad (64)$$

where we have introduced the phase shift $\delta(k)$ for s -wave scattering

$$f(k) = \frac{1}{2ik} (e^{2i\delta(k)} - 1) \quad \Leftrightarrow \quad \frac{1}{f(k)} = \frac{k}{\tan \delta(k)} - ik. \quad (65)$$

The form (64) can also be written, up to a global phase factor $e^{i\delta(k)}$ that is unimportant here, as

$$\bar{\psi}_{\mathbf{k}}(r) = \frac{\sin[kr + \delta(k)]}{kr}. \quad (66)$$

Scattering states for two centers. In the case of scattering by two pseudo-potential centers located at $+\mathbf{R}/2$ and $-\mathbf{R}/2$ (i.e. the two particles M , assumed to be fixed), we can look for scattering states in the form

$$\psi_{\mathbf{k},\pm}(\mathbf{r}) = \frac{\sin[k|\mathbf{r} - \mathbf{R}/2| + \delta_{\pm}(k)]}{k|\mathbf{r} - \mathbf{R}/2|} \pm \frac{\sin[k|\mathbf{r} + \mathbf{R}/2| + \delta_{\pm}(k)]}{k|\mathbf{r} + \mathbf{R}/2|} \quad (67)$$

The index $\pm$ denotes here the symmetry of each state under exchange of the centers: $\mathbf{R}/2 \leftrightarrow -\mathbf{R}/2$. Indeed, as in § 2, we can look for the eigenstates of the Hamiltonian in the form of even or odd functions of $\mathbf{r}$, it being understood that the phase shift for an even state, $\delta_+(k)$ (the same for each of the two scattering centers), is *a priori* different from the phase shift for an odd state, $\delta_-(k)$ (again the same for each scattering center).

The Bethe–Peierls condition imposes

$$-\frac{1}{ka} \sin[\delta_{\pm}(k)] = \cos[\delta_{\pm}(k)] \pm \frac{\sin[kR + \delta_{\pm}(k)]}{kR} \quad (68)$$

which can be solved to give

$$\tan[\delta_{\pm}(k)] = -\frac{kR \pm \sin(kR)}{\frac{R}{a} \pm \cos(kR)}. \quad (69)$$

To evaluate the change of the density of states of the light particle induced by the heavy particles, let us suppose that the light particle is contained in a large sphere of radius $R_0 \gg R$, and that its wave function

$\psi_{\mathbf{k},\pm}(\mathbf{r})$ must vanish on the surface of this sphere. Let us use the following expansion in the arguments of the sines appearing in (67)

$$r \gg R : \quad |\mathbf{r} \pm \mathbf{R}/2| \approx r \pm \frac{1}{2} R \cos \theta \quad (70)$$

where θ is the angle between $\mathbf{r}$ and $\mathbf{R}$, and more simply take $|\mathbf{r} \pm \mathbf{R}/2| \approx r$ as the denominator of (67). We then find that the condition that $\psi_{\mathbf{k},\pm}(\mathbf{r})$ vanish at $r = R_0$ is satisfied for all θ if and only if

$$\sin[kR_0 + \delta_+(k)] = 0 \quad \text{or} \quad \cos[kR_0 + \delta_-(k)] = 0 \quad (71)$$

i.e. two sets of possible values for k :

$$\boxed{k_{n,+}R_0 + \delta_{n,+} = n\pi \quad k_{n,-}R_0 + \delta_{n,-} = (n + 1/2)\pi} \quad (72)$$

Recall also that in the absence of a scattering potential, the quantization conditions in a sphere of radius R_0 are $k_n R_0 = n\pi$ [resp. $k_n R_0 = (n + 1/2)\pi$] for waves of even [resp. odd] angular momentum ℓ .

Fermi energy for the light particles. We now study the energy required to fill all the energy levels of the light particles up to a given value $\mu = \hbar^2 k_F^2 / 2m$. The change of energy due to the presence of the two scattering centers is

$$\Delta E(R) = -\frac{\hbar^2}{2m} (\kappa_+^2 + \kappa_-^2) + \frac{\hbar^2}{2m} \sum_{k_F} [(k_{n,+}^2 + k_{n,-}^2) - (k_{n,+}^2 + k_{n,-}^2)_0] \quad (73)$$

Using

$$k_{n,+}^2 = \frac{1}{R_0^2} (n\pi - \delta_{n,+})^2 \approx \left(\frac{n\pi}{R_0}\right)^2 - \frac{2n\pi}{R_0^2} \delta_{n,+} \quad (74)$$

this change of energy can be written as

$$\Delta E(R) = -\frac{\hbar^2}{2m} (\kappa_+^2 + \kappa_-^2) - \frac{\hbar^2}{m\pi} \int_0^{k_F} k [\delta_+(k) + \delta_-(k)] dk. \quad (75)$$

The interaction energy between the two heavy particles is then

$$\boxed{V(R) = \Delta E(R) - \Delta E(+\infty) = -\frac{\hbar^2 k_F^2}{2m} v(k_F R)} \quad (76)$$

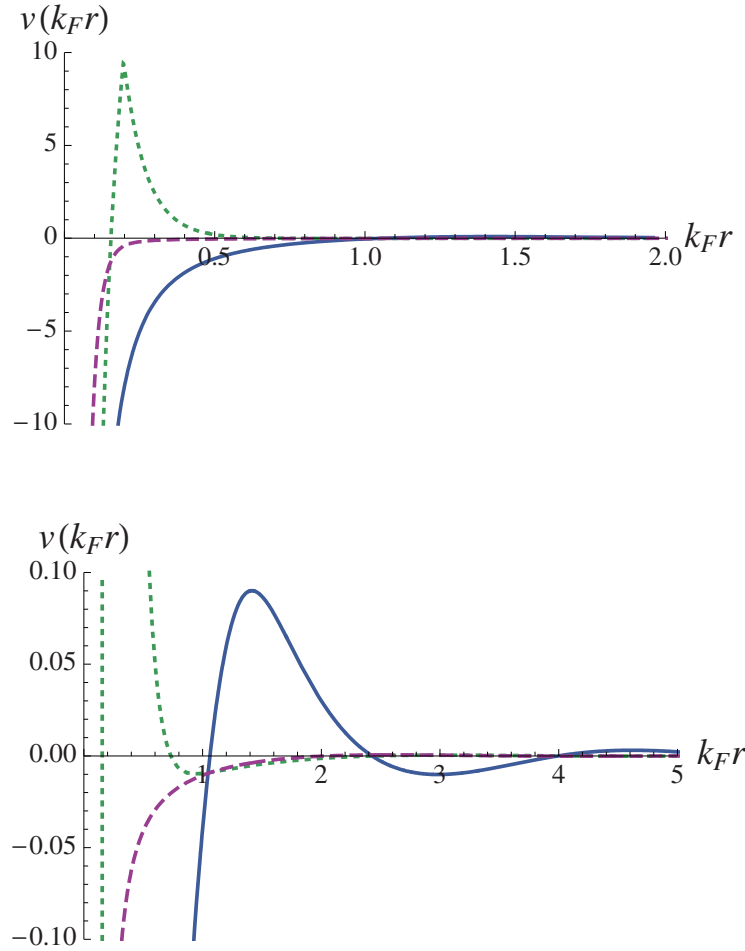


Figure III.13. Effective interaction energy $v(k_F R)$ between two heavy particles immersed in a bath of polarized fermionic particles. Dashed line: $(ak_F)^{-1} = -5$, solid line: unitary regime $(ak_F)^{-1} = 0$, dotted line: $(ak_F)^{-1} = 5$. The lower figure is an enlargement of the upper figure. Figures taken from Nishida (2009).

where the dimensionless quantity $v(k_F R)$ characterizes the physical properties of the problem. This quantity, itself dependent on the dimensionless parameter $k_F a$, is plotted in figure III.13, extracted from Nishida (2009) and has the following characteristics:

- In the unitary regime $a = \infty$, the scale invariance of the three-body problem is broken, since the fermionic bath introduces its own length scale k_F^{-1} . Figure III.13 shows that $v(k_F R)$ exhibits damped oscillations with this characteristic length scale.
- In the regime of positive and relatively small values of a ($k_F a < 1$), the fermionic bath creates a repulsive potential comparable to a hard core at $r \approx a$.
- In the regime of negative and relatively small values of a ($k_F |a| < 1$), the bath creates an essentially attractive potential, which takes significant values for $r \lesssim |a|$. In the limit $a \rightarrow 0_-$, Nishida (2009) shows that one recovers the RKKY (Ruderman–Kittel–Kasuya–Yosida) potential describing the interaction between two magnetic impurities in a Fermi liquid.

This study by Nishida (2009) has recently been taken up by Sun & Cui (2019) with a focus on the case of ^{133}Cs impurities immersed in a ^6Li bath. We will return to this mixture in the next chapter.

4-3 N heavy particles and one light particle

The $mMM \cdots M$ case is also a direct generalization of the formalism set up in § 2. Consider N particles of large mass, held fixed at the points $\mathbf{R}_1, \dots, \mathbf{R}_N$. A light particle of mass m moves within this set of scattering centers, and we look for the possible bound states of this particle. One possible example, studied by Christianen, Cirac, et al. (2022), is that of a ^6Li atom moving in an assembly of ^{133}Cs atoms.

The wave function of the light particle associated with a negative energy E (hence a bound state) can be written as

$$\psi(\mathbf{r}) = \sum_{j=1}^N A_j \frac{e^{-\kappa|\mathbf{r}-\mathbf{R}_j|}}{|\mathbf{r}-\mathbf{R}_j|}, \quad E = -\frac{\hbar^2 \kappa^2}{2m}. \quad (77)$$

This wave function is the generalization of the wave function (27) used in the case $N = 2$. Away from the points $\mathbf{r} = \mathbf{R}_j$, it is a solution of the Schrödinger equation for a free particle of negative energy, $\nabla^2 \psi = \kappa^2 \psi$ and we must now ensure that the Bethe–Peierls boundary condition is satisfied at all points $\mathbf{R}_j$.

Let us take a particular point $\mathbf{R}_i$. The term in $|\mathbf{r} - \mathbf{R}_i|^{-1}$ that appears in (77) when we take the limit $\mathbf{r} \rightarrow \mathbf{R}_i$ is

$$\text{term in } |\mathbf{r} - \mathbf{R}_i|^{-1} : \quad A_i \quad (78)$$

Similarly, the term in $|\mathbf{r} - \mathbf{R}_i|^0$ in this limit $\mathbf{r} \rightarrow \mathbf{R}_i$ is

$$\text{term in } |\mathbf{r} - \mathbf{R}_i|^0 : \quad -\kappa A_i + \sum_{j \neq i} A_j \frac{e^{-\kappa R_{ij}}}{R_{ij}} \quad (79)$$

The Bethe–Peierls condition states that these two terms must be in the ratio $-1/a$, which reads

$$-\frac{1}{a} A_i = -\kappa A_i + \sum_{j \neq i} A_j \frac{e^{-\kappa R_{ij}}}{R_{ij}}. \quad (80)$$

This condition must be satisfied for all indices $i = 1, \dots, N$, which means that the coefficients A_i must satisfy a system of N equations in N unknowns:

$$[\mathcal{M}][A_i] = 0 \quad (81)$$

where $[\mathcal{M}]$ denotes the $N \times N$ matrix defined by

$$\boxed{\mathcal{M}_{ii} = \frac{1}{a} - \kappa \quad i \neq j : \quad \mathcal{M}_{ij} = \frac{e^{-\kappa R_{ij}}}{R_{ij}}} \quad (82)$$

For this system to have a solution other than the trivial one, $A_i = 0$ for all i , the determinant of the matrix $[\mathcal{M}]$ must vanish:

$$\boxed{\det[\mathcal{M}] = 0} \quad (83)$$

which provides, for a given set of positions $\mathbf{R}_j$, a series of possible positive values for κ , and therefore a series of bound states for the light particle.

4-4 Dilute system: recovering a binary potential

We continue our study of the $mMM \cdots M$ case, and in this section we place ourselves in the case $a > 0$, i.e. when there is a bound state between the light particle and a heavy particle. We also assume that the gas of heavy particles is dilute, with an average distance between heavy particles that is larger than a . This case has been studied in detail by Petrov, Astrakharchik, et al. (2007) and we will follow their approach here.

If the heavy particles are infinitely far apart, the ground level of the light particle is N -fold degenerate and has energy $E_0 = -\hbar^2/2ma^2$, i.e. $\kappa = 1/a$. The light particle can in fact bind to one of the N heavy particles, without the $N - 1$ remaining particles playing a role.

Let us now take into account in a perturbative way the possible coupling between the effects of these heavy particles. The N -fold degeneracy of the energy level E_0 is lifted, and we obtain a series of N energy states around E_0 . Let us introduce $x \equiv \frac{1}{a} - \kappa$, which we treat as a small parameter. This variable appears directly in the N diagonal coefficients of the matrix $[\mathcal{M}]$. Moreover, the off-diagonal coefficients of this matrix can be expanded in the form

$$i \neq j : \quad \mathcal{M}_{ij} = \frac{e^{-\kappa R_{ij}}}{R_{ij}} \approx G_{ij} + x H_{ij}, \quad (84)$$

where

$$G_{ij} = \frac{e^{-R_{ij}/a}}{R_{ij}}, \quad H_{ij} = e^{-R_{ij}/a}. \quad (85)$$

These coefficients G_{ij} and H_{ij} are exponentially small when the average distance between heavy particles becomes greater than a . The determinant of the matrix $[\mathcal{M}]$ can therefore be expanded as a polynomial in the variable

x , in which we keep only the dominant terms, using $G_{ij}, H_{ij} \ll x \ll 1$:

$$0 = \det[\mathcal{M}] = \begin{vmatrix} x & \cdots & G_{ij} + xH_{ij} & \cdots \\ \vdots & x & & \vdots \\ \cdots & G_{ij} + xH_{ij} & \cdots & x \end{vmatrix} \quad (86)$$

$$\approx x^N - \frac{1}{2}x^{N-2} \sum'_{i,j} (G_{ij} + xH_{ij})^2 \quad (87)$$

$$\approx x^N - x^{N-1} \sum'_{i,j} G_{ij}H_{ij} - \frac{1}{2}x^{N-2} \sum'_{i,j} G_{ij}^2 \quad (88)$$

where the sums run over all pairs (i, j) excluding the case $i = j$ (this is the meaning of the prime on the summation sign). The factor $\frac{1}{2}$ avoids double-counting of (i, j) and (j, i) . The neglected terms¹ involve higher powers of $e^{-R_{ij}/a}$. We thus obtain N values of x , and therefore of κ , which we denote by x_α and κ_α ($\alpha = 1, \dots, N$).

Now suppose we have N light particles, treated as polarized fermions, i.e. $m \cdots m M \cdots M$. The ground state of the $N + N$ particle system is obtained by arranging the N light particles in the N states we have just identified, and we are interested in the energy of this ground state:

$$E = - \sum_{\alpha=1}^N \frac{\hbar^2 \kappa_\alpha^2}{2m} = - \frac{\hbar^2}{2m} \left(\frac{N}{a^2} - \frac{2}{a} \sum_{\alpha} x_\alpha + \sum_{\alpha} x_\alpha^2 \right) \quad (89)$$

This quantity can be evaluated from the well-known relations giving the sums of the roots of a polynomial of degree N . From (88), we find:

$$\sum_{\alpha} x_\alpha = \sum'_{i,j} G_{ij}H_{ij} \quad \sum_{\alpha,\beta} x_\alpha x_\beta = - \sum'_{i,j} G_{ij}^2 \quad (90)$$

from which we deduce

$$\sum_{\alpha} x_\alpha^2 = \sum'_{i,j} G_{ij}^2 + \left(\sum'_{i,j} G_{ij}H_{ij} \right)^2 \quad (91)$$

¹In particular, we neglect terms such as $e^{-R_{ij}/a} e^{-R_{jk}/a}$, which are only significant if the three heavy particles i, j, k are within a neighborhood of size a .

where the second term on the right-hand side is exponentially smaller than the first.

We then arrive at the energy of the ground state of N light particles:

$$E \approx E_0 + \frac{1}{2} \sum'_{i,j} U(R_{ij}) \quad \text{with} \quad E_0 = -N \frac{\hbar^2}{2ma^2} \quad (92)$$

where the binary potential $U(R)$ is identical to that appearing in (60):

$$U(R) = \frac{2\hbar^2}{maR} \left(1 - \frac{a}{2R} \right) e^{-2R/a} \quad (93)$$

This is a repulsive potential between the heavy particles, the energy being minimized by placing the mM dimers infinitely far apart.

In conclusion, while the $mM \cdots M$ case can give rise to a collective bound state by lowering the energy with respect to mM (with the $N - 1$ other M particles held fixed at infinity), this is not the case if we try to put as many light particles as heavy particles. The Pauli principle forces some of the m particles into antibonding orbitals, which destabilizes the $N + N$ structure. An interesting question, but beyond the scope of this course, concerns the general case $N_m + N_M$, addressed for example by Givois, Tononi, et al. (2022), who predict the formation of density waves in a one-dimensional model.

Chapter IV

The Efimov effect for a light–heavy–heavy system

In this chapter, we continue our study of the three-body problem, composed of two heavy particles of mass M and one light particle of mass m (figure IV.1). As in the previous chapter, we assume that the heavy particles do not interact with each other, apart from a hard-core potential that prevents them from approaching closer than R_0 . The mM interaction is described by the Bethe–Peierls boundary condition for a scattering length a , which can be positive, negative, or infinite for the resonant case.

In the previous chapter, we assumed that the heavy particles were at rest at $\pm \mathbf{R}/2$, and we determined the possible energy states of the light particle, in particular its ground-state energy $E(R) \leq 0$. We now turn to the dynamics of the heavy particles, using the Born–Oppenheimer approximation (Efimov 1973; Fonseca, Redish, et al. 1979); this means that we consider that these two heavy particles evolve in the effective potential:

$$V(R) = E(R) \quad \text{if } R > R_0 \quad (1)$$

$$V(R) = +\infty \quad \text{if } R < R_0 \quad (2)$$

where the hard core at R_0 (with $R_0 \ll |a|$) prevents the “fall to the center” that can occur for a $1/R^2$ potential (see Chapters 1 and 2). We will now see that the two heavy particles can bind to each other thanks to the exchange of the light particle: the fact that this light particle can jump from one heavy atom to the other creates an effective attractive interaction between these two heavy atoms.

The Born–Oppenheimer approximation is based on the inequality $m \ll M$, which means that the time scale associated with the motion of the light

particle is much shorter than that associated with the heavy atoms. This ensures that the light particle follows the motion of the heavy particles adiabatically. Compared with the standard adiabatic approximation, in the Born–Oppenheimer approximation we make the additional assumption that we can neglect the role of the scalar and vector geometric potentials (the latter being at the origin of the Berry phase). We will return to the role of these potentials in Chapter 6, when we analyze the origin of the “three-body parameter”, which generalizes the notion of hard core when the three particles are identical.

Let us recall the main results of the previous chapter concerning the energy $E(R)$ of the ground state of the light particle, depending on the value of the scattering length a (figure IV.2):

- In the case $a = \pm\infty$, the energy $E(R)$ varies as $1/R^2$, with a coefficient that involves the root of the transcendental equation $x = e^{-x}$. This root is denoted by $\Omega \approx 0.567\,143$, and we found

$$a = \pm\infty : \quad E(R) = -\frac{\hbar^2 \Omega^2}{2mR^2}. \quad (3)$$

- For a scattering length $a < 0$, the energy $E(R)$ is strictly zero for $R \geq |a|$. Below this value, it is given by

$$a < 0, \quad R < |a| : \quad E(R) = -\frac{\hbar^2}{2m} \left[\frac{1}{|a|} - \frac{W(e^{R/|a|})}{R} \right]^2 \quad (4)$$

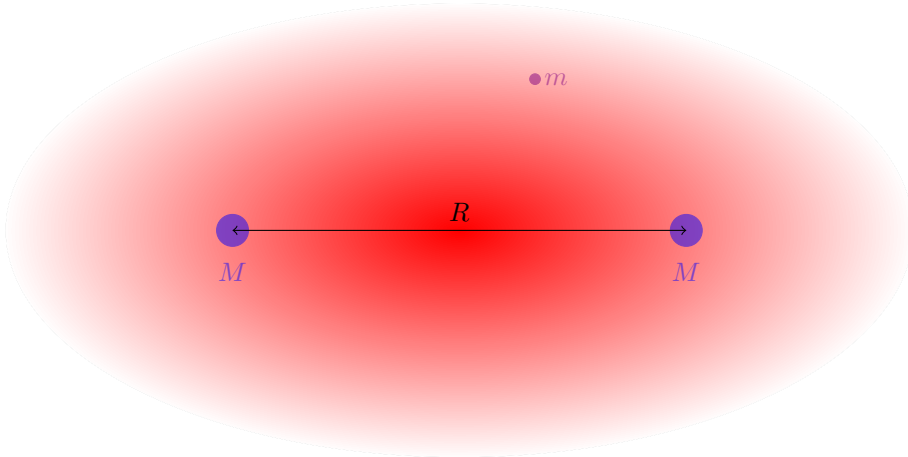


Figure IV.1. The mMM problem studied in this chapter. The MM interaction is assumed to be entirely due to the presence of the light particle, apart from a hard-core interaction that prevents the two heavy particles from approaching closer than R_0 .

where $W(x)$ is the Lambert function, solution of $We^W = x$. Recall that there is no mM bound dimer in this case for an mM interaction described by the pseudo-potential (i.e. by the Bethe–Peierls boundary condition).

- For a scattering length $a > 0$, we have shown for the bonding orbital that

$$a > 0 : \quad E(R) = -\frac{\hbar^2}{2m} \left[\frac{1}{a} + \frac{W(e^{-R/a})}{R} \right]^2. \quad (5)$$

In particular, for $R \rightarrow +\infty$, we find the energy of the bound dimer mM :

$$E_{\text{dim}} = -\frac{\hbar^2}{2ma^2}. \quad (6)$$

Recall that the condition $m \ll M$ implies that the reduced mass of the system mM is close to m .

To analyze the motion of the two bodies of mass M , we place ourselves as always in the reference frame of their center of mass and we are inter-

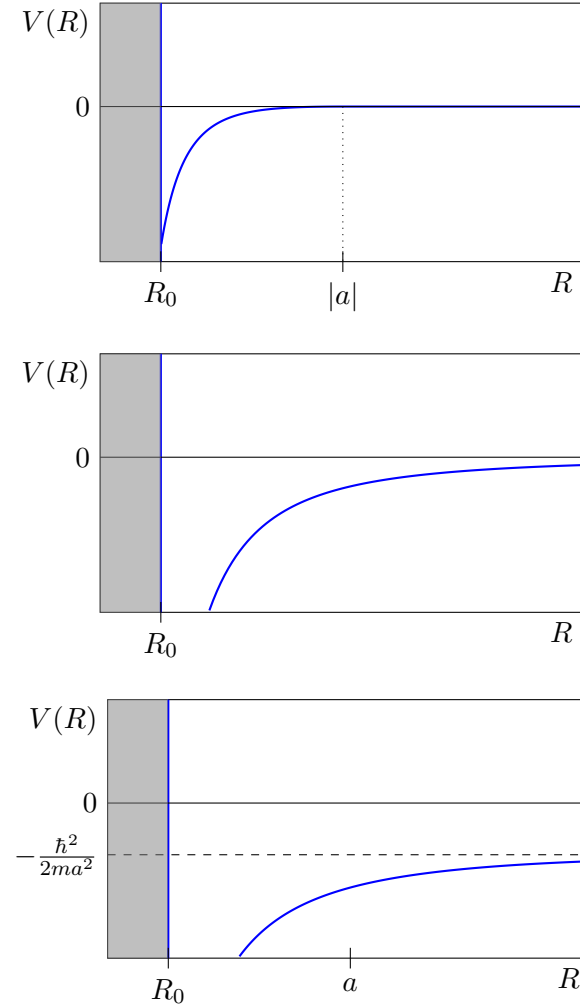


Figure IV.2. The three possible cases for the effective potential $V(R)$ generated between the two heavy particles by exchange of the light particle [Eqs. (1-2)]. Top: case $a < 0$, for which $V(R)$ is strictly zero for $R > |a|$ [Eq. (4)]. Middle: resonant case $a = \pm\infty$ leading to $V(R) \propto 1/R^2$ outside the hard core [Eq. (3)]. Bottom: case $a > 0$, for which the bound dimer mM of energy $-\hbar^2/2ma^2$ exists [Eq. (5)].

ested in the dynamics of the relative particle of coordinates $\mathbf{R}$, of reduced mass $M/2$, and subjected to the potential $V(R)$ defined in (1-2). Since this potential is rotationally invariant, we look for an eigenbasis common to the Hamiltonian, $\hat{L}^2$ and $\hat{L}_z$. The angular part is given by a spherical harmonic, and the Schrödinger equation for the reduced radial wave function $u(R) = R\psi(R)$ reads, for a given scattering length a ,

$$-\frac{\hbar^2}{M}u''(R) + \left(V(R) + \frac{\hbar^2\ell(\ell+1)}{MR^2}\right)u(R) = \mathcal{E}u(R). \quad (7)$$

We are now going to look at possible bound states, with energy $\mathcal{E} < 0$. Recall that if the heavy particles are polarized bosons (resp. fermions), only even ℓ (resp. odd) channels are allowed. If these particles are distinguishable, by their spin state for example, there is no constraint on ℓ .

In practice, since we are mainly interested in the ground state of the system (with M/m and a fixed), we will concentrate on the $\ell = 0$ states for bosons and $\ell = 1$ for polarized fermions, the other angular momentum channels corresponding to significantly higher energies.

1 The Efimov effect for $a = \infty$

1-1 The Thomas collapse

The article by Thomas (1935) is one of the very first applications of quantum physics to the three-body problem, in this case in a nuclear physics context. Thomas was interested in the stability of the tritium nucleus (one proton, two neutrons) and showed that the ground-state energy of this system could not be written solely in terms of the p - n scattering length, but had necessarily to involve the finite range of the nuclear forces.

We will not reproduce here the whole of Thomas's argument, which is relatively involved. We will restrict ourselves to the case of two heavy particles of mass M , assumed to be spinless bosons and not interacting with each other. The light particle of mass m interacts resonantly with each heavy particle.

As already mentioned, a simple way of describing the quasi-resonant interaction between two particles (in this case mM) is to take a square po-

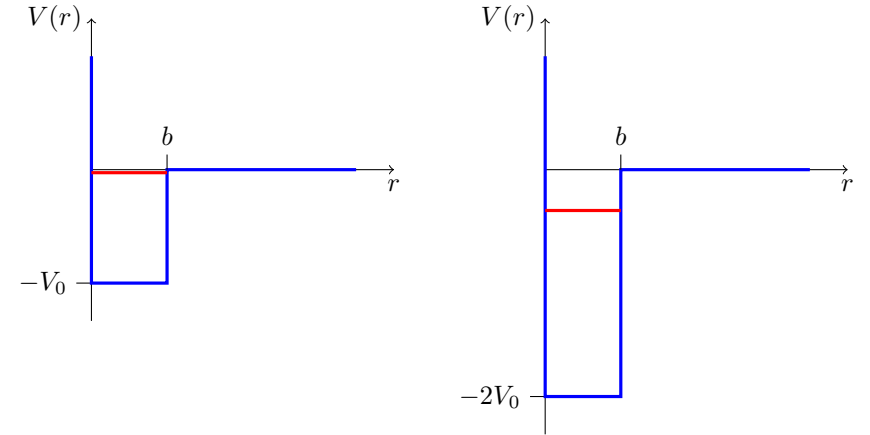


Figure IV.3. Left: square potential well at the threshold for the appearance of the first bound state, with $k_0b \approx \pi/2$, $k_0 = \sqrt{2mV_0}/\hbar$. Right: potential well with the same range b , but twice the depth. This well admits a bound state of energy $\propto V_0$.

tential well $V(r)$ of depth V_0 and range b , and place it in the vicinity of the threshold for the appearance of the first bound state:

$$k_0b \approx \frac{\pi}{2} \quad \text{with} \quad k_0 = \sqrt{2mV_0}/\hbar. \quad (8)$$

The limit of a potential of zero range and fixed scattering length (Bethe-Peierls boundary condition) is then obtained by taking $b \rightarrow 0$ and $(V_0, k_0) \rightarrow \infty$ while maintaining

$$a = b - \frac{\tan(k_0b)}{k_0} \quad (9)$$

constant (the 2021 lecture series, Chapter 3, §3.1). Recall once again that $m \ll M$, which means that the reduced mass of the pair mM is approximately equal to m (this was not the case for the problem considered by Thomas).

If we place the two heavy particles at the same point in space (this is possible because we have assumed that they do not interact, so we forget

about the hard core at R_0 for a moment), the potential felt by the light particle is doubled: $V(r) \rightarrow 2V(r)$, i.e. a potential with range b and depth $2V_0$. This potential then admits a bound state of energy proportional to $-V_0$ (in fact $\approx -0.36 V_0$, figure IV.3), so that its energy tends to $-\infty$ when we take the limit of a zero-range potential: this is the result obtained by Thomas.

We therefore need to take into account the range of the potential (or some other “three-body parameter”) if the problem is not to be singular. In what follows, the radius R_0 of the hard-core potential between the two heavy particles will play this role.

1-2 The case of bosons: s wave

We now return to the three-body problem described in the Born–Oppenheimer approximation, concentrating here on the most “spectacular” case, where the scattering length a is infinite, i.e. where the bound state of the dimer mM is about to appear.

In this case, the potential $V(R)$ to be taken into account was given in (3). It is attractive and varies as $1/R^2$ at all length scales. For a channel with non-zero angular momentum, we must add the centrifugal potential $V_{\text{centrif}}(R) = \hbar^2 \ell(\ell+1)/MR^2$ [cf. (7)]. Using the notation of Chapters 1 and 2 with $g = -\hbar^2 \Omega^2/2m$, the total potential is:

$$R > R_0 : \quad V_{\text{tot}}(R) = V(R) + V_{\text{centrif}}(R) = \alpha \frac{\hbar^2}{MR^2} \quad (10)$$

with

$$\alpha = -\frac{M}{2m} \Omega^2 + \ell(\ell+1) \quad (11)$$

Since this potential varies as $1/R^2$ out to arbitrarily large distances, we can carry over the conclusions of Chapter 2 unchanged:

- A negative energy state can exist in the ℓ angular momentum channel if $\alpha < -1/4$, i.e.:

$$\text{Bound state if: } \frac{M}{2m} \Omega^2 > \ell(\ell+1) + \frac{1}{4} = \left(\ell + \frac{1}{2}\right)^2. \quad (12)$$

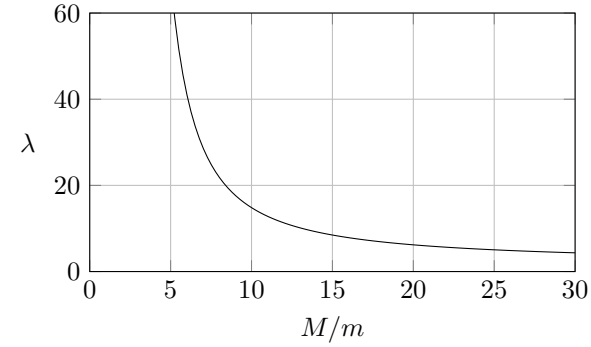


Figure IV.4. Variation of the scale parameter with the mass ratio M/m , calculated in the Born–Oppenheimer approximation. For a comparison with the exact result, see for example Petrov (2012).

Let us look at the $\ell = 0$ channel, which leads to the lowest possible energy states. Using $\Omega^2 \approx 0.322$, this condition becomes $M/m > 1.6$, which is obviously satisfied here since we have assumed $M \gg m$ to use the Born–Oppenheimer approach. There is therefore always at least one three-body bound state in the case of heavy bosonic particles.

- The regularization of $V(R)$ at short distances is ensured by the assumption of a hard-core potential of radius R_0 between the two heavy particles. In what follows, we will take R_0 to be of the order of the van der Waals radius R_{vdW} . In reality, the two heavy atoms can approach each other more closely than this, but the physics involved then goes beyond the universality we are trying to describe here by modeling the mM interactions by the pseudo-potential.
- Once this regularization has been carried out, we can determine the ground state of the motion of the two heavy particles. Above this ground state, we find infinitely many bound states whose energies form, to a good approximation (the better the closer we get to the dissociation limit), a geometric sequence of common ratio $1/\lambda^2$ with (for

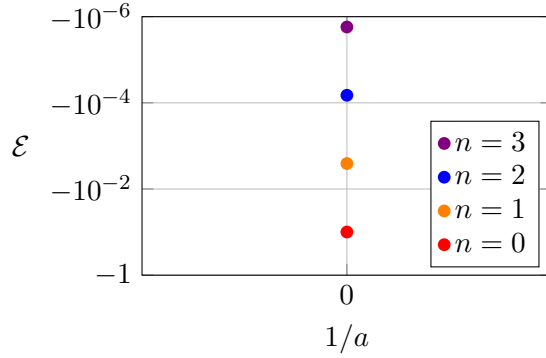


Figure IV.5. Resonant case: numerical calculation of the energies $\mathcal{E}$ of the first bound states of the mMM trimer using Eq. (7). Here we take $a = \infty$ and $M/m = 20$, corresponding approximately to the ratio $M(^{133}\text{Cs})/m(^6\text{Li}) = 22.2$. The energies (expressed in units of $\hbar^2/MR_0^2$) form, to a very good approximation, a geometric sequence of common ratio $e^{-2\pi/|s_0|} \approx 1/38$ ($|s_0| \approx 1.7$).

$\ell = 0$)

$$\lambda = e^{\pi/|s_0|} \quad \text{with} \quad s_0 = \left(\alpha + \frac{1}{4}\right)^{1/2} \in i\mathbb{R} \quad (13)$$

or

$$\lambda = e^{\pi/|s_0|} \quad \text{with} \quad |s_0| = \left(\frac{M}{2m}\Omega^2 - \frac{1}{4}\right)^{1/2} \quad (14)$$

The variation of the scaling parameter λ with M/m is plotted in figure IV.4.

This brings us to the conclusion initially reached by Efimov: while the two-body potential admits no bound states ($a = \infty$), it is possible to produce infinitely many three-body bound states, these states being connected to one another by scale invariance. We have plotted in figure IV.5 the positions of the first four bound states in the case $M/m = 20$, $\ell = 0$, corresponding approximately to the situation encountered experimentally for a mixture of ^6Li and ^{133}Cs . The scaling law $\mathcal{E}_n/\mathcal{E}_{n+1} \approx e^{2\pi/|s_0|} \approx 38$ with $|s_0| \approx 1.7$ for this mass ratio M/m is well satisfied.

1-3 The three-body parameter R_0

Above we introduced the length R_0 , which we equated to a hard core preventing the two heavy particles from approaching arbitrarily close to each other. The introduction of such a parameter is necessary in the three-body problem to ensure the regularity of the solution.

This additional parameter, beyond the two-body scattering length, is generically called the *three-body parameter*. We will retain this name here, even though in the case we are interested in, it is more a property of the MM binary system. The precise determination of this parameter for the mMM case was carried out by Wang, Wang, et al. (2012), using Lennard-Jones potentials to model the mM and MM interactions. These authors derived a universal law for this parameter by relating it to the van der Waals radius R_{vdW} of the MM interaction [see also the article by Zhao, Han, et al. (2019), which proposes a simple result in the case of a resonance in a_{MM}]. We will return to the physical origin of this universality in Chapter 6, considering the case of three identical particles.

1-4 The case of polarized fermions: p -wave

For polarized fermions, the quantum number ℓ associated with the angular momentum can only take odd values. The lowest-energy state is obtained for the channel $\ell = 1$, and the condition (12) then reads $\frac{M}{2m}\Omega^2 > \frac{9}{4}$, or equivalently

$$p\text{-wave polarized fermions:} \quad \frac{M}{m} > 14.0 \quad (15)$$

This is a strong constraint that considerably reduces the choice of atomic species that can be used. A possible candidate triplet is ^{171}Yb – ^{171}Yb – ^6Li leading to $M/m = 28.5$ (Khranov, Hansen, et al. 2014). Note that we obtained the result (15) analytically using the Born–Oppenheimer approximation. An exact numerical treatment, of the type we will discuss in the next chapter, leads to a very similar limit: $M/m = 13.606\,966$ (Kartavtsev & Malykh 2007).

The other angular momentum channels $\ell \geq 3$ cannot be used in practice, unless the mass of an atomic species is artificially modified by confining it

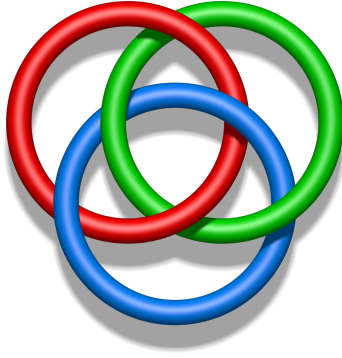


Figure IV.6. Borromean rings: these three rings cannot be separated by continuous deformation, but opening one of the circles frees the other two as well (figure: Wikipedia).

in an optical lattice, for example.

2 Around the resonance: $a < 0$ or $a > 0$

2-1 The case $a < 0$ and Borromean states

We now turn to the case where the scattering length characterizing the mM interaction is negative. In the pseudo-potential model, this means that, although attractive, this interaction is too weak to bind the mM dimer. We will now see that if $|a|$ is large enough, i.e. if $1/a$ is not too far from 0, we can still observe bound states of the trimer, i.e. three-body states with negative $\mathcal{E}$ energy.

This situation is often referred to as Borromean, by analogy with the rings shown in figure IV.6. The three particles taken together can form a stable structure, but no pair of two particles can form a bound state.

To simplify the analysis, we will concentrate in what follows on the case of bosons, limiting ourselves to the channel of angular momentum $\ell = 0$. In the introduction we recalled the potential $V(R)$ in this case [cf. (4)] and this

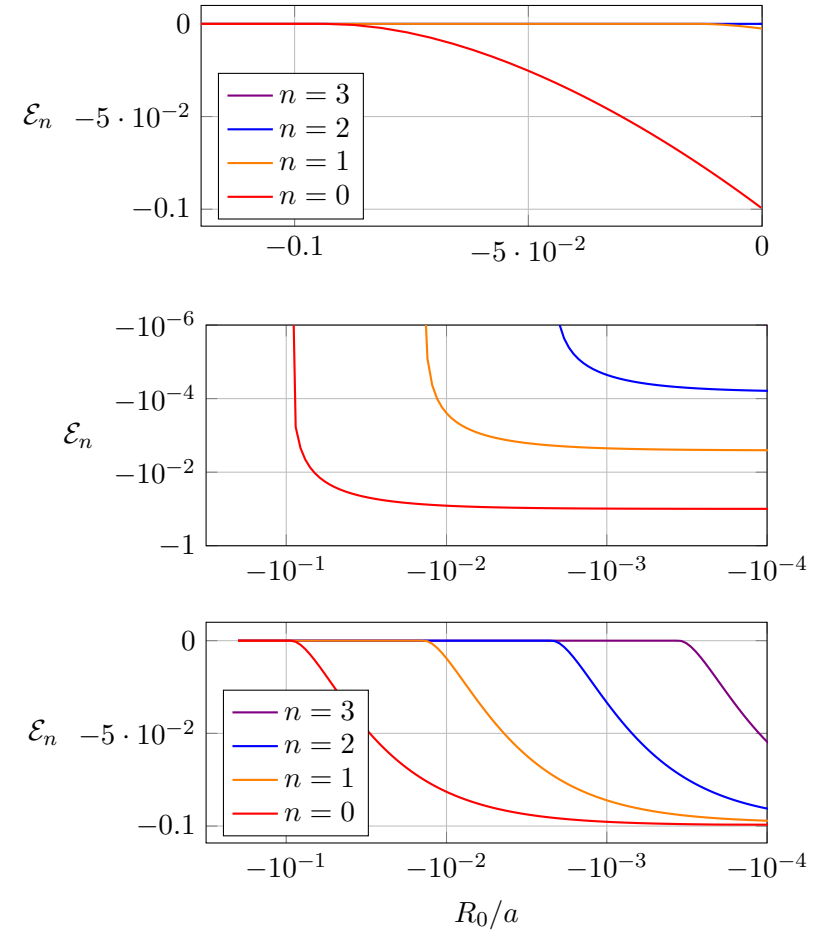


Figure IV.7. Borromean case ($a < 0$): variation of the energies $\mathcal{E}_n(a)$ of the first bound states of the trimer mM as a function of the scattering length a , assumed here to be negative, for $M/m = 20$. The same data are plotted in lin-lin (top), log-log (middle) and semi-log (bottom) coordinates. Energies are expressed in units of $\hbar^2/MR_0^2$. To improve the readability of the lower plot, the energy of level n has been multiplied by λ^{2n} with $\lambda = e^{\pi/|s_0|} \approx 6.2$.

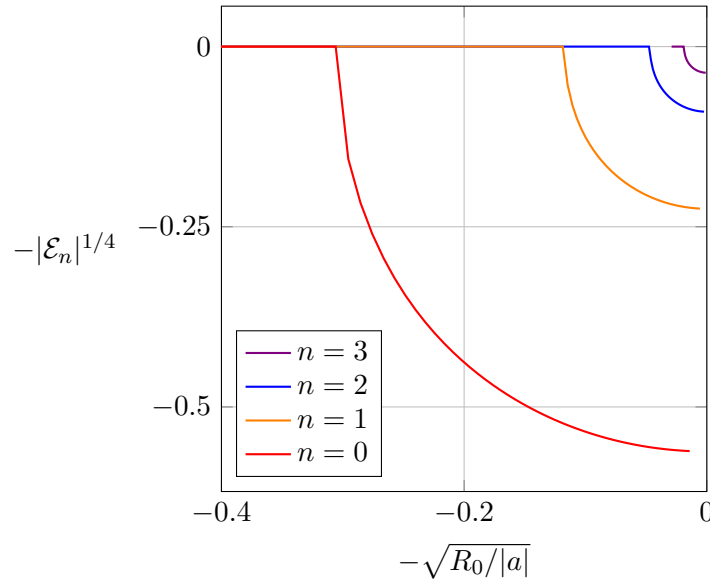


Figure IV.8. Borromean case ($a < 0$): variation of $|\mathcal{E}_n|^{1/4}$ with $\sqrt{R_0/|a|}$ for $M/m = 20$. The energy is expressed in units of $\hbar^2/MR_0^2$.

potential is plotted in figure IV.2. Figure IV.7 shows the result of a numerical search for the eigenstates u_n and associated eigenenergies $\mathcal{E}_n$ of the radial Schrödinger equation (7) for angular momentum $\ell = 0$ and $M/m = 20$.

More precisely, we plot in linear or logarithmic coordinates the variation with $1/a$ of the energy of the ground level $n = 0$ and of the first three excited states $n = 1, 2, 3$. One conclusion that is immediately apparent from this figure is that the mMM trimer is not always stable. For $R_0/a < -0.093$, i.e. $|a| < 10.8 R_0$, there are no mMM bound states. The first bound state $n = 0$ appears for $a \approx -10.8 R_0$ and remains the only solution until $a \approx -72.5 R_0$, for which value a first excited bound state ($n = 1$) also appears. A second excited state appears for $a \approx -455 R_0$ and so on. The closer we get to the resonant limit $|a| = +\infty$, the greater the number of bound states. Rather than the energy, we may prefer to plot the wave number $\kappa = \sqrt{M|\mathcal{E}|/\hbar}$ as a function of R_0/a , which is done in figure IV.8 (in fact $\sqrt{\kappa} \propto |\mathcal{E}|^{1/4}$ is plotted

as a function of $\sqrt{1/a}$, in order to compress the curves a little further and to distinguish the various branches more clearly).

Careful examination of figure IV.7 reveals a scaling law (homothety) for various quantities. For example, we find the scaling law $\mathcal{E}_{n-1}/\mathcal{E}_n \approx 38$ when $|a| \rightarrow \infty$, already obtained in the previous section for this value of M/m . We also observe a homothety on the critical values $a_-^{(n)}$ at which the different bound states appear, with $a_-^{(n)}/a_-^{(n-1)} \approx 6.2$. We will now account for these scaling symmetries and show the general result:

$$\mathcal{E}_{n-1}(a) = \lambda^2 \mathcal{E}_n(\lambda a) \quad \text{with} \quad \lambda = e^{\pi/|s_0|} \quad (16)$$

The two homotheties mentioned above can be deduced by taking the special cases $|a| = +\infty$ for the first, and $\mathcal{E}_n = 0$ for the second (recall that for the mass ratio M/m chosen for figure IV.7, we have $|s_0| \approx 1.72$ and $\lambda \approx 6.2$).

We will now explain the origin of these two homotheties. The arguments used are similar to those developed in Chapter 2, but they require a slight adjustment because the potential is not proportional to $1/R^2$ up to $R = \infty$.

To progress, we first note that in the domain $x = R/|a| \ll 1$, the Lambert function is $W(e^{R/|a|}) \approx W(1) = \Omega$ and the expression¹ of $E(R; a)$ simplifies to

$$R_0 < R \ll |a| : \quad E(R; a) \approx -\Omega^2 \frac{\hbar^2}{2mR^2}. \quad (17)$$

In this domain, we find essentially the same potential as for $|a| = \infty$. The strongly bound mMM states in this potential, i.e. those such that $|\mathcal{E}| \gg \hbar^2/ma^2$, are not much affected by the cutoff of the potential for $R > |a|$. On the other hand, all the weakly bound states of the resonant case, of energy $|\mathcal{E}| \lesssim \hbar^2/ma^2$, are expected to disappear as a result of this cutoff. We therefore understand that a finite number of mMM bound states remain (instead of the infinite number of states found for $|a| = +\infty$).

Recall also that the reduced radial wave function $u_n(R)$ of every state vanishes at $R = R_0 \ll |a|$. From what we saw in Chapter 2, we know that

¹We write explicitly the dependence of the quantities E , V , u_n on the scattering length a , because this dependence will play an important role in what follows.

for a sufficiently excited state (in practice $n = 2$ or 3 is enough), this wave function also vanishes at the point $R \approx \lambda R_0$ with $\lambda = e^{\pi/|s_0|}$, provided that this point itself remains well below $|a|$.

We can then carry out the following reasoning. Let us start from the n th eigenstate (with $n > 0$) for the scattering length a , whose reduced radial wave function u_n satisfies the Schrödinger equation for $\ell = 0$:

$$\left[-\frac{\hbar^2}{M} \frac{d^2}{dR^2} + V(R; a) \right] u_n(R; a) = \mathcal{E}_n(a) u_n(R; a). \quad (18)$$

Let us consider the eigenvalue problem for the scattering length a/λ and look at the function

$$\begin{aligned} R > R_0 &: & v(R) &= u_n(\lambda R; a), \\ R < R_0 &: & v(R) &= 0. \end{aligned} \quad (19)$$

As we pointed out, this function vanishes at R_0 , since u_n has a node (approximately) at λR_0 : it is therefore admissible as a wave function for our problem; more precisely, if $u_n(R; a)$ has n nodes in the interval $]R_0, +\infty[$, the function $v(R)$ will have $n - 1$ nodes on this same interval. Furthermore, using the property of the potential $V(R; a)$ deduced from the expression (4) involving the Lambert function $W(e^{R/|a|})$:

$$R > R_0: \quad V(\lambda R; a) = \frac{1}{\lambda^2} V\left(R; \frac{a}{\lambda}\right), \quad (20)$$

we see that $v(R)$ satisfies the eigenvalue equation:

$$\left[-\frac{\hbar^2}{M} \frac{d^2}{dR^2} + V\left(R; \frac{a}{\lambda}\right) \right] v(R) = \lambda^2 \mathcal{E}_n(a) v(R). \quad (21)$$

The function $v(R)$ is therefore a solution of the radial Schrödinger equation for the scattering length a/λ with the eigenvalue $\lambda^2 \mathcal{E}_n(a)$ and it satisfies the boundary condition $v(R_0) = 0$. Since this function has $n - 1$ nodes on the interval $]R_0, +\infty[$, we deduce that it is equal to $u_{n-1}(R; a/\lambda)$ (up to a multiplicative constant) and that we have the relation between the eigenenergies:

$$\mathcal{E}_{n-1}(a/\lambda) = \lambda^2 \mathcal{E}_n(a), \quad (22)$$

which is the result announced in (16).

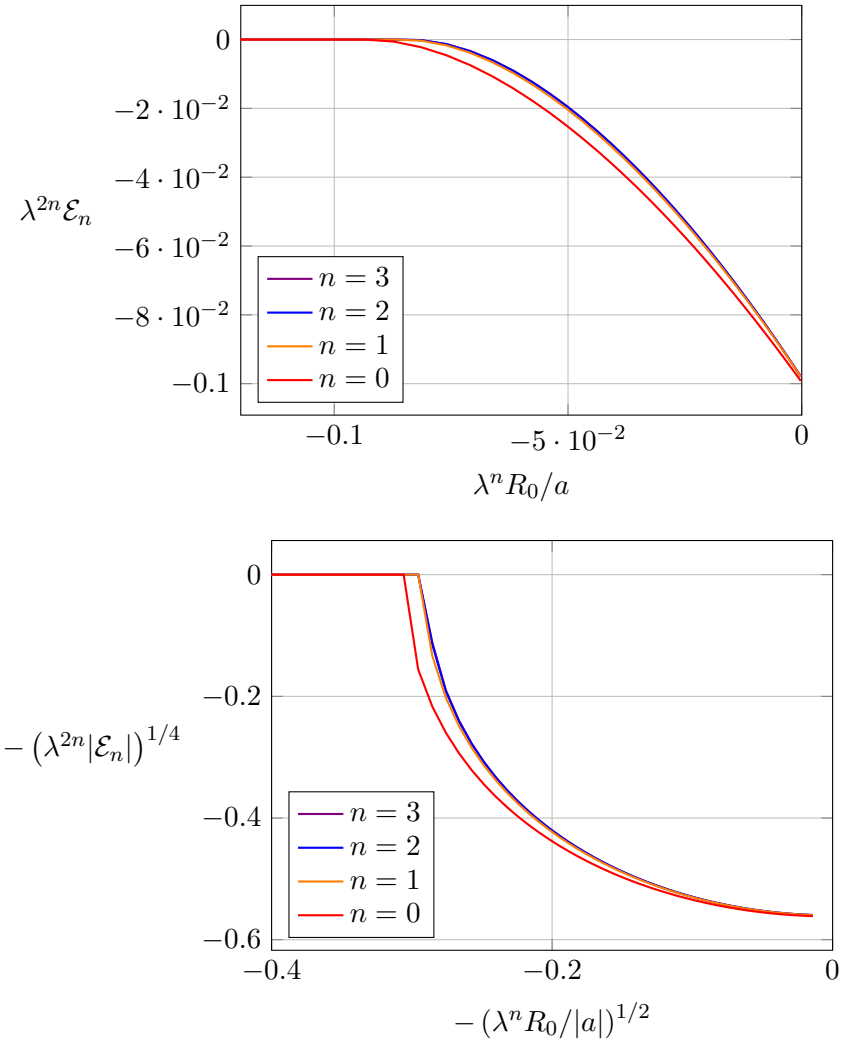


Figure IV.9. Checking the scaling law (16) for scattering lengths $a < 0$. The calculation is made for $M/m = 20$ and the energies are expressed in units of $\hbar^2 / M R_0^2$.

To check this scaling law, we have taken the energies $\mathcal{E}_n(a)$ already shown in figure IV.7 and replotted them in figure IV.9 in the form $[x = \lambda^n R_0/a, y = \lambda^{2n} \mathcal{E}_n(a)]$. This law is remarkably well satisfied: the curves for $n = 2$ and $n = 3$ are almost indistinguishable, and the $n = 1$ curve is very close to them. Only the ground state $n = 0$ shows a noticeable difference, but, as we pointed out above, we did not expect the scaling law to hold accurately for it.

An immediate consequence of this scaling law concerns the points of appearance $a_-^{(n)}$ of the trimers, at which $\mathcal{E}_n$ vanishes. We find the scaling law

$$a_-^{(n)} = \lambda a_-^{(n-1)}, \quad (23)$$

a relation that we anticipated in figure IV.7. We shall see that this relation can be tested experimentally and is a strong signature of the universality of Efimov physics.

2-2 The case $a > 0$ and dimer-trimer competition

We now turn to the branch $a > 0$ for which we know that there is a bound state of the dimer mM , with energy $E_{\text{dim}} = -\hbar^2/2ma^2$. For a three-body bound state to be stable, it is therefore not enough for its energy to be negative, contrary to what we used for $a < 0$. Its energy must be lower than E_{dim} ; otherwise it is energetically preferable to break up the trimer into an mM dimer on the one hand and an M particle at rest far from the dimer on the other.

To analyze the problem of the formation of a three-body bound state mMM in the Born–Oppenheimer approximation, we can follow an approach very similar to that used for $a < 0$. To begin with, we note that the mM interaction potential given in (5) can always be put into the form:

$$R < R_0 : V(R) = +\infty \quad (24)$$

$$R_0 < R : V(R) = -\frac{\hbar^2}{2mR^2} \mathcal{F}(R/a) \quad (25)$$

with

$$\mathcal{F}(x) = [W(e^{-x}) + x]^2. \quad (26)$$

When $R \rightarrow +\infty$, the potential $V(R)$ (plotted in figure IV.2) tends to E_{dim} . This means that the bound trimer, in order to be the ground state of the three-body system, must have an energy lower than E_{dim} . Furthermore, the difference $V(R) - E_{\text{dim}}$ varies as $e^{-R/a}$ as R increases, so that the potential able to bind the dimer is of finite range, of the order of a : we know immediately that there can be only a finite number of bound states in such a potential.

The result of the numerical search for mMM bound states in the Born–Oppenheimer approximation is shown in figure IV.10. It confirms the existence of a finite (or zero) number of states for any value of $a > 0$. For $a = 100 R_0$ for example, we find four bound states ($n = 0, 1, 2, 3$), of energy $\mathcal{E}_n < E_{\text{dim}}$. This means that if we had prepared a trimer in an energy state $\mathcal{E}_n$ with $n > 3$ at the point $|a| = +\infty$, and then adiabatically reduced a to the value $100 R_0$, this trimer would have dissociated to give an mM dimer and a free M atom.

To interpret the results shown in figure IV.10, we note that the demonstration of the scaling law (16),

$$\mathcal{E}_{n-1}(a) = \lambda^2 \mathcal{E}_n(\lambda a) \quad \text{for } n \text{ large enough}, \quad (27)$$

given in the case $a < 0$ in §2-1 remains valid in the case $a > 0$ since the generic form (24,25) of the potential is unchanged. In fact, since the relevant quantity here is the difference between $\mathcal{E}_n$ and the energy of the dimer, we will rewrite this law in the form:

$$\boxed{\mathcal{E}_{n-1}(a) - E_{\text{dim}}(a) = \lambda^2 [\mathcal{E}_n(\lambda a) - E_{\text{dim}}(\lambda a)] \quad \text{for } n \text{ large enough}} \quad (28)$$

This rewriting is possible because $E_{\text{dim}}(a) \propto 1/a^2$ in the pseudo-potential model used here. The test of this scaling law is shown in figure IV.11. We see that this law is indeed satisfied for large enough n , but that it does not hold for $n = 0, 1, 2$, in contrast with the case $a < 0$ (see figure IV.9). However, we will see in §3 that it is difficult to observe mMM states in practice for a quantum number n beyond 2. This scaling law on the $a > 0$ side is therefore less relevant experimentally than its equivalent for $a < 0$.

Notation. In what follows, we will denote by $a_*^{(n)}$ (following tradition) the (positive) value of the scattering length a for which the energy of the

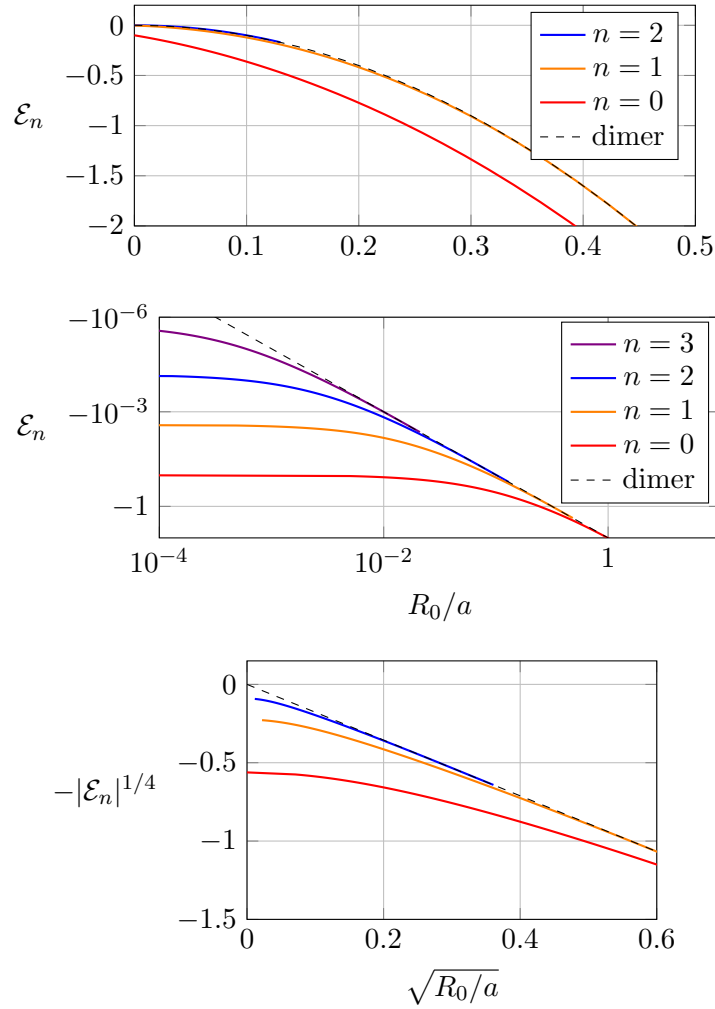


Figure IV.10. Dimer–trimer competition for $a > 0$: variation of the energies $\mathcal{E}_n(a)$ of the first bound states of the mMM trimer as a function of the scattering length a , assumed here to be positive, for $M/m = 20$. The same data are plotted in different coordinate systems. Energies are expressed in units of $\hbar^2/MR_0^2$. The energy of the dimer is $-\frac{\hbar^2}{2ma^2} = -\frac{M}{2m} \frac{R_0^2}{a^2} \frac{\hbar^2}{MR_0^2}$.

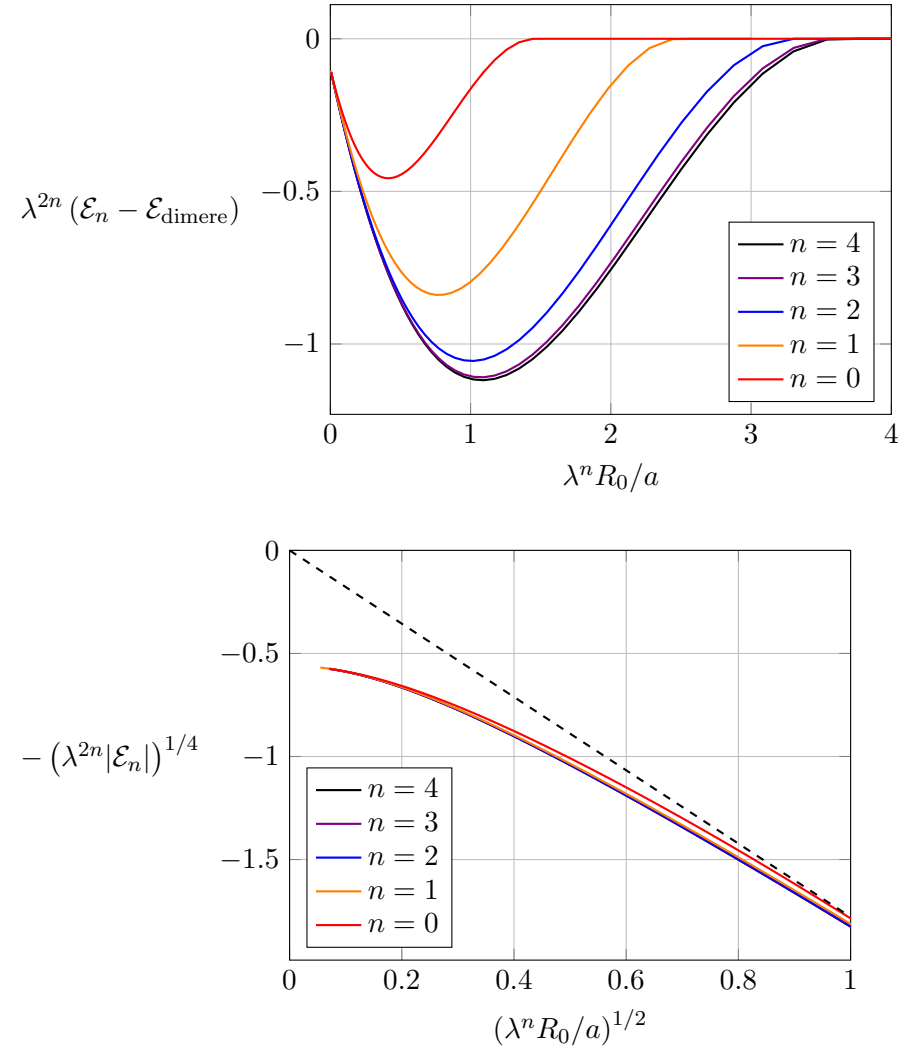


Figure IV.11. Checking the scaling law (28) for scattering lengths $a > 0$. The calculation is made for $M/m = 20$ and the energies are expressed in units of $\hbar^2/MR_0^2$.

n th trimer is equal to that of the mM dimer. Like $a_-^{(n)}$, this quantity $a_*^{(n)}$ is a function of R_0 . One might wonder why the notation $a_+^{(n)}$ has not been used for this crossing point between the energy of the trimer and that of the dimer. The reason is that the notation $a_+^{(n)}$ is instead used to denote a minimum of the three-body loss rate (also on the $a > 0$ side of the resonance), as we will see in Chapter 6.

2-3 Complete curves

To summarize what we have found on both sides, $a < 0$ and $a > 0$, of the $|a| = +\infty$ resonance, we have collected in figure IV.12 the results already shown separately. These curves are presented on a logarithmic scale, with an x axis that is a little unusual in that it represents $-\ln(R_0/|a|)$ on the $a < 0$ side and $+\ln(R_0/a)$ on the $a > 0$ side. The gap between $R_0/a = -10^{-5}$ and $R_0/a = +10^{-5}$, which would be infinite in “true” logarithmic coordinates, has been replaced by a segment of finite length. These same data are plotted in linear coordinates in figure IV.13.

Figure IV.12 shows that the levels become closer to each other as the M/m ratio increases. This narrowing is due to the decrease of the scale factor $\lambda = e^{\pi/|s_0|}$ as $|s_0| \approx \Omega\sqrt{M/2m}$ increases [cf. eq. (14)].

Note also that the remarkable points on either side of the resonance, $a_-^{(n)}$ and $a_*^{(n)}$, are each proportional to R_0 and to λ^{-n} , where λ depends on the ratio M/m . For example, we find (cf. figures IV.9 and IV.11):

$$\frac{M}{m} = 20 : \quad \lambda^n \frac{R_0}{a_-^{(n)}} \approx -0.0815 \quad \lambda^n \frac{R_0}{a_*^{(n)}} \approx +3.540 \quad (29)$$

from which we deduce:

$$\text{For } \frac{M}{m} = 20 : \quad \frac{a_-^{(n)}}{a_*^{(n)}} \approx -43 \quad \text{for } n \geq 3. \quad (30)$$

Checking the link between these parameters a_- and a_* , corresponding to the two sides of the resonance $|a| = +\infty$, is a very important test of the universality of the Efimov effect. Helfrich, Hammer & Petrov (2010) studied the variation of this ratio with M/m , and we have reproduced their results in figure IV.14.

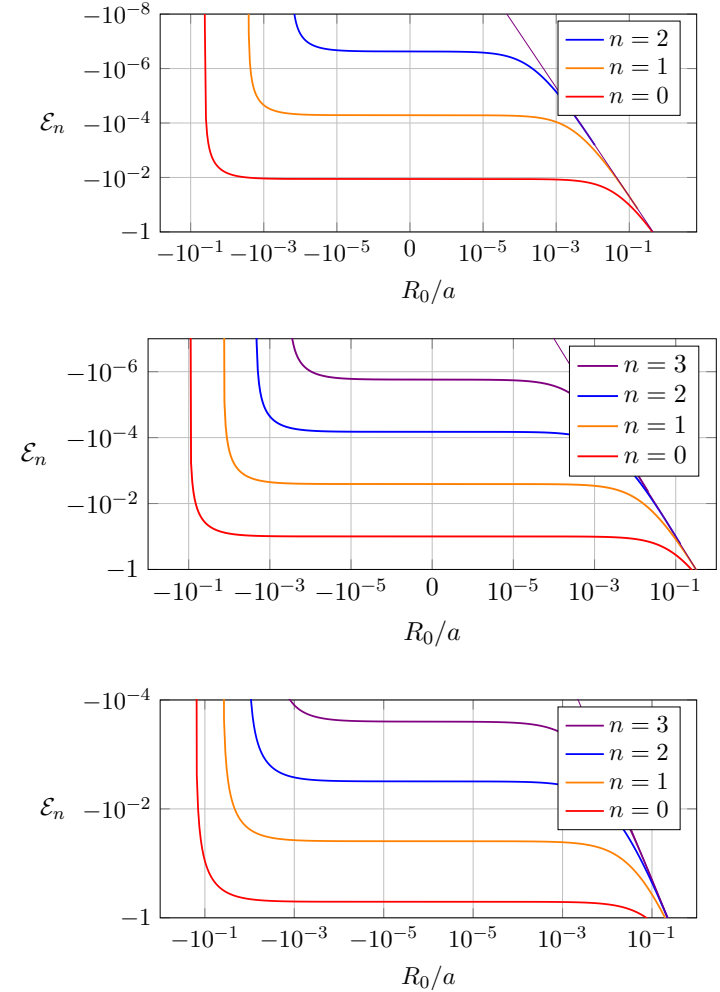


Figure IV.12. Variation of the energies $\mathcal{E}_n(a)$ of the first bound states of the mMM trimer as a function of the scattering length a , for $M/m = 10$ (top), 20 (middle) and 40 (bottom). The data are plotted in log-log coordinates (see the text for a precise description of the x axis). Energies are expressed in units of $\hbar^2/MR_0^2$.

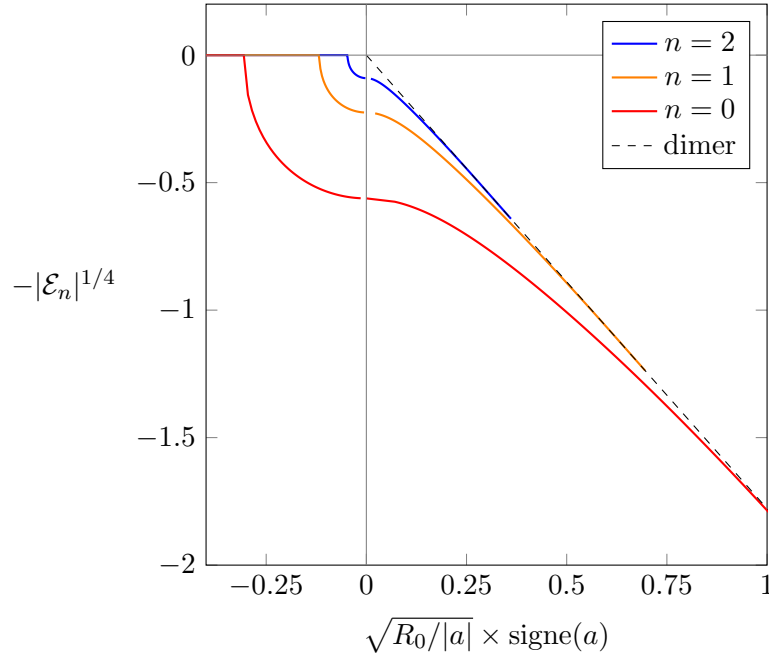


Figure IV.13. Variation of $-|\mathcal{E}_n|^{1/4}$ with $\sqrt{R_0/|a|}$ for the first bound states of the mMM trimer ($M/m = 20$).

3 Experiments on the light-heavy-heavy case

3-1 Experiments on atomic gas mixtures

The first manifestations of Efimov physics in gases of cold atoms were observed by Kraemer, Mark, et al. (2006) on a cesium gas. This was a homonuclear system, the theoretical description of which is more complicated than that of the mMM system considered so far. We therefore postpone the description of the results of Kraemer, Mark, et al. (2006) to Chapter 6 and concentrate here on more recent experiments, carried out in Heidelberg (Pires, Ulmanis, et al. 2014) and in Chicago (Tung, Jiménez-García, et al. 2014), in which three branches of trimers were observed, with (approximately) the

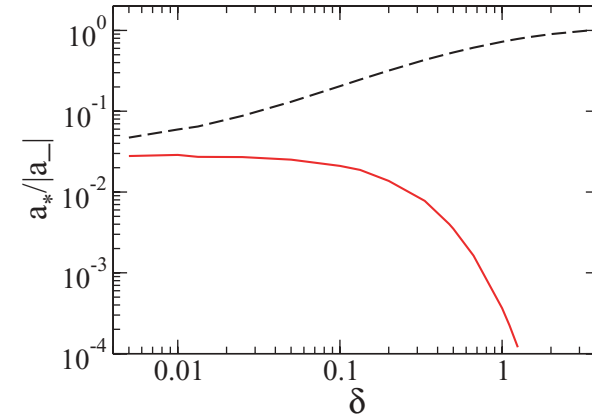


Figure IV.14. Red solid curve: variation of the ratio $a_*^{(n)}/|a_-^{(n)}|$ (for n sufficiently large) with the mass ratio $\delta \equiv m/M$. For $m/M = 1/20$, we find $a_*^{(n)}/|a_-^{(n)}| \sim 1/40$ [cf. (30)]. Black dashed curve: ratio $a_*^{(n+1)}/|a_-^{(n)}|$. Figure taken from Helfrich, Hammer & Petrov (2010).

expected scaling ratio.

It should be noted that in addition to the Heidelberg and Chicago experiments, which we will look at in detail, other mixtures have been studied in search of physics related to the universality discovered by Efimov:

- Barontini, Weber, et al. (2009) [see also Barontini, Weber, et al. (2010)] have published results tending to establish the formation of K-K-Rb and K-Rb-Rb trimers related to “Efimovian” physics on the $a < 0$ side ($a_- \stackrel{?}{=} -246(14) a_0$). They studied a mixture of ^{41}K and ^{87}Rb (Fano-Feshbach resonance at 38.4 G). They also described a possible three-body resonance on the $a > 0$ side ($a_* \stackrel{?}{=} 667(1) a_0$).
- Bloom, Hu, et al. (2013) studied a very similar mixture (^{40}K and ^{87}Rb), but they did not observe any resonance on the $a < 0$ side that could have been attributed to an Efimov effect [see also Hu, Bloom, et al. (2014)]. On the $a > 0$ side, they observed an Efimovian process in the relaxation of an mM dimer colliding with an M atom, corresponding

to $a_* = 230(10) a_0$, but this peak was not at the position of the resonance predicted by Barontini, Weber, et al. (2009) [see also the more recent work by Wacker, Jørgensen, et al. (2016) and Kato, Wang, et al. (2017)].

- Williams, Hazlett, et al. (2009) observed a peak in the three-body recombination signal in a ^6Li gas with three equally populated spin components. This same system was used by Lompe, Ottenstein, et al. (2010) to highlight Efimov trimers formed by photoassociation.
- Maier, Eisele, et al. (2015) studied a ^7Li - ^{87}Rb mixture and demonstrated a resonance attributable to an Efimov effect.

3-2 Fano-Feshbach resonance for ^6Li - ^{133}Cs

The Heidelberg and Chicago experiments were conducted with a mixture of cesium atoms in the role of the heavy particle ($M = 133$) and lithium in the role of the light particle ($m = 6$), giving a mass ratio of $M/m = 22.2$. This system exhibits several Feshbach resonances for the mM two-body problem. The two groups worked at a magnetic field close to 840 gauss, for which a broad resonance occurs.

The detailed study of the parameters of this resonance is described by Ulmanis, Häfner, Pires, Kuhnle, Weidemüller, et al. (2015). It is based on a dimer photoassociation technique, as shown in figure IV.15. The dimer binding energy is measured as a function of the magnetic field, and should vanish at resonance. Near resonance, on the $a > 0$ side, this energy can be approximated by $-\hbar^2/2m_r a^2$, where $m_r \approx 5.7$ is the reduced mass of the two-body system. The experimental result for the measurement of this binding energy is shown in figure IV.16, with the simple prediction $-\hbar^2/2m_r a^2$ as well as the result of a more sophisticated model taking into account several coupled collision channels. The result for the mM scattering length takes the “traditional” form

$$a = a_{\text{bg}} \left(1 - \frac{\Delta}{B - B_{\text{res}}} \right) \quad (31)$$

with $a_{\text{bg}} = -29.4 a_0$, $\Delta = -58.21 \text{ G}$ and $B_{\text{res}} = 842.829 \text{ G}$.

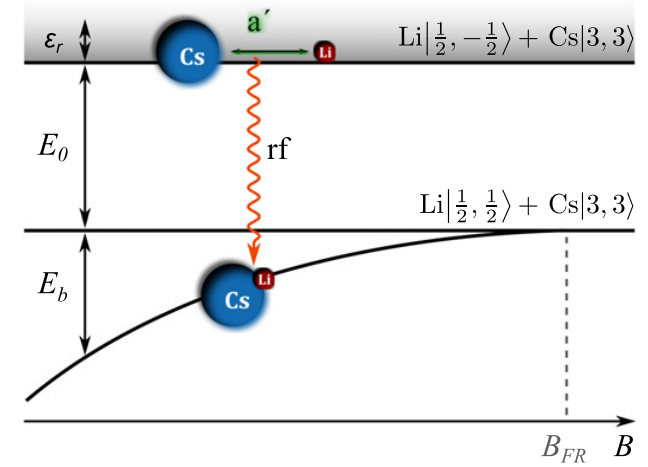


Figure IV.15. Photoassociation of mM dimers in a mixture of ^6Li and ^{133}Cs . Figure taken from Ulmanis, Häfner, Pires, Kuhnle, Weidemüller, et al. (2015).

We show in figure IV.16 the result of Ulmanis, Häfner, Pires, Kuhnle, Weidemüller, et al. (2015) for the measurement of the loss of Cs atoms in the vicinity of the resonance. The authors conclude that these two measurements are in relatively good agreement with each other, with the measurement based on photoassociation giving results ten times more accurate.

3-3 The formation of trimers on the $a < 0$ side

The two 2014 experiments carried out in Heidelberg and Chicago focused on the $a < 0$ side of the resonance (i.e. $B > B_{\text{res}}$). The principle is simple: when the scattering length is close to one of the $a_-^{(n)}$ thresholds corresponding to the appearance of a trimer (figure IV.17), one observes a significant loss of atoms linked to three-body recombination: the three atoms couple temporarily to form an Efimov state, which then decays into a strongly bound dimer and an isolated atom. The energy released by the formation of the dimer is converted into kinetic energy of the two partners, which escape from the trap (D’Incao & Esry 2005b; D’Incao & Esry 2006b). The theoret-

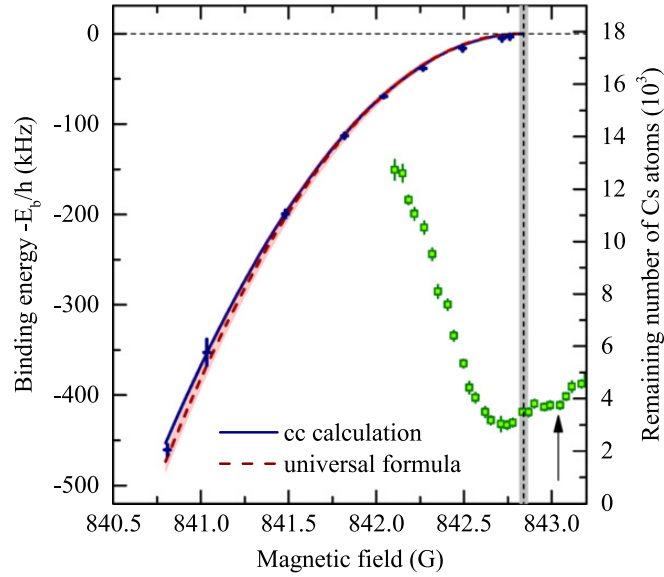


Figure IV.16. Blue crosses: binding energy of mM dimers in a mixture of ^6Li and ^{133}Cs . Green squares: Cs atom loss signal. The shaded vertical band gives the position of the resonance and its uncertainty ($B_{\text{res}} = 842.829 \text{ G}$). Figure taken from Ulmanis, Häfner, Pires, Kuhnle, Weidemüller, et al. (2015).

ical description of the recombination process will be given in more detail later in this course; in what follows, we simply assume that this process is maximal when a is close to one of the $a_-^{(n)}$.

Several typical loss signals are shown in figure IV.18. This figure, corresponding to data from the Chicago group, shows the decrease in the number of lithium atoms for two values of the magnetic field: $B = 848.0 \text{ G}$ for the top figure (i.e. relatively far from resonance), $B = 842.7 \text{ G}$ for the bottom figure (i.e. very close to resonance). These data were obtained for a pure lithium gas (open symbols) and for a lithium-cesium mixture (filled symbols). The data for pure lithium are almost independent of the value of B , whereas those for the mixture show a spectacular increase in the decay rate at short times for data acquired close to resonance.

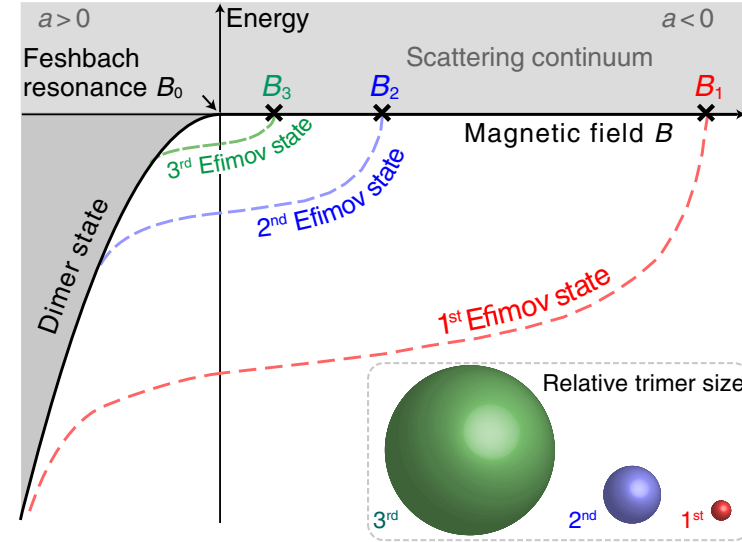


Figure IV.17. Principle of Efimov trimer detection: we look for magnetic fields B_j for which the scattering length is negative and equal to one of the threshold values $a_-^{(n)}$ for the appearance of a trimer. Note that the x axis is oriented in the direction of increasing magnetic fields, and therefore decreasing values of $1/a$, which is the opposite of the convention used in figures IV.7, IV.10 and IV.12. Figure taken from Tung, Jiménez-García, et al. (2014).

Note that the losses of cesium atoms are always very significant in this magnetic field domain, independently of the presence of lithium atoms. This is because the Cs–Cs scattering length is negative and of large absolute value: $|a_{\text{Cs Cs}}| > 1000 a_0$.

When we plot the number of lithium atoms remaining in the trap after a given time τ as a function of the magnetic field (and therefore of the scattering length $a_{\text{Li Cs}}$), we observe three successive resonances corresponding to the three values of B_j shown in figure IV.17. Figure IV.19 shows the data obtained in Chicago.

The detailed analysis of the experimental data from Heidelberg and Chicago was carried out by Ulmanis, Häfner, Pires, Kuhnle, Weidemüller,

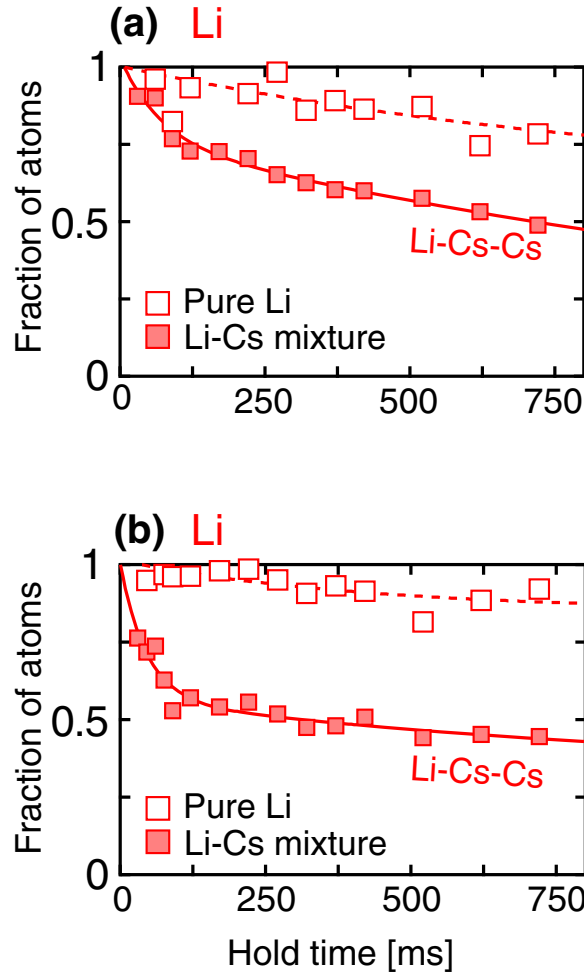


Figure IV.18. Decay in the number of atoms in an optical trap initially containing 20 000 to 30 000 ^6Li atoms and (for solid symbols) 40 000 to 50 000 ^{133}Cs atoms. The temperature of the cloud is of the order of 350 nK. Top: $B = 848.0$ G, relatively far from the resonance in $a_{\text{Li Cs}}$. Bottom: $B = 842.7$ G, close to resonance. Figure taken from Tung, Jiménez-García, et al. (2014).

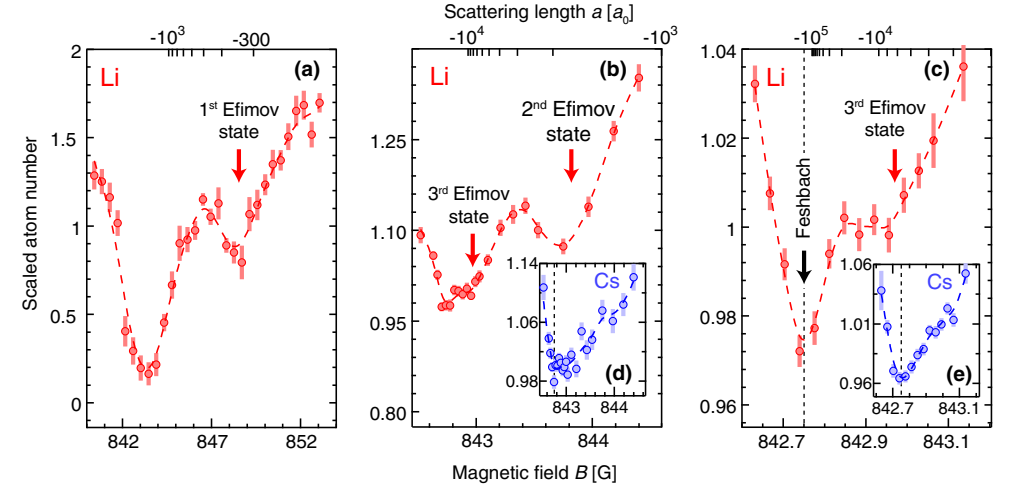


Figure IV.19. Variation in the number of lithium atoms in the optical trap after a waiting time τ , with $\tau = 225$ ms for the left-hand figure ($T = 800$ nK) and $\tau = 115$ ms for the other two ($T = 360$ nK for the middle figure and $T = 270$ nK for the right-hand figure). Figure taken from Tung, Jiménez-García, et al. (2014).

et al. (2015), thanks to the precise determination of the position of the Fano-Feshbach resonance in $a_{\text{Li Cs}}$ obtained from figure IV.16. Table IV.1 summarizes the results of this analysis. The expected universal value of the ratio $a_-^{(n)}/a_-^{(n-1)}$ [cf. eq. (23)] is $\lambda = 4.9$ (Braaten & Hammer 2006; D’Incao & Esry 2006a). Note that this value is obtained from a complete numerical calculation of the three-body problem (while continuing to neglect the mM interaction). The approximate value deduced from the Born–Oppenheimer treatment described above is $\lambda_{\text{BO}} = 5.6$.

3-4 Discussions and extensions

In the above treatment, we have completely neglected the interaction between the two heavy atoms. This approximation is valid for certain mixtures (Li–Rb for example), but is highly questionable for the Li–Cs mixture studied in Heidelberg and Chicago. The Cs–Cs scattering length is in fact

i	Magnetic field (G)	$a_{-}^{(i)} (10^3 a_0)$	$a_{-}^{(i)} / a_{-}^{(i-1)}$
0 (ground)	848.90 (6)(3) ^a	-0.311 (3)(1)(1)	—
1	843.85 (1)(3) ^a	-1.71 (2)(5)(4)	5.48 (7)(16)(10)
2	843.03 (5)(3) ^a	-8.54 (2.12)(1.27)(97)	5.00 (1.24)(76)(46)
0	848.55 (12)(3) ^b	-0.329 (6)(2)(1)	—
1	843.82 (4)(3) ^b	-1.76 (7)(5)(4)	5.35 (24)(16)(10)
2	842.97 (3)(3) ^b	-12.2 (2.6)(2.6)(1.9)	6.93 (1.50)(1.48)(97)

Table IV.1. Magnetic field values measured at Heidelberg (a) and Chicago (b) for the appearance of Efimov trimers in a ^6Li - ^{133}Cs mixture, on the $a < 0$ side of the resonance. The resulting ratios $a_{-}^{(i)} / a_{-}^{(i-1)}$ are close to the expected “universal” value. Table taken from Ulmanis, Häfner, Pires, Kuhnle, Weidemüller, et al. (2015).

large in absolute value ($> 1000 a_0$) over the entire magnetic field range explored around the resonance at 843 G.

This problem has been tackled in detail by Petrov & Werner (2015) [see also Wang, Wang, et al. (2012) and Mikkelsen, Jensen, et al. (2015)] who have compared the two limiting cases $a_{MM} = 0$ and $a_{MM} = \infty$. The result is remarkable: the parameters underlying the Efimov scaling law, $|s_0|$ and $\lambda = e^{\pi/|s_0|}$, vary very little between the two cases. Petrov & Werner (2015) find:

$$a_{mM} = \infty, a_{MM} = 0 : \quad |s_0| = 1.98277, \lambda = 4.87661 \quad (32)$$

and [see also Yamashita, Bellotti, et al. (2013)]

$$a_{mM} = \infty, a_{MM} = \infty : \quad |s_0| = 2.00308, \lambda = 4.79887. \quad (33)$$

On the other hand, Petrov & Werner (2015) show that the three-body loss rate is considerably increased in the case of the Li-Cs mixture by the fact that the MM interactions are quasi-resonant (cf. figure IV.20).

Petrov & Werner (2015) have also studied theoretically the effect of temperature on the three-body loss signal. A typical result, comparing the $T = 0$ and $T = 400 \text{ nK}$ cases, is shown in figure IV.20. It can be seen that

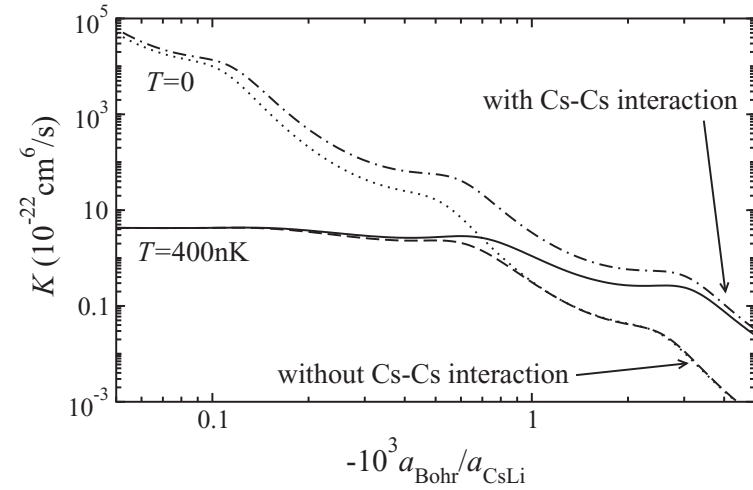


Figure IV.20. Variation of the three-body loss rate in a Li-Cs mixture, with and without the Cs-Cs interaction, and for two different temperatures, $T = 0$ and $T = 400 \text{ nK}$. Figure taken from Petrov & Werner (2015) (see that article for the parameters of the calculation).

a non-zero temperature tends to smooth out the resonances of the loss signal, and can also shift them relative to the $T = 0$ case. Similar results have been obtained independently by Mikkelsen, Jensen, et al. (2015). In the Ulmanis, Häfner, Pires, Werner, et al. (2016) paper, the Heidelberg group presents experimental data taken at lower temperatures (120 nK) than in the original 2014 experiments, which confirm the trends just described.

Following the experimental publications by the Heidelberg and Chicago groups, the study of the mMM Efimov effect has been the subject of numerous theoretical studies, in particular to go beyond the description of interactions in terms of contact potential. Finite range effects have been studied in particular by Zinner & Nygaard (2015), Acharya, Ji, et al. (2016), and Wu, Han, et al. (2016).

Ulmanis, Häfner, Pires, Kuhnle, Wang, et al. (2016) have added an interesting measurement on the Li-Cs mixture by repeating the initial experiments around another Feshbach resonance located near $B = 889 \text{ G}$. Under

these conditions, the scattering length $a_{\text{Cs Cs}} = 190 a_0$ is positive, which means that weakly bound Cs_2 dimers can play a significant role. This leads to the disappearance of the resonance for the ground Efimov state and a change in the scaling factor to $\lambda = 4.0(3)$ [see also Häfner, Ulmanis, et al. (2017)]. A detailed theoretical treatment of three-body relaxation in this configuration, in particular the line shape likely to appear (Fano profile), was proposed by Giannakeas & Greene (2018) and Giannakeas & Greene (2021).

The two Feshbach resonances mentioned so far for the Li–Cs pair (843 G and 889 G) are broad resonances, for which the description of the interaction in terms of a scattering length (with no significant contribution from the effective range) is appropriate. Johansen, DeSalvo, et al. (2017) compared the results obtained for the resonance at 889 G and another, much narrower resonance² at 893 G. One of the main conclusions of this study is a very significant shift of the position of the resonance with respect to the “naive” prediction. A complementary theoretical analysis of a narrow resonance for the Li–Cs–Cs problem has recently been proposed by Li, Yudkin, et al. (2022).

4 The universal trimers of Kartavtsev & Malykh

4-1 Back to the case of fermions

We now return to the case where the heavy particles are polarized fermions, so that their accessible states must involve only the odd relative angular momentum channels.

As we indicated in § 1-4, when we place ourselves at resonance, i.e. $a = \pm\infty$, two cases are possible for a zero-range mM interaction:

- For M/m greater than the critical value $13.606\,966\cdots$, infinitely many states can appear in the $\ell = 1$ channel in the potential α/R^2 ($\alpha < 0$) that emerges from the problem. As for bosons, we need to introduce a *three-body parameter*, in our approach the hard core at R_0 , to prevent the

²The parameters characterizing these resonances are $s_{\text{res}} = 0.66$ for $B = 843$ G and 889 G, and $s_{\text{res}} = 0.05$ for $B = 893$ G (cf. the 2021 lecture series, Chapter 6).

“fall to the center” and to ensure that the system admits a ground state of finite negative energy. Above this ground state, we find infinitely many bound states, with energies forming, to a very good approximation, a geometric sequence $E_{n+1} = E_n/\lambda^2$.

- For M/m smaller than the critical value $13.606\,966\cdots$, no three-body bound state exists for $a = \pm\infty$.

Following a seminal work by Petrov (2003) on three-body recombination in these systems, Kartavtsev & Malykh (2007) took up this problem from the $a > 0$ side of the resonance and showed that the effective interaction resulting from the exchange of the light particle [described by the potential (5) in the Born–Oppenheimer approximation] could give rise to bound trimers for a mass ratio below the critical value 13.6. These trimers are called universal because it is not necessary to introduce a three-body parameter to define their energy (we will come back to this point in § 4-3). Their binding energy depends only on the scattering length a characterizing the mM interaction (recall that any MM interaction is neglected here).

Recall also that we are assuming here an mM interaction characterized only by the scattering length a , which in practice corresponds to the case of a broad Fano–Feshbach resonance. The case of a narrow resonance with $1/a = 0$ is discussed by Castin & Tignone (2011a).

4-2 Born–Oppenheimer approach

At a semi-quantitative level, the result of Kartavtsev & Malykh (2007) can be recovered using the Born–Oppenheimer approach followed so far. We place ourselves in the case of a mass ratio below the critical value of the $a = \infty$ case [i.e. $M/m < 14.0$ for the Born–Oppenheimer treatment, cf. (15)] and ask the following question: can there be a bound state in the effective potential created by the light particle, including the centrifugal barrier for the wave $\ell = 1$? Let us recall the expression of this total potential for $a < 0$:

$$\begin{aligned} a < 0, R < |a| : \quad & V_{\text{tot}}(R) = -\frac{\hbar^2}{2m} \left[\frac{1}{|a|} - \frac{W(e^{R/|a|})}{R} \right]^2 + \frac{2\hbar^2}{MR^2} \\ a < 0, R > |a| : \quad & V_{\text{tot}}(R) = \frac{2\hbar^2}{MR^2} \end{aligned} \quad (34)$$

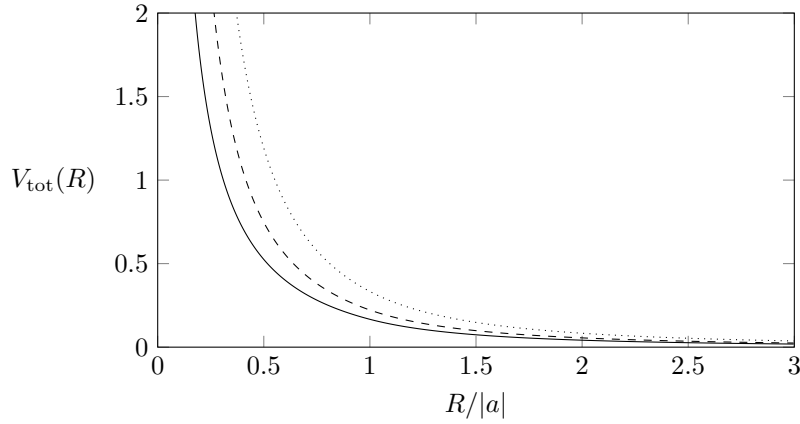


Figure IV.21. Total potential (in units of $\hbar^2/ma^2$) for the channel $\ell = 1$ in the case $a < 0$, calculated using the Born–Oppenheimer approximation. From top to bottom, $M/m = 6, 9, 12$.

and for $a > 0$:

$$a > 0: \quad V_{\text{tot}}(R) = -\frac{\hbar^2}{2m} \left[\frac{1}{a} + \frac{W(e^{-R/a})}{R} \right]^2 + \frac{2\hbar^2}{MR^2}. \quad (35)$$

For $a < 0$, this potential is plotted in figure IV.21 for different values of M/m . It is always a decreasing function of R , which rules out the existence of a bound state in this potential. Note that this potential is in any case always greater than the potential obtained in the case $a = \pm\infty$ for the same value of the ratio M/m . Since we know that there is no bound state in the case $a = \pm\infty$, there can be none in the case $a < 0$ either.

The interesting situation is obtained for $a > 0$. As can be seen in figure IV.22, the potential $V_{\text{tot}}(R)$ is not always a monotonic function of R . It can have an absolute minimum when the ratio M/m exceeds ~ 7 , while retaining a limit $V_{\text{tot}}(R) \rightarrow +\infty$ when $R \rightarrow 0$. When $R \rightarrow \infty$, the potential $V_{\text{tot}}(R)$ tends to $-\hbar^2/(2ma^2)$, which corresponds to the energy of the mM dimer when it is far from the other M particle.

This form of the potential for $a > 0$ opens up the possibility of obtaining

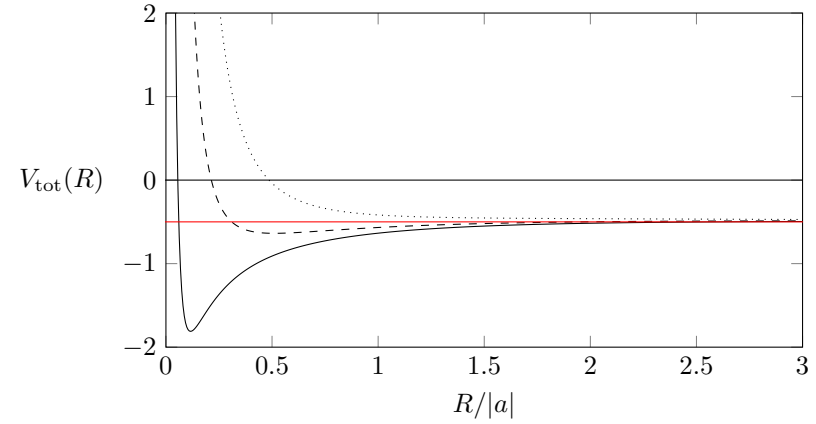


Figure IV.22. Total potential (in units of $\hbar^2/ma^2$) for the channel $\ell = 1$ in the case $a > 0$, calculated using the Born–Oppenheimer approximation. From top to bottom, $M/m = 5, 8, 11$.

bound states, i.e. states whose energy is strictly less than the energy of the dimer $-\hbar^2/(2ma^2)$. It is possible to use the Born–Oppenheimer approach to determine the threshold on M/m above which such a bound state appears. However, the result is very sensitive to the shape of the potential and it is safer to use a precise numerical method, as was done by Kartavtsev & Malykh (2007).

Note that even when the threshold for the existence of a bound state is not reached, the non-monotonic form of the potential, with a local minimum likely to host a quasi-bound state, can give rise to a scattering resonance. This phenomenon was observed by Jag, Zaccanti, et al. (2014) for a ${}^6\text{Li}$ – ${}^{40}\text{K}$ mixture (mass ratio $M/m = 6.7$).

4-3 Kartavtsev–Malykh results and extensions

Kartavtsev & Malykh (2007) used a treatment of the three-body problem similar to that we shall see in the next chapter, involving the solution of hyper-radial equations [see also Petrov (2003)]. For the case $a > 0$, they

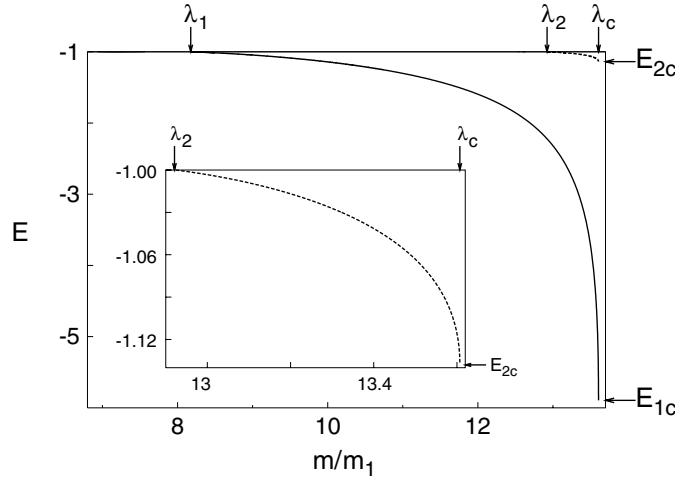


Figure IV.23. Energies of the “universal” bound states for the mMM problem in the case where the M particles are non-interacting polarized fermions and the scattering length a characterizing the mM interaction is positive. The energies E are measured in units of $\hbar^2/(2m_r a^2)$, and the abscissa is the ratio M/m (denoted m/m_1 here). Figure taken from Kartavtsev & Malykh (2007).

arrived at the following conclusions when the particles M are polarized fermions:

- For $M/m < \lambda_1 = 8.173$, there is no bound state for the mMM problem.
- For $\lambda_1 = 8.173 < M/m < \lambda_2 = 12.917$, there is (in the absence of an additional three-body parameter, see §4-3) one and only one bound state, of energy $\alpha_1 \hbar^2/(2m_r a^2)$, with the dimensionless coefficient α_1 plotted in figure IV.23 and $m_r = mM/(m + M)$.
- For $\lambda_2 = 12.917 < M/m < \lambda_c = 13.607$, there are two bound states, of energies $\alpha_j \hbar^2/(2m_r a^2)$, with the coefficients α_j , $j = 1, 2$, plotted in figure IV.23.
- For $13.607 < M/m$, there can be an arbitrarily large number of bound states when $1/a \rightarrow 0_+$: this is the Efimov effect. Determining the en-

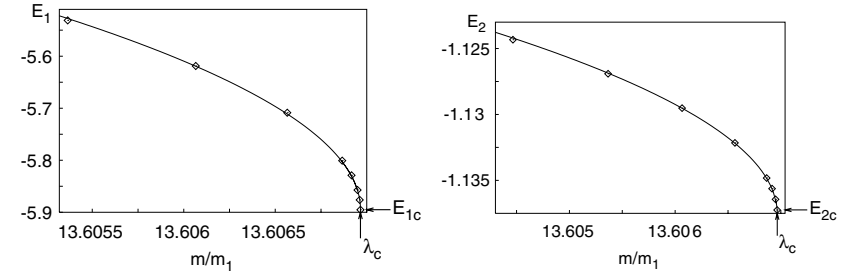


Figure IV.24. Same caption as for figure IV.23. Figure taken from Kartavtsev & Malykh (2007).

ergies of these bound states requires the introduction of a three-body parameter, for example the hard-core radius R_0 .

The states found in the range $8.173 < M/m < 13.607$ have a total angular momentum $L = 1$. They are called universal since their energy depends only on the two-body problem mM and does not require the introduction of an additional parameter related to the three-body problem. An enlargement of the energy behavior of these states in the vicinity of the critical point λ_c is shown in figure IV.24.

To date, Kartavtsev–Malykh trimers have not been observed experimentally. As indicated by Endo, García-García, et al. (2016), a well-suited system could be a mixture of ${}^6\text{Li}$ and ${}^{53}\text{Cr}$, both fermionic with $M/m = 8.8$.

Note on the absence of a three-body parameter. For $M/m > 8.619$, Kartavtsev & Malykh (2016) showed that, for the zero-range model used here, there is an ambiguity in the definition of the three-particle wave function, since two independent solutions, each square-integrable, are available. This ambiguity is already present in the one-body problem in the $1/R^2$ potential. We have seen that the equation $u''(R) - \frac{\alpha}{R^2}u(R) = 0$ has two solutions $u(R) = R^{s_{\pm}+1}$ with $s_{\pm} = -\frac{1}{2} \pm \sqrt{\alpha + \frac{1}{4}}$. For $-1/4 < \alpha < 3/4$, both solutions are acceptable on the simple criterion of integrability at $R = 0$.

Kartavtsev & Malykh (2016) then introduced an additional parameter,

which we denote by B_3 , to fix the amplitude of the s_- solution, which diverges at $R = 0$, relative to the s_+ solution, which converges at $R = 0$. The original article by Kartavtsev & Malykh (2007), whose results we described above, corresponded to the implicit choice $B_3 = 0$. The spectra expected when non-zero values of B_3 are taken into account are given by Kartavtsev & Malykh (2016), since a third trimer may appear in a small region of parameter space.

This problem was taken up again by Endo, Naidon, et al. (2012), then more recently by Naidon, Pricoupenko, et al. (2022) with a potential V_{mM} of non-zero range b . In this model, Naidon, Pricoupenko, et al. (2022) showed that the zero-range limit for V_{mM} leads naturally to the choice $B_3 = 0$, thus to the results of Kartavtsev & Malykh (2007).

Endo, Naidon, et al. (2012) have shown the existence of a continuous transition (*crossover*) towards non-universal trimers when the parameter a/b is varied. This approach based on a non-zero mM potential also makes it possible to specify the conditions under which Kartavtsev–Malykh trimers can be observed and leads to a very narrow range of suitable scattering lengths: $a \gtrsim 100b$ (Naidon, Pricoupenko, et al. 2022). Naidon, Pricoupenko, et al. (2022) also took into account a possible direct p -wave interaction³ for MM , and showed that it can lead to the formation of additional trimers, potentially easier to observe.

Finally, it should be noted that Endo, García-García, et al. (2016) have shown that the interaction between Kartavtsev–Malykh trimers is repulsive at low energies: it is therefore possible to form a stable Fermi-liquid phase with them if the m particle is itself a fermion, provided that $M/m \lesssim 9.5$. Blume (2012) has indeed found that beyond this value, the formation of an $mMMM$ tetramer (also universal) can become energetically favorable.

³The problem of three identical polarized fermions interacting only in the p wave has been treated by Jona-Lasinio, Pricoupenko, et al. (2008).

Chapter V

The Efimov problem for three identical bosons

In this chapter we discuss the “real” Efimov effect, as studied in the original publication by Efimov (1970). We consider three identical particles, which we will assume to be of spin zero or polarized bosons, and we are interested in the situation where only the binary interaction between particles is relevant. We assume that this interaction is characterized by the scattering length a (positive or negative) and focus on the case where $|a|$ is very large compared with the range b of the potential.

In the following treatment, we will in fact take a potential of zero range (the pseudo-potential), treating the interactions via the Bethe–Peierls boundary conditions that we have already encountered in previous chapters. The slightly more general case of a separable binary potential is briefly dealt with in the appendix.

The result found by Efimov is remarkable: for $a = \pm\infty$, while there is no two-body bound state (at least in the pseudo-potential model), we find infinitely many three-body bound states, with energies forming a geometric sequence. As already explained, this geometric sequence must be truncated on the side of very negative energies, since we require this system to have a ground state. This requires the introduction of a three-body parameter that we will call R_0 .

Once the three-body parameter is fixed, the entire spectrum of the problem can be deduced (figure V.1). On the $a < 0$ side, when we decrease the value of $|a|$, we see the different trimer states disappear one after the other because their binding energy vanishes. On the $a > 0$ side, when we

decrease the value of a , the trimer states enter into competition with the “dimer plus free particle” state, and they too eventually disappear. Efimovian physics is therefore truly a physics of scattering resonance, in the vicinity of the point $a = \pm\infty$.

Unlike the mMM case, for which the Born–Oppenheimer approximation made it possible to carry out practically all the calculations analytically, the case of three identical particles is much more complicated to deal with. In what follows, we will first give details of the solution in the strictly resonant case, which will allow us to return to the $1/r^2$ interaction that has been the guiding principle throughout this year’s course. We will then outline the treatment away from resonance, but without carrying out the explicit calculations, which in any case require a substantial numerical effort if reasonable accuracy is to be obtained.

In his work in the 1970s, Efimov envisaged an application of his model to nuclear physics. In particular, he mentioned an assembly of three α particles (two protons, two neutrons) that could form an excited state of the ^{12}C carbon nucleus. It turned out that the resonance conditions needed to reach $|a| \gg b$ (where b is the range of the two-body potential) were not met in this case. It was not until 1994 that the helium trimer was observed (Schöllkopf & Toennies 1994), a state that (almost) qualifies as an Efimov trimer, followed by experiments on gases of cold atoms with the pioneering work of R. Grimm’s group in Innsbruck (Kraemer, Mark, et al. 2006).

As we wrote above, we will not carry out all the calculations here to ar-

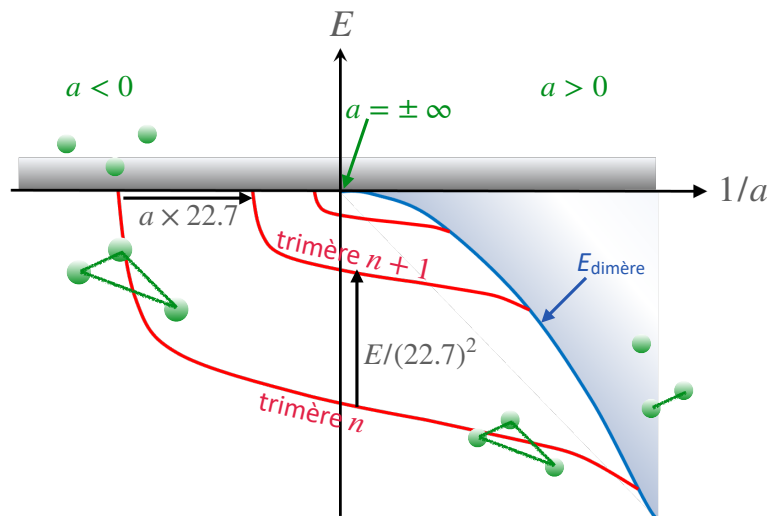


Figure V.1. Schematic diagram of the spectrum of dimers and trimers, for a zero-range interaction described by the scattering length a . The introduction of a three-body parameter R_0 is necessary to fix the position of the levels on the vertical axis ($1/a = 0$). The rest of the diagram follows universally from this.

rive at the final energy diagram. These calculations can be found in several review articles written over the last twenty years, including those used as a basis for this chapter: Nielsen, Fedorov, et al. (2001), Braaten & Hammer (2006), Naidon & Endo (2017), Greene, Giannakeas, et al. (2017) and D’Incao (2018).

1 Parameterization of space

In all its generality, the three-body problem in three-dimensional space consists of finding the eigenfunctions $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ of the Hamiltonian, depending on nine space variables. It is of course impossible to tackle such a prob-

lem head-on, and it is imperative to take into account the various symmetries of the system in order to simplify it.

To begin with, we can let ourselves be guided by the solution of the two-body problem: starting from the six space variables $\{\mathbf{r}_1, \mathbf{r}_2\}$, the separation into center-of-mass and relative variables

$$\{\mathbf{r}_1, \mathbf{r}_2\} \longrightarrow \{\mathbf{R}_{12}, \mathbf{r}_{12}\} \quad (1)$$

with

$$\mathbf{R}_{12} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \quad \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \quad (2)$$

reduces the problem to the three components of $\mathbf{r}_{12}$, since the motion of the center of mass $\mathbf{R}_{12}$ is that of a free particle. Then, by taking into account the rotational symmetry of the two-body interaction, the problem is reduced to a one-dimensional one, involving only $r_{12} = |\mathbf{r}_{12}|$.

For the three-body problem, things are not so simple. Separating off the motion of the center of mass allows us to go from nine to six variables, but it is then difficult to simplify the general problem any further. We will see in this section, however, that for a zero-range interaction described by the Bethe–Peierls boundary condition, the nine-variable problem can be reduced to one with only two variables.

1-1 Bethe–Peierls boundary condition

We consider three particles of mass m interacting in pairs via the pseudopotential associated with the scattering length a . This interaction is taken into account using the Bethe–Peierls boundary conditions, which impose the behavior of the total wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ when two particles approach each other. For example, when the position of particle 3 is fixed as well as the midpoint $\mathbf{R}_{12}$ of the segment (1-2), and when the distance r_{12} tends towards 0 (figure V.2), we impose:

$$r_{12} \rightarrow 0: \quad \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \left(\frac{1}{r_{12}} - \frac{1}{a} \right) \Phi(\mathbf{R}_{12}, \mathbf{r}_3) + \mathcal{O}(r_{12}). \quad (3)$$

In an expansion in powers of r_{12} , the Bethe–Peierls condition therefore imposes a relation between the first two coefficients of the expansion, that of

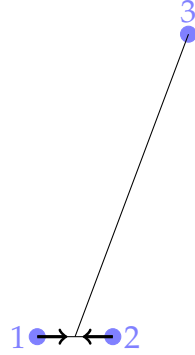


Figure V.2. An example of a situation where the Bethe–Peierls boundary condition (3) comes into play.

$(r_{12})^{-1}$ and that of $(r_{12})^0$, without constraining the subsequent coefficients [terms in $(r_{12})^n$ with $n \geq 1$].

Once the Bethe–Peierls boundary condition has been imposed, the Hamiltonian governing the evolution of the three particles is purely kinetic. The search for eigenstates of the three-body system therefore involves solving the eigenvalue equation:

$$-\frac{\hbar^2}{2m} \left(\sum_{j=1}^3 \nabla_{\mathbf{r}_j}^2 \right) \Psi = E \Psi. \quad (4)$$

1-2 Jacobi coordinates

As with the two-body problem, the total system is translationally invariant. We can therefore separate the motion of the center of mass

$$\mathbf{R}_{123} = \frac{1}{3} (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3), \quad (5)$$

which is that of a free particle of mass $3m$, from the relative motion of the three particles. There is no simple choice of relative coordinates that fully

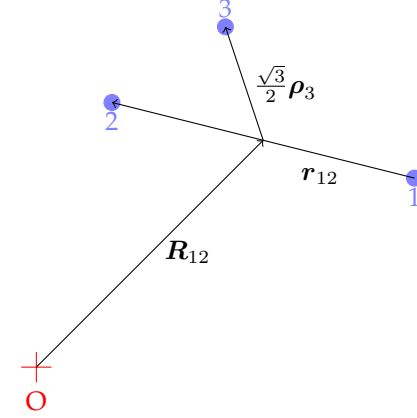


Figure V.3. One of the Jacobi coordinate systems for the three-body problem. We have chosen here the one that singles out the (1, 2) pair.

respects the symmetry between the three particles. Here we will use the Jacobi system (see figure V.3). By singling out particle 3 with respect to the pair (1, 2), this system amounts to the change of variables

$$\{\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\} \longrightarrow \{\mathbf{R}_{123}, \mathbf{r}_{12}, \boldsymbol{\rho}_3\} \quad (6)$$

where $\mathbf{R}_{123}$ and $\mathbf{r}_{12}$ have already been defined above and where

$$\frac{\sqrt{3}}{2} \boldsymbol{\rho}_3 = \mathbf{r}_3 - \mathbf{R}_{12}. \quad (7)$$

The reason for the coefficient $\sqrt{3}/2$ will appear in a moment¹.

¹We have adopted the same coordinate system as Naidon & Endo (2017). There is also a choice in the literature [see for example Greene, Giannakeas, et al. (2017)] corresponding to a different “distribution” of this factor $\sqrt{3}/2$, which consists in setting

$$\tilde{\mathbf{r}}_{12} = \left(\frac{\sqrt{3}}{2} \right)^{1/2} (\mathbf{r}_1 - \mathbf{r}_2) \quad \tilde{\boldsymbol{\rho}}_3 = \left(\frac{\sqrt{3}}{2} \right)^{-1/2} (\mathbf{r}_3 - \mathbf{R}_{12}), \quad (8)$$

so that the Delves and Jacobi angles are unchanged, and the corresponding hyperradius reads $\tilde{R}^2 = \tilde{r}_{12}^2 + \tilde{\rho}_3^2 = \frac{\sqrt{3}}{2} R^2$ where R is defined in (29). For the term associated with the hyper-

Once the coordinates have been chosen, we need to rewrite the eigenvalue equation (4). A simple calculation gives the sum of the Laplacians

$$\sum_{j=1}^3 \nabla_{\mathbf{r}_j}^2 = \frac{1}{3} \nabla_{\mathbf{R}_{123}}^2 + 2 (\nabla_{\mathbf{r}_{12}}^2 + \nabla_{\boldsymbol{\rho}_3}^2). \quad (10)$$

The term in $\frac{1}{3} \nabla_{\mathbf{R}_{123}}^2$ corresponds to the kinetic energy of the center of mass. The motion of the center of mass is not affected by the Bethe–Peierls boundary condition and its eigenfunctions are plane waves $e^{i\mathbf{K} \cdot \mathbf{R}_{123}}$ of energy $\hbar^2 K^2 / 6m$. In all that follows, we assume that we have placed ourselves in the frame of the center of mass of the three-body system, which amounts to choosing $\mathbf{K} = 0$, and we omit the contribution $\frac{1}{3} \nabla_{\mathbf{R}_{123}}^2$. From now on, we thus work with the unknown function $\Psi(\mathbf{r}_{12}, \boldsymbol{\rho}_3)$, which is a solution of

$$-\frac{\hbar^2}{m} (\nabla_{\mathbf{r}_{12}}^2 + \nabla_{\boldsymbol{\rho}_3}^2) \Psi = E \Psi \quad (11)$$

which must be solved taking into account the Bethe–Peierls boundary conditions. Note the advantage of the factor $\sqrt{3}/2$ in the definition (7) of $\boldsymbol{\rho}_3$, which yields a form of the Laplacian that is symmetric in the two variables $\mathbf{r}_{12}$ and $\boldsymbol{\rho}_3$.

The three Jacobi coordinate systems. As we have said, there is no simple choice of coordinate system that respects the symmetry between the three particles. The choice $\{\mathbf{r}_{12}, \boldsymbol{\rho}_3\}$ made above singles out particle 3. We can of course make equivalent choices by singling out particle 1: $\{\mathbf{r}_{23}, \boldsymbol{\rho}_1\}$, or particle 2: $\{\mathbf{r}_{31}, \boldsymbol{\rho}_2\}$. In what follows we will need the formulae for passing from one of these coordinate systems to another (rotation angle $\pm 2\pi/3$):

$$\begin{pmatrix} \mathbf{r}_{23} \\ \boldsymbol{\rho}_1 \end{pmatrix} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ +\sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} \mathbf{r}_{12} \\ \boldsymbol{\rho}_3 \end{pmatrix} \quad (12)$$

and

$$\begin{pmatrix} \mathbf{r}_{31} \\ \boldsymbol{\rho}_2 \end{pmatrix} = \begin{pmatrix} -1/2 & +\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} \mathbf{r}_{12} \\ \boldsymbol{\rho}_3 \end{pmatrix}. \quad (13)$$

radius in the Hamiltonian [see for example (32)], we must then make the substitution:

$$-\frac{\hbar^2}{m} \frac{\partial^2}{\partial R^2} \longrightarrow -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial R^2} \quad \text{with} \quad \mu = m/\sqrt{3}. \quad (9)$$

When it comes to imposing the Bethe–Peierls boundary conditions, we will have to take, for example, the limit $r_{12} \rightarrow 0$, keeping $\mathbf{R}_{12}$ and $\mathbf{r}_3$ fixed, which will lead to the following for the other two coordinate systems:

$$\mathbf{r}_{23} \rightarrow -\frac{\sqrt{3}}{2} \boldsymbol{\rho}_3, \quad \boldsymbol{\rho}_1 \rightarrow -\frac{\boldsymbol{\rho}_3}{2} \quad (14)$$

and

$$\mathbf{r}_{31} \rightarrow \frac{\sqrt{3}}{2} \boldsymbol{\rho}_3, \quad \boldsymbol{\rho}_2 \rightarrow -\frac{\boldsymbol{\rho}_3}{2}. \quad (15)$$

1-3 Faddeev components

Fixing a parameterization of space by one of the three sets of Jacobi coordinates, $(\mathbf{r}_{12}, \boldsymbol{\rho}_3)$ for example, and then looking directly for the eigenfunctions $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \equiv \Psi(\mathbf{r}_{12}, \boldsymbol{\rho}_3)$ leads to difficult calculations, even for the zero-range potential considered here. One reason for this is that this choice of coordinates, which singles out particle 3, is not “democratic”, to use the expression of Nielsen, Fedorov, et al. (2001). More prosaically, it does not facilitate consideration of the Bethe–Peierls boundary conditions for each of the three possible pairs. For the pair (1, 2), this boundary condition in the coordinate system $(\mathbf{R}_{12}, \mathbf{r}_{12}, \boldsymbol{\rho}_3)$ is of course very simple, since it involves taking the limit (figure V.2):

$$\text{Pair (1, 2):} \quad \mathbf{r}_{12} \rightarrow 0 \quad \text{with} \quad \mathbf{R}_{12}, \boldsymbol{\rho}_3 \text{ constant.} \quad (16)$$

But taking into account the boundary condition for the pairs (2, 3) and (3, 1) is less immediate.

To make it easier to take account of the three boundary conditions simultaneously, we will look for the Ψ function in the form:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \chi(\mathbf{r}_{12}, \boldsymbol{\rho}_3) + \chi(\mathbf{r}_{23}, \boldsymbol{\rho}_1) + \chi(\mathbf{r}_{31}, \boldsymbol{\rho}_2), \quad (17)$$

where we have introduced the two Jacobi coordinate systems singling out particle 1 and particle 2 respectively. The function $\chi(\mathbf{r}, \boldsymbol{\rho})$ is called a Faddeev component and its precise construction is detailed in the appendix to this chapter (§5). The structure of equation (17) has the merit of being symmetric by construction under exchange of the three particles, which

is necessary since we are interested here in the problem of three identical bosons².

In this form, each of the three functions $\chi(\mathbf{r}_{ij}, \boldsymbol{\rho}_k)$ appearing in (17) “takes charge” of the short-range divergent behavior of the wave function for the pair (i, j) . Specifically, we impose

$$\chi(\mathbf{r}, \boldsymbol{\rho}) \text{ diverges as } \frac{1}{r} \text{ when } r \rightarrow 0. \quad (18)$$

We will therefore use the expansion

$$r \rightarrow 0 : \quad \chi(\mathbf{r}, \boldsymbol{\rho}) = \frac{A(\boldsymbol{\rho})}{r} + B(\boldsymbol{\rho}) + \mathcal{O}(r) \quad (19)$$

with the coefficients of r^{-1} and r^0 calculated from:

$$A(\boldsymbol{\rho}) = \lim_{r \rightarrow 0} [r \chi(\mathbf{r}, \boldsymbol{\rho})] \quad B(\boldsymbol{\rho}) = \lim_{r \rightarrow 0} \left[\frac{\partial (r \chi(\mathbf{r}, \boldsymbol{\rho}))}{\partial r} \right]. \quad (20)$$

As we indicated above, the Bethe–Peierls boundary condition relates the dominant term in $1/r_{ij}$ to the next order of the expansion, the constant term in $-1/a$. More precisely, in the limit $r_{12} \rightarrow 0$:

$$\text{Term in } (r_{12})^{-1} : \quad \lim_{r \rightarrow 0} [r \chi(\mathbf{r}, \boldsymbol{\rho}_3)] \quad (21)$$

and for the term in $(r_{12})^0$:

$$\lim_{r \rightarrow 0} \left[\frac{\partial (r \chi(\mathbf{r}, \boldsymbol{\rho}_3))}{\partial r} \right] + \chi\left(-\frac{\sqrt{3}}{2} \boldsymbol{\rho}_3, -\frac{1}{2} \boldsymbol{\rho}_3\right) + \chi\left(+\frac{\sqrt{3}}{2} \boldsymbol{\rho}_3, -\frac{1}{2} \boldsymbol{\rho}_3\right) \quad (22)$$

where we have used the limit on the various Jacobi coordinates given in (14-15).

For our problem, the Bethe–Peierls boundary condition therefore reads, for any value of $\boldsymbol{\rho}$,

$$\lim_{r \rightarrow 0} \left[\frac{\partial [r \chi(\mathbf{r}, \boldsymbol{\rho})]}{\partial r} \right] + \chi\left(-\frac{\sqrt{3}}{2} \boldsymbol{\rho}, -\frac{1}{2} \boldsymbol{\rho}\right) + \chi\left(+\frac{\sqrt{3}}{2} \boldsymbol{\rho}, -\frac{1}{2} \boldsymbol{\rho}\right) = -\frac{1}{a} \lim_{r \rightarrow 0} [r \chi(\mathbf{r}, \boldsymbol{\rho})] \quad (23)$$

²There may exist situations in which each Faddeev component is well defined, but $\chi(\mathbf{r}_{12}, \boldsymbol{\rho}_3) + \chi(\mathbf{r}_{23}, \boldsymbol{\rho}_1) + \chi(\mathbf{r}_{31}, \boldsymbol{\rho}_2) = 0$. One then speaks of *spurious solutions* (Nielsen, Fedorov, et al. 2001). We will not encounter any here.

Furthermore, the function $\chi(\mathbf{r}, \boldsymbol{\rho})$ satisfies an eigenvalue equation identical to (11):

$$-\frac{\hbar^2}{m} (\nabla_{\mathbf{r}}^2 + \nabla_{\boldsymbol{\rho}}^2) \chi(\mathbf{r}, \boldsymbol{\rho}) = E \chi(\mathbf{r}, \boldsymbol{\rho}) \quad (24)$$

which corresponds, as already mentioned, to a purely kinetic energy since interactions are taken into account here via the boundary condition (23).

1-4 Hyperradius and Delves angle

At this stage, equation (11), or its counterparts for the other two Jacobi coordinate systems, is an equation in six space variables, which can be parameterized in many ways once a Jacobi coordinate system has been adopted. We will use the following choice³ which specifies the size and shape of the triangle formed by the three particles and then defines the orientation of this triangle in three-dimensional space:

- The hyperradius R , defined by

$$R^2 = r_{12}^2 + \rho_3^2 = \frac{2}{3} (r_{12}^2 + r_{23}^2 + r_{31}^2), \quad (29)$$

³Another choice commonly used in the literature to deal with non-zero-range potentials is to use R , the three Euler angles, and the two angles θ and φ defining the coordinates r_{ij} [see for example Greene, Giannakeas, et al. (2017)]:

$$r_{ij} = \frac{R}{\sqrt{2}} [1 + \sin \theta \sin(\varphi + \nu_{ij})]^{-1/2} \quad (25)$$

with $\nu_{ij} = -\pi/6, -5\pi/6, +\pi/2$ for $(i, j) = (1, 2), (2, 3), (3, 1)$. The kinetic energy operator then reads $\hat{H}_{\text{kin}} = \hat{T}_R + \hat{T}_1 + \hat{T}_2 + \hat{T}_3$, with $\hat{T}_R$ unchanged with respect to (32) and

$$\hat{T}_1 = -\frac{4\hbar^2}{mR^2} \frac{1}{\sin(2\theta)} \frac{\partial}{\partial \theta} \sin(2\theta) \frac{\partial}{\partial \theta} \quad (26)$$

$$\hat{T}_2 = -\frac{2\hbar^2}{mR^2} \frac{1}{\sin^2(\theta)} \left(i \frac{2\partial}{\partial \varphi} - \frac{1}{2\hbar} \cos \theta \hat{J}_z \right)^2 \quad (27)$$

$$\hat{T}_3 = \frac{2\hat{J}_x^2}{mR^2(1 - \sin \theta)} + \frac{2\hat{J}_y^2}{mR^2(1 + \sin \theta)} + \frac{2\hat{J}_z^2}{mR^2}. \quad (28)$$

where $\hat{\mathbf{J}}$ is the total angular momentum of the system. In the angular momentum subspace $J = 0$, the dependence on the Euler angles disappears and the eigenstates of the Hamiltonian are functions of the three variables R, θ, φ (D’Incao & Esry 2005a).

provides information about the nature of the grouping of the three particles: R becomes large as soon as one particle moves away from the other two; a small value of the hyperradius is therefore obtained if, and only if, the three particles are close to each other. Note that the hyperradius (29) is identical for the three Jacobi coordinate systems, since it makes the three variables $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ play identical roles.

- The *Delves angle* α is defined by

$$r_{12} = R \sin \alpha, \quad \rho_3 = R \cos \alpha, \quad 0 \leq \alpha \leq \pi/2. \quad (30)$$

Strictly speaking, we should denote this Delves angle by α_3 , since it gives information about the position of particle 3 relative to the pair 1–2. We can of course also define α_1 and α_2 , but we will not need them in what follows⁴. The Delves angle indicates whether we are dealing with a rather elongated triangle (small values of α) or a rather flattened triangle (α close to $\pi/2$). More precisely, if $\alpha \equiv \alpha_3$ is close to 0, particle 3 is far from the pair 1–2; if α is close to $\pi/2$, particle 3 is close to the midpoint of 1–2 (see figure V.4). On the other hand, when α is close to $\pi/4$, the shape of the triangle is not well defined: it may be elongated if particle 3 is close to 1 or 2, or quasi-equilateral.

- The Jacobi angle $\beta = (\hat{\mathbf{r}}_{12}, \hat{\mathbf{\rho}}_3)$ (which should also have an index 3 to remove any ambiguity). Knowing the hyperradius and the two angles α and β makes it possible to completely specify the size and shape of the triangle formed by the three particles (figure V.5).
- The three remaining angular parameters correspond to the three Euler angles needed to specify the orientation of this triangle in space.

Once we have defined the coordinate system (R, α, Ω) , where Ω denotes collectively the Jacobi angle β and the three Euler angles, we can write the kinetic Hamiltonian $-(\hbar^2/m)(\nabla_{\mathbf{r}}^2 + \nabla_{\mathbf{\rho}}^2)$ involved in (24) in a relatively compact form (Pack & Parker 1987; Yuen 2020):

$$\hat{H}_{\text{kin}} = \hat{T}_R + \hat{T}_\alpha + \hat{T}_\Omega \quad (31)$$

with, for the hyperradial part,

$$\hat{T}_R = -\frac{\hbar^2}{m} \frac{1}{R^5} \frac{\partial}{\partial R} R^5 \frac{\partial}{\partial R}, \quad (32)$$

⁴Note the remarkable relation $\sin^2 \alpha_1 + \sin^2 \alpha_2 + \sin^2 \alpha_3 = 3/2$.

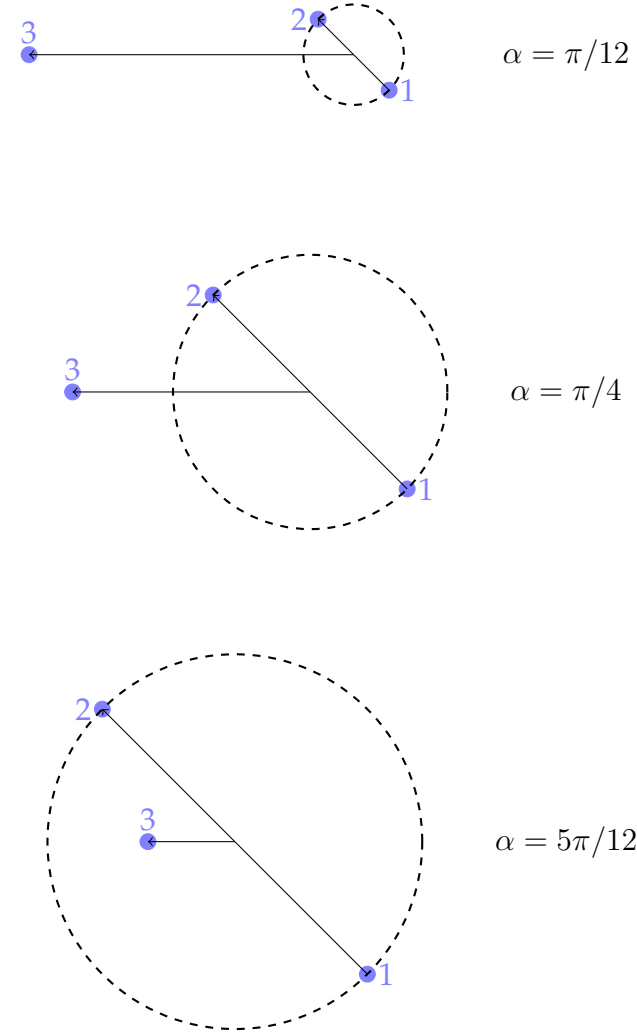


Figure V.4. Three possible configurations for the same hyperradius R and different Delves angles α . The positions of particles 1 and 2 are not completely determined by the knowledge of R and α : we only know that they lie on the dotted circle, diametrically opposite each other.

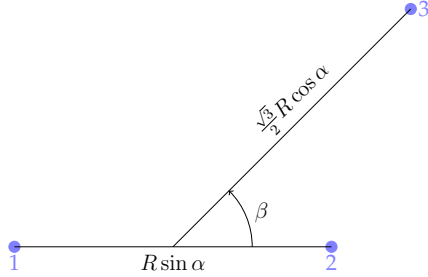


Figure V.5. Determining the shape of the triangle formed by the three particles from the parameters R, α, β .

and for the Delves angle part:

$$\hat{T}_\alpha = -\frac{\hbar^2}{mR^2} \frac{1}{\sin^2(2\alpha)} \frac{\partial}{\partial \alpha} \sin^2(2\alpha) \frac{\partial}{\partial \alpha}. \quad (33)$$

We will not write here the explicit form of $\hat{T}_\Omega$ as a function of the angle β and the Euler angles, but we simply give its structure in terms of the two operators $\hat{\mathbf{L}}$ and $\hat{\mathbf{J}}$, where $\hat{\mathbf{L}}$ denotes the angular momentum of the dimer aligned along $\mathbf{r}$ and $\hat{\mathbf{J}}$ the total angular momentum of the three bodies:

$$\hat{T}_\Omega = \frac{1}{mR^2} \left[\frac{(\hat{\mathbf{J}} - \hat{\mathbf{L}})^2}{\cos^2 \alpha} + \frac{\hat{\mathbf{L}}^2}{\sin^2 \alpha} \right]. \quad (34)$$

When the interactions between the particles are described by any binary potential $V(r_{ij})$, the distances r_{ij} involve R, α and β . The same applies to the eigenstates of the total Hamiltonian (kinetic plus interactions), so that the three terms $\hat{T}_R, \hat{T}_\alpha$ and $\hat{T}_\Omega$ all give a non-trivial contribution. In the case of an interaction described by the pseudo-potential, since the Hamiltonian is purely kinetic, we can immediately place ourselves in the eigensubspace corresponding to $J = L = 0$, which is the only one to give rise to the Efimov effect.

We therefore restrict the search for functions $\chi(\mathbf{r}, \rho)$ to functions of R and α only (or equivalently of $r = R \sin \alpha$ and $\rho = R \cos \alpha$ only). Furthermore, given the structure of $\hat{T}_R$ and $\hat{T}_\alpha$, it is convenient to make the change

of function

$$\chi(r, \rho) = \frac{\Phi(R, \alpha)}{R^{5/2} \sin(2\alpha)} \quad (35)$$

and we arrive at the eigenvalue equation:

$$\left[-\frac{\hbar^2}{m} \left[\partial_R^2 + \frac{1}{R^2} \left(\partial_\alpha^2 + \frac{1}{4} \right) \right] \right] \Phi(R, \alpha) = E \Phi(R, \alpha) \quad (36)$$

We still need to specify the boundary conditions to be imposed on $\Phi(R, \alpha)$.

First of all, it should be noted that the change of function (35) requires the behavior of $\Phi(R, \alpha)$ to be clearly defined at the zeros of $\sin(2\alpha)$ in the denominator, i.e. at $\alpha = 0$ and $\alpha = \pi/2$:

- When $\alpha \rightarrow 0$ at constant R , the variable $r = R \sin \alpha$ tends to 0 and we know that $\chi(r, \rho)$ must diverge as $1/r$. It is therefore sufficient to require $\Phi(R, \alpha)$ to be regular at $\alpha = 0$; it need not vanish at this point.
- When $\alpha \rightarrow \pi/2$ at constant R , the variable $\rho = R \cos \alpha$ tends to 0, which means that particle 3 comes to sit at the midpoint of the segment 1–2 (figure V.4). The function $\chi(r, \rho)$ is regular at this point⁵, and it is therefore necessary to require that the numerator of (35) vanish at least linearly in $\alpha - \pi/2$ at this point:

$$\Phi(R, \frac{\pi}{2}) = 0 \quad (37)$$

Moreover, the boundary condition (23) translates into

$$\left[\frac{\partial \Phi(R, \alpha)}{\partial \alpha} \right]_{\alpha \rightarrow 0} + \frac{8}{\sqrt{3}} \Phi(R, \frac{\pi}{3}) = -\frac{R}{a} \Phi(R, 0) \quad (38)$$

The contribution of $\alpha = 0$ corresponds to the case where particles 1 and 2 move towards each other (figure V.6, left), and the contribution $\alpha = \pi/3$ corresponds to the case where particle 3 can come into contact with either particle 1 or particle 2 (figure V.6, right).

⁵Unless $R \rightarrow 0$, but this case, in which the three particles coincide, is “of zero measure”.

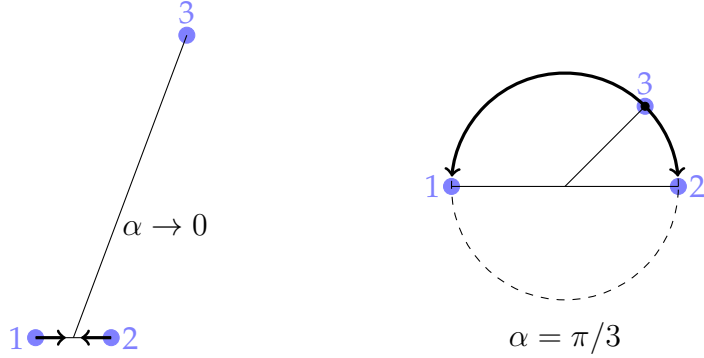


Figure V.6. The two values of the Delves angle α that can bring one particle on top of another, and thus enter the Bethe–Peierls boundary condition (38).

2 The solution in the resonant case

2-1 Separation of variables for $a = \pm\infty$

The structure of the eigenvalue equation (36) lends itself well to the search for eigenfunctions in factorized form of the type $g_1(R) \times g_2(\alpha)$. But the boundary condition (38) is generally not compatible with this factorization. There are nevertheless two cases where this factorization is possible, the resonant case $a = \pm\infty$ and the non-interacting case $a = 0$. We will concentrate here on the resonant case and then check that the non-interacting case gives the expected (trivial) result.

Let us place ourselves in the resonant case and look for a solution of (36-37-38) in the form

$$\Phi(R, \alpha) = \phi(R) F(\alpha). \quad (39)$$

Thanks to the choice $a = \infty$, the boundary conditions (37-38) do not involve the unknown function $\phi(R)$, but only $F(\alpha)$:

$$F(\pi/2) = 0 \quad (40)$$

and

$$\left[\frac{dF}{d\alpha} \right]_{\alpha \rightarrow 0} + \frac{8}{\sqrt{3}} F(\pi/3) = 0. \quad (41)$$

The eigenvalue equation (36) reads

$$-\left[\frac{d^2\phi}{dR^2} + \frac{\phi(R)}{4R^2} \right] F(\alpha) - \frac{\phi(R)}{R^2} \frac{d^2F}{d\alpha^2} = \frac{mE}{\hbar^2} \phi(R) F(\alpha). \quad (42)$$

The procedure is then standard. One first solves the eigenvalue equation for one of the unknown functions, in this case $F(\alpha)$:

$$\boxed{-\frac{d^2F}{d\alpha^2} = s^2 F(\alpha)} \quad (43)$$

where the (real) eigenvalue s^2 must be chosen so as to satisfy the boundary conditions (40-41). The result obtained is then inserted into (42) to determine the solution for the hyperradius:

$$\boxed{-\frac{d^2\phi}{dR^2} + \frac{s^2 - 1/4}{R^2} \phi(R) = \epsilon \phi(R) \quad \text{with} \quad \epsilon = \frac{mE}{\hbar^2}} \quad (44)$$

Here again we find a one-dimensional Schrödinger equation in the $1/r^2$ potential! The question we address in the next section is whether the coefficient s^2 can be negative, so that this potential is attractive and can give rise to bound states.

2-2 Angular equation and the Efimov effect

The solution of the eigenvalue equation for the angular variable, $F'' + s^2 F = 0$ with s^2 real (positive, negative or zero), compatible with the first boundary condition $F(\pi/2) = 0$, reads, up to a multiplicative constant,

$$F(\alpha) = \sin \left[s \left(\frac{\pi}{2} - \alpha \right) \right]. \quad (45)$$

We insert this form into the second boundary condition (41):

$$s \cos(s\pi/2) = \frac{8}{\sqrt{3}} \sin(s\pi/6) \quad (46)$$

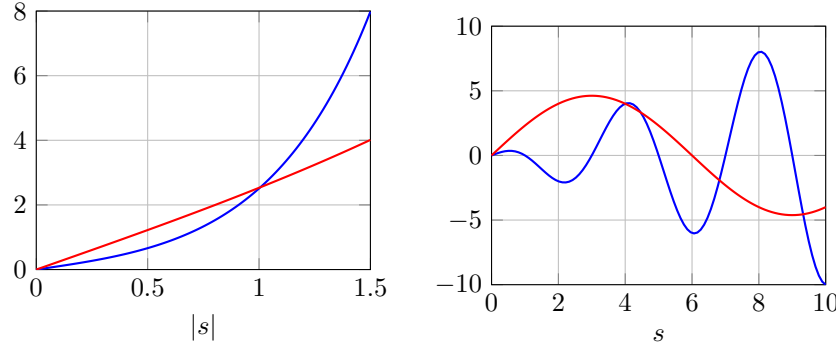


Figure V.7. Left: search for the solutions of (46) with $s^2 < 0$, with this equation rewritten in the form (48) for the variable $|s|$; it has a unique solution given by (47). Right: search for the solutions of (46) with $s^2 > 0$. On each graph, the blue and red curves correspond respectively to the left- and right-hand sides of equations (46) and (48).

where s is real or pure imaginary.

The numbers s satisfying (46) come in pairs $(s, -s)$, the solution $s = 0$ having to be discarded, since it leads to an identically vanishing function $F(\alpha)$. A simple numerical study shows that equation (46) has two types of solution (see also the graphical solution in figure V.7):

- A pair of purely imaginary solutions

$$s_0 = \pm i |s_0| \quad \text{with} \quad |s_0| = 1.00624 \dots \quad (47)$$

equation (46) then being rewritten as

$$|s_0| \cosh(|s_0| \pi / 2) = \frac{8}{\sqrt{3}} \sinh(|s_0| \pi / 6) \quad (48)$$

where all the quantities are real. The equation for the hyperradius then reads

$$-\frac{d^2 \phi}{dR^2} - \frac{|s_0|^2 + 1/4}{R^2} \phi(R) = \epsilon \phi(R) \quad (49)$$

- An infinite family of solutions $\pm s_j$ with s_j real and positive, $j \geq 1$.

As we have seen several times in previous chapters, the condition for the eigenvalue equation (44) on the variable R to admit a bound state, i.e. an eigenvalue $\epsilon < 0$, is that the coefficient of the term in $1/R^2$, here $s^2 - 1/4$, be strictly less than $-1/4$. Hence s^2 must be negative, which selects one and only one type of solution, $s_0 = \pm i |s_0|$, leading to the eigenvalue equation (49).

Once this solution has been identified, the whole procedure developed in the previous chapters applies without modification. From equation (49), we know that:

- It is necessary to introduce a boundary condition at small values of R , for example a hard core at R_0 , to prevent the “fall to the center”. We thus obtain a ground state of energy $E_0 < 0$, whose wave function $\phi(R)$ has no node other than at R_0 .
- Once this condition has been imposed, we obtain infinitely many bound states whose energies form, to a very good approximation, a geometric sequence

$$\frac{E_n}{E_{n+1}} \approx \lambda^2 \quad \text{with} \quad \lambda = e^{\pi/|s_0|} \approx 22.7, \quad \lambda^2 \approx 515 \quad (50)$$

- The zero-energy wave function is log-periodic:

$$\phi(R) = \sin[|s_0| \ln(R/R_0)] \quad (51)$$

and we find this structure for the bound states as well, as long as we restrict ourselves to values of R small compared with their outer turning point.

Note that the angular wave function $F(\alpha)$ found in (45), which can be rewritten as $\sinh[|s_0|(\frac{\pi}{2} - \alpha)]$ in the Efimovian case, is relatively sharply peaked around $\alpha = 0$, which indicates that the trimers obtained in this case have the shape of an elongated triangle, as shown in figure V.8 (Naidon & Endo 2017).

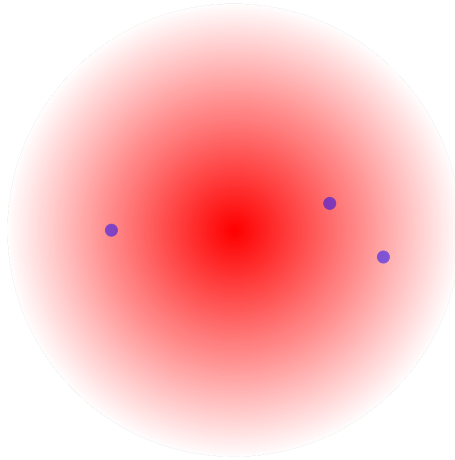


Figure V.8. A typical configuration of an Efimov trimer, corresponding to a small value of the Delves angle α , and therefore an elongated triangle. The state of the three particles is invariant under rotation, which is represented by the red halo. The three blue dots represent a possible (and relatively probable, given a global rotation) result of a measurement of the positions.

2-3 Consistency check: the case without interaction

We were able to solve the eigenvalue problem (36-37-38) in the case $a = \infty$ because it was possible to find the solutions in a factorized form. There is another situation where this is also the case: $a = 0$. We will now check that the expected results are obtained in the absence of interaction.

When the scattering length vanishes (or, more precisely, tends to 0 from below), i.e. when the particles do not interact with each other, the boundary condition (38) imposes

$$a = 0 \quad \Rightarrow \quad \Phi(R, 0) = 0. \quad (52)$$

Here again we look for the solutions of (36) in the factorized form

$$\Phi(R, \alpha) = \phi(R) F(\alpha) \quad (53)$$

with boundary conditions (37-53):

$$F(0) = 0, \quad F(\pi/2) = 0. \quad (54)$$

Here too, the function $F(\alpha)$ must be a solution of the eigenvalue equation $F'' + s^2 F = 0$, and the boundary conditions (54) lead immediately to

$$F(\alpha) = \sin(s\alpha) \quad \text{with} \quad s = 2j, \quad j \in \mathbb{N}^*. \quad (55)$$

We insert this form into (36) to deduce the equation satisfied by $\phi(R)$:

$$-\frac{d^2\phi}{dR^2} + \frac{4j^2 - 1/4}{R^2} \phi(R) = \epsilon \phi(R). \quad (56)$$

This corresponds to a Schrödinger equation for the repulsive (centrifugal-type) potential $(4j^2 - 1/4)/R^2$. All the eigenvalues ϵ are therefore non-negative, and there is no bound state in this case. This is of course the expected result in the absence of interaction.

3 The solution in the general case

3-1 Separation of angular and radial variables

When the scattering length a is neither zero nor infinite, taking into account the boundary condition (38) requires the manipulation of two-variable functions, which is numerically complicated.

In practice, a powerful approach is to assume, in a first step, that R is a fixed parameter in order to solve the angular problem described by the variable α , and then, in a second step, to insert the result into the equation for R . The underlying physical idea is that the Delves angle α is a fast variable and the hyperradius a slow variable, which allows the corresponding approximations to be made in the second step.

Mathematically, this approach is made possible by the fact that the boundary condition (38) is local in R , i.e. it involves only the values of the function $\Phi(R, \alpha)$ at a given point R , but not its partial derivatives with respect to R .

We therefore seek to solve (36) with boundary conditions (37-38) by writing the solution in the form

$$\Phi(R, \alpha) = \sum_i \phi_i(R) F_i(\alpha; R) \quad (57)$$

where F_i are functions of α at R fixed, solutions of the eigenvalue equation

$$\boxed{-\frac{d^2 F_i(\alpha; R)}{d\alpha^2} = s_i^2(R) F_i(\alpha; R)} \quad (58)$$

and satisfying the boundary conditions (37-38), always at fixed R .

Once the set of eigenfunctions F_i and eigenvalues s_i^2 is known, we insert the form (57) into the eigenvalue equation (36) and obtain an infinite set of coupled equations for the $\phi_i(R)$:

$$-\frac{d^2 \phi_i}{dR^2} + \frac{s_i^2(R) - 1/4}{R^2} \phi_i(R) + \sum_j \hat{O}_{ij}(R) \phi_j(R) = \epsilon \phi_i(R). \quad (59)$$

The operators $\hat{O}_{ij}(R)$ have a structure which is usual in the adiabatic approximation formalism; they involve the scalar products of the functions $F_i(\alpha; R)$ and $F_j(\alpha; R)$ and their derivatives with respect to R . They describe the “rotation” of the basis vectors on which the expansion is performed, i.e. the R dependence of the angular functions F_i . The term $i = j$ corresponds to a *geometric potential* (scalar and vector) that adds to the *hyperspherical potential* $[s_i^2(R) - 1/4]/R^2$ appearing in the evolution (59) of the wave function $\phi_i(R)$. The off-diagonal terms $i \neq j$ describe couplings between the different channels.

We will not discuss in this chapter the form of the operators $\hat{O}_{ij}(R)$ [see for example Braaten & Hammer (2006), eqs. (114)-(116) for a detailed expression], but we will come back to it in the next chapter when discussing the value of the three-body parameter for a van der Waals interaction.

At resonance, or for zero interaction (see the previous section), the functions $F_i(\alpha; R)$ are in fact independent of R , and all the $\hat{O}_{ij}(R)$ then vanish. Away from these particular values of the scattering length a , the operators $\hat{O}_{ij}(R)$ are non-zero and, depending on the accuracy required in the numerical calculation, a certain number of them can be taken into account. To lowest order, the hyperspherical adiabatic approximation consists in neglecting all the operators $\hat{O}_{ij}(R)$ and keeping only

$$\boxed{-\frac{d^2 \phi_i}{dR^2} + \frac{s_i^2(R) - 1/4}{R^2} \phi_i(R) \approx \epsilon \phi_i(R)} \quad (60)$$

All the physics of the problem—at least for the zero-angular-momentum states to which we have restricted ourselves—is then contained in the eigenvalues $s_i^2(R)$ of the angular problem, which define the hyperspherical potentials.

3-2 Hyperspherical potentials

The search for eigenvalues $s_i^2(R)$ and eigenfunctions $F_i(\alpha; R)$ for the eigenvalue equation (58) with boundary conditions (37-38) is carried out in the same way as for the resonant case in §2. We look for the eigenfunction at fixed R in the form

$$F(\alpha; R) = \sin \left[s(R) \left(\frac{\pi}{2} - \alpha \right) \right] \quad (61)$$

which automatically ensures that F is a solution of $F'' + s^2 F = 0$ with the boundary condition $F(\pi/2; R) = 0$. Taking into account the boundary condition (38) imposes:

$$-s \cos(s\pi/2) + \frac{8}{\sqrt{3}} \sin(s\pi/6) = -\frac{R}{a} \sin(s\pi/2) \quad (62)$$

which is solved numerically for each value of R/a .

Here we are interested in the smallest eigenvalue $s_{\min}^2(R)$ of (58):

- For $a > 0$, this eigenvalue is negative for all values of R , so $s_{\min}(R)$ is pure imaginary.
- For $a < 0$, $s_{\min}^2(R)$ is negative for small values of R ($R \lesssim |a|$) and $s_{\min}^2(R)$ is positive for larger values.

The variation of $s_{\min}^2(R)$ in these two cases is shown in figure V.9 (top) [see also figures 4 and 5 in Nielsen, Fedorov, et al. (2001)]. Note that the two solutions for $a > 0$ and $a < 0$ tend to $-|s_0|^2$ when $R \ll |a|$ with $|s_0| = 1.00624 \dots$, which recovers the case $a = \pm\infty$ discussed in the previous section and which gives rise to the Efimov effect. When we take the opposite limit $R \gg |a|$ for $a < 0$, we find the result $s = 2$ corresponding to the lowest value of the case without interaction [cf. (55)]. When $R \gg a$ with $a > 0$, the

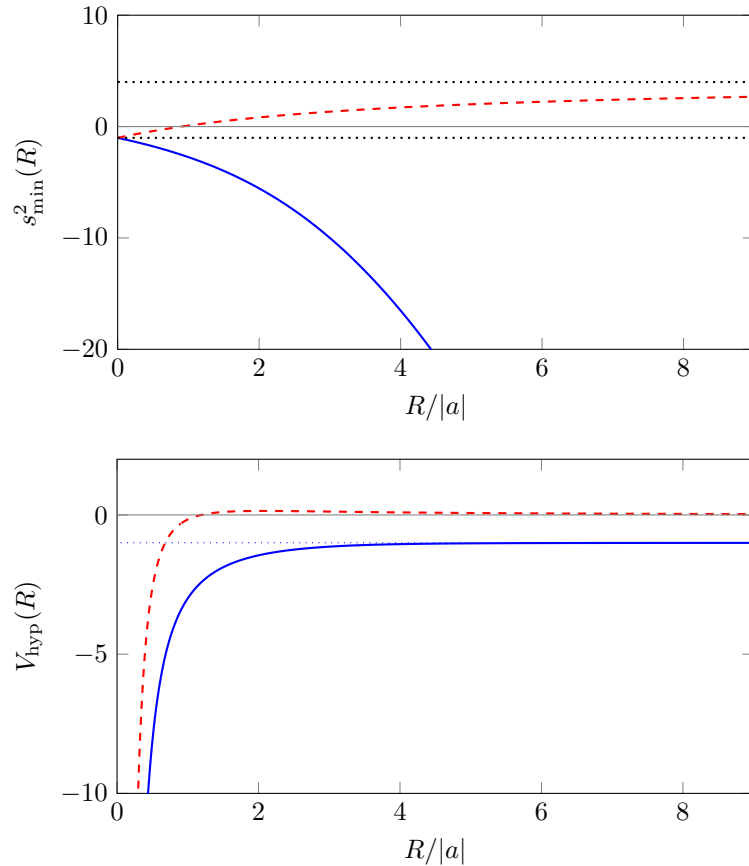


Figure V.9. Top: the first eigenvalue $s_{\min}^2(R)$ for $a > 0$ (solid blue curve) and for $a < 0$ (dashed red curve). The two dotted lines indicate the zero-interaction limit ($s = 2$, see (55)) and the resonant case $s_0 = i \times 1.00624$. Bottom: the associated hyperspherical potential $V_{\text{hyp}}(R) = [s_{\min}^2(R) - 1/4]/R^2$, in units of $\hbar^2/ma^2$. In the case $a > 0$, we recover the dimer energy $-\hbar^2/ma^2$ in the limit $R \rightarrow \infty$ (dotted line).

value $s_{\min}^2(R)$ tends to $-\infty$, corresponding to the formation of the bound state of the dimer.

Figure V.9 (bottom) shows the associated hyperspherical potentials:

$$V_{\text{hyp}}(R) = \frac{\hbar^2}{m} \frac{s_{\min}^2(R) - 1/4}{R^2} \quad (63)$$

For $R \ll |a|$, the fact that $s_{\min}^2(R)$ tends to $-(1.00624)^2$ means that we recover the potential in $1/R^2$ of the resonant case. At large values of R , $V(R)$ tends to 0 for $a < 0$ and to the energy of the bound state of the dimer, $-\hbar^2/ma^2$, for $a > 0$.

We have concentrated here on the smallest eigenvalue $s_{\min}^2(R)$ of (58). All the other eigenvalues are strictly positive (whatever the sign of a) and they lead for $R \ll a$ to a repulsive hyperspherical potential varying as $1/R^2$ (Braaten & Hammer 2006). Consequently, only the potential associated with the lowest eigenvalue can give rise to “universal” three-body bound states.

3-3 Universality for the three-boson problem

Once we have fixed the three-body parameter which regularizes the problem for $a = \pm\infty$, we can use the hyperspherical formalism to determine the variations with a of the eigenstates of the system.

The general form of this variation is very similar to that found in the previous chapter in the Born–Oppenheimer approximation for the mMM problem. We find a series of energy branches corresponding to the different bound states of the trimer. As in the mMM case, the diagram possesses a remarkable scale invariance: the knowledge of one branch in the $(1/a, E)$ plane allows us to deduce all the others by a simple homothety with center $(0, 0)$. The only difference from the mMM case is that the homothety ratio is now fixed, and determined by $\lambda = e^{\pi/|s_0|}$ with $|s_0| = 1.00624$, whereas it was a function of M/m in the previous case.

We have plotted in figure V.10 this energy branch for one of the trimer states, in the $(\sqrt{1/|a|}, |E|^{1/4})$ coordinate system already used in Chapter 4 for the mMM problem. The solid curve is the result of an accurate numerical calculation (Braaten, Hammer & Kusunoki 2003; Naidon

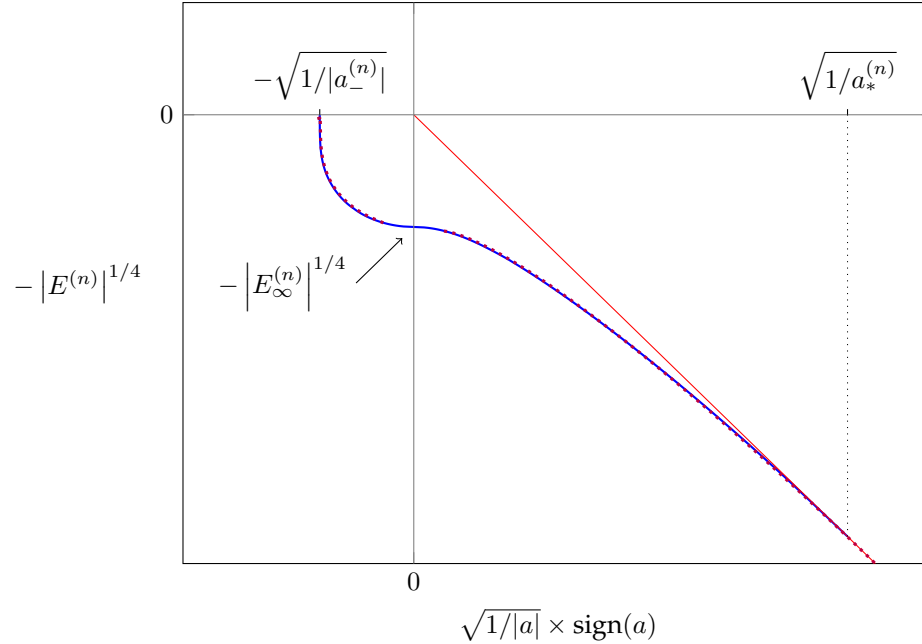


Figure V.10. Solid curve: accurate numerical calculation of the energy branch $\mathcal{E}^{(n)}$ of the n th Efimov trimer as a function of $1/a$. Dotted line: solution of the one-channel Schrödinger equation (60) for the hyperspherical potential (63). The scattering length a and the energy $\mathcal{E}^{(n)}$ are defined here up to a multiplicative constant, which depends on the three-body parameter R_0 . The red line on the $a > 0$ side represents the dimer of energy $E = -\hbar^2/ma^2$. The energy branch of the $(n+1)$ th trimer can be deduced from this curve by a homothety of center O and ratio $1/\lambda$. The solid curve was plotted using the parameterization provided by Naidon & Endo (2017) [their equation (2.40)].

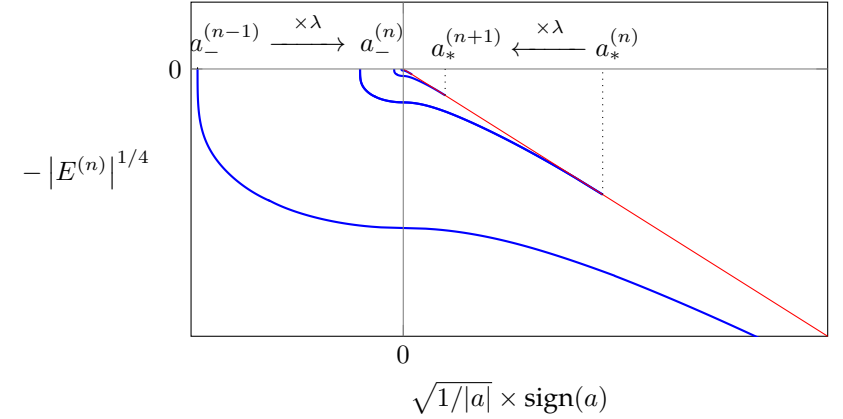


Figure V.11. The energies of the Efimov trimers in the vicinity of a resonance as a function of $1/a$. The red line on the $a > 0$ side represents the dimer with energy $E = -\hbar^2/ma^2$.

& Endo 2017). The dotted curve represents the solution of the one-channel Schrödinger equation (60), taking into account only the hyperspherical potential $V_{\text{hyp}}(R)$ of the lowest channel given in (63) and plotted in figure V.9. We can see that this one-channel approximation, which amounts to neglecting the contributions of all the $\mathcal{O}_{ij}$ operators, is excellent for our model of a zero-range binary interaction.

Figure V.11 also shows a representation of the stacking of the different branches. Let us summarize the main features of these two diagrams:

- On the $a < 0$ side of the resonance, we find the thresholds $a_-^{(n)}$, $n = 0, 1, \dots$, for the appearance of the trimers, which form a geometric sequence of common ratio $\lambda \approx 22.7$. For each threshold, we predict a peak in the three-body recombination rate L_3 in an atomic gas, to which we will return in the next chapter.
- At resonance, the energies of the trimers form a geometric sequence of common ratio $\lambda^2 \approx 515$ [cf. (50)].
- On the $a > 0$ side of the resonance, the energy of the n th trimer meets

that of the dimer (plus a free atom at rest) at a value $a_*^{(n)}$. A resonance in the inelastic atom–dimer relaxation rate β_{AD} is expected at these points $a_*^{(n)}$. The values of $a_*^{(n)}$ also form a geometric sequence of common ratio λ .

- The values of $a_-^{(n)}$ and $a_*^{(n)}$ (on either side of the resonance) are related by [see for example Braaten & Hammer (2006) and Xie, Van de Graaff, et al. (2020) and figure V.10]:

$$\frac{a_-^{(n)}}{a_*^{(n)}} \approx 21.3 \quad \Longleftrightarrow \quad \frac{a_-^{(n-1)}}{a_*^{(n)}} \approx 0.94 \quad (64)$$

The value of $a_-^{(n)}$ and the wave number at resonance $\kappa_\infty^{(n)}$, defined by $E_\infty^{(n)} = -\hbar^2 (\kappa_\infty^{(n)})^2 / m$, are related by (Naidon & Endo 2017):

$$a_-^{(n)} \kappa_\infty^{(n)} \approx 1.51 \quad (65)$$

As in the mMM case, these scaling laws are better satisfied the larger n is.

4 A first example: the helium trimer

Following Efimov's predictions, physicists searched for systems in which the required conditions could be achieved, with both atoms and nuclei. The interactions had to occur essentially at low energy, describable by s -wave scattering, and the associated scattering length a had to be large compared with the range b of the potentials involved, which is *a priori* an exceptional situation: we usually have $a \sim b$.

Quantum gases, with their Fano–Feshbach scattering resonances, are of course ideal candidates for testing this physics, since they make it possible to achieve arbitrarily large scattering lengths at temperatures several orders of magnitude below the energy scale $\hbar^2 / mb^2$. In the next chapter, we will describe in detail a number of experiments carried out with these gases since 2005. In this section, we will present the results for an atom that quickly appeared very promising: helium (Lim, Duffy, et al. 1977).

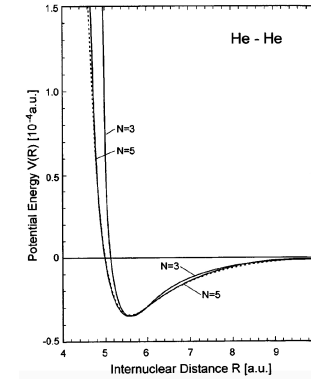


Figure V.12. The interaction potential between two helium atoms in their ground state. The number N indicates the order of the calculation in a multipole expansion of the interaction [see the 2021 lecture series, Chapter 1, for more details]. Figure taken from Tang & Toennies (2003).

4-1 A good candidate: the helium atom

The interaction potential between two helium atoms is well known. We described it in the 2021 lecture series. Its range, characterized by the van der Waals length R_{vdW} , is 0.27 nm and the scattering length $a = 9.04$ nm is ≈ 30 times greater. This potential well, plotted in figure V.12, admits one and only one bound state, which was observed for the first time by Schöllkopf & Toennies (1994) in an atom interferometry experiment that we briefly recall below. The binding energy of this dimer ($\sim 10^{-7}$ eV) is much lower than the depth of the potential well between the two atoms ($\sim 10^{-3}$ eV), indicating that it is only very marginally bound (Grisenti, Schöllkopf, et al. 2000). The average distance between the two atoms is ~ 5 nm, comparable to the scattering length and much greater than R_{vdW} .

In the experiment by Schöllkopf & Toennies (1994), a supersonic beam of helium is formed from a high-pressure container (15 bar) with a hole 5 microns in diameter. The beam leaving this hole propagates in a vacuum, cools as a result of the supersonic expansion and thus becomes quasi-monokinetic ($\Delta v/v \lesssim 5\%$). The wavelength associated with each type of particle (atom, dimer, trimer), $\lambda_{dB} = h/mv$, is then well defined. Thus, for

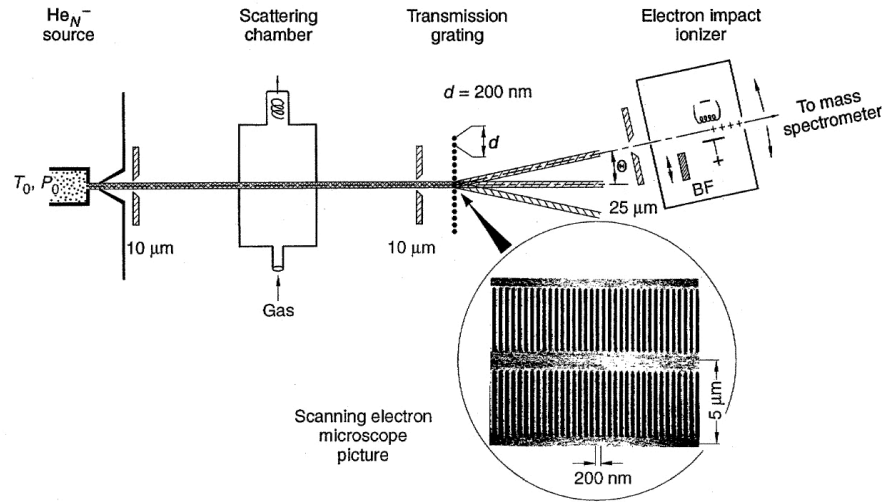


Figure V.13. Experimental setup using matter-wave diffraction by a grating to detect the presence of helium dimers and trimers in a supersonic beam of atomic helium. Figure taken from Schöllkopf & Toennies (1994).

a temperature of 30 K, we have $\lambda_{dB} = 0.18$ nm for He atoms.

This beam is collimated by two 10 micron wide slits, located 47 cm apart, and then passes through a periodic grating on which the particles can be diffracted (figure V.13). The grating period is $d = 200$ nm and diffraction peaks are expected to be observed at angles $\theta_n \approx n\lambda_{dB}/d$.

An example of the signal is shown in figure V.14. It shows a main peak on the left, corresponding to non-diffracted particles. On the right, for an angle θ_1 , the large peak corresponds to the first order ($n = 1$) diffraction of the atoms. Between these two large peaks is the signal of interest. We see two peaks at $\theta_2 = \theta_1/2$ and $\theta_3 = \theta_1/3$, which correspond to particles whose wavelengths are respectively 2 and 3 times shorter than those of the atoms. These are the dimer and the trimer respectively, which travel at the same speed as the atoms, owing to collisions at the exit of the source, but have masses 2 and 3 times larger.

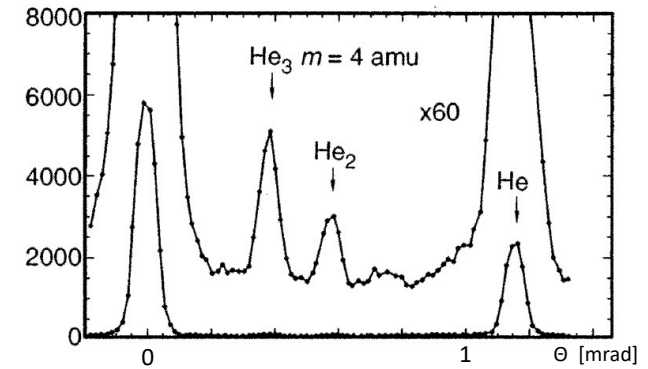


Figure V.14. Angular distribution of the particles diffracted by the grating. Since the beam is monokinetic, comparison of the diffraction angles gives a direct indication of the mass of the diffracted particles. The large peak on the left corresponds to the non-diffracted beam, and the large peak on the right to the first order of diffraction for helium atoms. The two small intermediate peaks reveal the existence of He₂ dimers and He₃ trimers. Figure taken from Schöllkopf & Toennies (1994).

4-2 The ground state of the He₃ trimer

The Schöllkopf & Toennies (1994) experiment therefore reveals the existence of a He₃ bound trimer. The very good knowledge of the interaction potential between two helium atoms provides a good understanding of the structure of this trimer. Its size is of the order of a nanometer—much smaller than that of the dimer—and its structure is close to an equilateral triangle.

Figure V.15 shows the usual curve giving the binding energy of the trimer in the $(1/a, E)$ plane. This curve was obtained by taking the true potential (leading to the scattering length $a = 9.04$ nm) and multiplying it by a dimensionless factor ζ . We observe the following elements (Braaten & Hammer 2006):

- For $\zeta = 1$ (the “true” potential), we expect two bound trimers: one of energy -131.84 mK and size ~ 1 nm [the one observed by Schöllkopf

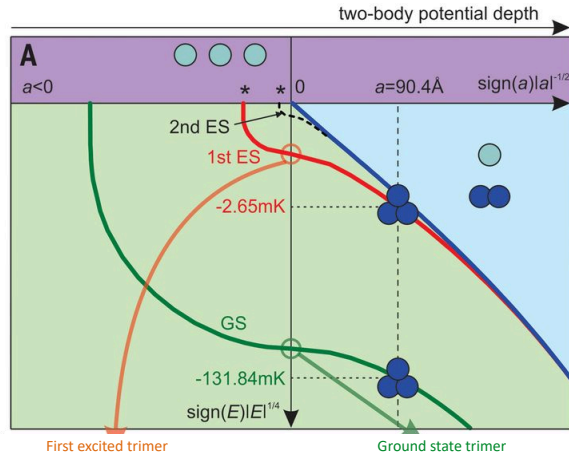


Figure V.15. Helium dimer and trimer: energy diagram calculated for the two-body interaction potential $\zeta V(r)$. For $\zeta = 1$, we obtain the “true” He–He interaction potential. The scattering resonance $a = \pm\infty$ is obtained for $\zeta = 0.97$. Figure adapted from Kunitski, Zeller, et al. (2015).

& Toennies (1994)], and another, much more weakly bound, of energy $E = -2.65$ mK and size ~ 8 nm.

- When ζ is decreased, the scattering length becomes infinite for $\zeta = 0.97$. The dimer state then disappears and there are infinitely many trimer states. The ratio between the energies of the ground-state trimer and the first excited trimer is 570 (to be compared with the factor 515 expected for the zero-range model).
- The branch of the ground-state trimer disappears for $\zeta \approx 0.9$.
- When ζ is increased above 1, we see that unlike in the case of the zero-range potential, the branch of the ground-state trimer does not join the dimer branch, whereas the branch of the excited trimer does.

This raises the question of the Efimovian nature of the ground-state trimer. As pointed out by Braaten & Hammer (2006), the fact that going from $a = 9$ nm to $a = \infty$ gives “almost” the right ratio between the energies of the ground-state trimer and the first excited trimer argues in favor

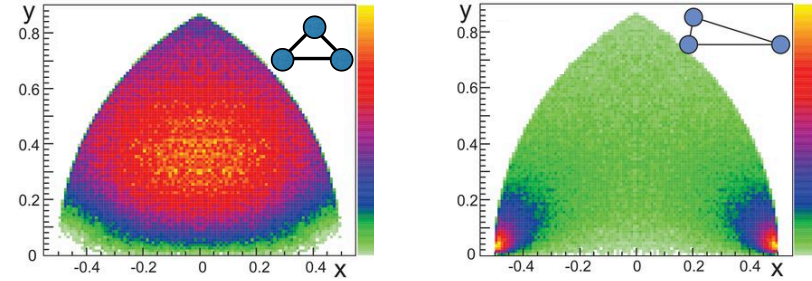


Figure V.16. Distribution of atoms in a helium trimer. By convention, the two atoms furthest apart are placed in the bottom left and right corners. The color encodes the probability density for finding the third atom. Left: theoretical prediction for the ground-state trimer. Right: theoretical prediction for the excited trimer. Figure adapted from Kunitski, Zeller, et al. (2015).

of a positive answer. However, the behavior at $\zeta > 1$ is different from that expected: the scattering length a_* does not exist.

Perhaps more problematically, the geometry of this trimer is not what would be expected for an Efimov trimer, namely an elongated isosceles triangle. This “defect” is illustrated in figure V.16, left. To produce this figure, the two atoms furthest apart within the trimer are placed in the bottom left and right corners. The probability density for finding the third atom is shown in false color. For an elongated Efimov-type trimer, we expect to find this third atom close to one of the two bottom corners. For the ground-state trimer, a very different distribution is observed. For the excited trimer, on the other hand, the predicted distribution corresponds well to that expected for an Efimov trimer (figure V.16, right). This point naturally led the experimenters to try to identify this excited trimer.

4-3 The excited He_3 trimer

In the search for the excited He_3 trimer, an initial series of experiments was carried out in the Göttingen group. One strategy that was explored is shown in figure V.17. It consists in carrying out the diffraction experiment with the grating tilted, so as to take advantage of a “sieve” effect. If

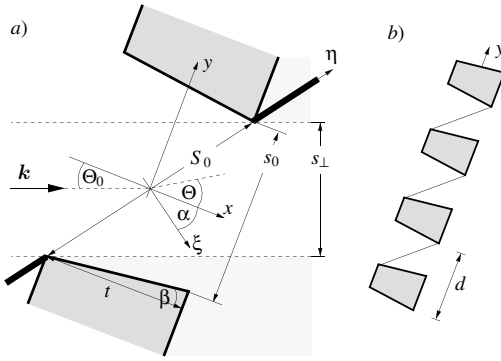


Figure V.17. Diffraction experiment carried out with an inclined grating, to filter the size of the diffracted objects. Figure taken from Brühl, Kalinin, et al. (2005).

the object to be diffracted is too large, it is unlikely to be transmitted by the diffraction grating and a drop in the signal should be observed.

Brühl, Kalinin, et al. (2005) concluded from their experiment that the size of the trimer they observed was always compatible with the size of the ground-state trimer, which was significantly smaller than the size of the dimer. They were thus able to place an upper limit of the order of 6 % on the proportion of excited trimers, whereas they were expecting a proportion of at least 10 %. Their conclusion was as follows: “We feel that the difference between the expectation of 10% and the experimental upper limit of 6% is sufficient to entertain the possibility that the $^4\text{He}_3$ Efimov state does, in fact, not exist despite the over 40 theory publications which have appeared since 1977.”

The search for the excited trimer was taken up in a different way by Kunitski, Zeller, et al. (2015). After selecting the trimers using a matter-wave diffraction experiment like that of Schöllkopf & Toennies (1994), they ionized the three atoms with a very short laser pulse (30 fs) and characterized the Coulomb explosion that followed this ionization. Once the three ions had been detected with position resolution, solving the classical equations of motion made it possible to determine the initial spatial distribution of the atoms (figure V.18).

Kunitski, Zeller, et al. (2015) observed a bimodal distribution, corre-

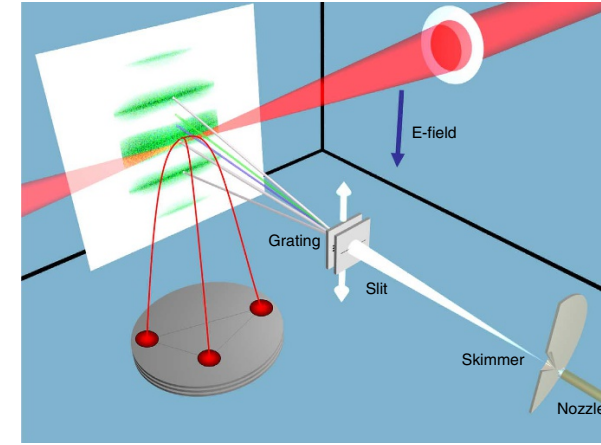


Figure V.18. Coulomb explosion of a helium trimer. Figure taken from Voigtsberger, Zeller, et al. (2014).

sponding to the sum of two radically different distributions. The weight of the two components varies strongly with the pressure of the supersonic beam (figure V.19). At relatively high pressure, only the ground-state trimer is formed. Since it corresponds to closely spaced atoms, a large energy (~ 5 eV) is released when the atoms are suddenly ionized. At low pressure, by contrast, there is a significant contribution from the excited trimer, which gives rise to a much lower Coulomb energy (~ 0.57 eV). This unexpected variation in the fraction of excited trimers with beam pressure explains the negative result of the Brühl, Kalinin, et al. (2005) experiment. Forty years after its existence was predicted by Lim, Duffy, et al. (1977), the excited helium trimer was finally observed!

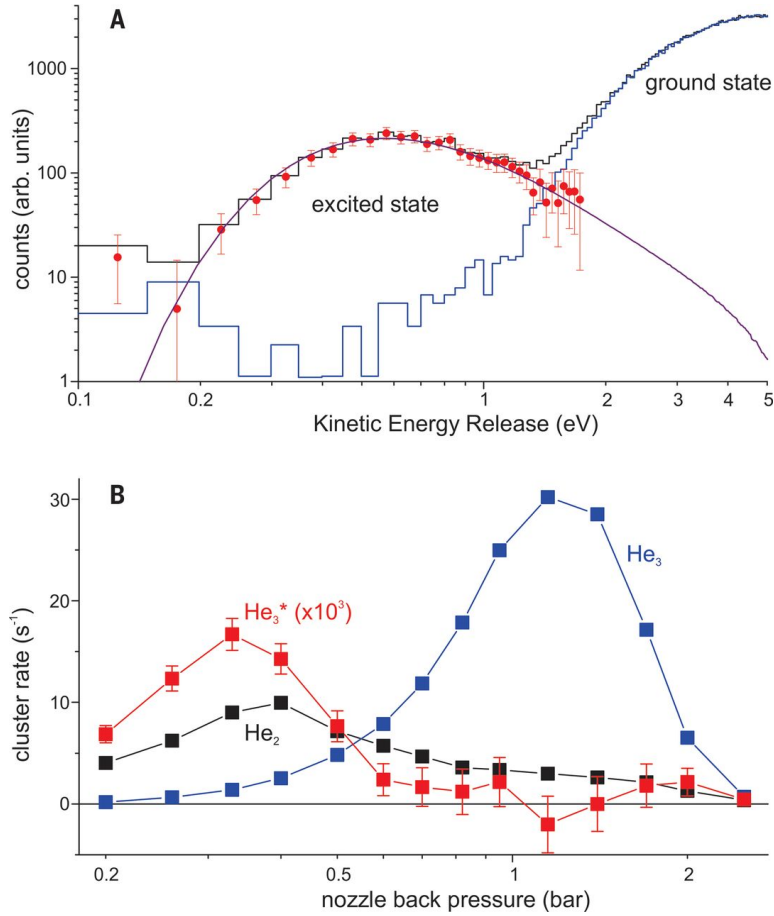


Figure V.19. Top: bimodal distribution of the energy released during the Coulomb explosion of Efimov trimers. The black curve was obtained in the low-pressure regime, $P = 0.33$ bar, for which both trimers are present. The blue curve was obtained in the high-pressure regime, where only the ground-state trimer is formed. The red dots represent the difference between the black and blue curves. Bottom: contributions of the ground-state and excited trimers as a function of the helium beam pressure. Figure taken from Kunitski, Zeller, et al. (2015).

5 Appendix: Skorniakov–Ter-Martirosian eq.

5-1 Definition of Faddeev components

Let us consider a three-body wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ solution of the Schrödinger equation

$$(\hat{H}_0 + \hat{V}) |\Psi\rangle = E |\Psi\rangle \quad (66)$$

where $\hat{H}_0$ is the kinetic energy operator for the three particles and $\hat{V}$ is the sum of the three binary potentials.

$$\hat{V} = \hat{V}_{12} + \hat{V}_{23} + \hat{V}_{31}. \quad (67)$$

At this stage, we consider regular potentials, and we can take the zero-range limit later. The function Ψ , solution of (66), satisfies

$$|\Psi\rangle = \hat{G}_0 \sum_{(ij)} \hat{V}_{ij} |\Psi\rangle \quad \text{with} \quad \hat{G}_0 = \frac{1}{E - \hat{H}_0}. \quad (68)$$

We restrict ourselves here to solutions of negative energy (bound states), so that there is no problem associated with possible poles of $\hat{H}_0$.

The Faddeev components introduced in §1-3 are defined as

$$|\chi_1\rangle = \hat{G}_0 \hat{V}_{23} |\Psi\rangle \quad |\chi_2\rangle = \hat{G}_0 \hat{V}_{31} |\Psi\rangle \quad |\chi_3\rangle = \hat{G}_0 \hat{V}_{12} |\Psi\rangle \quad (69)$$

According to (68), we therefore have

$$|\Psi\rangle = |\chi_1\rangle + |\chi_2\rangle + |\chi_3\rangle \quad (70)$$

and the three Faddeev components satisfy

$$\hat{H}_0 |\chi_3\rangle + \hat{V}_{12} (|\chi_1\rangle + |\chi_2\rangle + |\chi_3\rangle) = E |\chi_3\rangle \quad (71)$$

and the two equations deduced from it by circular permutation. Equation (71) can also be written as

$$|\chi_3\rangle = \hat{G}_0 \hat{V}_{12} |\chi_3\rangle + \hat{G}_0 \hat{V}_{12} (|\chi_1\rangle + |\chi_2\rangle) \quad (72)$$

and we will use this expression in §5-3 to deal with the case of a separable potential.

5-2 Separable one-body potential

A one-body potential is said to be separable when its action on a state $|\psi\rangle$ is that of a projector, up to a multiplicative factor [see the 2021 lecture series, Chapter 5, §3]:

$$\hat{V} = V_0 |\phi_0\rangle\langle\phi_0|, \quad (73)$$

i.e. in the position representation⁶

$$\hat{V} \psi(\mathbf{r}) = \alpha V_0 \phi_0(\mathbf{r}) \quad \text{with} \quad \alpha = \int \phi_0^*(\mathbf{r}) \psi(\mathbf{r}) d^3r \quad (76)$$

and in terms of momentum (or rather wave vector, to avoid factors of $\hbar$):

$$\hat{V} \tilde{\psi}(\mathbf{q}) = \alpha V_0 \tilde{\phi}_0(\mathbf{q}) \quad \text{with} \quad \alpha = \int \tilde{\phi}_0^*(\mathbf{q}) \tilde{\psi}(\mathbf{q}) \frac{d^3q}{(2\pi)^3}. \quad (77)$$

The state $|\phi_0\rangle$ is chosen to be normalized:

$$\int |\phi_0(\mathbf{r})|^2 d^3r = 1 \quad \int |\tilde{\phi}_0(\mathbf{q})|^2 \frac{d^3q}{(2\pi)^3} = 1. \quad (78)$$

Note that a separable potential is in general non-local, since $\hat{V} \psi(\mathbf{r})$ depends on the values of ψ at all points in space through the scalar product α . An exception corresponds to the choice $|\phi_0\rangle = |\mathbf{r}_0\rangle$, which corresponds to a contact interaction at the point $\mathbf{r}_0$.

The search for possible bound states ($E < 0$) of a separable potential is very simple in the momentum representation. Let us take $V_0 < 0$ and define for a particle of mass m_r

$$V_0 = -\frac{\hbar^2 k_0^2}{2m_r} \quad E = -\frac{\hbar^2 \kappa^2}{2m_r}. \quad (79)$$

⁶We use the conventions

$$\langle \mathbf{r} | \mathbf{q} \rangle = e^{i\mathbf{q} \cdot \mathbf{r}}, \quad \langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}'), \quad \langle \mathbf{q} | \mathbf{q}' \rangle = (2\pi)^3 \delta(\mathbf{q} - \mathbf{q}'), \quad (74)$$

so that the closure relations in momentum and position space read

$$\hat{1} = \int |\mathbf{q}\rangle\langle\mathbf{q}| \frac{d^3q}{(2\pi)^3} = \int |\mathbf{r}\rangle\langle\mathbf{r}| d^3r. \quad (75)$$

The Schrödinger equation $(\hat{H}_0 + \hat{V}) |\psi\rangle = E |\psi\rangle$ with $\hat{H}_0 = \hat{p}^2/2m_r$ gives:

$$\frac{\hbar^2 q^2}{2m_r} \tilde{\psi}(\mathbf{q}) + \alpha V_0 \tilde{\phi}_0(\mathbf{q}) = E \tilde{\psi}(\mathbf{q}) \quad (80)$$

which leads to

$$\tilde{\psi}(\mathbf{q}) = \alpha \frac{k_0^2}{q^2 + \kappa^2} \tilde{\phi}_0(\mathbf{q}) \quad (81)$$

For this solution to be acceptable, we need to check that it is self-consistent, i.e. that it gives back the correct scalar product α . This selects the only possible energy, as the solution of

$$\frac{1}{k_0^2} = \int \frac{|\tilde{\phi}_0(\mathbf{q})|^2}{q^2 + \kappa^2} \frac{d^3q}{(2\pi)^3} \quad (82)$$

5-3 Three-body problem and separable potentials

A binary potential $\hat{V}_{12}$ is said to be separable if its action on the relative variable is as described above, while leaving the center-of-mass variable untouched. We assume here that the three-body potential $\hat{V}$ is a sum of separable binary potentials $\hat{V}_{ij}$. It is then possible to simplify considerably the search for the energies of the bound states of the three-body problem [see for example Naidon, Endo & Ueda (2014), Naidon & Endo (2017), and Greene, Giannakeas, et al. (2017)].

Let us consider equation (72), which we now put into a readily usable form. The state $|\chi_3\rangle$ is defined as a function of the two Jacobi coordinates $\mathbf{r}_{12}, \boldsymbol{\rho}_3$:

$$\langle \mathbf{r}_{12}, \boldsymbol{\rho}_3 | \chi_3 \rangle = \chi(\mathbf{r}_{12}, \boldsymbol{\rho}_3). \quad (83)$$

To exploit the separability of $\hat{V}_{12}$, we write (72) in momentum space. The conjugate momenta of a given set of Jacobi coordinates, for example

$$\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1 \quad \boldsymbol{\rho}_3 = \frac{2}{\sqrt{3}} \left[\mathbf{r}_3 - \frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2) \right], \quad (84)$$

are written as

$$\mathbf{q}_{12} = \frac{1}{2} (\mathbf{k}_2 - \mathbf{k}_1) \quad \mathbf{Q}_3 = \frac{1}{\sqrt{3}} \left[\mathbf{k}_3 - \frac{1}{2} (\mathbf{k}_1 + \mathbf{k}_2) \right]. \quad (85)$$

We define the Fourier transform of $\chi(\mathbf{r}_{12}, \boldsymbol{\rho}_3)$ with respect to the two variables $\mathbf{r}_{12}, \boldsymbol{\rho}_3$:

$$\tilde{\chi}(\mathbf{q}_{12}, \mathbf{Q}_3) = \int e^{-i(\mathbf{q}_{12} \cdot \mathbf{r}_{12} + \mathbf{Q}_3 \cdot \boldsymbol{\rho}_3)} \chi(\mathbf{r}_{12}, \boldsymbol{\rho}_3) d^3 r_{12} d^3 \rho_3 \quad (86)$$

and we use the expression for $\hat{H}_0$ in terms of these variables:

$$\hat{H}_0 = -\frac{\hbar^2}{m} (\nabla_{\mathbf{r}_{12}}^2 + \nabla_{\boldsymbol{\rho}_3}^2). \quad (87)$$

We set

$$E = -\frac{\hbar^2 \kappa^2}{m} \quad V_0 = -\frac{\hbar^2 k_0^2}{m}, \quad (88)$$

and we can write (72) as

$$\tilde{\chi}(\mathbf{q}_{12}, \mathbf{Q}_3) = \frac{-m/\hbar^2}{q_{12}^2 + Q_3^2 + \kappa^2} \left[{}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \chi_3 \rangle + \sum_{j=1,2} {}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \chi_j \rangle \right] \quad (89)$$

In the expression above, and in the rest of this section, we use a superscript $^{(k)}$ to specify the coordinate system $i = 1, 2, 3$ used for each ket $|\mathbf{q}_{ij}, \mathbf{Q}_k\rangle$. The first term in the bracket can be calculated directly

$$\begin{aligned} {}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \chi_3 \rangle &= V_0 {}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | [(|\phi_0\rangle\langle\phi_0|)^{(12)} \otimes \hat{1}_3] | \chi_3 \rangle \\ &= V_0 \tilde{\phi}_0(\mathbf{q}_{12}) \langle \phi_0, \mathbf{Q}_3 | \chi_3 \rangle \\ &= V_0 \tilde{\phi}_0(\mathbf{q}_{12}) \int \tilde{\phi}_0^*(\mathbf{q}') \tilde{\chi}(\mathbf{q}', \mathbf{Q}_3) \frac{d^3 q'}{(2\pi)^3}. \end{aligned} \quad (90)$$

The other two terms in the bracket require a little more work. Let us start by noting that these two contributions are equal because of the symmetry of the problem. For example, let us look at the contribution of $i = 2$, for which we introduce a closure relation for the Jacobi coordinates associated with $i = 2$:

$${}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \chi_2 \rangle = \int {}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \mathbf{q}'_{31}, \mathbf{Q}'_2 \rangle^{(2)} \tilde{\chi}(\mathbf{q}'_{31}, \mathbf{Q}'_2) \frac{d^3 q'_{31} d^3 Q'_2}{(2\pi)^6}. \quad (91)$$

To calculate the matrix element appearing in this expression, we need to go from the momenta $(\mathbf{q}_{31}, \mathbf{Q}_2)$ to the momenta $(\mathbf{q}_{12}, \mathbf{Q}_3)$. One can check

that

$$\mathbf{q}_{12} = -\frac{1}{2}\mathbf{q}_{31} + \frac{\sqrt{3}}{2}\mathbf{Q}_2 \quad \mathbf{Q}_3 = -\frac{\sqrt{3}}{2}\mathbf{q}_{31} - \frac{1}{2}\mathbf{Q}_2 \quad (92)$$

from which we deduce

$$|\mathbf{q}'_{31}, \mathbf{Q}'_2\rangle^{(2)} = |-\frac{1}{2}\mathbf{q}'_{31} + \frac{\sqrt{3}}{2}\mathbf{Q}'_2, -\frac{\sqrt{3}}{2}\mathbf{q}'_{31} - \frac{1}{2}\mathbf{Q}'_2\rangle^{(3)} \quad (93)$$

The matrix element appearing in (91) then reads

$$\begin{aligned} {}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \mathbf{q}'_{31}, \mathbf{Q}'_2 \rangle^{(2)} &= V_0 \tilde{\phi}_0(\mathbf{q}_{12}) \tilde{\phi}_0^* \left(-\frac{1}{2}\mathbf{q}'_{31} + \frac{\sqrt{3}}{2}\mathbf{Q}'_2 \right) \\ &\times (2\pi)^3 \delta \left(\mathbf{Q}_3 + \frac{\sqrt{3}}{2}\mathbf{q}'_{31} + \frac{1}{2}\mathbf{Q}'_2 \right). \end{aligned} \quad (94)$$

The integral over $\mathbf{q}'_{31}$ in (91) drops out because of the presence of the Dirac distribution, and we arrive at

$$\begin{aligned} {}^{(3)}\langle \mathbf{q}_{12}, \mathbf{Q}_3 | \hat{V}_{12} | \chi_2 \rangle &= \frac{2}{\sqrt{3}} V_0 \tilde{\phi}_0(\mathbf{q}_{12}) \times \\ &\int \tilde{\phi}_0^* \left[\frac{1}{\sqrt{3}}(\mathbf{Q}_3 + 2\mathbf{Q}'_2) \right] \tilde{\chi} \left[\frac{-1}{\sqrt{3}}(2\mathbf{Q}_3 + \mathbf{Q}'_2), \mathbf{Q}'_2 \right] \frac{d^3 Q'_2}{(2\pi)^3}. \end{aligned} \quad (95)$$

We now look for the solution $\chi(\mathbf{q}_{12}, \mathbf{Q}_3)$ in a form directly inspired by the solution (81) of the two-body problem:

$$\tilde{\chi}(\mathbf{q}_{12}, \mathbf{Q}_3) = \frac{k_0^2}{q_{12}^2 + Q_3^2 + \kappa^2} \tilde{\phi}_0(\mathbf{q}_{12}) \mathcal{F} \left(\frac{2}{\sqrt{3}}\mathbf{Q}_3 \right) \quad (96)$$

where $\mathcal{F}$ is the function to be determined. To simplify the notation, we assume that the function $\phi_0(\mathbf{r})$ is rotationally invariant, so that $\tilde{\phi}_0(\mathbf{q})$ is also rotationally invariant and depends only on $q = |\mathbf{q}|$. Substituting the form (96) into the set of equations (89,90,95) and setting $\mathbf{Q} = 2\mathbf{Q}_3/\sqrt{3}$, $\mathbf{Q}' = 2\mathbf{Q}'_2/\sqrt{3}$, we arrive at the equation of Skorniakov & Ter-Martirosian (1957):

$$\boxed{\mathcal{A}(Q, \kappa) \mathcal{F}(Q) = 2 \int \mathcal{B}(Q, Q', \kappa) \mathcal{F}(Q') \frac{d^3 Q'}{(2\pi)^3}} \quad (97)$$

with

$$\mathcal{A}(Q, \kappa) = \frac{1}{k_0^2} - \int \frac{|\tilde{\phi}_0(q)|^2}{q^2 + \frac{3}{4}Q^2 + \kappa^2} \frac{d^3 q}{(2\pi)^3} \quad (98)$$

and

$$\mathcal{B}(\mathbf{Q}, \mathbf{Q}', \kappa) = \frac{\tilde{\phi}_0^* \left(\left| \mathbf{Q}' + \frac{1}{2} \mathbf{Q} \right| \right) \tilde{\phi}_0 \left(\left| \mathbf{Q} + \frac{1}{2} \mathbf{Q}' \right| \right)}{Q^2 + Q'^2 + \mathbf{Q} \cdot \mathbf{Q}' + \kappa^2}. \quad (99)$$

We have therefore reduced the three-body problem to the determination of the function $\mathcal{F}(\mathbf{Q})$, solution of the integral equation (97).

We can recover the case of a contact potential by taking $|\phi_0\rangle = |\mathbf{r}_0 = 0\rangle$, which amounts to taking $\tilde{\phi}_0(\mathbf{q})$ independent of $\mathbf{q}$ in the above. Note that it is then necessary to introduce an ultraviolet cutoff—equivalent to the three-body parameter—to regularize the integrals appearing in (97), see for example the appendix to the review article by Naidon & Endo (2017) as well as Pricoupenko (2012) and Petrov (2012).

Chapter VI

The Efimov effect explored with gases of cold atoms

This final chapter is devoted to a description of the main experimental manifestations of the Efimov effect in ultracold atomic gases. This detailed exploration has been made possible by the use of scattering resonances, known in this context as Fano–Feshbach resonances, which allow the scattering length a to be adjusted to a value considerably larger (in absolute value) than the range b of the interatomic potentials.

In these experiments, Efimov trimers are characterized essentially by a signal of atom or dimer losses. The loss rate goes through a maximum or a minimum at very specific points of the energy diagram $E(a)$ shown in figure VI.1. We will describe in detail the processes at play in § 1 and show how it has been possible to observe the main characteristics of Efimov physics on either side of the resonance, which amounts to linking the physics for $a < 0$ to that for $a > 0$ (§ 2).

It should be noted that it is also possible to use spectroscopic methods (incoherent or coherent) based on a photo-association process to study different aspects of the Efimov effect. We will not go into this here, and refer the interested reader to Lompe, Ottenstein, et al. (2010), Nakajima, Horikoshi, et al. (2011), Machtey, Shotan, et al. (2012), Yudkin, Elbaz, Giannakeas, et al. (2019), and Yudkin, Elbaz & Khaykovich (2020).

Experiments carried out between 2006 and 2010 on gases of cold atoms have revealed an unexpected property. The three-body parameter R_0 was expected to take *a priori* random values, at least in the zero-range interaction model. In fact, for the van der Waals interactions in $-C_6/r^6$ that are domi-

nant in this low-temperature domain, one finds that the three-body parameter is closely related to the van der Waals radius, $R_{\text{vdW}} = \frac{1}{2} (mC_6/\hbar^2)^{1/4}$. We will discuss the origin of this link using the formalism of the hyperspherical approach (§ 3).

The last part (§ 4) will be devoted to the presentation of some effects going beyond the one initially considered by Efimov. We will be particularly interested in the case of fermions, possibly accompanied by an additional particle to bind them. Our presentation will be far from exhaustive; we therefore refer readers with a specific interest in the quantum few-body problem to the special issue of the Comptes Rendus de Physique de l'Académie des Sciences of January 2011 and to recent review articles by Naidon & Endo (2017), Greene, Giannakeas, et al. (2017), and D'Incao (2018).

1 The three-body recombination rate

1-1 Scaling laws for the coefficient L_3

Most of the experiments carried out to date on cold atomic gases use an atom loss signal to detect the thresholds for the appearance of Efimov trimers. These losses occur in particular when three atoms (assumed here to be identical bosons) are next to each other, with the possibility of forming

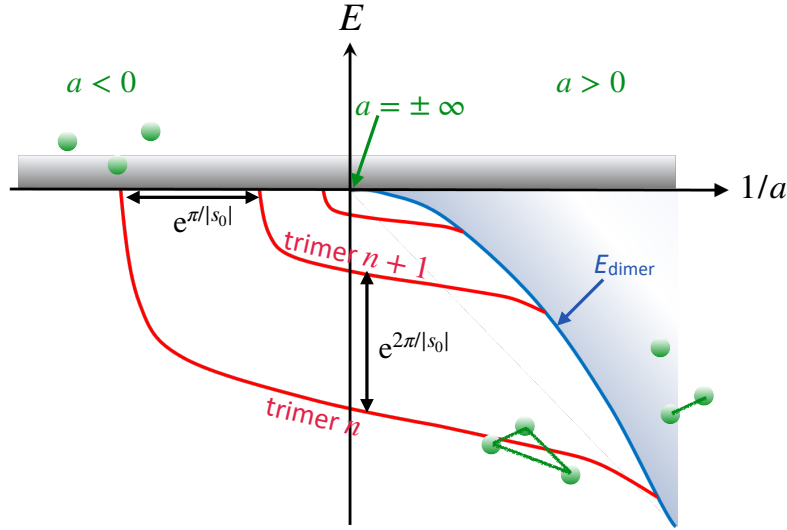


Figure VI.1. Schematic representation of the energies E of the Efimov trimers as a function of $1/a$ (not to scale). The purely imaginary number s_0 has modulus $|s_0| = 1.00624$ (see Chapter 5).

a molecule. For a uniform atomic gas of average density ρ_A , the decrease in the number of atoms N_A obeys the law

$$\frac{dN_A}{dt} = -\frac{g^{(3)}}{3!} L_3 \rho_A^2 N_A. \quad (1)$$

In this equation, the factor $g^{(3)}$ accounts for the bosonic bunching that must be taken into account if the gas is non-degenerate (Hanbury Brown and Twiss effect): it corresponds to the sum of the different contributions linked to the exchange symmetry of the three bosons and is therefore $g^{(3)} = 3! = 6$. For a pure condensate, there are no density-density correlations and $g^{(3)} = 1$. See Kagan, Svistunov, et al. (1985) and Söding, Guéry-Odelin, et al. (1999) for more details.

A simple dimensional analysis, possibly supplemented by a more quan-

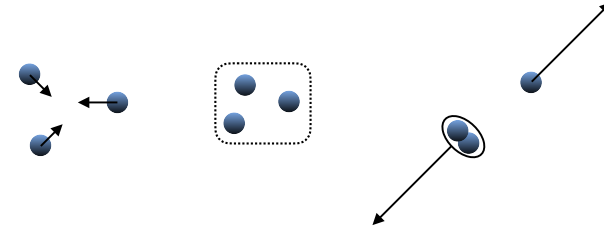


Figure VI.2. Three-body recombination assisted by the intermediate formation of a near-zero-energy Efimov state on the $a < 0$ side of the resonance ($a \approx a_-^{(n)}$). The final state contains a strongly bound dimer not described by the pseudo-potential approach.

titative treatment (Fedichev, Reynolds, et al. 1996), shows that, for zero-range interactions, the loss coefficient L_3 reads

$$L_3 = 3 C(a) \frac{\hbar a^4}{m} \quad (2)$$

In this expression, the coefficient C is a dimensionless number depending on the ratio a/R_0 , where R_0 is the three-body parameter needed to regularize the problem near the origin. In the absence of any Efimovian effect, Fedichev, Reynolds, et al. (1996) had predicted $C = 3.9$.

When we take into account the effects linked to Efimov physics, the processes involved in this three-body recombination differ depending on whether we are interested in the $a < 0$ or $a > 0$ part, and we will therefore describe them in detail in what follows.

Note that the measurement of L_3 in a gas of trapped cold atoms is generally affected by temperature. In particular, the limit $\sim \hbar a^4/m$ is replaced by $\sim \hbar \lambda^4/m$ when the thermal wavelength λ becomes less than a . We will not discuss these finite-temperature effects here, and refer the interested reader for example to Rem, Grier, et al. (2013) and Eismann, Khaykovich, et al. (2016), in which the heating that accompanies these recombination processes is taken into account in the gas dynamics.

1-2 Part $a < 0$ of the resonance

On this side of the resonance, trimers form directly from a collision between three free atoms (figure VI.2). At the formation threshold, where the scattering length approaches one of the $a_-^{(n)}$, these trimers have almost zero energy and a large spatial extent, and therefore a strong overlap with the wave function of the free atoms. Once such a trimer has formed, it can decay, releasing a free atom and a strongly bound dimer (not described by the pseudo-potential approach, but present in real interatomic potentials). We therefore expect an increase in L_3 around each value $a = a_-^{(n)}$.

This effect was originally predicted by Esry, Greene, et al. (1999a) and detailed references can be found in recent review articles by Naidon & Endo (2017), Greene, Giannakeas, et al. (2017) and D’Incao (2018). Analysis of three-body recombination and the formation of strongly bound dimers leads to the following expression¹ for the coefficient L_3 (Braaten & Hammer 2004):

$$a < 0 : \quad C(a) \approx C' \frac{\sinh(2\eta)}{\sin^2 [|s_0| \ln(a/a_-^{(0)})] + \sinh^2 \eta} \quad (3)$$

with $C' \approx 4590$. This result depends on an adjustable parameter, the dimensionless number η , called the *inelasticity parameter*.

The physical meaning of the parameter η is relatively simple: to take three-body losses into account and establish the result (3), we solve the Schrödinger equation for the hyperradial wave function $\phi(R)$, modifying the boundary condition at short distances. So far, we have assumed for $R \ll |a|, k^{-1}$:

$$\phi(R) \sim \frac{1}{\sqrt{R}} \sin [|s_0| \ln(R/R_0)] \sim \frac{1}{\sqrt{R}} \left[e^{i|s_0| \ln(R/R_0)} - e^{-i|s_0| \ln(R/R_0)} \right] \quad (4)$$

where the two terms inside the bracket can be interpreted as the outgoing and incoming waves in a three-body collision: in this collision, the hyperradius initially has a large value compared with all the characteristic lengths

¹The structure of this expression is very similar to that giving the transmission of a Fabry–Perot optical cavity, known as the Airy function. This similarity is not accidental, of course, as the two problems are formally similar.

of the problem. It decreases towards values of the order of the range of the potentials, which corresponds to the physical situation where the three particles are relatively close to each other. It then returns to infinity, which means that at least one of the three particles is far from the other two. An inelastic collision is described by requiring that the outgoing flux from the collision be strictly smaller than the incoming flux, which amounts to the boundary condition

$$\phi(R) \sim \frac{1}{\sqrt{R}} \left[e^{-2\eta} e^{i|s_0| \ln(R/R_0)} - e^{-i|s_0| \ln(R/R_0)} \right]. \quad (5)$$

The determination of (3) from this new boundary condition is described by Braaten & Hammer (2004) and Braaten & Hammer (2006).

The parameter η varies with the atomic species and with the strength of the transitions leading to the strongly bound dimers. We check in figure VI.3 that this coefficient L_3 (normalized by the “bare” value $3\hbar a^4/m$) goes through a maximum whenever a equals one of the $a_-^{(n)}$ (the argument of the sine is then a multiple of π).

The *recombination length* is defined as (Esry, Greene, et al. 1999a):

$$\rho_3 = (\mu L_3 / \hbar)^{1/4} \quad (6)$$

where $\mu = m/\sqrt{3}$ is the reduced three-body mass. We expect the resonances described above to be clearly visible only if this length is smaller than the thermal wavelength of the particles, which means that we have to work with sufficiently cold gases (see for example figure VI.9). This condition is more difficult to fulfill for the excited trimers than for the ground state $n = 0$, since L_3 increases with n (the expression for L_3 involves a^4).

1-3 Part $a > 0$ of the resonance

In this case, the existence of the weakly bound dimer of energy $-\hbar^2/ma^2$ opens up a new pathway for three-body recombination (figure VI.4): three colliding free atoms can give rise to one of these dimers, with the third atom flying off on its own. Such a process can be analyzed entirely within the framework of our pseudo-potential approach, since it does not involve strongly bound states. The result of the calculation of the coefficient L_3

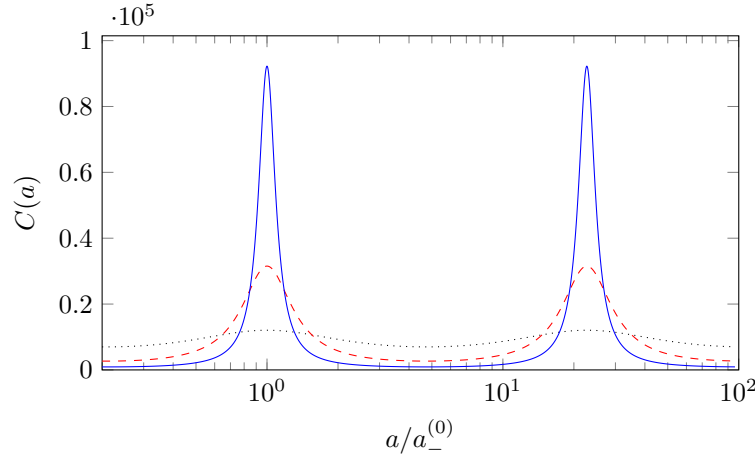


Figure VI.3. Normalized three-body recombination loss coefficient, $C(a) \equiv L_3/(3\hbar a^4/m)$, on the $a < 0$ side of the resonance with $\eta = 0.1$ (solid blue line), $\eta = 0.3$ (dashed red line) and $\eta = 1$ (dashed black line).

therefore does not involve an adjustable parameter (unlike the case $a < 0$ where η is involved) and we find (Esry, Greene, et al. 1999b; Bedaque, Braaten, et al. 2000; Petrov 2004; Braaten & Hammer 2007a; D’Incao 2018):

$$a > 0 \text{ (weakly bound dimers)} : \quad C(a) \approx C'' \sin^2 \left[|s_0| \ln \left(\frac{a}{a_+^{(1)}} \right) \right] \quad (7)$$

with²

$$a_+^{(0)} \approx 0.20 a_*^{(1)} \quad C'' \approx 67.1. \quad (8)$$

The vanishing of this rate for the values $a_+^{(n)} = a_+^{(0)} e^{n\pi/|s_0|}$ can be interpreted as a destructive interference effect between the different paths leading to the production of the dimer during a collision of three atoms. In such

²In this case, we locate $a_+^{(0)}$ relative to $a_*^{(1)}$ rather than to $a_*^{(0)}$. Indeed, when we go beyond the zero-range limit and consider a true potential of the van der Waals type, the branch of the $n = 0$ trimer does not cross the dimer branch, which means that the point $a_*^{(0)}$ is pushed to infinity (see the discussion at the end of § 2-1).

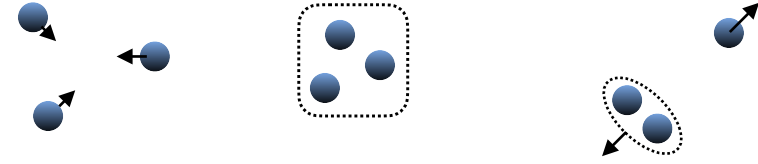


Figure VI.4. Three-body recombination assisted by the intermediate formation of a near-zero-energy Efimov state on the $a > 0$ side of the resonance. The final state involves the weakly bound dimer of energy $-\hbar^2/ma^2$. The normalized recombination rate $C(a)$ exhibits minima ($a_+^{(n)}$) and maxima ($a_p^{(n)}$) corresponding to an interference process between the different channels leading to this final state. Unlike the case of $a < 0$, the calculation of this rate can be done entirely within the framework of the pseudo-potential model and does not require the introduction of an additional parameter (apart from R_0).

a process, the hyperradius is initially very large, decreases and then returns to infinity. Several channels corresponding to the hyperspherical potentials can simultaneously make a significant contribution and the $\sin^2[\dots]$ term in (7) can be understood as a Stückelberg oscillation, resulting from the coupling between these different channels. The review article by D’Incao (2018) provides a detailed description of these different pathways.

Note that in the literature we also find the notation $a_p^{(n)}$ for the maximum of the function $\sin^2[\dots]$ involved in (7). Each maximum $a_p^{(n)}$ lies halfway (in logarithmic coordinates) between two successive minima $a_+^{(n)}$ and $a_+^{(n+1)}$, so that

$$a_p^{(n)} = a_+^{(n)} \sqrt{22.7} \approx a_*^{(n+1)}. \quad (9)$$

The variation of $C(a)$ for $a > 0$ is plotted in figure VI.5.

1-4 Link between the two sides of the resonance

In the universal regime, we can relate the remarkable points on the $a < 0$ side, i.e. the threshold values $a_-^{(n)}$ for the existence of a trimer, and the

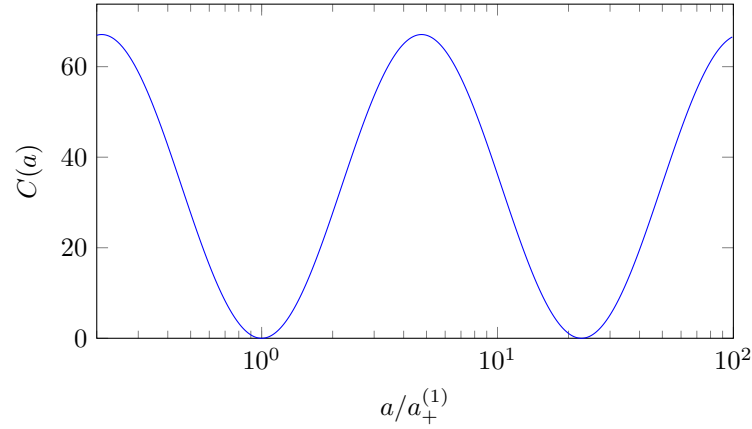


Figure VI.5. Normalized three-body recombination loss coefficient, $C(a) \equiv L_3/(3\hbar a^4/m)$, on the $a > 0$ side of the resonance. The value of $a_+^{(n)}$ is $\approx 4.5 a_*^{(n)} \approx 0.20 a_*^{(n+1)}$, where $a_*^{(n)}$ denotes the crossing point between the dimer and the n th branch of the trimer. In the model that leads to this prediction, recombination occurs only into the weakly bound dimer that exists on this side of the resonance.

remarkable points on the $a > 0$ side, i.e. the “dimer–trimer” crossing $a_*^{(n)}$, or the minimum of the three-body recombination rate $a_+^{(n)}$. The result of Braaten & Hammer (2006) [their equations (200) and (201)], refined by Golin, Mora, et al. (2008) [their equation (19)], gives

$$\boxed{\frac{a_-^{(n)}}{a_*^{(n)}} \approx -21.31} \quad (10)$$

which means that $a_-^{(n)}$ is actually close (in absolute value) to $a_*^{(n+1)}$:

$$\frac{a_-^{(n)}}{a_*^{(n+1)}} \approx -0.939 = -\frac{1}{1.065}. \quad (11)$$

From this relation we deduce the link between a_- and a_+ , which are the quantities most easily accessible from a measurement of the three-body re-

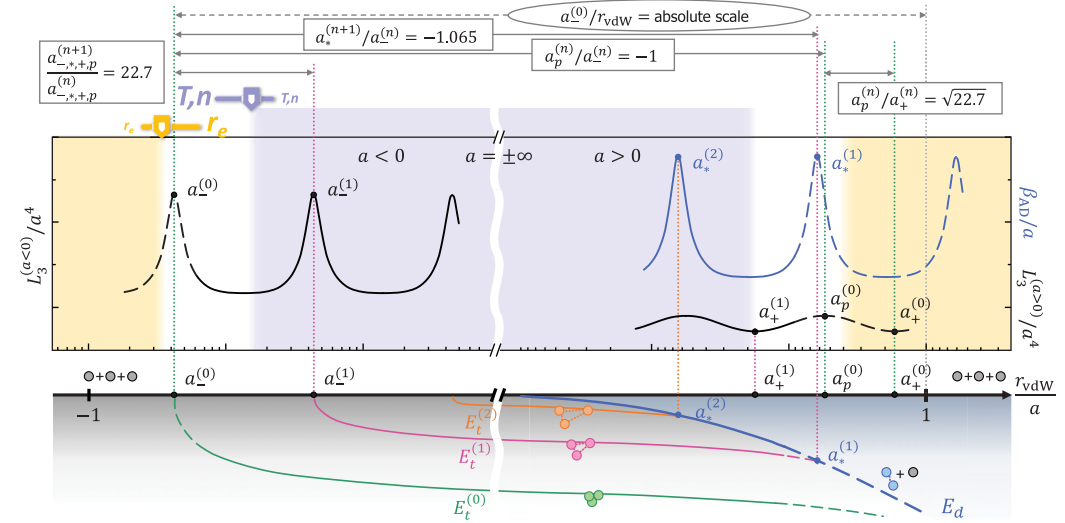


Figure VI.6. Links between the $a < 0$ and $a > 0$ sides for the main characteristics of Efimov physics. Figure taken from Xie, Van de Graaff, et al. (2020).

combination rate between atoms of the gas:

$$\boxed{\frac{a_-^{(n)}}{a_+^{(n)}} = -4.7} \quad (12)$$

These main relations are summarized in figure VI.6, taken from Xie, Van de Graaff, et al. (2020).

2 Observation of some main features

2-1 First observation on cesium

In the field of cold atomic gases, the first clear demonstration of an Efimov effect was made by Kraemer, Mark, et al. (2006). The experiment

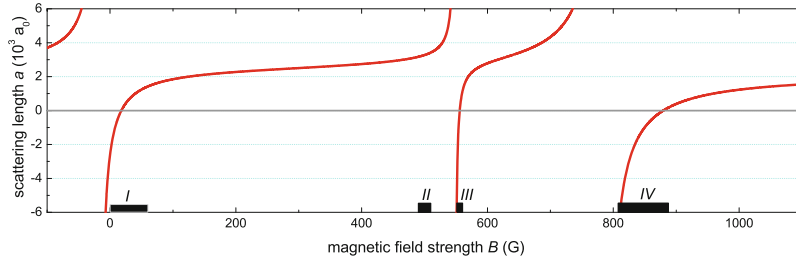


Figure VI.7. Theoretical prediction for the scattering length $a(B)$ of a cesium gas in the $|f = 3, m_f = 3\rangle$ state, when only the couplings to zero-angular-momentum dimers are taken into account. Figure taken from Ferlaino, Zenesini, et al. (2011).

was carried out on a cesium gas prepared in its lowest hyperfine state³ $|f = 3, m_f = 3\rangle$ around a Feshbach resonance. The cesium atom lends itself well to this type of experiment for two reasons:

- The “background” scattering length a_{bg} , i.e. its value well away from any resonance [cf. the 2021 lecture series], is large compared with the range R_{vdW} : $a \approx 2200 a_0 \approx 20 R_{vdW}$, which ensures that we will generally be dealing with broad resonances, for which the universality associated with the pseudo-potential description is guaranteed. When we take into account only the couplings to molecular states of zero angular momentum, we arrive at the $a(B)$ diagram of figure VI.7.
- As cesium is a heavy element, relativistic effects play an important role in the dynamics of electronic coupling. This adds significant coupling with molecular states of non-zero angular momentum, and thus enriches the $a(B)$ diagram. A zoom on the low-magnetic-field region (marked by the symbol *I* in figure VI.7) is shown in figure VI.8.

Kraemer, Mark, et al. (2006) studied the variation of the three-body recombination rate around $B = 7.5$ G, where a takes large absolute and negative values. Their main result is shown in figure VI.9. For the low-temperature points (10 nK), there is a sharp increase of the three-body re-

³Recall that the ^{133}Cs nucleus has spin $i = 7/2$, so that the hyperfine coupling with the spin $1/2$ of the valence electron gives rise to two states, $f = 3$ and $f = 4$.

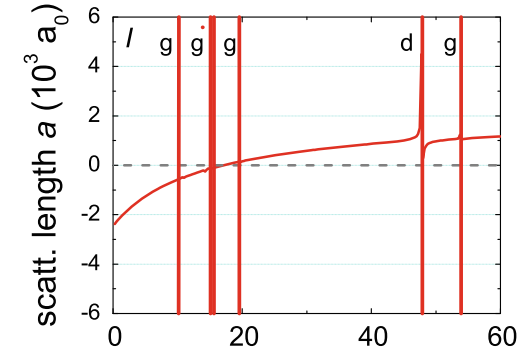


Figure VI.8. Theoretical prediction for the scattering length $a(B)$ of a cesium gas in the $|f = 3, m_f = 3\rangle$ state, when couplings to dimers of non-zero angular momentum are added. The x axis indicates the magnetic field, expressed in gauss. Figure taken from Ferlaino, Zenesini, et al. (2011).

combination rate in the vicinity of $a_-^{(0)} = -872(22) a_0$, corresponding to the threshold for the appearance of the ground state Efimov trimer. The red solid line in figure VI.9 corresponds to a fit by the theoretical prediction (3) for $\eta = 0.10(3)$.

It is interesting to compare the properties of the trimer observed by Kraemer, Mark, et al. (2006) and those of the ground-state trimer He_3 observed by Schöllkopf & Toennies (1994) (see previous chapter). As shown by Lee, Koehler, et al. (2007), these two trimers have in common the fact that their energy branch, extended on the side of small and positive a values, never crosses the dimer branch [see also Bruch & Sawada (1973) and Yudkin, Elbaz & Khaykovich (2020)]. From this point of view, neither the He_3 trimer nor the Cs_3 trimer of Kraemer, Mark, et al. (2006) satisfies all the criteria that can be imposed on an Efimovian structure. On the other hand, the state observed by Kraemer, Mark, et al. (2006) is undoubtedly a Borromean state since it exists in a zone $a < 0$ for which there is no dimer in a weakly bound state (there are of course strongly bound Cs_2 dimers, but that is a different matter). By comparison, He_3 was observed for $a > 0$, i.e. in a zone where the weakly bound He_2 dimer exists: it was therefore not a Borromean state.

It should also be noted that the Kraemer, Mark, et al. (2006) experiment

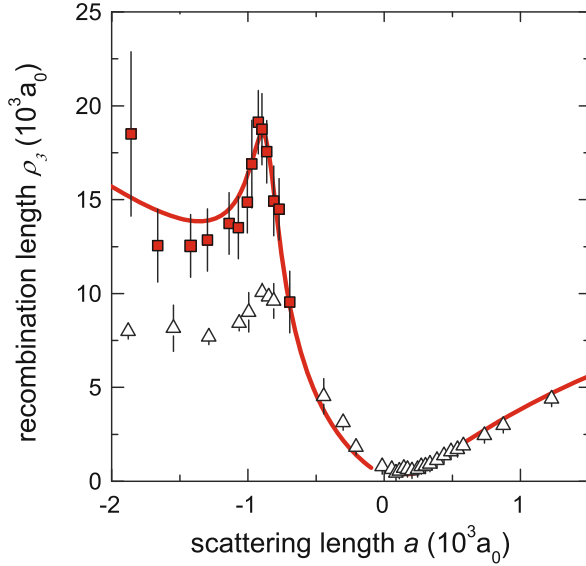


Figure VI.9. Three-body recombination length [defined in (6)] measured by Kraemer, Mark, et al. (2006). The red squares (resp. black triangles) correspond to a temperature of 10 nK (resp. 200 nK). Figure adapted from Ferlaino, Zenesini, et al. (2011).

continuously explored a magnetic field zone leading to scattering lengths on either side of $a = 0$. In addition to the remarkable peak shown in figure VI.9 obtained for $a < 0$, the authors also observed peaks on the $a > 0$ side. However, it is important to point out that a universal relation between the two domains is not expected in this case. These universal relations hold between the $a < 0$ and $a > 0$ regions flanking an $a = \pm\infty$ resonance, not a zero of a .

2-2 Connecting the regions $a < 0$ and $a > 0$

In 2009, several experimental groups announced that they had succeeded in connecting the two domains $a > 0$ and $a < 0$ located around a resonance

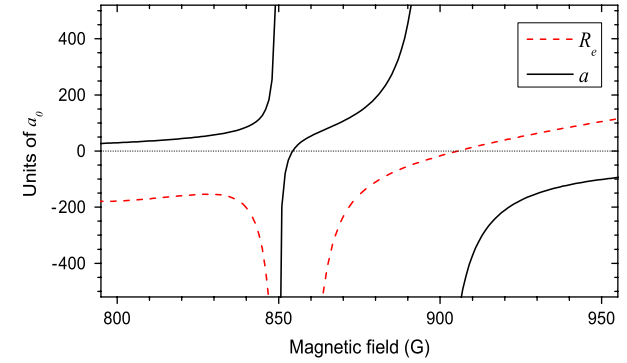


Figure VI.10. Scattering length and effective range for the ^7Li Feshbach resonance. Figure extracted from Gross, Shotan, et al. (2009).

$a = \infty$: Knoop, Ferlaino, et al. (2009), Gross, Shotan, et al. (2009), Zaccanti, Deissler, et al. (2009) and Pollack, Dries, et al. (2009). For the last two, one may also consult the partial re-analysis of the data in Roy, Landini, et al. (2013) and Dyke, Pollack, et al. (2013).

Here we shall concentrate on the Gross, Shotan, et al. (2009) experiment. It was carried out on a gas of ^7Li atoms (bosons) prepared in the state that connects to $|f = 1, m = 0\rangle$ at zero field (the ground level of the ^7Li atom is split into two hyperfine sublevels, $f = 1$ and $f = 2$). Two Feshbach resonances, at 846 G and 894 G, come into play (figure VI.10), giving a region in which a diverges while the effective range r_e keeps a relatively small value (broad resonance). This configuration is therefore well suited to the search for Efimovian universality.

Figure VI.11 shows the result obtained by Gross, Shotan, et al. (2009) for the measurement of the L_3 coefficient on either side of the resonance.

- On the $a < 0$ side (corresponding to the large values of B), L_3 goes through a maximum at $a_-^{(0)} = -264(11) a_0$, and a fit of the measurements to (3) gives $\eta_- = 0.236(42)$. This result gives $|a_-^{(0)}| \sim 8.5 r_e$, so that the universal regime has been reached. The temperature of the gas (1 μK) does not allow us to observe the next resonance, expected

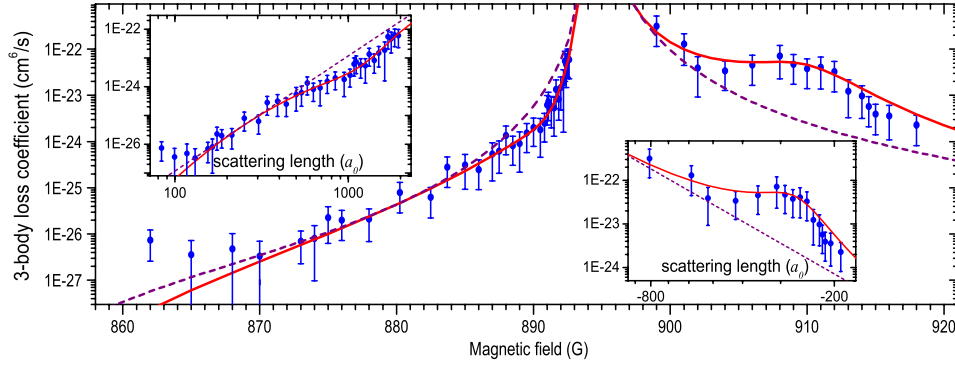


Figure VI.11. Three-body loss rate through a Feshbach resonance for a ^7Li gas. Figure extracted from Gross, Shotan, et al. (2009).

at a value of $|a|$ 22.7 times larger.

- On the $a > 0$ side (corresponding to small values of B), we see the start of the oscillating behavior expected for L_3 [cf. (7)]. In particular, we find a pronounced minimum of L_3 around $a_+^{(1)} = 1160 a_0$, corresponding to the destructive interference mentioned in § 1-3.

We stated in § 1-4 the link between the two sides of the resonance:

$$\frac{a_-^{(n)}}{a_+^{(n)}} = -4.7 \quad \text{or equivalently} \quad \frac{a_-^{(n)}}{a_+^{(n+1)}} = -\frac{4.7}{22.7} = -0.21. \quad (13)$$

The values found experimentally $a_-^{(0)} = -264 a_0$ and $a_+^{(1)} = 1160 a_0$ lead to the ratio -0.23 , close to that expected if we assume that the two measurements refer to two consecutive trimers. As Gross, Shotan, et al. (2009) write in their conclusion, “*This seems like an observation of the long hunted universal behavior of a three-body observable in a physical system with resonantly enhanced two-body interactions*”!

Let us also indicate the result obtained by Zaccanti, Deissler, et al. (2009) and Pollack, Dries, et al. (2009) after the reanalysis mentioned above and explained by Naidon & Endo (2017):

- The Zaccanti, Deissler, et al. (2009) experiment, carried out on ^{39}K , led to $a_-/a_+ = -3.1 (0.3)$ [value before re-analysis $-6.7 (0.6)$].
- The Pollack, Dries, et al. (2009) experiment, carried out on ^7Li , led to $a_-/a_+ = -2.8 (0.3)$ [value before re-analysis $-2.5 (0.6)$].

These results lie significantly further from the universal limit, probably owing to effects related to the effective range r_e , which was relatively large in these experiments. See the detailed discussion in Xie, Van de Graaff, et al. (2020).

2-3 Efimov’s geometric sequence

The observation of two successive loss resonances on the same side of the Feshbach resonance makes it possible to test directly the scaling factor 22.7 of Efimov’s theory. Zaccanti, Deissler, et al. (2009) and Pollack, Dries, et al. (2009) carried out initial measurements to test this law on ^{39}K and ^7Li atoms [see also Williams, Hazlett, et al. (2009) for the observation of an excited trimer].

Here we describe a more recent experiment carried out in Innsbruck by Huang, Sidorenkov, et al. (2014) on ^{133}Cs . In this experiment, particular care was taken to evaluate finite-temperature effects and to extrapolate the measured quantities to zero temperature. The experiment was carried out on a Feshbach resonance at a much higher field (around 800 G) than that used by Kraemer, Mark, et al. (2006). This broad resonance, coupled with good control of the gas temperature in the nanokelvin range, makes it possible to achieve large scattering lengths, up to $10^5 a_0$.

In the Huang, Sidorenkov, et al. (2014) experiment, the gas is prepared close to quantum degeneracy in a hybrid trap (magnetic plus optical), at a temperature between 7 and 10 nK. The ground-state size of the trap is $\sim 5 \mu\text{m}$, to be compared with the expected size of the second trimer, $\sim 1 \mu\text{m}$: there is enough room for this trimer, but the next one (22.7 times larger) would not fit into this trap...

Figure VI.12 shows the main result of Huang, Sidorenkov, et al. (2014) with a sharp peak in the three-body loss coefficient around $a = -17\,000 a_0$. The ground-state trimer had previously been observed by the same group

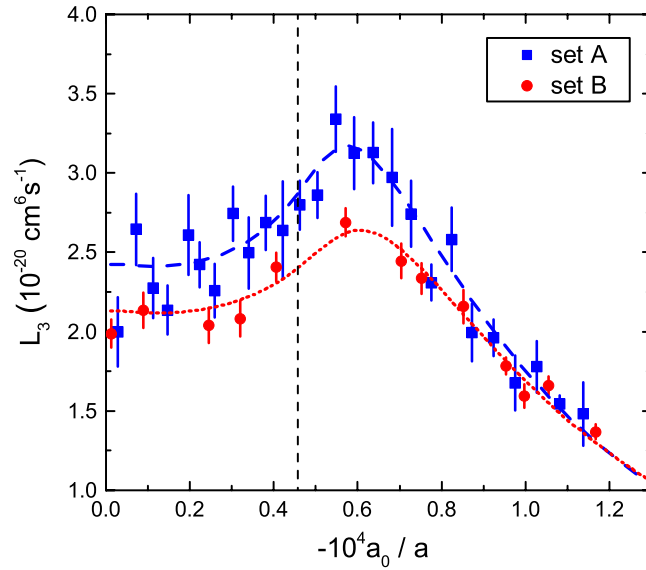


Figure VI.12. Observation of the second Efimov trimer for cesium around 800 G. A fit to a theoretical model taking into account the non-zero temperature of the gas leads to $a_-^{(1)} = -20\,190\,(1200)\,a_0$, i.e. $a_-^{(1)}/a_-^{(0)} = 21.0\,(1.3)$. Set A: $T = 8.7\,\text{nK}$; set B: $T = 10.0\,\text{nK}$. Figure extracted from Huang, Sidorenkov, et al. (2014).

(Berninger, Zenesini, et al. 2011), and it forms at $a_-^{(0)} = -963\,(11)\,a_0$, giving a ratio of 17.7, whereas Efimov universality predicts 22.7.

This deviation from Efimov’s “universal” prediction may be due (at least in part) to effects related to the non-zero temperature of the gas. For the $a_-^{(0)}$ position of the ground-state trimer, the temperature effects are not very significant. To predict the threshold value $a_-^{(1)}$ for the next trimer, Huang, Sidorenkov, et al. (2014) used the model developed by Rem, Grier, et al. (2013). They analyzed their experimental data, keeping the position $a_-^{(1)}$ and the temperature as adjustable parameters. The fit gave a temperature very close to that measured directly and gave the value $a_-^{(1)} = -20\,190\,(1200)\,a_0$, a factor of 21.0 (1.3) above $a_-^{(0)}$. This is remarkably close to Efimov’s universal value (1.3 σ difference). In any case, a non-

negligible deviation from the scaling law is expected for the first trimers $n = 0$ and $n = 1$, in particular because of non-zero-range effects (Schmidt, Rath, et al. 2012).

To conclude this section, we should point out that this Efimovian geometric sequence has also been demonstrated in mMM mixtures: the experiment is then less demanding, because the common ratio of the geometric sequence is considerably reduced as one moves towards mass ratios $m/M \ll 1$ (see Chapter 4).

2-4 The dimer–trimer crossing

An important feature of the energy diagram on the $a > 0$ side of the resonance is the set of points $\{a_*^{(n)}\}$, where the energy of the trimer becomes equal to the energy of the dimer (the third atom being almost at rest, infinitely far from the dimer). If we start from an atom–dimer mixture, we expect the loss rate β_{AD} for this mixture to be maximal at such a point: during an atom–dimer collision, the partners spend a long time in each other’s vicinity, which favors the transition to other, more deeply bound states (figure VI.13). The argument is the same as the one that leads to an increase of the three-body loss rate on the $a < 0$ side of the resonance, at the points $a_-^{(n)}$.

The first evidence of losses in an atom–dimer mixture due to this effect was published by Knoop, Ferlaino, et al. (2009). We will focus here on more recent experiments by the Boulder group, described by Chapurin, Xie, et al. (2019) and Xie, Van de Graaff, et al. (2020), which have made it possible to verify Efimov universality between the a_* value and the other remarkable points in the energy diagram.

Xie, Van de Graaff, et al. (2020) worked with a ^{39}K gas prepared in the hyperfine state $|f = 1, m_f = -1\rangle$ around $B = 33.6$ gauss. In the 2021 lecture series we described the properties of the corresponding Fano–Feshbach resonance. This resonance has the advantage of having a fairly small effective range ($r_e \approx 130\,a_0$ at resonance), which makes it possible to increase the range of universality of Efimovian effects. Chapurin, Xie, et al. (2019) had studied the $a < 0$ side of this resonance and found $a_-^{(0)} = -908\,(11)\,a_0$ and $\eta = 0.25\,(1)$ (figure VI.14).

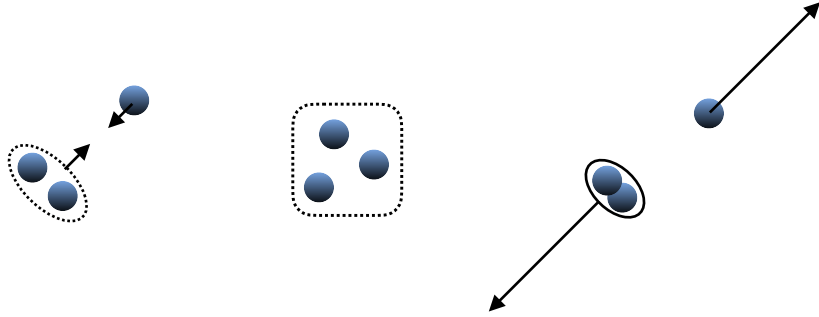


Figure VI.13. Inelastic atom–dimer collision assisted by the intermediate formation of an Efimov state on the $a > 0$ side of the resonance. The initial state involves the weakly bound dimer of energy $-\hbar^2/ma^2$ and the final state contains a strongly bound dimer, not described by the pseudo-potential model. The rate of this process is maximal for $a = a_*^{(n)}$, when the energy of the weakly bound dimer coincides with that of the Efimov trimer.

Dimers are formed by “magneto-association”, obtained by rapidly crossing the Fano–Feshbach resonance towards the $a > 0$ side. The number of dimers can decrease simply through a spin flip of one of the constituent atoms, which breaks up the dimer. It can also decrease through collisions with atoms, which is the process of interest, and which leads to an evolution of the number of dimers N_D in the presence of an atomic density ρ_A according to the law

$$\frac{dN_D}{dt} = -\beta_{AD} \rho_A N_D. \quad (14)$$

The rate β_{AD} describing this process is plotted in figure VI.15, together with a fit to the law proposed by Braaten & Hammer (2007b) [see also Braaten & Hammer (2009) and Helfrich & Hammer (2009)]:

$$\beta_{AD} = C \frac{\sinh(2\eta)}{\sin^2[s_0 \ln(a/a_*)] + \sinh^2(\eta)} \frac{\hbar a}{m} \quad (15)$$

The structure of this expression is very similar to that proposed in (3) for three-body recombination; this is natural, since the two expressions describe the same physics, with the formation of strongly bound structures,

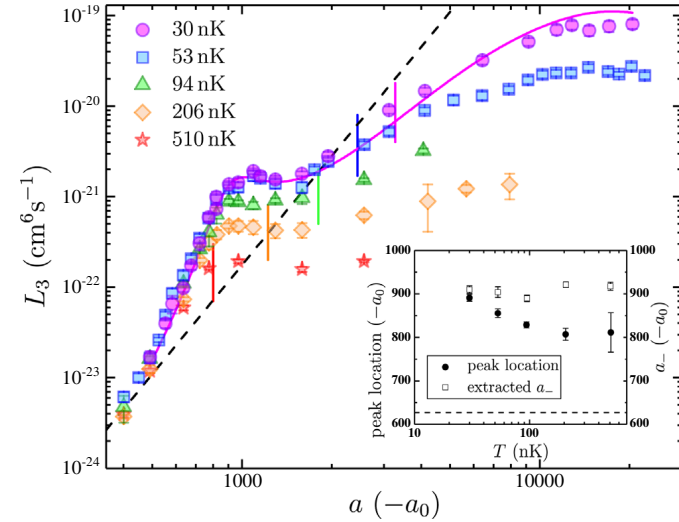


Figure VI.14. Three-body relaxation rate in a ^{39}K gas on side $a < 0$ for the Fano–Feshbach resonance located around $B = 33.6$ Gauss. One finds $a_- = -908(11) a_0$. Figure taken from Chapurin, Xie, et al. (2019).

not included in the initial pseudo-potential model and accounted for by the parameter η .

The result of the Xie, Van de Graaff, et al. (2020) analysis, extrapolated to zero temperature, gives $a_*^{(1)} = 884(14) a_0$ and $\eta = 0.28(2)$. The same authors also measured the three-body recombination rate L_3 (i.e. with no dimer present) on the $a > 0$ side and obtained the almost sinusoidal oscillation (after division of L_3 by a^4) shown in figure VI.16, as expected from (7). We deduce the position of the first minimum $a_+^{(0)} = 246(6) a_0$ and the first maximum $a_p^{(0)} = 876(28) a_0$.

Let us summarize all the results obtained by Chapurin, Xie, et al. (2019) and Xie, Van de Graaff, et al. (2020) (in units of a_0):

$$a_+^{(0)} = 246 \quad a_p^{(0)} = 876 \quad a_*^{(1)} = 884 \quad a_-^{(0)} = -908 \quad (16)$$

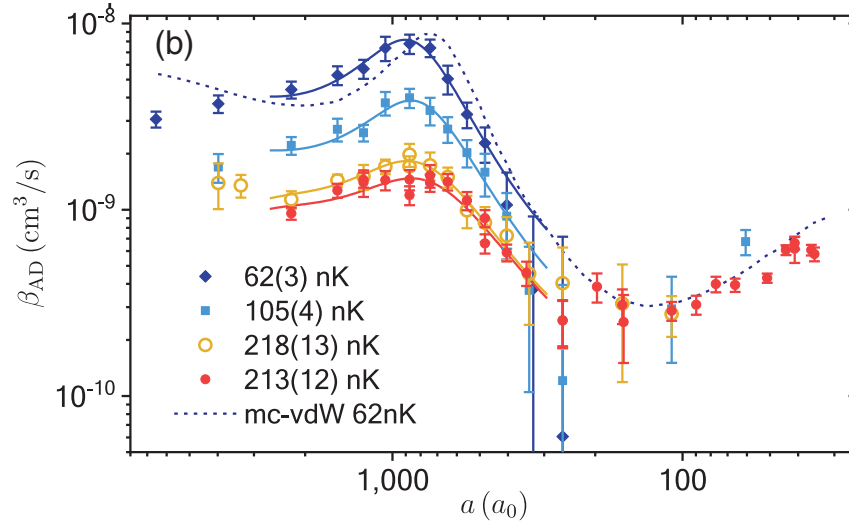


Figure VI.15. Two-body (atom–dimer) loss rate in the vicinity of $a_*^{(1)}$ in a ^{39}K gas. Figure taken from Xie, Van de Graaff, et al. (2020).

This set is a remarkable test of Efimov’s universality with the different ratios

$$\frac{a_*^{(1)}}{a_-^{(0)}} = \frac{884}{-908} = -0.97 \quad \text{Expected value: } -1.065 \quad (17)$$

$$\frac{a_p^{(0)}}{a_-^{(0)}} = \frac{876}{-908} = -0.96 \quad \text{Expected value: } -1 \quad (18)$$

$$\frac{a_p^{(0)}}{a_+^{(0)}} = \frac{876}{246} = 3.56 \quad \text{Expected value: } 4.76 \quad (19)$$

Note that for the last ratio, the relatively small value of $a_+^{(0)}$ (compared with the effective range r_e) makes it difficult to reach the universal value, which may explain the observed deviation.

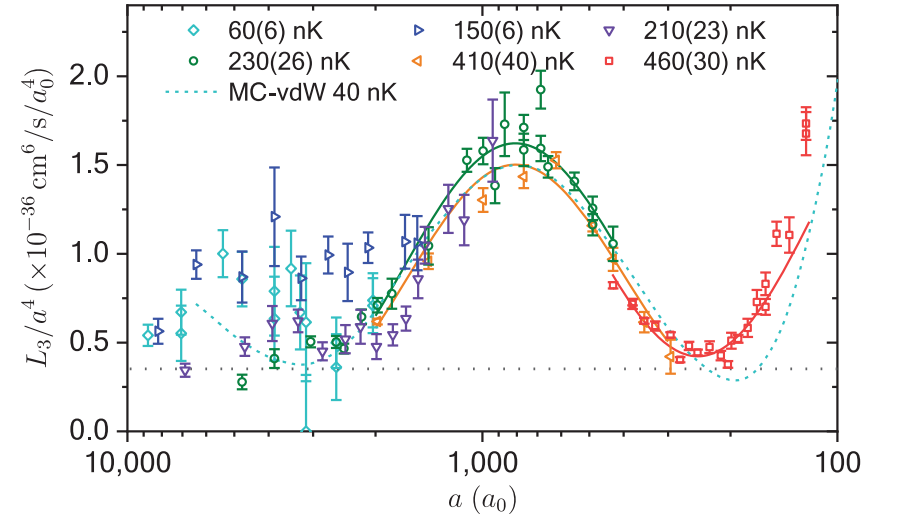


Figure VI.16. Three-body loss rate in a ^{39}K gas on the $a > 0$ side. Figure extracted from Xie, Van de Graaff, et al. (2020).

3 The three-body parameter

3-1 A surprising coincidence?

In the approach we have presented here, based on a zero-range interaction, the three-body parameter R_0 is an *ad hoc* parameter, unrelated to the other physical quantities of the problem. It was initially expected that the same would apply to the van der Waals interaction at play in cold atom gases. It was therefore a surprise when, after compiling experimental values of R_0 for different Fano–Feshbach resonances of a given atomic species – cesium – (Gross, Shotan, et al. 2010; Berninger, Zenesini, et al. 2011) as well as for other atomic species, it was found that these values were closely related to the van der Waals length

$$R_{\text{vdW}} = \frac{1}{2} \left(\frac{mC_6}{\hbar^2} \right)^{1/4}. \quad (20)$$

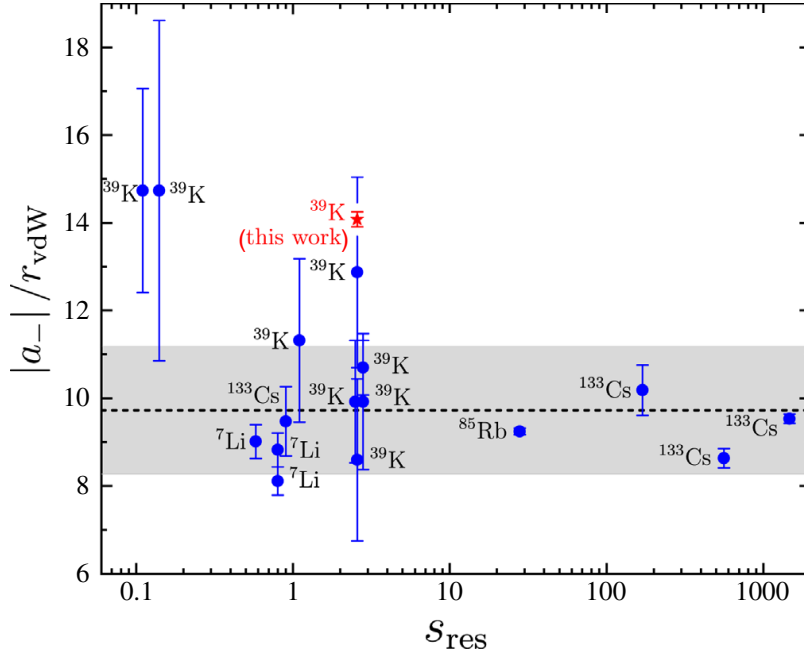


Figure VI.17. Values of the ratio $a_-^{(0)}/R_{\text{vdW}}$ for the first Efimov trimer for different atomic species, as a function of the width s_{res} of the Fano–Feshbach resonance. The gray area corresponds to $a_-^{(0)}/R_{\text{vdW}} = -9.7 \pm 1.5$. Figure taken from Chapurin, Xie, et al. (2019).

For example, if we look at the $a_-^{(0)}$ peak of the three-body recombination rate on the $a < 0$ side of the resonance, we see that the position of this peak seems to be “locked” around $-10 R_{\text{vdW}}$, with a few exceptions, notably on the side of very narrow Fano–Feshbach resonances (see figure VI.17 for more details).

To clarify the situation theoretically, Wang, D’Incao, et al. (2012) studied the behavior of this ratio $a_-^{(0)}/R_{\text{vdW}}$ for different two-body potentials, varying the number of bound states in these potentials [see also Mestrom, Wang, et al. (2017)]. Their results are shown in figure VI.18; they were

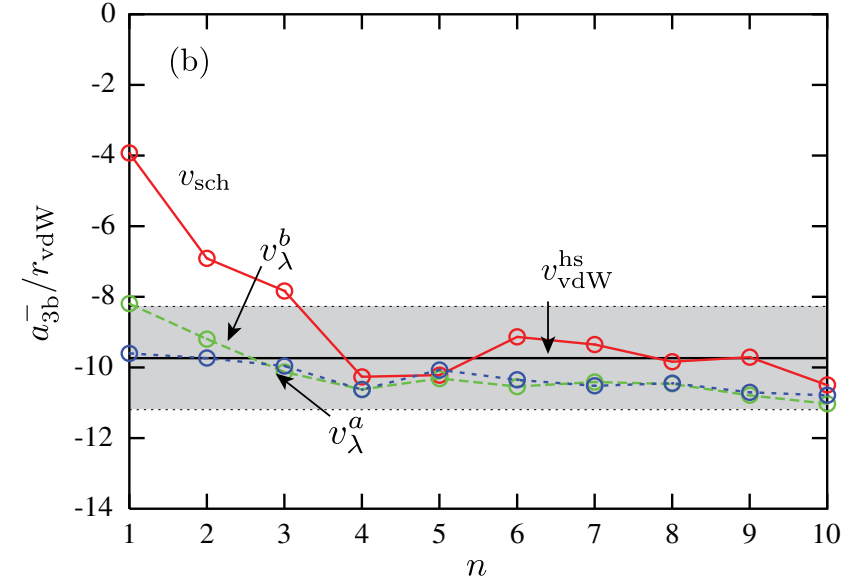


Figure VI.18. Values of the ratio $a_-^{(0)}/R_{\text{vdW}}$ for the first Efimov trimer calculated for different two-body interaction potentials. Figure extracted from Wang, D’Incao, et al. (2012).

obtained for

$$V_\lambda^a(r) = -\frac{C_6}{r^6} + \frac{C_{12}}{r^{12}} \quad C_{12} \equiv \lambda^6 C_6 \quad (21)$$

$$V_\lambda^b(r) = -\frac{C_6}{r^6} \exp(-\lambda^6/r^6) \quad (22)$$

$$V_{\text{vdW}}^{\text{hs}}(r) = B_{\text{hs}} \Theta(r_{\text{hs}} - r) - \frac{C_6}{r^6} \Theta(r - r_{\text{hs}}) \quad (23)$$

These potentials all vary as r^{-6} at long distances⁴. This leads to the tight clustering observed experimentally: $a_-^{(0)} \sim -10 R_{\text{vdW}}$. The fourth potential used in figure VI.18, $V_{\text{sch}}(r)$, decreases exponentially fast at infinity and will not be discussed here.

⁴For the van der Waals potential with a hard core, $V_{\text{vdW}}^{\text{hs}}(r)$ (“hs” = “hard sphere”), the parameters are adjusted so as to sit at the threshold for the appearance of the first bound state.

The link found between the three-body parameter and R_{vdW} is therefore not fortuitous: it is recovered theoretically and we now need to understand its physical origin.

3-2 Back to the hyperspherical approach

To understand the origin of this link between the three-body parameter and R_{vdW} , we will return to the approach described in the previous chapter for dealing with the three-body problem. Once the transition to the reference frame of the center of mass has been made, the problem is described by six variables: the hyperradius R , with

$$R^2 = \frac{2}{3} (r_{12}^2 + r_{23}^2 + r_{31}^2) \quad (24)$$

and five angles:

- the two angles α (Delves) and β (Jacobi), which determine the shape of the triangle (up to a homothety),
- the three Euler angles, which determine the orientation of the triangle in space.

In what follows, we denote by Ω the quintuplet formed by these five angles, a given configuration of the triangle in the laboratory frame thus being defined by (R, Ω) .

The hyperspherical approach takes as its starting point the Schrödinger equation in the form (D’Incao, Greene, et al. 2009)

$$\left[-\frac{\partial^2}{\partial R^2} + \hat{H}_{\text{ang}}(\Omega; R) \right] \Phi(R, \Omega) = \mathcal{E} \Phi(R, \Omega) \quad \text{with} \quad \mathcal{E} = \frac{mE}{\hbar^2} \quad (25)$$

where the operator $\hat{H}_{\text{ang}}(\Omega; R)$ involves derivatives with respect to the five angles of Ω (generalized angular momentum operator), and also contains the interaction potentials between the three particles. The hyperradius R plays the role of an external parameter in $\hat{H}_{\text{ang}}(\Omega; R)$: this operator is local in R and does not contain derivatives with respect to R .

We start by solving the eigenvalue problem for the hyperangle Ω at fixed R , and find a series of eigenfunctions and eigenvalues parameterized by R :

$$\hat{H}_{\text{ang}}(\Omega; R) F_i(\Omega; R) = \epsilon_i(R) F_i(\Omega; R), \quad (26)$$

For all R , these functions F_i form an orthonormal basis of the functions of Ω , with

$$\langle F_i(R) | F_j(R) \rangle = \int F_i^*(\Omega; R) F_j(\Omega; R) d^5\Omega = \delta_{i,j}. \quad (27)$$

Once this first stage has been completed, we look for the solution of the initial equation (25) in the general form

$$\Phi(R, \Omega) = \sum_j \phi_j(R) F_j(\Omega; R), \quad (28)$$

where the functions $\phi_j(R)$ are unknown at this stage. To determine them, we insert this form into (25) and project the result onto a particular F_i , to find

$$-\frac{d^2 \phi_i}{dR^2} + \epsilon_i(R) \phi_i(R) + [\dots] = \mathcal{E} \phi_i(R). \quad (29)$$

In this expression, the term $[\dots]$ appears because of the R dependence of the functions $F_j(\Omega; R)$; more precisely, with the notation used in (27),

$$[\dots] = -2 \sum_j \frac{d\phi_j}{dR} \langle F_i | \partial_R F_j \rangle - \sum_j \phi_j(R) \langle F_i | \partial_R^2 F_j \rangle \quad (30)$$

The simplest approach is to neglect the term $[\dots]$ altogether. This corresponds to the Born–Oppenheimer approximation in molecular physics and is also what we presented in Chapter 5, §4.1: the hyperspherical potential that we introduced then, $[s_i^2(R) - 1/4]/R^2$, was none other than the $\epsilon_i(R)$ term that appears in (29).

Conversely, if we keep the infinite system of coupled equations for the ϕ_j , we have an exact description of the problem. In practice, the description is all the better the higher the index j at which the system is truncated.

An intermediate approach, which will guide us here, consists in keeping only one unknown function ϕ_i while taking into account the corrections coming from the R dependence of $F_i(\Omega; R)$ in (30). After a relatively simple calculation [see for example Dalibard, Gerbier, et al. (2011) or the 2014

lecture series, Chapter 3, §4], we arrive at the following simple form for the equation satisfied by ϕ_i :

$$\left\{ \left[-i \frac{d}{dR} - \mathcal{A}_i(R) \right]^2 + \epsilon_i(R) + \mathcal{V}_i(R) \right\} \phi_i(R) = \mathcal{E} \phi_i(R) \quad (31)$$

where two geometric potentials $\mathcal{A}_i$ and $\mathcal{V}_i$ appear:

$$\mathcal{A}_i(R) = i \langle F_i(R) | \partial_R F_i(R) \rangle \quad \mathcal{V}_i(R) = \sum_{j \neq i} |\langle \partial_R F_i(R) | F_j(R) \rangle|^2 \quad (32)$$

If the variable R lived in a space of dimension greater than 1, the potential $\mathcal{A}_i$ would be a “vector potential” and would describe a possible Berry phase. For the problem of interest here, where the variable R is one-dimensional, $\mathcal{A}_i$ plays no role: it can be eliminated by a gauge change on the function ϕ_i , by setting $\tilde{\phi}_i(R) = \phi_i(R) e^{-i\chi(R)}$ with $\chi(R) = \int_0^R \mathcal{A}_i(R') dR'$. The “scalar potential” $\mathcal{V}_i(R)$, on the other hand, plays an important role. Let us note straight away that it is always positive, and larger the more rapidly the angular state $|F_i(R)\rangle$ varies with R .

3-3 Emergence of a hard core at $\sim 2R_{\text{vdW}}$

To assess quantitatively the role of the geometric potential defined in the previous section, it is interesting to examine the results of Wang, D’Incao, et al. (2012) already cited, as well as those of Naidon, Endo & Ueda (2014) [with their erratum Naidon, Endo & Ueda (2021)]. These authors considered two types of two-body potentials

$$V_{\text{soft}}(r) = -\frac{C_6}{r^6 + \sigma^6} \quad \text{and} \quad V_{\text{LJ}}(r) = -\frac{C_6}{r^6} + \frac{C_{12}}{r^{12}}. \quad (33)$$

For a fixed C_6 , they varied the number of bound states by changing σ or C_{12} , and then calculated the resulting total potential $W_i(R) = \epsilon_i(R) + \mathcal{V}_i(R)$ for the lowest-energy channel $i = 0$. The calculation was carried out in the unitary case ($a = \infty$) for which the adiabatic potential $\epsilon_0(R)$ is equal to $-(|s_0|^2 + 1/4)/R^2$ if the range of the two-body potential can be neglected.

The result plotted in figure VI.19 is striking. As soon as the number of bound states exceeds 3, the form of $W_i(R)$ becomes almost independent

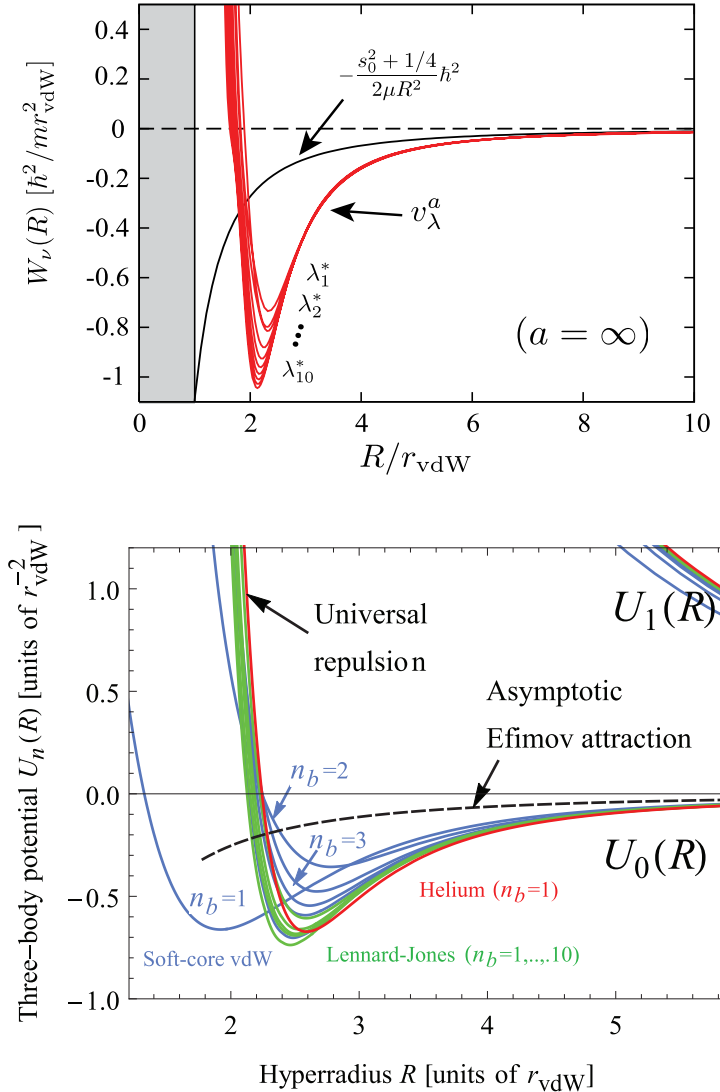


Figure VI.19. Total potential $W_i(R) = \epsilon_i(R) + \mathcal{V}_i(R)$ for channel $i = 0$. The calculation is made at unitarity, i.e. for $a = \infty$. Figures taken from Wang, D’Incao, et al. (2012) (top) and Naidon, Endo & Ueda (2014) (bottom).

of this number of bound states and therefore of the depth of the original two-body potential $V(r)$. More precisely:

- For $R \gtrsim 10R_{\text{vdW}}$, we recover the Efimov potential determined in the previous chapter for a zero-range interaction, $-(|s_0|^2 + 1/4)/R^2$.
- For $2R_{\text{vdW}} \lesssim R \lesssim 10R_{\text{vdW}}$, the potential $W_i(R)$ is significantly deeper than the Efimov potential for a zero-range interaction.
- For $R \approx 2R_{\text{vdW}}$, a hard core emerges, even if the initial two-body potential $V(r)$ is strictly monotonic, as is the case for $V_{\text{soft}}(r)$.

All that remains is to understand why the potential $W_0(R)$ makes this quasi-hard core appear at short distances. The explanation given by Wang, D’Incao, et al. (2012) and Naidon, Endo & Ueda (2014) is based on the optimal shape of the trimer as a function of the hyperradius R :

- When $R \gg R_{\text{vdW}}$, the optimal shape is the same as for a zero-range potential: it is an elongated triangle with two particles close together and the third much further away.
- When the hyperradius becomes of the order of a few R_{vdW} , the optimal shape of the triangle is closer to an equilateral triangle. Indeed, the elongated shape would imply having two particles at a distance much smaller than R_{vdW} , which is unlikely, as can be seen from the solution of the two-body problem shown in figure VI.20 [see also the 2021 lecture series, Chapter 4, §4].

The shape of the triangle therefore varies rapidly in the neighborhood $R \sim 2R_{\text{vdW}}$, which creates a large geometric scalar potential $\mathcal{V}_0(R)$ [cf. (32)].

Note that this explanation is based on an analysis of a one-channel binary potential. In experiments on cold atomic gases, Fano–Feshbach resonances are used to approximate the $a = \infty$ situation and the parameters of the resonance, such as its width and background scattering length, can play a significant role. See Schmidt, Rath, et al. (2012), Wang & Julienne (2014), and Langmack, Schmidt, et al. (2018) for a detailed treatment of this case.

The case of narrow Feshbach resonances is special because of the effective range $\gg R_{\text{vdW}}$ which appears in the problem (Petrov 2004). Recourse

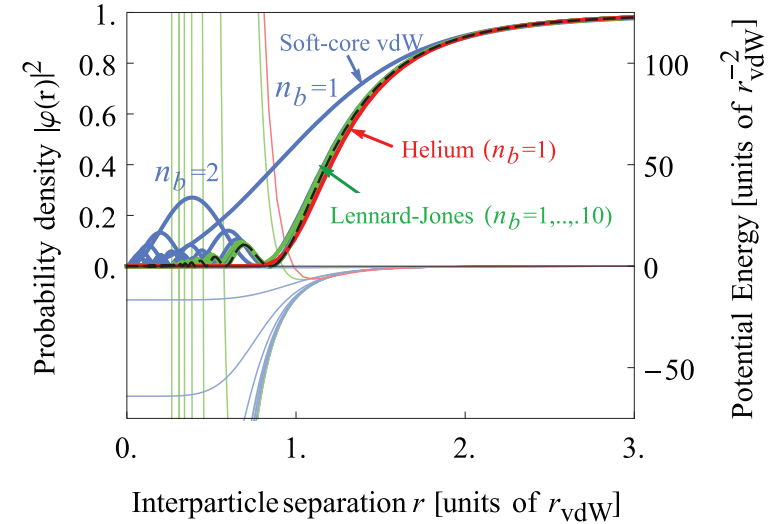


Figure VI.20. Probability density of the zero-energy two-body wave function for the different potentials given in (33). As soon as there are several bound states for these potentials, the probability of finding the two atoms at a distance less than R_{vdW} becomes very low. The thin lines indicate the potentials used for the calculation. The calculation is made for $a = \infty$. Figure taken from Naidon, Endo & Ueda (2014).

to a three-body parameter to regularize the situation is then no longer necessary, and Gogolin, Mora, et al. (2008) have been able to provide an analytical solution of the three-body problem in this case [see also Castin & Tignone (2011b), Endo & Castin (2016), Secker, Ahmed-Braun, et al. (2021), and Kraats, Ahmed-Braun, et al. (2022) and references therein]. Several recent experiments have been conducted in this regime, including Johansen, DeSalvo, et al. (2017), Yudkin, Elbaz, Giannakeas, et al. (2019), Xie, Van de Graaff, et al. (2020), Li, Yudkin, et al. (2022), and Etrych, Martirosyan, et al. (2022).

4 Beyond the standard Efimov effect

The original work by Efimov (1970) concerned three identical bosons in resonant interaction and it is this case that we have concentrated on in these last two chapters. To conclude this presentation, we will now review a few different situations, in terms of the statistical nature or the number of particles involved. Given the space available, our discussion will necessarily be fragmentary, and we refer the interested reader to Naidon & Endo (2017), which presents in detail many extensions of Efimov's problem.

4-1 Three identical fermions

Let us start with the simple case where we replace the three identical bosons of the Efimov effect by three polarized fermions. There is then no longer any binary interaction in the s wave, and we must turn to binary interactions in the p wave ($\ell = 1$), for which the scattering amplitude $f_1(k)$ reads [see the 2021 lecture series, Chapter 3, §2.3]:

$$\frac{1}{f_1(k)} \approx -\frac{1}{k^2 v} + \frac{k_e}{2} - ik, \quad (34)$$

where v is the scattering volume and k_e an effective range term (always negative near resonance). The counterpart of $|a| = \infty$ for an s -wave resonance is here an infinite scattering volume v . A weakly bound state of the dimer appears on the $v > 0$ side of the resonance.

This problem was studied by Jona-Lasinio, Pricoupenko, et al. (2008) [see also Levinsen, Cooper, et al. (2008) and Braaten, Hagen, et al. (2012)]. These authors showed that for the channel of angular momentum 1, there could be two bound trimers, one of each parity, for v chosen sufficiently close to the resonance $v = \infty$. These trimers can be Borromean in nature, i.e. exist for large negative values of the scattering volume, for which there is no weakly bound two-body state. The position of these trimers is universal in that it depends only on the parameters of the two-body problem, in this case the values of v , k_e and the range b of the potential (figure VI.21).

There is therefore no Efimov effect in this case, i.e. no emergence of an infinite series of three-body bound states at the dimer formation threshold. Furthermore, it is not necessary to introduce a three-body param-

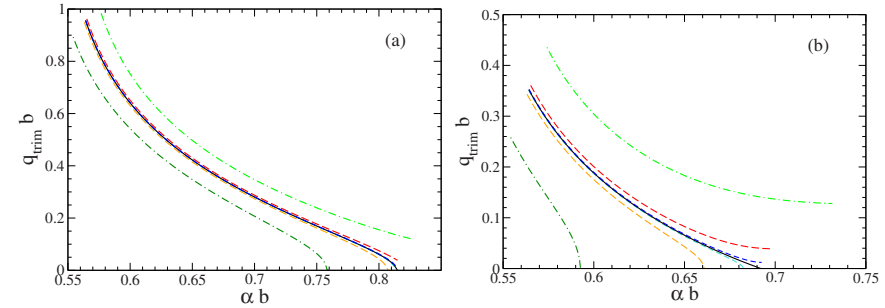


Figure VI.21. Wave number q defining the energy $-\hbar^2 q^2/m$ of the trimer formed from three identical fermions. The effective range is given here as $\alpha \equiv -k_e/2$. The parameter b denotes the range of the potential, obtained here by modeling a Fano–Feshbach resonance with Gaussian coupling between the open and closed channels. Figure on the left (resp. right): positive (resp. negative) parity. Black solid line: $v = \infty$; blue dashed line: $v = \pm 10^4 b^3$; red/orange dashed line: $v = \pm 10^3 b^3$; green dashed line: $v = \pm 10^2 b^3$. Figures taken from Jona-Lasinio, Pricoupenko, et al. (2008).

ter to describe the energy of the two universal trimers mentioned above. This problem has recently been taken up by Chen & Greene (2022), who confirmed the conclusions of Jona-Lasinio, Pricoupenko, et al. (2008) for Lennard–Jones-type potentials ($-r^{-6} + r^{-12}$).

4-2 Three distinguishable particles

When three distinguishable particles are considered, the wave function does not have to be symmetrized or antisymmetrized, which relaxes a constraint present for indistinguishable particles. For the same interaction strength, the ground-state energy of the system of three distinguishable particles is therefore necessarily lower than or equal to that calculated for bosons or fermions.

If the three s -wave interactions are resonant ($|a_{ij}| = \infty$) and the three masses are equal, we find the same result as for three identical bosons because of the symmetry of the system. In particular, we have the scaling

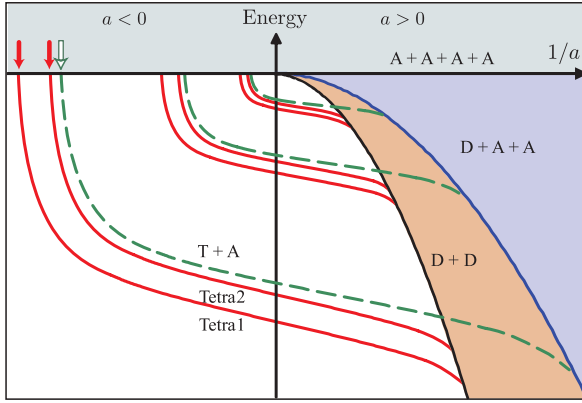


Figure VI.22. The two universal tetramer branches attached to each Efimov trimer branch. Figure taken from Ferlaino, Knoop, et al. (2009).

parameter $\lambda = e^{\pi/|s_0|} \approx 22.7$ with $|s_0| = 1.00624$.

If two interactions are resonant and the third is zero, for example $|a_{12}| = |a_{13}| = +\infty$ and $a_{23} = 0$, we formally find the mMM case studied in Chapters 3 and 4. If the relation $m \ll M$ does not hold, the Born–Oppenheimer approach is no longer valid, but a treatment similar to that adopted in Chapter 5 is still possible. We then find an Efimov effect, with a scaling parameter $\lambda = e^{\pi/|s_0|} \approx 2000$ with $|s_0| = 0.414$ (Naidon & Endo 2017). The very high value of this parameter λ makes experimental verification difficult.

4-3 Four identical bosons

We continue our discussion with the case of four identical bosons, of zero spin or polarized. Here too, the first question that arises is that of a genuine four-body Efimov effect, i.e. the existence of an infinite number of bound states of tetramers at the threshold $a_-^{(0)}$ of the first Efimov trimer, on the $a < 0$ side. This question was in fact addressed very shortly after Efimov’s publication by Amado & Greenwood (1973) and the answer is negative.

However, this result does not completely settle the question. Although

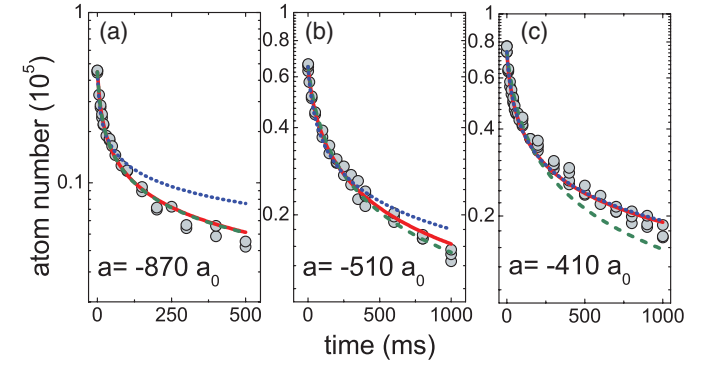


Figure VI.23. Decay in the number of cesium atoms in the vicinity of the threshold for the appearance of the first Efimov trimer. Dashed line: three (four) body losses only. Solid line: prediction deduced from (36). Figure taken from Ferlaino, Knoop, et al. (2009).

an Efimovian series of tetramers does not exist, there may be one or more tetramers attached to each Efimov trimer. This is a four-particle structure, with an energy that is negative and lower than that of the trimer. The prediction of such “universal” tetramers was made by Hammer & Platter (2007), then refined by Stecher, D’Incao, et al. (2009). There are two branches of tetramers attached to each branch of trimers (figure VI.22). These tetramers are described as universal because, once the position of the trimer is known, their energy can be calculated without the need to introduce a four-body parameter. This statement requires a few precautions for the ground-state trimer, since the corresponding tetramers are smaller than it and may therefore be sensitive to short-range physics [see Naidon & Endo (2017)].

These tetramers are Borromean in nature, in the sense that they can exist for a scattering length smaller in absolute value than the (negative) scattering length $a_-^{(n)}$ for which the trimer appears. The prediction of Stecher, D’Incao, et al. (2009) is

$$a_{4b1}^{(0)} = 0.43 a_-^{(0)} \quad a_{4b2}^{(0)} = 0.90 a_-^{(0)} \quad (35)$$

The existence of these tetramers has been confirmed by Ferlaino, Knoop, et

al. (2009) in an experiment that takes precise advantage of this Borromean nature. The Innsbruck researchers studied the loss of atoms in a cesium trap in the vicinity of the trimer appearance threshold $a_-^{(0)} = -870 a_0$. They observed two values of a for which the losses could be explained by the sum of a three-body law and a four-body law (figure VI.23):

$$\frac{\dot{N}}{N} = -L_3 \rho^2 - L_4 \rho^3. \quad (36)$$

The values found for $a_{4b1}^{(0)}$ and $a_{4b2}^{(0)}$ are in good agreement with the prediction (35) [measured coefficients: 0.47 and 0.84].

4-4 N_f identical fermions and another particle

The $mMMM$ system, i.e. $N_f = 3$ identical fermions and another particle, as well as its generalization to $N_f = 4$, are the only known systems⁵ which exhibit a true Efimov effect. The $N_f = 3$ case has been studied by Castin, Mora, et al. (2010) and the $N_f = 4$ case by Bazak & Petrov (2017).

The question we address in this section can be formulated as follows: how many polarized fermions of mass M can be bound through the interaction with a single light particle of mass m ? To begin with, let us recall the important result obtained in Chapters 3 and 4 for the $N_f = 2$ case. We considered the three-body system mMM for a zero-range interaction with $|a| = +\infty$ and indicated that (Kartavtsev & Malykh 2007):

- an Efimov effect can occur when $M/m > 13.607$;
- for $8.173 < M/m < 13.607$, there exist on the $a > 0$ side one (or two) “universal” trimers, whose energy does not depend on a three-body parameter.

To study the $mMMM$ problem, i.e. with an additional M fermion, Castin, Mora, et al. (2010) worked at unitarity for a zero-range mM binary interaction. The MM interactions between two identical fermions are assumed to be negligible (they could only be odd-wave interactions, which

⁵In particular, the mMM system with M bosonic does not exhibit this property (Adhikari & Fonseca 1981). The same is true for the $mmMM$ four-fermion system (Endo & Castin 2015).

are weak at low temperature). We therefore consider the purely kinetic Hamiltonian

$$\hat{H} = - \sum_{i=1}^4 \frac{\hbar^2}{2m_i} \nabla_i^2 \quad (37)$$

with Bethe–Peierls boundary conditions at the points where the light particle m comes into contact with one of the fermions M . The question is whether this Hamiltonian admits negative-energy states in which the three heavy particles are bound together by the light particle.

As for the three-body problem, it is useful, for an N -body problem (with $N = N_f + 1$), first to isolate the three variables of the center of mass (which we take to be at rest in what follows), and then to separate the remaining $d = 3N - 3$ variables into

- one variable R , the hyperradius, giving the length scale of the problem;
- $d - 1 = 3N - 4$ hyperangles, denoted collectively by Ω , defining the spatial arrangement of the N bodies (up to a homothety) and the orientation of this arrangement in space.

The general expression for the kinetic energy operator in d dimensions can be written in terms of these variables (see for example Greene, Gianakeas, et al. (2017)):

$$\hat{H} = \hat{T}_R + \frac{\hbar^2}{2m_r R^2} \hat{\Lambda}_\Omega^2 \quad (38)$$

where the radial kinetic energy operator is

$$\hat{T}_R = - \frac{\hbar^2}{2m_r} \left(\frac{\partial^2}{\partial R^2} + \frac{d-1}{R} \frac{\partial}{\partial R} \right) \quad (39)$$

and where $\hat{\Lambda}_\Omega$ is the “grand angular momentum” operator for the d -dimensional system. This operator involves the hyperangles and first- and second-order derivatives with respect to them⁶, but not the hyperradius R .

⁶For example, in dimension $d = 3$, we have the well-known expression as a function of the polar angle θ and the azimuthal angle φ :

$$\hat{\Lambda}^2 = \frac{\hat{L}^2}{\hbar^2} = - \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}. \quad (40)$$

Note that the precise definition of the pair “hyperradius, reduced mass” varies from author to author by numerical factors of order unity. In what follows, we will not go into quantitative calculations, and we will therefore not need to specify this choice. For an explicit construction of hyperangles, the hyperradius and the associated reduced mass, see Greene, Giannakeas, et al. (2017).

In general, when a is not infinite or zero, Bethe–Peierls boundary conditions couple hyperradius and hyperangles, which makes the problem particularly complex. In the case $|a| = +\infty$ (or in the case without interaction $a = 0$), the Bethe–Peierls boundary conditions only involve hyperangles. This is a signature of the scale invariance of the system, already mentioned several times in previous chapters: there is no length scale to compare with R in order to obtain a dimensionless equation. Thus, for the three-body problem, we arrived in Chapter 5 at the equation translating these boundary conditions for the angular part $F(\alpha)$ of the wave function:

$$|a| = +\infty : \quad \left[\frac{dF}{d\alpha} \right]_{\alpha \rightarrow 0} + \frac{8}{\sqrt{3}} F\left(\frac{\pi}{3}\right) = 0. \quad (41)$$

The treatment of Castin, Mora, et al. (2010) therefore starts from the fact that we can then look for the eigenstates of $\hat{H}$ in a factorized form:

$$\Phi(R, \Omega) = \frac{\phi(R)}{R^{(d-1)/2}} F(\Omega) \quad \text{with for } N = 4 : \quad \frac{d-1}{2} = 4. \quad (42)$$

The first step is to solve the eigenvalue problem for the angular part $F(\Omega)$, taking into account the Bethe–Peierls boundary conditions:

$$\hat{\Lambda}_{\Omega}^2 F(\Omega) = \lambda F(\Omega). \quad (43)$$

Once this (tricky!) stage has been completed, the radial equation then simply reads

$$-\frac{d^2\phi}{dR^2} + \frac{s^2 - 1/4}{R^2} \phi(R) = \epsilon \phi(R) \quad (44)$$

where [cf. Eq. (C-13) of Werner & Castin (2006)]

$$s^2 = \lambda + \frac{1}{4}(d-2)^2 \quad (45)$$

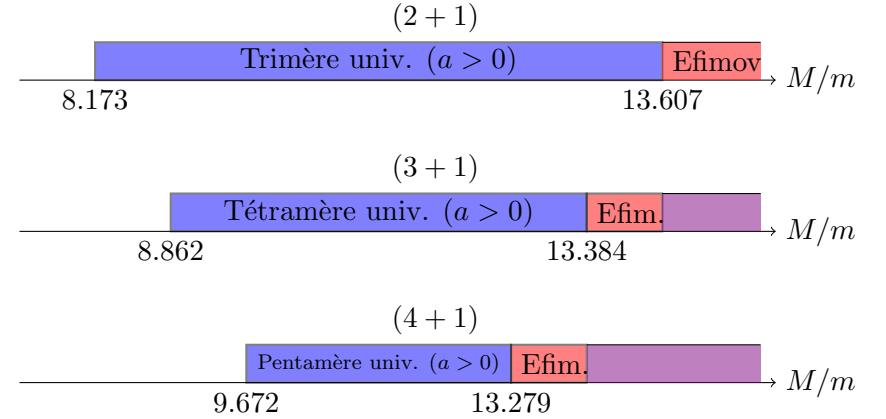


Figure VI.24. The possible bound states of N_f fermions of mass M in resonant binary interaction with a particle of mass m ($N_f = 2, 3, 4$). These data are taken from Kartavtsev & Malykh (2007), Castin, Mora, et al. (2010), Bazak & Petrov (2017), and Bazak (2020). The scale of the M/m axis is not linear. There is no Efimov effect for $N_f = 5$ or 6 (Bazak 2020).

is a number that depends on M/m but not on R , and where we have set $\epsilon = 2m_{\tau}E/\hbar^2$.

We now find ourselves in familiar territory: if negative values of s^2 are possible, an Efimov effect will appear. The result of Castin, Mora, et al. (2010) for $N = N_f + 1 = 4$ is that this effect can indeed occur when

$$13.384 < \frac{M}{m} \quad (46)$$

This condition is (slightly) less restrictive than the one found for the mMM problem. There is therefore an interval of values of M/m , $[13.384, 13.607]$, over which the four-body problem is Efimovian whereas the three-body problem is not (see figure VI.24). For $M/m > 13.607$, it is difficult to state general results for the $(3+1)$ problem, since solving the Efimovian $(2+1)$ problem requires the introduction of a non-universal three-body parameter. We have shown this region in purple in figure VI.24.

We can also look for a universal tetramer for lower values of M/m , similar to the universal trimer(s) of Kartavtsev & Malykh (2007). Such a tetramer exists on the interval $[8.862, 13.384]$ (Blume 2012; Bazak 2020).

As announced in the introduction to this section, the $(4 + 1)$ problem, i.e. $N_f = 4$ fermions of mass M and a light particle of mass m , also leads to an original Efimov effect with the formation of pentamers, in a (small) range of values of M/m for which there are no Efimov trimers, nor Efimov tetramers (Bazak & Petrov 2017). It can be shown, on the other hand, that there are no Efimov states for the $(5 + 1)$ and $(6 + 1)$ systems (Bazak 2020). These results are also summarized in figure VI.24.

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