Chapter 5
The Unitary Gas and its Symmetry Properties

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Abstract   The physics of atomic quantum gases is currently taking advantage of a powerful tool, the possibility to fully adjust the interaction strength between atoms using a magnetically controlled Feshbach resonance. For fermions with two internal states, formally two opposite spin states ↑ and ↓, this allows to prepare long lived strongly interacting three-dimensional gases and to study the BEC–BCS crossover. Of particular interest along the BEC–BCS crossover is the so-called unitary gas, where the atomic interaction potential between the opposite spin states has virtually an infinite scattering length and a zero range. This unitary gas is the main subject of the present chapter: it has fascinating symmetry properties, from a simple scaling invariance, to a more subtle dynamical symmetry in an isotropic harmonic trap, which is linked to a separability of the N-body problem in hyperspherical coordinates. Other analytical results, valid over the whole BEC–BCS crossover, are presented, establishing a connection between three recently measured quantities, the tail of the momentum distribution, the short range part of the pair distribution function and the mean number of closed channel molecules. The chapter is organized as follows. In Sect. 5.1, we introduce useful concepts, and we present a simple definition and basic properties of the unitary gas, related to its scale invariance. In Sect. 5.2, we describe various models that may be used to describe the BEC–BCS crossover, and in particular the unitary gas, each model having its own advantage and shedding some particular light on the unitary gas properties: scale invariance and a virial theorem hold within the zero-range model, relations between the derivative of the energy with respect to the inverse scattering length and the short range pair correlations or the

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tail of the momentum distribution are easily derived using the lattice model, and the same derivative is immediately related to the number of molecules in the closed channel (recently measured at Rice) using the two-channel model. In Sect. 5.3, we describe the dynamical symmetry properties of the unitary gas in a harmonic trap, and we extract their physical consequences for many-body and few-body problems.

5.1 Simple Facts About the Unitary Gas

5.1.1 What is the Unitary Gas?

First, the unitary gas is ... a gas. As opposed to a liquid, it is a dilute system with respect to the interaction range b: its mean number density ρ satisfies the constraint

$$\rho b^3 \ll 1. \tag{5.1}$$

For a rapidly decreasing interaction potential $V(r)$, b is the spatial width of $V(r)$. In atomic physics, where $V(r)$ may be viewed as a strongly repulsive core and a Van der Waals attractive tail $-C_6/r^6$, one usually assimilates b to the Van der Waals length $(mC_6/\hbar^2)^{1/4}$.

The intuitive picture of a gas is that the particles mainly experience binary scattering, the probability that more than two particles are within a volume b^3 being negligible. As a consequence, what should really matter is the knowledge of the scattering amplitude f_k of two particles, where k is the relative momentum, rather than the r dependence of the interaction potential $V(r)$. This expectation has guided essentially all many-body works on the BEC–BCS crossover: One uses convenient models for $V(r)$ that are very different from the true atomic interaction potential, but that reproduce correctly the momentum dependence of f_k at the relevant low values of k, such as the Fermi momentum or the inverse thermal de Broglie wavelength, these relevant low values of k having to satisfy $kb \ll 1$ for this modelization to be acceptable.

Second, the unitary gas is such that, for the relevant values of the relative momentum k, the modulus of f_k reaches the maximal value allowed by quantum mechanics, the so-called unitary limit [1]. Here, we consider s-wave scattering between two opposite-spin fermions, so that f_k depends only on the modulus of the relative momentum. The optical theorem, a consequence of the unitarity of the quantum evolution operator [1], then implies

$$\mathrm{Im}\, f_k = k|f_k|^2. \tag{5.2}$$

Dividing by $|f_k|^2$, and using $f_k/|f_k|^2 = 1/f_k^*$, one sees that this fixes the value of the imaginary part of $1/f_k$, so that it is strictly equivalent to the requirement that there exists a real function $u(k)$ such that

$$f_k = -\frac{1}{ik + u(k)} \qquad (5.3)$$

for all values of k. We then obtain the upper bound $|f_k| \le 1/k$. Ideally, the unitary gas saturates this inequality for all values of k:

$$f_k^{\text{unitary}} = -\frac{1}{ik}. \qquad (5.4)$$

In reality, Eq. 5.4 cannot hold for all k. It is thus important to understand over which range of k Eq. 5.4 should hold to have a unitary gas, and to estimate the deviations from Eq. 5.4 in that range in a real experiment. To this end, we use the usual low-k expansion of the denominator of the scattering amplitude [1], under validity conditions specified in [2]:

$$u(k) = \frac{1}{a} - \frac{1}{2}r_e k^2 + \dots \qquad (5.5)$$

The length a is the scattering length, the length r_e is the effective range of the interaction. Both a and r_e can be of arbitrary sign. Even for $1/a = 0$, even for an everywhere non-positive interaction potential, r_e can be of arbitrary sign. As this last property seems to contradict a statement in the solution of problem 1 in Sect. 131 of [3], we have constructed an explicit example depicted in Fig. 5.1, which even shows that the effective range may be very different in absolute value from the true potential range b, i.e. r_e/b for $a^{-1} = 0$ may be in principle an arbitrarily large and negative number. Let us assume that the ... in Eq. 5.5 are negligible if $kb \ll 1$, an assumption that will be revisited in Sect. 5.2.3.3. Noting k_{typ} a typical relative momentum in the gas, we thus see that the unitary gas is in practice obtained as a double limit, a *zero range* limit

$$k_{\text{typ}}b \ll 1, k_{\text{typ}}|r_e| \ll 1 \qquad (5.6)$$

and an *infinite scattering length* limit:

$$k_{\text{typ}}|a| \gg 1. \qquad (5.7)$$

At zero temperature, we assume that $k_{\text{typ}} = k_F$, where the Fermi momentum is conventionally defined in terms of the gas total density ρ as for the ideal spin-1/2 Fermi gas:

$$k_F = (3\pi^2\rho)^{1/3}. \qquad (5.8)$$

In a trap, ρ and thus k_F are position dependent. Condition (5.7) is well satisfied experimentally, thanks to the Feshbach resonance. The condition $k_F b \ll 1$ is also well satisfied at the per cent level, because $b \approx$ the Van der Waals length is in the nanometer range. Up to now, there is no experimental tuning of the effective range
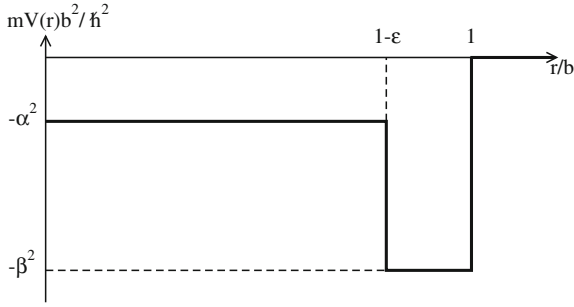
Fig. 5.1 A class of non-positive potentials (of compact support of radius b) that may lead to a negative effective range in the resonant case $a^{-1} = 0$. The resonant case is achieved when the three parameters α, β and ε satisfy $\tan[(1-\varepsilon)\alpha] \tan(\varepsilon\beta) = \alpha/\beta$. Then from Smorodinskii's formula, see Problem 1 in Sect. 131 of [3], one sees that $r_e/b \leq 2$. One also finds that $r_e/b \sim -\cos^2\theta/(\pi\varepsilon)^2 \to -\infty$ when $\varepsilon \to 0$ with $\alpha = \pi$, $\beta\varepsilon \to \theta$, where $\theta = 2.798386\ldots$ solves $1 + \theta\tan\theta = 0$

r_e, and there are cases where $k_F|r_e|$ is not small. However, to study the BEC–BCS crossover, one uses in practice the so-called broad Feshbach resonances, which do not require a too stringent control of the spatial homogeneity of the magnetic field, and where $|r_e| \sim b$; then Eq. 5.6 is also satisfied.

We note that the assumption $k_{\text{typ}} = k_F$, although quite intuitive, is not automatically correct. For example, for bosons, as shown by Efimov [4], an effective three-body attraction takes place, leading to the occurrence of the Efimov trimers; this attraction leads to the so-called problem of *fall to the center* [3], and one has $1/k_{\text{typ}}$ of the order of the largest of the two ranges b and $|r_e|$. Eq. 5.6 is then violated, and an extra length scale, the three-body parameter, has to be introduced, breaking the scale invariance of the unitary gas. Fortunately, for three fermions, there is no Efimov attraction, except for the case of different masses for the two spin components: if two fermions of mass $m_\uparrow$ interact with a lighter particle of mass $m_\downarrow$, the Efimov effect takes place for $m_\uparrow/m_\downarrow$ larger than $\simeq 13.607$ [5, 6]. If a third fermion of mass $m_\uparrow$ is added, a four-body Efimov effect appears at a slightly lower mass ratio $m_\uparrow/m_\downarrow \simeq 13.384$ [7]. In what follows we consider the case of equal masses, unless specified otherwise.

At non-zero temperature $T > 0$, another length scale appears in the unitary gas properties, the thermal de Broglie wavelength λ_{dB}, defined as

$$\lambda_{\text{dB}}^2 = \frac{2\pi\hbar^2}{mk_BT}. \tag{5.9}$$

At temperatures larger than the Fermi temperature $T_F = \hbar^2 k_F^2/(2mk_B)$, one has to take $k_{\text{typ}} \sim 1/\lambda_{\text{dB}}$ in the conditions Eq. 5.7. In practice, the most interesting regime is however the degenerate regime $T < T_F$, where the non-zero temperature does not bring new conditions for unitarity.

5.1.2 Some Simple Properties of the Unitary Gas

As is apparent in the expression of the two-body scattering amplitude Eq. 5.4, there is no parameter or length scales issuing from the interaction. As a consequence, for a gas in the trapping potential $U(\mathbf{r})$, the eigenenergies E_i of the N-body problem only depend on $\hbar^2/m$ and on the spatial dependence of $U(\mathbf{r})$: the length scale required to get an energy out of $\hbar^2/m$ is obtained from the shape of the container.

This is best formalized in terms of a spatial scale invariance. Qualitatively, if one changes the volume of the container, even if the gas becomes arbitrarily dilute, it remains at unitarity and strongly interacting. This is of course not true for a finite value of the scattering length a: If one reduces the gas density, $\rho^{1/3}a$ drops eventually to small values, and the gas becomes weakly interacting.

Quantitatively, if one applies to the container a similarity factor λ in all directions, which changes its volume from V to $\lambda^3 V$, we expect that each eigenenergy scales as

$$E_i \rightarrow \frac{E_i}{\lambda^2} \tag{5.10}$$

and each eigenwavefunction scales as

$$\psi_i(\mathbf{X}) \rightarrow \frac{\psi_i(\mathbf{X}/\lambda)}{\lambda^{3N/2}}. \tag{5.11}$$

Here $\mathbf{X} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is the set of all coordinates of the particles, and the λ-dependent factor ensures that the wavefunction remains normalized. The properties (5.10, 5.11), which are at the heart of what the unitary gas really is, will be put on mathematical grounds in Sect. 5.2 by replacing the interaction with contact conditions on ψ. Simple consequences may be obtained from these scaling properties, as we now discuss.

In a harmonic isotropic trap, where a single particle has an oscillation angular frequency ω, taking as the scaling factor the harmonic oscillator length $a_{\mathrm{ho}} = [\hbar/(m\omega)]^{1/2}$, one finds that

$$\frac{E_i}{\hbar\omega} = \mathscr{F}_i(N) \tag{5.12}$$

where the functions $\mathscr{F}_i$ are universal functions, ideally independent of the fact that one uses lithium 6 or potassium 40 atoms, and depending only on the particle number.

In free space, the unitary gas cannot have a N-body bound state (an eigenstate of negative energy), whatever the value of $N \geq 2$. If there was such a bound state, which corresponds to a square integrable eigenwavefunction of the relative (Jacobi) coordinates of the particles, one could generate a continuum of such square integrable eigenstates using Eqs. 5.10, 5.11. This would violate a fundamental property of self-adjoint Hamiltonians [8]. Another argument is that the energy of a discrete universal bound state would depend only on $\hbar$ and m, which is impossible by dimensional analysis.

At thermal equilibrium in the canonical ensemble in a box, say a cubic box of volume $V = L^3$ with periodic boundary conditions, several relations may be obtained if one takes the thermodynamic limit $N \to +\infty$, $L^3 \to +\infty$ with a fixed density ρ and temperature T, and if one assumes that the free energy F is an extensive quantity. Let us consider for simplicity the case of equal population of the two spin states, $N_\uparrow = N_\downarrow$. Then, in the thermodynamic limit, the free energy per particle $F/N \equiv f$ is a function of the density ρ and temperature T. If one applies a similarity of factor λ and if one change T to T/λ^2 so as to keep a constant ratio $E_i/(k_B T)$, that is a constant occupation probability for each eigenstate, one obtains from Eq. 5.10 that

$$f(\rho/\lambda^3, T/\lambda^2) = f(\rho, T)/\lambda^2. \tag{5.13}$$

At zero temperature, f reduces to the ground state energy per particle $e_0(\rho)$. From Eq. 5.13 it appears that $e_0(\rho)$ scales as $\rho^{2/3}$, exactly as the ground state energy of the ideal Fermi gas. One thus simply has

$$e_0(\rho) = \xi e_0^{\text{ideal}}(\rho) = \frac{3\xi}{5} \frac{\hbar^2 k_F^2}{2m} \tag{5.14}$$

where k_F is defined by Eq. 5.8 and ξ is a universal number. This is also a simple consequence of dimensional analysis [9]. Taking the derivative with respect to N or to the volume, this shows that the same type of relation holds for the zero temperature chemical potential, $\mu_0(\rho) = \xi \mu_0^{\text{ideal}}(\rho)$, and for the zero temperature total pressure, $P_0(\rho) = \xi P_0^{\text{ideal}}(\rho)$, so that

$$\mu_0(\rho) = \xi \frac{\hbar^2 k_F^2}{2m} \tag{5.15}$$

$$P_0(\rho) = \frac{2\xi}{5} \rho \frac{\hbar^2 k_F^2}{2m}. \tag{5.16}$$

At non-zero temperature, taking the derivative of Eq. 5.13 with respect to λ in $\lambda = 1$, and using $F = E - TS$, where E is the mean energy and $S = -\partial_T F$ is the entropy, as well as $\mu = \partial_N F$, one obtains

$$\frac{5}{3} E - \mu N = TS. \tag{5.17}$$

From the Gibbs-Duhem relation, the grand potential $\Omega = F - \mu N$ is equal to $-PV$, where P is the pressure of the gas. This gives finally the useful relation

$$PV = \frac{2}{3} E, \tag{5.18}$$

that can also be obtained from dimensional analysis [9], and that of course also holds at zero temperature (see above). All these properties actually also apply to the ideal

Fermi gas, which is obviously scaling invariant. The relation (5.18) for example was established for the ideal gas in [10].

Let us finally describe at a macroscopic level, i.e. in a hydrodynamic picture, the effect of the similarity Eq. 5.11 on the quantum state of a unitary gas, assuming that it was initially at thermal equilibrium in a trap. In the initial state of the gas, consider a small (but still macroscopic) element, enclosed in a volume dV around point $\mathbf{r}$. It is convenient to assume that dV is a fictitious cavity with periodic boundary conditions. In the hydrodynamic picture, this small element is assumed to be at local thermal equilibrium with a temperature T. Then one performs the spatial scaling transform Eq. 5.10 on each many-body eigenstate ψ of the thermal statistical mixture, which does not change the statistical weigths. How will the relevant physical quantities be transformed in the hydrodynamic approach?

The previously considered small element is now at position $\lambda\mathbf{r}$, and occupies a volume $\lambda^3 dV$, with the same number of particles. The hydrodynamic mean density profile after rescaling, ρ_λ, is thus related to the mean density profile ρ before scaling as

$$\rho_\lambda(\lambda\mathbf{r}) = \rho(\mathbf{r})/\lambda^3. \tag{5.19}$$

Second, is the small element still at (local) thermal equilibrium after scaling? Each eigenstate of energy E_{loc} of the locally homogeneous unitary gas within the initial cavity of volume dV is transformed by the scaling into an eigenstate within the cavity of volume $\lambda^3 dV$, with the eigenenergy E_{loc}/λ^2. Since the occupation probabilities of each local eigenstate are not changed, the local statistical mixture remains thermal provided that one rescales the temperature as

$$T_\lambda = T/\lambda^2. \tag{5.20}$$

A direct consequence is that the entropy of the small element of the gas is unchanged by the scaling, so that the local entropy *per particle s* in the hydrodynamic approach obeys

$$s_\lambda(\lambda\mathbf{r}) = s(\mathbf{r}). \tag{5.21}$$

Also, since the mean energy of the small element is reduced by the factor λ^2 due to the scaling, and the volume of the small element is multiplied by λ^3, the equilibrium relation Eq. 5.18 imposes that the local pressure is transformed by the scaling as

$$p_\lambda(\lambda\mathbf{r}) = p(\mathbf{r})/\lambda^5. \tag{5.22}$$

5.1.3 Application: Inequalities on ξ and Finite-Temperature Quantities

Using the previous constraints imposed by scale invariance of the unitary gas on thermodynamic quantities, in addition to standard thermodynamic inequalities, we

show that one can produce constraints involving both the zero-temperature quantity ξ and finite-temperature quantities of the gas.

Imagine that, at some temperature T, the energy E and the chemical potential μ of the non-polarized unitary Fermi gas have been obtained, in the thermodynamic limit. If one introduces the Fermi momentum Eq. 5.8 and the corresponding Fermi energy $E_F = \hbar^2 k_F^2/(2m)$, this means that on has at hand the two dimensionless quantities

$$A \equiv \frac{E}{N E_F} \tag{5.23}$$

$$B \equiv \frac{\mu}{E_F}. \tag{5.24}$$

As a consequence of Eq. 5.18, one also has access to the pressure P. We now show that the following inequalities hold at any temperature T:

$$\left(\frac{3}{5A}\right)^{2/3} B^{5/3} \leq \xi \leq \frac{5A}{3}. \tag{5.25}$$

In the canonical ensemble, the mean energy $E(N,T,V)$ is an increasing function of temperature for fixed volume V and atom number N. Indeed one has the well-known relation $k_B T^2 \partial_T E(N, T, V) = \mathrm{Var} H$, and the variance of the Hamiltonian is non-negative. As a consequence, for any temperature T:

$$E(N, T, V) \geq E(N, 0, V). \tag{5.26}$$

From Eq. 5.14 we then reach the upper bound on ξ given in Eq. 5.25.

In the grand canonical ensemble, the pressure $P(\mu, T)$ is an increasing function of temperature for a fixed chemical potential. This results from the Gibbs-Duhem relation $\Omega(\mu, T, V) = -V P(\mu, T)$ where Ω is the grand potential and V the volume, and from the differential relation $\partial_T \Omega(\mu, T) = -S$ where $S \geq 0$ is the entropy. As a consequence, for any temperature T:
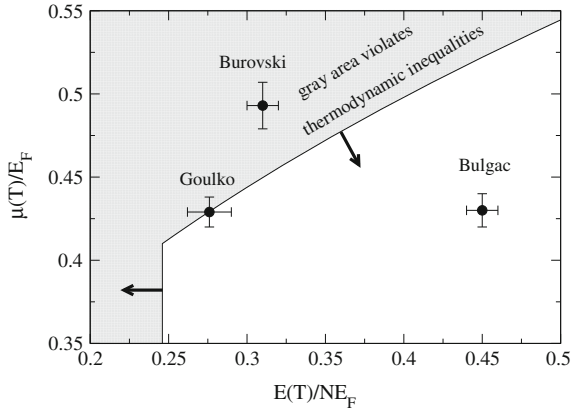
$$P(\mu, T) \geq P(\mu, 0). \tag{5.27}$$

For the unitary gas, the left hand side can be expressed in terms of A using (5.18). Eliminating the density between Eq. 5.15 and 5.16 we obtain the zero temperature pressure

$$P(\mu, 0) = \frac{1}{15\pi^2 \xi^{3/2}} \frac{\hbar^2}{m} \left(\frac{2m\mu}{\hbar^2}\right)^{5/2}. \tag{5.28}$$

This leads to the lower bound on ξ given in Eq. 5.25.

Let us apply Eq. 5.25 to the Quantum Monte Carlo results of [11]: at the critical temperature $T = T_c$, $A = 0.310(10)$ and $B = 0.493(14)$, so that

Fig. 5.2 For the spin balanced uniform unitary gas at thermal equilibrium: assuming $\xi = 0.41$ in Eq. 5.25 defines a zone (*shaded in gray*) in the plane energy–chemical potential that is forbidden at all temperatures. The black disks correspond to the unbiased Quantum Monte Carlo results of Burovski et al. [11], of Bulgac et al. [13], and of Goulko et al. [14] at the critical temperature. Taking the unknown exact value of ξ, which is below the fixed node upper bound 0.41 [12], will shift the forbidden zone boundaries as indicated by the arrows

$$0.48(3) \leq \xi_{[11]} \leq 0.52(2). \tag{5.29}$$

This deviates by two standard deviations from the fixed node result $\xi \leq 0.40(1)$ [12]. The Quantum Monte Carlo results of [13], if one takes a temperature equal to the critical temperature of [11], give $A = 0.45(1)$ and $B = 0.43(1)$; these values, in clear disagreement with [11], lead to the non-restrictive bracketing $0.30(2) \leq \xi_{[13]} \leq 0.75(2)$. The more recent work [14] finds $k_B T_c / E_F = 0.171(5)$ and at this critical temperature, $A = 0.276(14)$ and $B = 0.429(9)$, leading to

$$0.41(3) \leq \xi_{[14]} \leq 0.46(2). \tag{5.30}$$

Another, more graphical application of our simple bounds is to assume some reasonable value of ξ, and then to use Eq. 5.25 to construct a zone in the energy-chemical potential plane that is forbidden at all temperatures. In Fig. 5.2 , we took $\xi = 0.41$, inspired by the fixed node upper bound on the exact value of ξ [12]: the shaded area is the resulting forbidden zone, and the filled disks with error bars represent the in principle exact Quantum Monte Carlo results of various groups at $T = T_c$. It is apparent that the prediction of [11] lies well within the forbidden zone and thus violates thermodynamic inequalities. The prediction of [13] is well within the allowed zone, whereas the most recent prediction of [14] is close to the boundary between the forbidden and the allowed zones. If one takes a smaller value for ξ, the boundaries of the forbidden zone will shift as indicated by the arrows on the figure. All this shows that simple reasonings may be useful to test and guide numerical studies of the unitary gas.

5.1.4 Is the Unitary Gas Attractive or Repulsive?

According to a common saying, a weakly interacting Fermi gas ($k_F|a| \ll 1$) experiences an effective repulsion for a positive scattering length $a > 0$, and an effective attraction for a negative scattering length $a < 0$. Another common fact is that, in the unitary limit $|a| \to +\infty$, the gas properties do not depend on the sign of a. As the unitary limit may be apparently equivalently obtained by taking the limit $a \to +\infty$ or the limit $a \to -\infty$, one reaches a paradox, considering the fact that the unitary gas does not have the same ground state energy than the ideal gas and cannot be at the same time an attractive and repulsive state of matter.

This paradox may be resolved by considering the case of two particles in an isotropic harmonic trap. After elimination of the center of mass motion, and restriction to a zero relative angular momentum to have *s*-wave interaction, one obtains the radial Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\left[\psi''(r) + \frac{2}{r}\psi'(r)\right] + \frac{1}{2}\mu\omega^2 r^2 \psi(r) = E_{\mathrm{rel}}\psi(r), \qquad (5.31)$$

with the relative mass $\mu = m/2$. The interactions are included in the zero range limit by the $r = 0$ boundary conditions, the so-called Wigner-Bethe-Peierls contact conditions described in Sect. 5.2:

$$\psi(r) = A[r^{-1} - a^{-1}] + O(r) \qquad (5.32)$$

that correctly reproduce the free space scattering amplitude

$$f_k^{\mathrm{zero\,range}} = -\frac{1}{a^{-1} + ik}. \qquad (5.33)$$

The general solution of Eq. 5.31 may be expressed in terms of Whittaker M et W functions. For an energy E_{rel} not belonging to the non-interacting spectrum $\{(\frac{3}{2} + 2n)\hbar\omega, n \in \mathbb{N}\}$, the Whittaker function M diverges exponentially for large r and has to be disregarded. The small r behavior of the Whittaker function W, together with the Wigner-Bethe-Peierls contact condition, leads to the implicit equation for the relative energy, in accordance with [15]:

$$\frac{\Gamma\left(\frac{3}{4} - \frac{E_{\mathrm{rel}}}{2\hbar\omega}\right)}{\Gamma\left(\frac{1}{4} - \frac{E_{\mathrm{rel}}}{2\hbar\omega}\right)} = \frac{a_{\mathrm{ho}}^{\mathrm{rel}}}{2a} \qquad (5.34)$$

with the harmonic oscillator length of the relative motion, $a_{\mathrm{ho}}^{\mathrm{rel}} = [\hbar/(\mu\omega)]^{1/2}$.

The function $\Gamma(x)$ is different from zero $\forall x \in \mathbb{R}$ and diverges on each non-positive integers. Thus Eq. 5.34 immediately leads in the unitary case to the spectrum $E_{\mathrm{rel}} \in \{(2n + 1/2)\hbar\omega, n \in \mathbb{N}\}$. This can be readily obtained by setting in Eq. 5.31 $\psi(r) = f(r)/r$, so that f obeys Schrödinger's equation for a 1D harmonic oscillator,
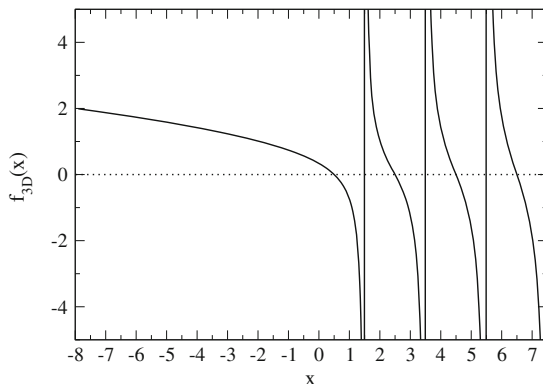
Fig. 5.3 For the graphical solution of Eq. 5.34, which gives the spectrum for two particles in a three-dimensional isotropic harmonic trap, plot of the function $f_{3D}(x) = \Gamma(\frac{3}{4} - \frac{x}{2})/\Gamma(\frac{1}{4} - \frac{x}{2})$, where x stands for $E_{rel}/(\hbar\omega)$

with the constraint issuing from Eq. 5.32 that $f(r = 0) \neq 0$, which selects the even 1D states.

The graphical solution of Eq. 5.34, see Fig. 5.3 , allows to resolve the paradox about the attractive or repulsive nature of the unitary gas. For example starting with the ground state wavefunction of the ideal gas case, of relative energy $E_{rel} = \frac{3}{2}\hbar\omega$, it appears that the two adiabatic followings (i) $a = 0^+ \rightarrow a = +\infty$ and (ii) $a = 0^- \rightarrow -\infty$ lead to *different* final eigenstates of the unitary case, to an excited state $E_{rel} = \frac{5}{2}\hbar\omega$ for the procedure (i), and to the ground state $E_{rel} = \frac{1}{2}\hbar\omega$ for procedure (ii).

The same explanation holds for the many-body case: the interacting gas has indeed several energy branches in the BEC–BCS crossover, as suggested by the toy model[1] of [16], see Fig. 5.4. Starting from the weakly attractive Fermi gas and ramping the scattering length down to $-\infty$ one explores a part of the ground energy branch, where the unitary gas is attractive; this ground branch continuously evolves into a weakly repulsive condensate of dimers [17] if $1/a$ further moves from 0^- to 0^+ and then to $+\infty$. The attractive nature of the unitary gas on the ground energy branch will become apparent in the lattice model of Sect. 5.2. On the other hand, starting from the weakly repulsive Fermi gas and ramping the scattering up to $+\infty$, one explores an effectively repulsive excited branch.

In the first experiments on the BEC–BCS crossover, the ground branch was explored by adiabatic variations of the scattering length and was found to be stable. The first excited energy branch was also investigated in the early work [18], and more recently in [19] looking for a Stoner demixing instability of the strongly repulsive two-component Fermi gas. A difficulty for the study of this excited branch

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[1] This toy model replaces the many-body problem with the one of a matterwave interacting with a single scatterer in a hard wall cavity of radius $\propto 1/k_F$.

Fig. 5.4 In the toy model
of [16], for the homogeneous
two-component unpolarized
Fermi gas, energy per
particle on the ground branch
and the first excited branch
as a function of the inverse
scattering length. The Fermi
wavevector is defined in
Eq. 5.8, $E_F = \hbar^2 k_F^2/(2m)$ is
the Fermi energy, and a is
the scattering length
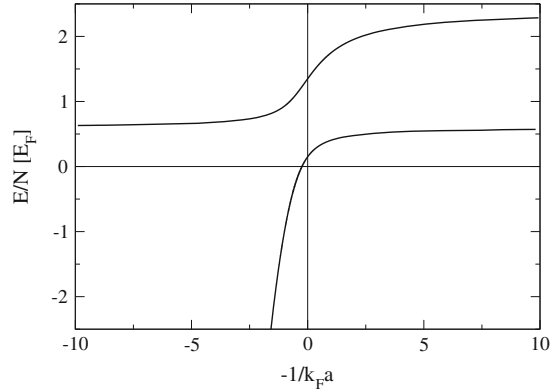
is its metastable character: Three-body collisions gradually transfer the gas to the
ground branch, leading e.g. to the formation of dimers if $0 < k_F a \lesssim 1$.

5.1.5 Other Partial Waves, Other Dimensions

We have previously considered the two-body scattering amplitude in the s-wave
channel. What happens for example in the p-wave channel? This channel is relevant
for the interaction between fermions in the same internal state, where a Feshbach
resonance technique is also available [20, 21]. Can one also reach the unitarity limit
Eq. 5.4 in the p-wave channel?

Actually the optical theorem shows that relation Eq. 5.3 also holds for the p-wave
scattering amplitude f_k. What differs is the low-k expansion of $u(k)$, that is now given
by

$$u(k) = \frac{1}{k^2 \mathcal{V}_s} + \alpha + \ldots, \tag{5.35}$$

where $\mathcal{V}_s$ is the scattering volume (of arbitrary sign) and α has the dimension of the
inverse of a length. The unitary limit would require $u(k)$ negligible as compared to
k. One can in principle tune $\mathcal{V}_s$ to infinity with a Feshbach resonance. Can one then
have a small value of α at resonance? A theorem for a compact support interaction
potential of radius b shows however that [22, 23]

$$\lim_{|\mathcal{V}_s| \to +\infty} \alpha \geq 1/b. \tag{5.36}$$

A similar conclusion holds using two-channel models of the Feshbach resonance
[23, 24]. α thus assumes a huge positive value on resonance, which breaks the scale
invariance and precludes the existence of a p-wave unitary gas. This does not prevent
however to reach the unitary limit in the *vicinity* of a particular value of k. For $\mathcal{V}_s$

large and negative, neglecting the ... in Eq. 5.35 under the condition $kb \ll 1$, one indeed has $|u(k)| \ll k$, so that $f_k \simeq -1/(ik)$, in a vicinity of

$$k_0 = \frac{1}{(\alpha|\mathcal{V}_s|)^{1/2}}. \tag{5.37}$$

Turning back to the interaction in the *s*-wave channel, an interesting question is whether the unitary gas exists in reduced dimensions.

In a one-dimensional system the zero range interaction may be modeled by a Dirac potential $V(x) = g\delta(x)$. If g is finite, it introduces a length scale $\hbar^2/(mg)$ that breaks the scaling invariance. Two cases are thus scaling invariant, the ideal gas $g = 0$ and the impenetrable case $1/g = 0$. The impenetrable case however is mappable to an ideal gas in one dimension, it has in particular the same energy spectrum and thermodynamic properties [25].

In a two-dimensional system, the scattering amplitude for a zero range interaction potential is given by [26]

$$f_k^{2D} = \frac{1}{\gamma + \ln(ka_{2D}/2) - i\pi/2} \tag{5.38}$$

where $\gamma = 0.57721566\ldots$ is Euler's constant and a_{2D} is the scattering length. For a finite value of a_{2D}, there is no scale invariance. The case $a_{2D} \to 0$ corresponds to the ideal gas limit. At first sight, the opposite limit $a_{2D} \to +\infty$ is a good candidate for a two-dimensional unitary gas; however this limit also corresponds to an ideal gas. This appears in the 2D version of the lattice model of Sect. 5.2 [27]. This can also be checked for two particles in an isotropic harmonic trap. Separating out the center of mass motion, and taking a zero angular momentum state for the relative motion, to have interaction in the *s*-wave channel, one has to solve the radial Schrödinger equation:

$$-\frac{\hbar^2}{2\mu}\left[\psi''(r) + \frac{1}{r}\psi'(r)\right] + \frac{1}{2}\mu\omega^2 r^2 \psi(r) = E_{\mathrm{rel}}\psi(r) \tag{5.39}$$

where $\mu = m/2$ is the reduced mass of the two particles, E_{rel} is an eigenenergy of the relative motion, and ω is the single particle angular oscillation frequency. The interactions are included by the boundary condition in $r = 0$:

$$\psi(r) = A\ln(r/a_{2D}) + O(r), \tag{5.40}$$

which is constructed to reproduce the expression of the scattering amplitude Eq. 5.38 for the free space problem.

The general solution of Eq. 5.39 may be expressed in terms of Whittaker functions M and W. Assuming that E_{rel} does not belong to the ideal gas spectrum $\{(2n + 1) \hbar\omega, n \in \mathbb{N}\}$, one finds that the M solution has to be disregarded because it diverges exponentially for $r \to +\infty$. From the small r behavior of the W solution, one obtains the implicit equation

Fig. 5.5 For the graphical solution of Eq. 5.41, which gives the spectrum for two interacting particles in a two-dimensional isotropic harmonic trap, plot of the function $f_{2D}(x) = \frac{1}{2}\psi[(1-x)/2] + \gamma$ where x stands for $E_{rel}/(\hbar\omega)$ and the special function ψ is the logarithmic derivative of the Γ function
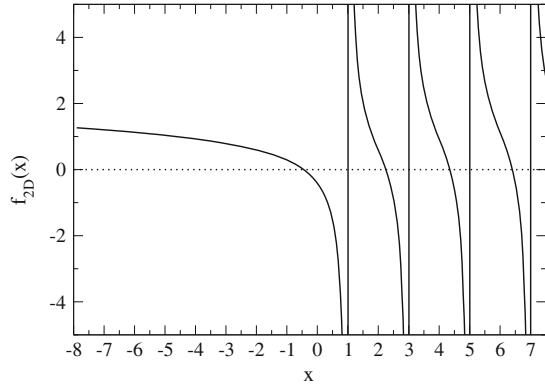
$$\frac{1}{2}\psi\left(\frac{\hbar\omega - E_{rel}}{2\hbar\omega}\right) + \gamma = -\ln(a_{2D}/a_{ho}^{rel}) \qquad (5.41)$$

where the relative harmonic oscillator length is $a_{ho}^{rel} = [\hbar/(\mu\omega)]^{1/2}$ and the digamma function ψ is the logarithmic derivative of the Γ function. If $a_{2D} \to +\infty$, one then finds that E_{rel} tends to the ideal gas spectrum $\{(2n+1)\hbar\omega, n \in \mathbb{N}\}$ from below, see Fig. 5.5, in agreement with the lattice model result that the 2D gas with a large and finite a_{2D} is a weakly attractive gas.

5.2 Various Models and General Relations

There are basically two approaches to model the interaction between particles for the unitary gas (and more generally for the BEC–BCS crossover).

In the first approach, see Sect. 5.2.1 and Sect. 5.2.3, one takes a model with a finite range b and a fixed (e.g. infinite) scattering length a. This model may be in continuous space or on a lattice, with one or several channels. Then one tries to calculate the eigenenergies, the thermodynamic properties from the thermal density operator $\propto \exp(-\beta H)$, etc, and the zero range limit $b \to 0$ should be taken at the end of the calculation. Typically, this approach is followed in numerical many-body methods, such as the approximate fixed node Monte Carlo method [12, 28, 29] or unbiased Quantum Monte Carlo methods [11, 13, 30]. A non-trivial question however is whether each eigenstate of the model is universal in the zero range limit, that is if the eigenenergy E_i and the corresponding wavefunction ψ_i converge for $b \to 0$. In short, the challenge is to prove that the ground state energy of the system does not tend to $-\infty$ when $b \to 0$.

In the second approach, see Sect. 5.2.2 , one directly considers the zero range limit, and one replaces the interaction by the so-called Wigner-Bethe-Peierls contact conditions on the N-body wavefunction. This constitutes what we shall call the *zero-range model*. The advantage is that only the scattering length appears in the

problem, without unnecessary details on the interaction, which simplifies the problem and allows to obtain analytical results. For example the scale invariance of the unitary gas becomes clear. A non-trivial question however is to know whether the zero-range model leads to a self-adjoint Hamiltonian, with a spectrum then necessarily bounded from below for the unitary gas (see Sect. 5.1.2), without having to add extra boundary conditions. For $N = 3$ bosons, due to the Efimov effect, the Wigner-Bethe-Peierls or zero-range model becomes self-adjoint only if one adds an extra three-body contact condition, involving a so-called three-body parameter. In an isotropic harmonic trap, at unitarity, there exists however a non-complete family of bosonic universal states, independent from the three-body parameter and to which the restriction of the Wigner-Bethe-Peierls model is hermitian [31, 32]. For equal mass two-component fermions, it is hoped in the physics literature that the zero-range model is self-adjoint for an arbitrary number of particles N. Surprisingly, there exist works in mathematical physics predicting that this is *not* the case when N is large enough [33, 34]; however the critical mass ratio for the appearance of an Efimov effect in the unequal-mass $3 + 1$ body problem given without proof in [34] was not confirmed by the numerical study[7], and the variational ansatz used in [33] to show that the energy is unbounded below does not have the proper fermionic exchange symmetry. This mathematical problem thus remains open.

5.2.1 Lattice Models and General Relations

5.2.1.1 The Lattice Models

The model that we consider here assumes that the spatial positions are discretized on a cubic lattice, of lattice constant that we call b as the interaction range. It is quite appealing in its simplicity and generality. It naturally allows to consider a contact interaction potential, opposite spin fermions interacting only when they are on the same lattice site. Formally, this constitutes a separable potential for the interaction (see Sect. 5.2.3 for a reminder), a feature known to simplify diagrammatic calculations [35]. Physically, it belongs to the same class as the Hubbard model, so that it may truly be realized with ultracold atoms in optical lattices [36], and it allows to recover the rich lattice physics of condensed matter physics and the corresponding theoretical tools such as Quantum Monte Carlo methods [11, 30].

The spatial coordinates $\mathbf{r}$ of the particles are thus discretized on a cubic grid of step b. As a consequence, the components of the wavevector of a particle have a meaning modulo $2\pi/b$ only, since the plane wave function $\mathbf{r} \rightarrow \exp(i\mathbf{k} \cdot \mathbf{r})$ defined on the grid is not changed if a component of $\mathbf{k}$ is shifted by an integer multiple of $2\pi/b$. We shall therefore restrict the wavevectors to the first Brillouin zone of the lattice:

$$\mathbf{k} \in \mathscr{D} \equiv \left[-\frac{\pi}{b}, \frac{\pi}{b} \right]^3 . \tag{5.42}$$

This shows that the lattice structure in real space automatically provides a cut-off in momentum space. In the absence of interaction and of confining potential, eigenmodes of the system are plane waves with a dispersion relation $\mathbf{k} \rightarrow \varepsilon_{\mathbf{k}}$, supposed to be an even and non-negative function of $\mathbf{k}$. We assume that this dispersion relation is independent of the spin state, which is a natural choice since the $\uparrow$ and $\downarrow$ particles have the same mass. To recover the correct continuous space physics in the zero lattice spacing limit $b \rightarrow 0$, we further impose that it reproduces the free space dispersion relation in that limit, so that

$$\varepsilon_{\mathbf{k}} \sim \frac{\hbar^2 k^2}{2m} \quad \text{for } kb \rightarrow 0. \tag{5.43}$$

The interaction between opposite spin particles takes place when two particles are on the same lattice site, as in the Hubbard model. In first quantized form, it is represented by a discrete delta potential:

$$V = \frac{g_0}{b^3} \delta_{\mathbf{r}_1, \mathbf{r}_2}. \tag{5.44}$$

The factor $1/b^3$ is introduced because $b^{-3} \delta_{\mathbf{r}, \mathbf{0}}$ is equivalent to the Dirac distribution $\delta(\mathbf{r})$ in the continuous space limit. To summarize, the lattice Hamiltonian in second quantized form in the general trapped case is

$$H = \sum_{\sigma=\uparrow,\downarrow} \int_{\mathscr{D}} \frac{d^3 k}{(2\pi)^3} \varepsilon_{\mathbf{k}} c_\sigma^\dagger(\mathbf{k}) c_\sigma(\mathbf{k}) + \sum_{\sigma=\uparrow,\downarrow} \sum_{\mathbf{r}} b^3 U(\mathbf{r}) (\psi_\sigma^\dagger \psi_\sigma)(\mathbf{r})$$
$$+ g_0 \sum_{\mathbf{r}} b^3 (\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow)(\mathbf{r}). \tag{5.45}$$

The plane wave annihilation operators $c_\sigma(\mathbf{k})$ in spin state σ obey the usual continuous space anticommutation relations $\{c_\sigma(\mathbf{k}), c_{\sigma'}^\dagger(\mathbf{k}')\} = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') \delta_{\sigma\sigma'}$ if $\mathbf{k}$ and $\mathbf{k}'$ are in the first Brillouin zone,[2] and the field operators $\psi_\sigma(\mathbf{r})$ obey the usual discrete space anticommutation relations $\{\psi_\sigma(\mathbf{r}), \psi_{\sigma'}^\dagger(\mathbf{r}')\} = b^{-3} \delta_{\mathbf{r}\mathbf{r}'} \delta_{\sigma\sigma'}$. In the absence of trapping potential, in a cubic box with size L integer multiple of b, with periodic boundary conditions, the integral in the kinetic energy term is replaced by the sum $\sum_{\mathbf{k}\in\mathcal{D}} \varepsilon_{\mathbf{k}} \tilde{c}_{\mathbf{k}\sigma}^\dagger \tilde{c}_{\mathbf{k}\sigma}$ where the annihilation operators then obey the discrete anticommutation relations $\{\tilde{c}_{\mathbf{k}\sigma}, \tilde{c}_{\mathbf{k}'\sigma'}^\dagger\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$ for $\mathbf{k}, \mathbf{k}' \in \mathscr{D}$.

The coupling constant g_0 is a function of the grid spacing b. It is adjusted to reproduce the scattering length of the true interaction. The scattering amplitude of two atoms on the lattice with vanishing total momentum, that is with incoming particles of opposite spin and opposite momenta $\pm \mathbf{k}_0$, reads

$$f_{k_0} = -\frac{m}{4\pi\hbar^2} \left[g_0^{-1} - \int_{\mathscr{D}} \frac{d^3 k}{(2\pi)^3} \frac{1}{E + i0^+ - 2\varepsilon_{\mathbf{k}}} \right]^{-1} \tag{5.46}$$

---

[2] In the general case, $\delta(\mathbf{k} - \mathbf{k}')$ has to be replaced with $\sum_{\mathbf{K}} \delta(\mathbf{k} - \mathbf{k}' - \mathbf{K})$ where $\mathbf{K} \in (2\pi/b)\mathbb{Z}^3$ is any vector in the reciprocal lattice.

as derived in details in [37] for a quadratic dispersion relation and in [38] for a general dispersion relation. Here the scattering state energy $E = 2\varepsilon_{\mathbf{k}_0}$ actually introduces a dependence of the scattering amplitude on the direction of $\mathbf{k}_0$ when the dispersion relation $\varepsilon_{\mathbf{k}}$ is not parabolic. If one is only interested in the expansion of $1/f_{\mathbf{k}_0}$ up to second order in k_0, e.g. for an effective range calculation, one may conveniently use the isotropic approximation $E = \hbar^2 k_0^2/m$ thanks to (5.43). Adjusting g_0 to recover the correct scattering length gives from Eq. 5.46 for $k_0 \to 0$:

$$\frac{1}{g_0} = \frac{1}{g} - \int_{\mathscr{D}} \frac{d^3k}{(2\pi)^3} \frac{1}{2\varepsilon_{\mathbf{k}}}, \tag{5.47}$$

with $g = 4\pi\hbar^2 a/m$. The above formula Eq. 5.47 is reminiscent of the technique of renormalization of the coupling constant [39, 40]. A natural case to consider is the one of the usual parabolic dispersion relation,

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}. \tag{5.48}$$

A more explicit form of Eq. 5.47 is then [41, 42]:

$$g_0 = \frac{4\pi\hbar^2 a/m}{1 - Ka/b} \tag{5.49}$$

with a numerical constant given by

$$K = \frac{12}{\pi} \int_0^{\pi/4} d\theta \ln(1 + 1/\cos^2\theta) = 2.442\ 749\ 607\ 806\ 335\ldots, \tag{5.50}$$

and that may be expressed analytically in terms of the dilog special function.

5.2.1.2 Simple Variational Upper Bounds

The relation Eq. 5.49 is quite instructive in the zero range limit $b \to 0$, for fixed non-zero scattering length a and atom numbers N_σ: In this limit, the lattice filling factor tends to zero, and the lattice model is expected to converge to the continuous space zero-range model, that is to the Wigner-Bethe-Peierls model described in Sect. 5.2.2. For each of the eigenenergies this means that

$$\lim_{b\to 0} E_i(b) = E_i, \tag{5.51}$$

where in the right hand side the set of E_i's are the energy spectrum of the zero range model. On the other hand, for a small enough value of b, the denominator in the right-hand side of Eq. 5.49 is dominated by the term $-Ka/b$, the lattice coupling constant g_0 is clearly negative, and the lattice model is attractive, as already pointed out in [43]. By the usual variational argument, this shows that the ground state energy of

the zero range interacting gas is below the one of the ideal gas, for the same trapping potential and atom numbers N_σ :

$$E_0 \leq E_0^{\text{ideal}}. \tag{5.52}$$

Similarly, at thermal equilibrium in the canonical ensemble, the free energy of the interacting gas is below the one of the ideal gas:

$$F \leq F^{\text{ideal}}. \tag{5.53}$$

As in [44] one indeed introduces the free-energy functional of the (here lattice model) interacting gas, $\mathscr{F}[\hat{\rho}] = \text{Tr}[H\hat{\rho}] + k_B T \text{Tr}[\hat{\rho} \ln \hat{\rho}]$, where $\hat{\rho}$ is any unit trace system density operator. Then

$$\mathscr{F}[\hat{\rho}_{\text{th}}^{\text{ideal}}] = F^{\text{ideal}}(b) + \text{Tr}[\hat{\rho}_{\text{th}}^{\text{ideal}} V], \tag{5.54}$$

where $\hat{\rho}_{\text{th}}^{\text{ideal}}$ is the thermal equilibrium density operator of the ideal gas in the lattice model, and V is the interaction contribution to the N-body Hamiltonian. Since the minimal value of $\mathscr{F}[\hat{\rho}]$ over $\hat{\rho}$ is equal to the interacting gas lattice model free energy $F(b)$, the left hand side of Eq. 5.5 is larger than $F(b)$. Since the operator V is negative for small b, because $g_0 < 0$, the right hand side of Eq. 5.53 is smaller than $F^{\text{ideal}}(b)$. Finally taking the limit $b \to 0$, one obtains the desired inequality. The same reasoning can be performed in the grand canonical ensemble, showing that the interacting gas grand potential is below the one of the ideal gas, for the same temperature and chemical potentials μ_σ :

$$\Omega \leq \Omega^{\text{ideal}}. \tag{5.55}$$

In [45], for the unpolarized unitary gas, this last inequality was checked to be obeyed by the experimental results, but it was shown, surprisingly, to be violated by some of the Quantum Monte Carlo results of [11]. For the particular case of the spatially homogeneous unitary gas, the above reasonings imply that $\xi \leq 1$ in Eq. 5.14, so that the unitary gas is attractive (in the ground branch, see Sect. 5.1.4). Using the BCS variational ansatz in the lattice model[3] [46] one obtains the more stringent upper bound [40]:

$$\xi \leq \xi_{\text{BCS}} = 0.5906\ldots \tag{5.56}$$

5.2.1.3 Finite-Range Corrections

For the parabolic dispersion relation, the expectation Eq. 5.51 was checked analytically for two opposite spin particles: for $b \to 0$, in free space the scattering amplitude

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[3] One may check, e.g. in the sector $N_\uparrow = N_\downarrow = 2$, that the BCS variational wavefunction, which is a condensate of pairs in some pair wavefunction, does not obey the Wigner-Bethe-Peierls boundary conditions even if the pair wavefunction does, so it looses its variational character in the zero-range model.

Fig. 5.6 Diamonds: the first low eigenenergies for three ($\uparrow\uparrow\downarrow$) fermions in a cubic box with a lattice model, as functions of the lattice constant b [42]. The box size is L, with periodic boundary conditions, the scattering length is infinite, the dispersion relation is parabolic Eq. 5.48. The unit of energy is $E_0 = (2\pi\hbar)^2/2mL^2$. Straight lines: Linear fits performed on the data over the range $b/L \leq 1/15$, except for the energy branch $E \simeq 2.89E_0$ which is linear on a smaller range. Stars in $b = 0$: Eigenenergies predicted by the zero-range model
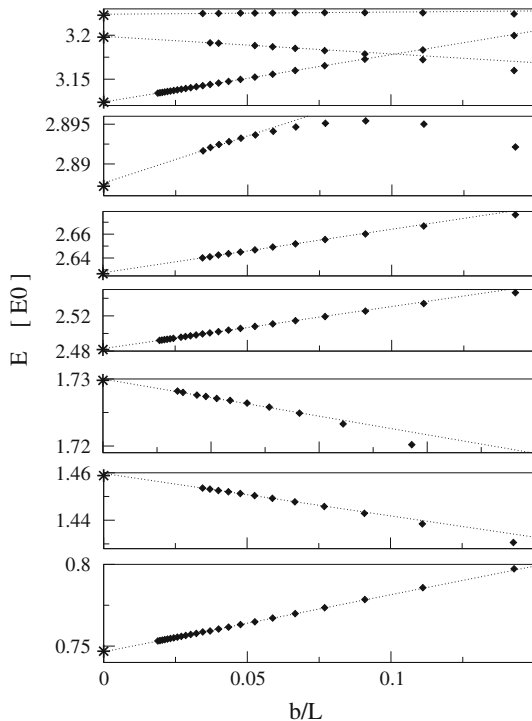
(5.46), and in a box the lattice energy spectrum, converge to the predictions of the zero-range model [42]. It was also checked numerically for $N = 3$ particles in a box, with two $\uparrow$ particles and one $\downarrow$ particle: as shown in Fig. 5.6, for the first low energy eigenstates with zero total momentum, a convergence of the lattice eigenenergies to the Wigner-Bethe-Peierls ones is observed, in a way that is eventually linear in b for small enough values of b. As discussed in [38], this asymptotic linear dependence in b is expected for Galilean invariant continuous space models, and the first order deviations of the eigenergies from their zero range values are linear in the effective range r_e of the interaction potential, as defined in Eq. 5.5, with model-independent coefficients:

$$\frac{dE_i}{dr_e}(b \to 0) \quad \text{is model-independent.} \tag{5.57}$$

However, for lattice models, Galilean invariance is broken and the scattering between two particles depends on their center-of-mass momentum; this leads to a breakdown of the universal relation (5.57), while preserving the linear dependence of the energy with b at low b [47].

A procedure to calculate r_e in the lattice model for a general dispersion relation $\varepsilon_{\mathbf{k}}$ in presented in Appendix 1. For the parabolic dispersion relation Eq. 5.47, its value was given in [46] in numerical form. With the technique exposed in Appendix 1, we

have now the analytical value:

$$r_e^{\text{parab}} = b\frac{12\sqrt{2}}{\pi^3}\arcsin\frac{1}{\sqrt{3}} = 0.336\,868\,47\ldots b. \tag{5.58}$$

The usual Hubbard model, whose rich many-body physics is reviewed in [48], was also considered in [46]: It is defined in terms of the tunneling amplitude between neighboring lattice sites, here $t = -\hbar^2/(2mb^2) < 0$, and of the on-site interaction $U = g_0/b^3$. The dispersion relation is then

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2}{mb^2}\sum_{\alpha=x,y,z}[1 - \cos(k_\alpha b)] \tag{5.59}$$

where the summation is over the three dimensions of space. It reproduces the free space dispersion relation only in a vicinity of $\mathbf{k} = \mathbf{0}$. The explicit version of Eq. 5.47 is obtained from Eq. 5.49 by replacing the numerical constant K by $K^{\text{Hub}} = 3.175911\ldots$. In the zero range limit this leads for $a \neq 0$ to $U/|t| \to -7.913552\ldots$, corresponding as expected to an *attractive* Hubbard model, lending itself to a Quantum Monte Carlo analysis for equal spin populations with no sign problem [11, 13]. The effective range of the Hubbard model, calculated as in Appendix 1, remarkably is negative [46]:

$$r_e^{\text{Hub}} \simeq -0.305718b. \tag{5.60}$$

It becomes thus apparent that an *ad hoc* tuning of the dispersion relation $\varepsilon_{\mathbf{k}}$ may lead to a lattice model with a zero effective range. As an example, we consider a dispersion relation

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}[1 - C(kb/\pi)^2], \tag{5.61}$$

where C is a numerical constant less than $1/3$. From Appendix 1 we then find that

$$r_e = 0 \quad \text{for} \quad C = 0.2570224\ldots \tag{5.62}$$

The corresponding value of g_0 is given by Eq. 5.49 with $K = 2.899952\ldots$.

As pointed out in [47], additionally fine-tuning the dispersion relation to cancel not only r_e but also another coefficient (denoted by B in [47]) may have some practical interest for Quantum Monte Carlo calculations that are performed with a non-zero b, by canceling the undesired linear dependence of thermodynamical quantities and of the critical temperature T_c on b.

5.2.1.4 Energy Functional, Tail of the Momentum Distribution and Pair Correlation Function at Short Distances

A quite ubiquitous quantity in the short-range or large-momentum physics of gases with zero range interactions is the so-called "contact", which, restricting here for

simplicity to thermal equilibrium in the canonical ensemble, can be defined by

$$C \equiv \frac{4\pi m}{\hbar^2} \left(\frac{dE}{d(-1/a)} \right)_S = \frac{4\pi m}{\hbar^2} \left(\frac{dF}{d(-1/a)} \right)_T .$$

(5.63)

For zero-range interactions, this quantity C determines the large-k tail of the momentum distribution

$$n_\sigma(\mathbf{k}) \underset{k \to \infty}{\sim} \frac{C}{k^4}$$

(5.64)

as well as the short-distance behavior of the pair distribution function

$$\int d^3 R g^{(2)}_{\uparrow\downarrow} \left(\mathbf{R} + \frac{\mathbf{r}}{2}, \mathbf{R} - \frac{r}{2} \right) \underset{r \to 0}{\sim} \frac{C}{(4\pi r)^2} .$$

(5.65)

Here the spin-σ momentum distribution $n_\sigma(\mathbf{k})$ is normalised as $\int \frac{d^3 k}{(2\pi)^3} n_\sigma(\mathbf{k}) = N_\sigma$. The relations (5.63–5.65) were obtained in [49, 50]. Historically, analogous relations were first established for one-dimensional bosonic systems [51, 52] with techniques that may be straightforwardly extended to two dimensions and three dimensions [38]. Another relation derived in [49] for the zero-range model expresses the energy as a functional of the one-body density matrix:

$$E = \sum_{\sigma=\uparrow,\downarrow} \int \frac{d^3 k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left[n_\sigma(\mathbf{k}) - \frac{C}{k^4} \right] + \frac{\hbar^2 C}{4\pi m a} + \sum_{\sigma=\uparrow,\downarrow} \int d^3 r U(\mathbf{r}) \rho_\sigma(\mathbf{r})$$

(5.66)

where $\rho_\sigma(\mathbf{r})$ is the spatial number density.

One usually uses (5.64) to define C, and then derives (5.63). Here we rather take (5.63) as the definition of C. This choice is convenient both for the two-channel model discussed in Sect. 5.2.3 and for the rederivation of (5.64–5.66) that we shall now present, where we use a lattice model before taking the zero-range limit.

From the Hellmann-Feynman theorem (that was already put forward in [51]), the interaction energy E_{int} is equal to $g_0 (dE/dg_0)_S$. Since we have $d(1/g_0)/d(1/g) = 1$ [see the relation (5.47) between g_0 and g], this can be rewritten as

$$E_{\text{int}} = \frac{\hbar^4}{m^2} \frac{C}{g_0} .$$

(5.67)

Expressing $1/g_0$ in terms of $1/g$ using once again (5.47), adding the kinetic energy, and taking the zero-range limit, we immediately get the relation (5.66). For the integral over momentum to be convergent, (5.64) must hold (in the absence of mathematical pathologies).

To derive (5.65), we again use (5.67), which implies that the relation

$$\sum_{\mathbf{R}} b^3 g^{(2)}_{\uparrow\downarrow} (\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2) = \frac{C}{(4\pi)^2} |\phi(\mathbf{r})|^2$$

(5.68)

holds for $\mathbf{r} = \mathbf{0}$, were $\phi(\mathbf{r})$ is the zero-energy two-body scattering wavefunction, normalised in such a way that

$$\phi(\mathbf{r}) \simeq \frac{1}{r} - \frac{1}{a} \text{ for } r \gg b \tag{5.69}$$

[see [38] for the straightforward calculation of $\phi(\mathbf{0})$]. Moreover, in the regime where r is much smaller than the typical interatomic distances and than the thermal de Broglie wavelength (but not necessarily smaller than b), it is generally expected that the $\mathbf{r}$-dependence of $g_{\uparrow\downarrow}^{(2)}(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2)$ is proportional to $|\phi(\mathbf{r})|^2$, so that (5.68) remains asymptotically valid. Taking the limits $b \to 0$ and then $r \to 0$ gives the desired (5.65).

Alternatively, the link (5.64, 5.65) between short-range pair correlations and large-k tail of the momentum distribution can be directly deduced from the short-distance singularity of the wavefunction coming from the contact condition (5.75) and the corresponding tail in Fourier space [38], similarly to the original derivation in 1D [52]. Thus this link remains true for a generic out-of-equilibrium statistical mixture of states satisfying the contact condition [49, 38].

5.2.1.5 Absence of Simple Collapse

To conclude this section on lattice models, we try to address the question of the advantage of lattice models as compared to the standard continuous space model with a binary interaction potential $V(\mathbf{r})$ between opposite spin fermions. Apart from practical advantages, due to the separable nature of the interaction in analytical calculations, or to the absence of sign problem in the Quantum Monte Carlo methods, is there a true physical advantage in using lattice models?

One may argue for example that everywhere non-positive interaction potentials may be used in continuous space, such as a square well potential, with a range dependent depth $V_0(b)$ adjusted to have a fixed non-zero scattering and no two-body bound states. E.g. for a square well potential $V(\mathbf{r}) = -V_0 \theta(b - r)$, where $\theta(x)$ is the Heaviside function, one simply has to take

$$V_0 = \frac{\hbar^2}{mb^2} \left(\frac{\pi}{2}\right)^2 \tag{5.70}$$

to have an infinite scattering length. For such an attractive interaction, it seems then that one can easily reproduce the reasonings leading to the bounds Eqs. 5.52, 5.53. It is known however that there exists a number of particles N, in the unpolarized case $N_{\uparrow} = N_{\downarrow}$, such that this model in free space has a N-body bound state, necessarily of energy $\propto -\hbar^2/(mb^2)$ [28, 53, 54]. In the thermodynamic limit, the unitary gas is thus not the ground phase of the system, it is at most a metastable phase, and this prevents a derivation of the bounds Eqs. 5.52, 5.53. This catastrophe is easy to predict variationally, taking as a trial wavefunction the ground state of the ideal Fermi gas enclosed in a fictitious cubic hard wall cavity of size $b/\sqrt{3}$ [55]. In the large N limit,

the kinetic energy in the trial wavefunction is then $(3N/5)\hbar^2 k_F^2/(2m)$, see Eq. 5.14, where the Fermi wavevector is given by Eq. 5.8 with a density $\rho = N/(b/\sqrt{3})^3$, so that

$$E_{\text{kin}} \propto N^{5/3} \frac{\hbar^2}{mb^2}. \tag{5.71}$$

Since all particles are separated by a distance less than b, the interaction energy is exactly

$$E_{\text{int}} = -V_0(N/2)^2 \tag{5.72}$$

and wins over the kinetic energy for N large enough, $2800 \lesssim N$ for the considered ansatz. Obviously, a similar reasoning leads to the same conclusion for an everywhere negative, non-necessarily square well interaction potential.[4] One could imagine to suppress this problem by introducing a hard core repulsion, in which case however the purely attractive nature of V would be lost, ruining our simple derivation of Eqs. 5.52, 5.53.

The lattice models are immune to this catastrophic variational argument, since one cannot put more than two spin 1/2 fermions "inside" the interaction potential, that is on the same lattice site. Still they preserve the purely attractive nature of the interaction. This does not prove however that their spectrum is bounded from below in the zero range limit, as pointed out in the introduction of this section.

5.2.2 Zero-Range Model, Scale Invariance and Virial Theorem

5.2.2.1 The Zero-Range Model

The interactions are here replaced with contact conditions on the N-body wavefunction. In the two-body case, the model, introduced already by Eq. 5.32, is discussed in details in the literature, see e.g. [56] in free space where the scattering amplitude f_k is calculated and the existence for $a > 0$ of a dimer of energy $-\hbar^2/(2\mu a^2)$ and wavefunction $\phi_0(r) = (4\pi a)^{-1/2}\exp(-r/a)/r$ is discussed, μ being the reduced mass of the two particles. The two-body trapped case, solved in [15], was already presented in Sect. 5.1.4. Here we present the model for an arbitrary value of N.

For simplicity, we consider in first quantized form the case of a fixed number $N_\uparrow$ of fermions in spin state $\uparrow$ and a fixed number $N_\downarrow$ of fermions in spin state $\downarrow$, assuming that the Hamiltonian cannot change the spin state. We project the N-body state vector $|\Psi\rangle$ onto the non-symmetrized spin state with the $N_\uparrow$ first particles in

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[4] In fixed node calculations, an everywhere negative interaction potential is used [12, 28, 29]. It is unknown if N in these simulations exceeds the minimal value required to have a bound state. Note that the imposed nodal wavefunction in the fixed node method, usually the one of the Hartree-Fock or BCS state, would be however quite different from the one of the bound state.

spin state $\uparrow$ and the $N_\downarrow$ remaining particles in spin state $\downarrow$, to define a scalar N-body wavefunction:

$$\psi(\mathbf{X}) \equiv \left(\frac{N!}{N_\uparrow! N_\downarrow!}\right)^{1/2} \langle\uparrow, \mathbf{r}_1| \otimes \dots \langle\uparrow, \mathbf{r}_{N_\uparrow}|\langle\downarrow, \mathbf{r}_{N_\uparrow+1}| \otimes \dots \langle\downarrow, \mathbf{r}_N|\Psi\rangle \quad (5.73)$$

where $\mathbf{X} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ is the set of all coordinates, and the normalization factor ensures that ψ is normalized to unity.[5] The fermionic symmetry of the state vector allows to express the wavefunction on another spin state (with any different order of $\uparrow$ and $\downarrow$ factors) in terms of ψ. For the considered spin state, this fermionic symmetry imposes that ψ is odd under any permutation of the first $N_\uparrow$ positions $\mathbf{r}_1, \dots, \mathbf{r}_{N_\uparrow}$, and also odd under any permutation of the last $N_\downarrow$ positions $\mathbf{r}_{N_\uparrow+1}, \dots, \mathbf{r}_N$.

In the Wigner-Bethe-Peierls model, that we also call zero-range model, the Hamiltonian for the wavefunction ψ is simply represented by the same partial differential operator as for the ideal gas case:

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}_i} + U(\mathbf{r}_i)\right], \quad (5.74)$$

where U is the external trapping potential supposed for simplicity to be spin state independent. As is however well emphasized in the mathematics of operators on Hilbert spaces [8], an operator is defined not only by a partial differential operator, but also by the choice of its so-called *domain D(H)*. A naive presentation of this concept of domain is given in the Appendix 2. Here the domain does not coincide with the ideal gas one. It includes the following Wigner-Bethe-Peierls contact conditions: for any pair of particles i,j, when $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j| \to 0$ for a fixed position of their centroid $\mathbf{R}_{ij} = (\mathbf{r}_i + \mathbf{r}_j)/2$, there exists a function A_{ij} such that

$$\psi(\mathbf{X}) = A_{ij}(\mathbf{R}_{ij}; (\mathbf{r}_k)_{k \neq i,j})(r_{ij}^{-1} - a^{-1}) + O(r_{ij}). \quad (5.75)$$

These conditions are imposed for all values of $\mathbf{R}_{ij}$ different from the positions of the other particles $\mathbf{r}_k$, k different from i and j. If the fermionic particles i and j are in the same spin state, the fermionic symmetry imposes $\psi(\dots, \mathbf{r}_i = \mathbf{r}_j, \dots) = 0$ and one has simply $A_{ij} \equiv 0$. For i and j in different spin states, the unknown functions A_{ij} have to be determined from Schrödinger's equation, e.g. together with the energy E from the eigenvalue problem

$$H\psi = E\psi. \quad (5.76)$$

Note that in Eq. 5.76 we have excluded the values of $\mathbf{X}$ where two particle positions coincide. Since $\Delta_{\mathbf{r}_i} r_{ij}^{-1} = -4\pi\delta(\mathbf{r}_i - \mathbf{r}_j)$, including these values would require

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[5] The inverse formula giving the full state vector in terms of $\psi(\mathbf{X})$ is $|\Psi\rangle = \left(\frac{N!}{N_\uparrow! N_\downarrow!}\right)^{1/2} A|\uparrow\rangle^{N_\uparrow}|\downarrow\rangle^{N_\downarrow}|\psi\rangle$, where the projector A is the usual antisymmetrizing operator $A = (1/N!) \sum_{\sigma \in S_N} \varepsilon(\sigma) P_\sigma$.

a calculation with distributions rather than with functions, with regularized delta interaction pseudo-potential, which is a compact and sometimes useful reformulation of the Wigner-Bethe-Peierls contact conditions [6, 56, 57, 58].

As already pointed out below Eq. 5.75, $A_{ij} \equiv 0$ if i and j are fermions in the same spin state. One may wonder if solutions exist such that $A_{ij} \equiv 0$ even if i and j are in different spin states, in which case ψ would simply vanish when $r_{ij} \to 0$. These solutions would then be common eigenstates to the interacting gas and to the ideal gas. They would correspond in a real experiment to long lived eigenstates, protected from three-body losses by the fact that ψ vanishes when two particles or more approach each other. In a harmonic trap, one can easily construct such "non-interacting" solutions, as for example the famous Laughlin wavefunction of the Fractional Quantum Hall Effect. "Non-interacting" solutions also exists for spinless bosons. These non-interacting states actually dominate the ideal gas density of states at high energy [32, 55].

5.2.2.2 What is the Kinetic Energy?

The fact that the Hamiltonian is the same as the ideal gas, apart from the domain, may lead physically to some puzzles. E.g. the absence of interaction term may give the impression that the energy E is the sum of trapping potential energy and kinetic energy only. This is actually not so. The correct definition of the mean kinetic energy, valid for general boundary conditions on the wavefunction, is

$$E_{\mathrm{kin}} = \int d^{3N} X \frac{\hbar^2}{2m} |\partial_{\mathbf{X}} \psi|^2. \tag{5.77}$$

This expression in particular guaranties that $E_{\mathrm{kin}} \geq 0$. If $A_{ij} \neq 0$ in Eq. 5.75, one then sees that, although ψ is square integrable in a vicinity of $r_{ij} = 0$ thanks to the Jacobian $\propto r_{ij}^2$ coming from three-dimensional integration, the gradient of ψ diverges as $1/r_{ij}^2$ and cannot be square integrable. Within the zero-range model one then obtains an infinite kinetic energy

$$E_{\mathrm{kin}}^{\mathrm{WBP}} = +\infty. \tag{5.78}$$

Multiplying Eq. 5.76 by ψ and integrating over $\mathbf{X}$, one realizes that the total energy is split as the trapping potential energy,

$$E_{\mathrm{trap}} = \int d^{3N} X |\psi(\mathbf{X})|^2 \sum_{i=1}^{N} U(\mathbf{r}_i) \tag{5.79}$$

and as the sum of kinetic plus interaction energy:

$$E_{\mathrm{kin}} + E_{\mathrm{int}} = -\int d^{3N} X \frac{\hbar^2}{2m} \psi^* \Delta_{\mathbf{X}} \psi. \tag{5.80}$$

This means that the interaction energy is $-\infty$ in the Wigner-Bethe-Peierls model. All this means is that, in reality, when the interaction has a non-zero range, both the kinetic energy and the interaction energy of interacting particles depend on the interaction range b, and diverge for $b \to 0$, in such a way however that the sum $E_{\text{kin}} + E_{\text{int}}$ has a finite limit given by the Wigner-Bethe-Peierls model. We have seen more precisely how this happens for lattice models in Sect. 5.2.1.4, see the expression (5.67) of E_{int} and the subsequent derivation of (5.66).[6]

5.2.2.3 Scale Invariance and Virial Theorem

In the case of the unitary gas, the scattering length is infinite, so that one sets $1/a = 0$ in Eq. 5.75. The domain of the Hamiltonian is then imposed to be invariant by any isotropic rescaling Eq. 5.11 of the particle positions. To be precise, we define for any scaling factor $\lambda > 0$:

$$\psi_\lambda(\mathbf{X}) \equiv \frac{\psi(\mathbf{X}/\lambda)}{\lambda^{3N/2}}, \tag{5.81}$$

and we impose that $\psi_\lambda \in D(H)$ for all $\psi \in D(H)$. This is the precise mathematical definition of the scale invariance loosely introduced in Sect. 5.1.2. In particular, it is apparent in Eq. 5.75 that, for $1/a = 0$, ψ_λ obeys the Wigner-Bethe-Peierls contact conditions if ψ does. On the contrary, if ψ obeys the contact conditions for a finite scattering length a, ψ_λ obeys the contact condition for a different, fictitious scattering length $a_\lambda = \lambda a \neq a$ and $D(H)$ cannot be scaling invariant.

There are several consequences of the scale invariance of the domain of the Hamiltonian $D(H)$ for the unitary gas. Some of them were presented in Sect. 5.1.2, other ones will be derived in Sect. 5.3. Here we present another application, the derivation of a virial theorem for the unitary gas. This is a first step towards the introduction of a SO(2,1) Lie algebra in Sect. 5.3. To this end, we introduce the infinitesimal generator D of the scaling transform Eq. 5.81, such that[7]

$$\psi_\lambda(\mathbf{X}) = e^{-iD\ln\lambda}\psi(\mathbf{X}). \tag{5.82}$$

Taking the derivative of Eq. 5.81 with respect to λ in $\lambda = 1$, one obtains the hermitian operator

$$D = \frac{1}{2i}(\mathbf{X} \cdot \partial_{\mathbf{X}} + \partial_{\mathbf{X}} \cdot \mathbf{X}) = \frac{3N}{2i} - i\mathbf{X} \cdot \partial_{\mathbf{X}}. \tag{5.83}$$

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[6] For a continuous-space model with an interaction potential $V(r)$, we have [76, 38] $E_{\text{int}} = \frac{C}{(4\pi)^2} \int d^3r\, V(r)|\phi(r)|^2$ where C is still defined by (5.63) and $\phi(r)$ still denotes the zero-energy two-body scattering state normalised according to (5.69).

[7] The scaling transform (5.81) defines a unitary operator $T(\lambda)$ such that $\psi_\lambda = T(\lambda)\psi$. One has $T(\lambda_1)T(\lambda_2) = T(\lambda_1\lambda_2)$. To recover the usual additive structure as for the group of spatial translations, one sets $\lambda = \exp\theta$, so that $T(\theta_1)T(\theta_2) = T(\theta_1 + \theta_2)$ and $T(\theta) = \exp(-i\theta D)$ where D is the generator. This is why $\ln\lambda$ appears in Eq. 5.82.

The commutator of D with the Hamiltonian is readily obtained. From the relation $\Delta_{\mathbf{X}}\psi_\lambda(\mathbf{X}) = \lambda^{-2}(\Delta\psi)(\mathbf{X}/\lambda)$, one has

$$e^{iD\ln\lambda}(H - H_{\text{trap}})e^{-iD\ln\lambda} = \frac{1}{\lambda^2}(H - H_{\text{trap}}) \tag{5.84}$$

where $H_{\text{trap}} = \sum_{i=1}^{N} U(\mathbf{r}_i)$ is the trapping potential part of the Hamiltonian. It remains to take the derivative in $\lambda = 1$ to obtain

$$i[D, H - H_{\text{trap}}] = -2(H - H_{\text{trap}}). \tag{5.85}$$

The commutator of D with the trapping potential is evaluated directly from Eq. 5.83:

$$i[D, H_{\text{trap}}] = \sum_{i=1}^{N} \mathbf{r}_i \cdot \partial_{\mathbf{r}_i} U(\mathbf{r}_i). \tag{5.86}$$

This gives finally

$$i[D, H] = -2(H - H_{\text{trap}}) + \sum_{i=1}^{N} \mathbf{r}_i \cdot \partial_{\mathbf{r}_i} U(\mathbf{r}_i). \tag{5.87}$$

The standard way to derive the virial theorem in quantum mechanics [59], in a direct generalization of the one of classical mechanics, is then to take the expectation value of $[D, H]$ in an eigenstate ψ of H of eigenenergy E. This works here for the unitary gas because the domain $D(H)$ is preserved by the action of D. On one side, by having H acting on ψ from the right or from the left, one trivially has $\langle [D, H] \rangle_\psi = 0$. On the other side, one has Eq. 5.87, so that

$$E = \sum_{i=1}^{N} \left\langle U(\mathbf{r}_i) + \frac{1}{2}\mathbf{r}_i \cdot \partial_{\mathbf{r}_i} U(\mathbf{r}_i) \right\rangle_\psi. \tag{5.88}$$

This relation was obtained with alternative derivations in the literature (see [60] and references therein). One of its practical interests is that it gives access to the energy from the gas density distribution [61]. As already mentioned, the scale invariance of the domain of H is crucial to obtain this result. If $1/a$ is non zero, a generalization of the virial relation can however be obtained, that involves $dE/d(1/a)$, see [62, 63].

5.2.3 Two-Channel Model and Closed-Channel Fraction

5.2.3.1 The Two-Channel Model

The lattice models or the zero-range model are of course dramatic simplifications of the real interaction between two alkali atoms. At large interatomic distances, much larger than the radius of the electronic orbitals, one may hope to realistically represent this interaction by a function $V(r)$ of the interatomic distance, with a van der Waals

attractive tail $V(r) \simeq -C_6/r^6$, a simple formula that actually neglects retardation effects and long-range magnetic dipole–dipole interactions. As discussed below the gas phase condition Eq. 5.1, this allows to estimate b with the so-called van der Waals length, usually in the range of 1-10 nm.

At short interatomic distances, this simple picture of a scalar interaction potential $V(r)$ has to be abandoned. Following quantum chemistry or molecular physics methods, one has to introduce the various Born-Oppenheimer potential curves obtained from the solution of the electronic eigenvalue problem for fixed atomic nuclei positions. Restricting to one active electron of spin $1/2$ per atom, one immediately gets two ground potential curves, the singlet one corresponding to the total spin $S = 0$, and the triplet one corresponding to the total spin $S = 1$. An external magnetic field B is applied to activate the Feshbach resonance. This magnetic field couples mainly to the total electronic spin and thus induces *different* Zeeman shifts for the singlet and triplet curves. In reality, the problem is further complicated by the existence of the nuclear spin and the hyperfine coupling, that couples the singlet channel to the triplet channel for nearby atoms, and that induces a hyperfine splitting within the ground electronic state for well separated atoms.

A detailed discussion is given in [64, 65]. Here we take the simplified view depicted in Fig. 5.7: the atoms interact *via* two potential curves, $V_{\mathrm{open}}(r)$ and $V_{\mathrm{closed}}(r)$. At large distances, $V_{\mathrm{open}}(r)$ conventionally tends to zero, whereas $V_{\mathrm{closed}}(r)$ tends to a positive value V_∞, one of the hyperfine energy level spacings for a single atom in the applied magnetic field. In the two-body scattering problem, the atoms come from $r = +\infty$ in the internal state corresponding to $V_{\mathrm{open}}(r)$, the so-called open channel, with a kinetic energy $E \ll V_\infty$. Due to a coupling between the two channels, the two interacting atoms can have access to the internal state corresponding to the curve $V_{\mathrm{closed}}(r)$, but only at short distances; at long distances, the external atomic wavefunction in this so-called closed channel is an evanescent wave that decays exponentially with r since $E < V_\infty$.

Now assume that, in the absence of coupling between the channels, the closed channel supports a bound state of energy E_b, called in what follows *the molecular state or the closed-channel molecule*. Assume also that, by applying a judicious magnetic field, one sets the energy of this molecular state close to zero, that is to the dissociation limit of the open channel. In this case one may expect that the scattering amplitude of two atoms is strongly affected, by a resonance effect, given the non-zero coupling between the two channels. This is in essence how the Feshbach resonance takes place.

The central postulate of the theory of quantum gases is that the short range details of the interaction are unimportant, only the low-momentum scattering amplitude f_k between two atoms is relevant. As a consequence, any simplified model for the interaction, leading to a different scattering amplitude f_k^{model}, is acceptable provided that

$$f_k^{\mathrm{model}} \simeq f_k \qquad (5.89)$$
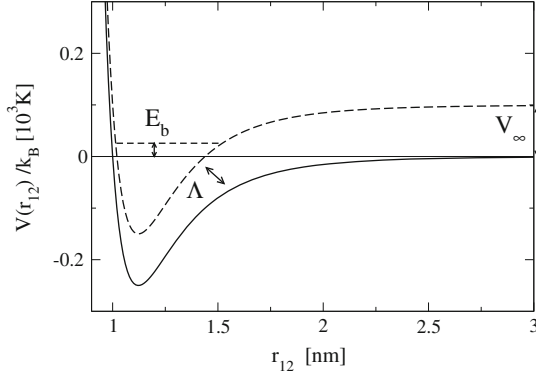
Fig. 5.7 Simple view of a Feshbach resonance. The atomic interaction is described by two curves (*solid line: open channel, dashed line: closed channel*). When one neglects the interchannel coupling Λ, the closed channel has a molecular state of energy E_b close to the dissociation limit of the open channel. The energy spacing V_∞ was greatly exaggerated, for clarity

for the relevant values of the relative momentum k populated in the gas. We insist here that we impose similar scattering amplitudes over some momentum range, not just equal scattering lengths a. For spin 1/2 fermions, typical values of k can be

$$k_{\text{typ}} \in \{a^{-1}, k_F, \lambda_{\text{dB}}^{-1}\} \tag{5.90}$$

where the Fermi momentum is defined in Eq. 5.8 and the thermal de Broglie wavelength in Eq. 5.9. The appropriate value of k_{typ} depends on the physical situation. The first choice $k_{\text{typ}} \sim a^{-1}$ is well suited to the case of a condensate of dimers ($a > 0$) since it is the relative momentum of two atoms forming the dimer. The second choice $k_{\text{typ}} \sim k_F$ is well suited to a degenerate Fermi gas of atoms (not dimers). The third choice $k_{\text{typ}} \sim \lambda^{-1}$ is relevant for a non-degenerate Fermi gas.

The strategy is thus to perform an accurate calculation of the "true" f_k, to identify the validity conditions of the simple models and of the unitary regime assumption Eq. 5.4. One needs a realistic, though analytically tractable, model of the Feshbach resonance. This is provided by the so-called *two-channel* models [65, 66, 67]. We use here the version presented in [68], which is a particular case of the one used in [64, 69] and Refs. therein: The open channel part consists of the original gas of spin 1/2 fermions that interact *via* a separable potential, that is in first quantized form for two opposite spin fermions, in position space:

$$\langle \mathbf{r}_1, \mathbf{r}_2 | V_{\text{sep}} | \mathbf{r}_1', \mathbf{r}_2' \rangle = \delta \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} - \frac{\mathbf{r}_1' + \mathbf{r}_2'}{2} \right) g_0 \chi(\mathbf{r}_2 - \mathbf{r}_1) \chi(\mathbf{r}_2' - \mathbf{r}_1'). \tag{5.91}$$

This potential does not affect the atomic center of mass, so it conserves total momentum and respects Galilean invariance. Its matrix element involves the product of a function of the relative position in the ket and of the same function of the relative position in the bra, hence the name *separable*. The separable potential is thus in

general non local. As we shall take a function χ of width $\approx b$ this is clearly not an issue. The coupling constant g_0 of the separable potential is well-defined by the normalization condition for χ, $\int d^3 r \chi(\mathbf{r}) = 1$. In the presence of this open channel interaction only, the scattering length between fermions, the so-called background scattering length a_{bg}, is usually small, of the order of the potential range b, hence the necessity of the Feshbach resonance to reach the unitary limit.

In the closed channel part, a single two-particle state is kept, the one corresponding to the molecular state, of energy E_b and of spatial range $\lesssim b$. The atoms thus exist in that channel not in the form of spin $1/2$ fermions, but in the form of bosonic spinless molecules, of mass twice the atomic mass. The coupling between the two channels simply corresponds to the possibility for each boson to decay in a pair of opposite spin fermions, or the inverse process that two opposite spin fermions merge into a boson, in a way conserving the total momentum. This coherent Bose-Fermi conversion may take place only if the positions $\mathbf{r}_1$ and $\mathbf{r}_2$ of the two fermions are within a distance b, and is thus described by a relative position dependent amplitude $\Lambda \chi(\mathbf{r}_1 - \mathbf{r}_2)$, where for simplicity one takes the same cut-off function χ as in the separable potential. It is important to realize that the Bose–Fermi conversion effectively induces an interaction between the fermions, which becomes resonant for the right tuning of E_b and leads to the diverging total scattering length a.

The model is best summarized in second quantized form [68], introducing the fermionic field operators $\psi_\sigma(\mathbf{r})$, $\sigma = \uparrow, \downarrow$, obeying the usual fermionic anticommutation relations, and the bosonic field operator $\psi_b(\mathbf{r})$ obeying the usual bosonic commutation relations:

$$
\begin{aligned}
H = \int d^3 r &\left[\sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger \left(-\frac{\hbar^2}{2m} \Delta_\mathbf{r} + U \right) \psi_\sigma + \psi_b^\dagger \left(E_b - \frac{\hbar^2}{4m} \Delta_\mathbf{r} + U_b \right) \psi_b \right] \\
&+ \Lambda \int d^3 r_1 d^3 r_2 \chi(\mathbf{r}_1 - \mathbf{r}_2) \left\{ \psi_b^\dagger [(\mathbf{r}_1 + \mathbf{r}_2)/2] \psi_\downarrow(\mathbf{r}_1) \psi_\uparrow(\mathbf{r}_2) + \text{h. c.} \right\} \\
&+ g_0 \int d^3 R d^3 r d^3 r' \chi(\mathbf{r}) \chi(\mathbf{r}') \psi_\uparrow^\dagger(\mathbf{R} - \mathbf{r}/2) \psi_\downarrow^\dagger(\mathbf{R} + \mathbf{r}/2) \psi_\downarrow(\mathbf{R} + \mathbf{r}'/2) \psi_\uparrow(\mathbf{R} - \mathbf{r}'/2),
\end{aligned}
$$
$$(5.92)$$

where $U(\mathbf{r})$ and $U_b(\mathbf{r})$ are the trapping potentials for the fermions and the bosons, respectively.

5.2.3.2 Scattering Amplitude and Universal Regime

In free space, the scattering problem of two fermions is exactly solvable for a Gaussian cut-off function $\chi(\mathbf{r}) \propto \exp[-r^2/(2b^2)]$ [64, 68]. A variety of parameterizations are possible. To make contact with typical notations, we assume that the energy E_b of the molecule in the closed channel is an affine function of the magnetic field B, a reasonable assumption close to the Feshbach resonance:

$$
E_b(B) = E_b^0 + \mu_b(B - B_0) \tag{5.93}
$$

where B_0 is the magnetic field value right on resonance and μ_b is the effective magnetic moment of the molecule. Then the scattering length for the model Eq. 5.92 can be exactly written as the celebrated formula

$$a = a_{\text{bg}}\left(1 - \frac{\Delta B}{B - B_0}\right), \tag{5.94}$$

where ΔB, such that $E_b^0 + \mu_b \Delta B = \Lambda^2/g_0$, is the so-called width of the Feshbach resonance. As expected, for $|B - B_0| \gg |\Delta B|$, one finds that a tends to the background scattering length a_{bg} solely due to the open channel interaction. With ΔB one forms a length R_* [70] which is always non-negative:

$$R_* \equiv \frac{\hbar^2}{m a_{\text{bg}} \mu_b \Delta B} = \left(\frac{\Lambda}{2\pi b E_b^0}\right)^2, \tag{5.95}$$

where the factor 2π is specific to our choice of χ. Physically, the length R_* is also directly related to the effective range on resonance:

$$r_e^{\text{res}} = -2R_* + \frac{4b}{\sqrt{\pi}}, \tag{5.96}$$

where the numerical coefficient in the last term depends on the choice of χ. The final result for the scattering amplitude for the model Eq. 5.92 is

$$-\frac{1}{f_k} = ik + \frac{e^{k^2 b^2}}{a}\left[1 - \left(1 - \frac{a}{a_{\text{bg}}}\right)\frac{k^2}{k^2 - Q^2}\right] - ik\ \text{erf}(-ikb) \tag{5.97}$$

where erf is the error function, that vanishes linearly in zero, and the wavevector Q, such that

$$Q^2 \equiv \frac{m}{\hbar^2 g_0}\left(g_0 E_b - \Lambda^2\right) = \frac{-1}{a_{\text{bg}} R_*(1 - a_{\text{bg}}/a)}, \tag{5.98}$$

may be real or purely imaginary.

The unitary limit assumption Eq. 5.4 implies that all the terms in the right hand side of Eq. 5.97 are negligible, except for the first one. We now discuss this assumption, restricting for simplicity to an infinite scattering length $a^{-1} = 0$ (i.e. a magnetic field sufficiently close to resonance) and a typical relative momentum $k_{\text{typ}} = k_F$ (i.e. a degenerate gas). To satisfy Eq. 5.89, with $f_k^{\text{model}} = -1/(ik)$, one should then have, in addition to the gas phase requirement $k_F b \ll 1$, that

$$\frac{k R_*}{|1 + k^2 a_{\text{bg}} R_*|} \ll 1\ \forall k \in [0, k_F]. \tag{5.99}$$

Table 5.1 summarizes the corresponding conditions to reach the unitary limit.[8, 9] Remarkably, the condition $k_F |r_e^{\text{res}}| \ll 1$ obtained in Eq. 5.6 from the expansion of

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[8] We discarded for simplicity the rather peculiar case where $k_F |a_{\text{bg}}| R_*$ is ≤ 1 but not $\ll 1$.

[9] An additional condition actually has to be imposed to have a universal gas, as we will see after Eq. 5.106.

Table 5.1 In the two-channel model, conditions deduced from Eq. 5.99 (supplementary to the gas phase condition $k_F b \ll 1$) to reach the unitary limit for a degenerate gas of spin 1/2 fermions of Fermi momentum k_F. It is assumed that the magnetic field is tuned right on resonance, so that the scattering length is infinite. The last column corresponds to narrow Feshbach resonances satisfying Eq. 5.100

	$k_F\sqrt{|a_{bg}|R_*} \ll 1$	$k_F\sqrt{|a_{bg}|R_*} > 1$
$a_{bg} > 0$	$k_F R_* \ll 1$	$(R_*/a_{bg})^{1/2} \ll 1$
$a_{bg} < 0$	$k_F R_* \ll 1$	unreachable

$1/f_k$ to order k^2 is not the end of the story. In particular, if $a_{bg} < 0$, $Q_{res}^2 \equiv -1/(a_{bg}R_*)$ is positive and $1/f_k$ diverges for $k = Q_{res}$; if the location of this divergence is within the Fermi sea, the unitary limit is not reachable. This funny case however requires huge values of $R_* a_{bg}$, that is extremely small values of the resonance width ΔB:

$$|\mu_b \Delta B| \lesssim \frac{\hbar^2 k_F^2}{2m}. \tag{5.100}$$

This corresponds to very narrow Feshbach resonances [71], whose experimental use requires a good control of the magnetic field homogeneity and is more delicate. Current experiments rather use broad Feshbach resonances such as on lithium 6, where $r_e^{res} = 4.7$ nm [72], $a_{bg} = -74$ nm, $R_* = 0.027$ nm [73], leading to $1/(|a_{bg}|R_*)^{1/2} = 700(\mu m)^{-1}$ much larger than $k_F \approx$ a few $(\mu m)^{-1}$, so that the unitary limit is indeed well reached.

5.2.3.3 Relation Between Number of Closed Channel Molecules and "Contact"

The fact that the two-channel model includes the underlying atomic physics of the Feshbach resonance allows to consider an observable that is simply absent from single channel models, namely the number of molecules in the closed channel, represented by the operator:

$$N_b \equiv \int d^3 \mathbf{r} \, \psi_b^\dagger(\mathbf{r}) \psi_b(\mathbf{r}) \tag{5.101}$$

where ψ_b is the molecular field operator. The mean number $\langle N_b \rangle$ of closed channel molecules was recently measured by laser molecular excitation techniques [74].

This mean number can be calculated from a two-channel model by a direct application of the Hellmann–Feynman theorem [75, 68] (see also [76]). The key point is that the only quantity depending on the magnetic field in the Hamiltonian Eq. 5.92 is the internal energy $E_b(B)$ of a closed channel molecule. At thermal equilibrium in the canonical ensemble, we thus have

$$\left(\frac{dE}{dB}\right)_S = \langle N_b \rangle \frac{dE_b}{dB}. \tag{5.102}$$

Close to the Feshbach resonance, we may assume that E_b is an affine function of B, see Eq. 5.93, so that the scattering length a depends on the magnetic field as in Eq. 5.94. Parameterizing E in terms of the inverse scattering length rather than B, we can replace dE/dB by $dE/d(1/a)$ times $d(1/a)/dB$. The latter can be calculated explicitly from (5.94). Thus

$$\langle N_b \rangle = \frac{C}{4\pi} R_* \left(1 - \frac{a_{\text{bg}}}{a}\right)^2, \tag{5.103}$$

where C is the contact defined in Eq. 5.63, and we introduced the length R_* defined in Eq. 5.95.

   If the interacting gas is in the universal zero range regime, its energy E depends on the interactions only via the scattering length, independently of the microscopic details of the atomic interactions, and its dependence with $1/a$ may be calculated by any convenient model. Then, at zero temperature, for the unpolarized case $N_\uparrow = N_\downarrow$, the equation of state of the homogeneous gas can be expressed as

$$e_0 = e_0^{\text{ideal}} f\left(\frac{1}{k_F a}\right), \tag{5.104}$$

where e_0 and e_0^{ideal} are the ground state energy per particle for the interacting gas and for the ideal gas with the same density, and the Fermi wavevector k_F was defined in Eq. 5.8. In particular, $f(0) = \xi$, where the number ξ was introduced in Eq. 5.14. Setting $\zeta \equiv -f'(0)$, we have for the homogeneous unitary gas

$$\frac{C^{\text{hom}}}{V} = \zeta \frac{2}{5\pi} k_F^4, \tag{5.105}$$

so that

$$\frac{\langle N_b \rangle^{\text{hom}}}{N} = \frac{3}{10} k_F R_* \zeta. \tag{5.106}$$

This expression is valid for a universal gas consisting mainly of fermionic atoms, which requires that $\langle N_b \rangle^{\text{hom}}/N \ll 1$, i. e. $k_F R* \ll 1$. This condition was already obtained in Sect. 5.2.3.2 for the broad resonances of the left column of Table 5.1. In the more exotic case of the narrow resonances of the second column of Table 5.1, this condition has to be imposed in addition to the ones of Table 5.1.

5.2.3.4   Application of General Relations: Various Measurements of the Contact

The relation (5.103) allowed us to extract in [68] the contact C of the trapped gas [related to the derivative of the total energy of the trapped gas *via* Eq. 5.63] from
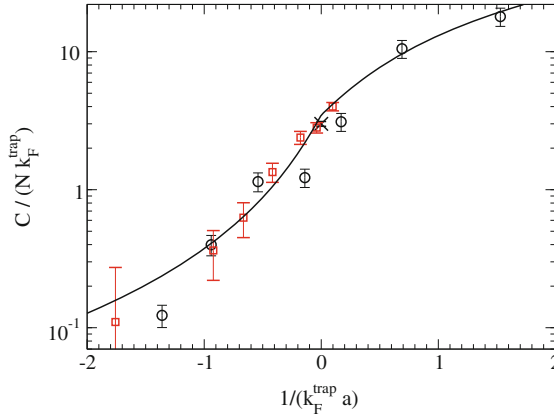
Fig. 5.8 The contact $C = \frac{dE}{d(-1/a)} \frac{4\pi m}{\hbar^2}$ of a trapped unpolarized Fermi gas. The circles are obtained from the measurements of $\langle N_b \rangle$ in [74], combined with the two channel model theory linking $\langle N_b \rangle$ to C [Eq. 5.103]. The cross was obtained in [78] by measuring the structure factor. The squares were obtained in [79] by measuring the momentum distribution. Solid line: zero-temperature theoretical prediction extracted from [29] as detailed in [68]. Here the Fermi wavevector k_F^{trap} of the trapped gas is defined by $\hbar^2 (k_F^{\mathrm{trap}})^2/(2m) = (3N)^{1/3} \hbar \bar{\omega}$, with $\bar{\omega}$ the geometric mean of the three oscillation frequencies ω_α and N the total atom number

the values of N_b measured in [74]. The result is shown in Fig. 5.8, together with a theoretical zero-temperature curve resulting from the local density approximation in the harmonically trapped case where $U(\mathbf{r}) = \frac{1}{2} m \sum_\alpha \omega_\alpha^2 x_\alpha^2$, the function f of (5.104) being obtained by interpolating between the fixed-node Monte-Carlo data of [29, 77] and the known asymptotic expressions in the BCS and BEC limits.[10]

While this is the first direct measurements of the contact in the BEC–BCS crossover, it has also been measured more recently:

- using Bragg scattering, *via* the large-momentum tail of the structure factor, directly related by Fourier transformation to the short-distance singularity Eq. 5.65 of the pair correlation function [78], see the cross at unitarity in Fig. 5.8
- *via* the tail of the momentum distribution Eq. 5.64 measured by abruptly turning off both trapping potential and interactions [79], see the squares in Fig. 5.8
- *via* (momentum resolved) radio-frequency spectroscopy [79, 80].

For the homogeneous unitary gas, the contact is conveniently expressed in terms of the dimensionless parameter ζ [see (5.105)]. The experimental value $\zeta = 0.91(5)$ was obtained by measuring the equation of state of the homogeneous gas with the technique proposed by [81] and taking the derivative of the energy with respect to the inverse scattering length [Eq. 5.63] (see [82] and the contribution of F. Chevy and C. Salomon in Chap. 11 of this volume). From the fixed-node Monte-Carlo calculations, one gets $\zeta \simeq 1$ by taking a derivative of the data of [29] for the function

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[10] See [68] for details. The cusp at unitarity is of course an artefact of this interpolation procedure.

f, while the data of [77] for the pair correlation function together with the relation (65) give $\zeta \simeq 0.95$.[11],[12]

In conclusion, the smallness of the interaction range leads to singularities; at first sight this may seem to complicate the problem as compared to other strongly interacting systems; however these singularities are well understood and have a useful consequence: the existence of exact relations resulting from the Hellmann-Feynman theorem [51] and from properties of the Fourier transform [52]. In particular this provides a "useful check on mutual consistency of various experiments", as foreseen in [83].

5.3 Dynamical Symmetry of the Unitary Gas

In this section, we present some remarkable properties of the unitary gas, derived from the zero-range model. The starting point is that the time evolution of the gas in a time dependent isotropic harmonic trap may be expressed exactly in terms of a gauge and scaling transform, see Sect. 5.3.1. This implies the existence of a SO(2,1) dynamical (or hidden) symmetry of the system, a formal property that we shall link to concrete consequences, such as the existence of an exactly decoupled bosonic degree of freedom (the breathing mode of the gas), see Sect. 5.3.2, or the separability of the *N*-body wavefunction in hyperspherical coordinates, see Sect. 5.3.3, which holds both in an isotropic harmonic trap and in free space and has several important consequences such as the analytical solution of the trapped three-body problem, see Sect. 5.3.4. In Sect. 5.3.5 we use the existence of the undamped breathing mode to rederive a remarkable property of the homogeneous unitary gas: its bulk viscosity vanishes. Section 5.3.6 concerns short-range scaling laws, which are related to the separability in hyperspherical coordinates, but hold for any scattering length and external potential.

5.3.1 Scaling Solution in a Time-Dependent Trap

In this section, we shall assume that the trapping potential $U(\mathbf{r})$ introduced in Eq. 5.74 is an isotropic harmonic potential. Whereas the hypothesis of harmonicity may be a good approximation in present experiments for small enough atomic clouds, the isotropy is not granted and requires some experimental tuning that, to our knowledge, remains to be done. On the other hand, we allow a general time dependence of the

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[11] This value is also compatible with the data of [77] for the one-body density matrix, whose short-range singular part is related by Fourier transformation to the large-*k* tail of the momentum distribution [38].

[12] At unitarity, the local density approximation can be done analytically, yielding a relation between the contact C of the trapped gas and the one of the homogeneous gas: $\frac{C}{Nk_F^{\mathrm{trap}}} = \frac{512}{175}\frac{\zeta}{\xi^{1/4}}$ [68].

trap curvature, so that Schrödinger's equation for the N-body wavefunction defined
in Eq. 5.73 is

$$i\hbar\partial_t\psi(\mathbf{X},t) = \left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{X}} + \frac{1}{2}m\omega^2(t)X^2\right]\psi(\mathbf{X},t), \qquad (5.107)$$

where we recall that $\mathbf{X}$ is the set of all particle coordinates, and $\omega(t)$ is the instanta-
neous angular oscillation frequency. The interaction between particles is described by
the contact conditions Eq. 5.75, written here for the unitary gas, that is for $a^{-1} = 0$:

$$\psi(\mathbf{X}) = \frac{A_{ij}(\mathbf{R}_{ij};(\mathbf{r}_k)_{k\neq i,j})}{r_{ij}} + O(r_{ij}). \qquad (5.108)$$

Let us consider the particular case, quite relevant experimentally, where the gas is
initially at equilibrium in a static trap $\omega(t=0) = \omega$. The gas is then in a statistical
mixture of stationary states, so we can assume that the initial N-body wavefunction
is an eigenstate of the Hamiltonian with energy E. At $t > 0$, the trap curvature is
varied, which leads to an arbitrary time dependent $\omega(t)$. In typical experiments, one
either sets abruptly $\omega(t)$ to zero, to perform a time of flight measurement, or one
modulates $\omega(t)$ at some frequency to study the gas collective modes. Can we predict
the evolution of the system? As shown in [58], the answer is yes, as we now explain.

In the absence of interactions, it is well known [84] that $\psi(\mathbf{X},t)$ is deduced from
the $t = 0$ wavefunction by a simple gauge plus scaling ansatz:

$$\psi(\mathbf{X},t) = \frac{e^{i\theta(t)}}{\lambda^{3N/2}(t)}\exp\left[\frac{im\dot{\lambda}(t)}{2\hbar\lambda(t)}X^2\right]\psi(\mathbf{X}/\lambda(t),0), \qquad (5.109)$$

where $\dot{\lambda}(t) = d\lambda(t)/dt$. At time $t = 0$, one clearly has $\theta(0) = 0$,

$$\lambda(0) = 1 \quad \text{and} \quad \dot{\lambda}(0) = 0. \qquad (5.110)$$

Inserting this ansatz into Schrödinger's equation (5.107), we obtain a Newton like
equation of motion for λ:

$$\ddot{\lambda}(t) = \frac{\omega^2}{\lambda^3(t)} - \omega^2(t)\lambda(t) \qquad (5.111)$$

to be solved with the initial conditions (5.110). We recall that ω stands for the *initial*
angular oscillation frequency. The equation (5.111) is well studied in the literature,
under the name of the Ermakov equation [85], and is in particular amenable to a linear
form: one recognizes an equation for the distance to the origin for a two-dimensional
harmonic oscillator of angular frequency $\omega(t)$, as obtained from Newton's equation
and from the law of equal areas. In particular, if $\omega(t) = \omega_{ct}$ is a constant over some
time interval, $\lambda(t)$ oscillates with a period π/ω_{ct} over that time interval.

The global phase $\theta(t)$ is given by

$$\theta(t) = -\frac{E}{\hbar} \int_0^t \frac{dt'}{\lambda^2(t')}. \tag{5.112}$$

This suggests that θ still evolves at the stationary pace $-E/\hbar$ provided that one introduces a modified time, as done in [86] in a bosonic mean field context:

$$\tau(t) = \int_0^t \frac{dt'}{\lambda^2(t')}. \tag{5.113}$$

We shall come back to this point below.

In presence of interactions, one has to check that the ansatz (5.109) obeys the contact conditions (5.108). First, the ansatz includes a scaling transform. As discussed in Sect. 5.2.2, this preserves the contact conditions and the domain of the Hamiltonian for the unitary gas. Second, the ansatz includes a quadratic gauge transform. Turning back to the definition of the contact conditions, we select an arbitrary pair of particles i and j and we take the limit $r_{ij} \to 0$ for a fixed centroid position $\mathbf{R}_{ij} = (\mathbf{r}_i + \mathbf{r}_j)/2$. In the gauge factor, the quantity $X^2 = \sum_{k=1}^N r_k^2$ appears. The positions $\mathbf{r}_k$ of the particles other than i and j are fixed. What matters is thus $r_i^2 + r_j^2$ that we rewrite as

$$r_i^2 + r_j^2 = 2R_{ij}^2 + \frac{1}{2}r_{ij}^2. \tag{5.114}$$

R_{ij} is fixed. r_{ij} varies but it appears squared in the gauge transform, so that

$$\exp\left[\frac{im\dot{\lambda}(t)}{2\hbar\lambda(t)}r_{ij}^2/2\right]\left[\frac{1}{r_{ij}} + O(r_{ij})\right] = \frac{1}{r_{ij}} + O(r_{ij}) \tag{5.115}$$

and the contact conditions are preserved by the gauge transform, even if the scattering length a was finite.

We thus conclude that the ansatz (5.109) gives the solution also for the unitary gas. This has interesting practical consequences. For measurements in position space, one has simple scaling relations, not only for the mean density $\rho_\sigma(\mathbf{r}, t)$ in each spin component σ:

$$\rho_\sigma(\mathbf{r}, t) = \frac{1}{\lambda^3(t)}\rho_\sigma(\mathbf{r}/\lambda(t), 0) \tag{5.116}$$

but also for higher order density correlation functions: for example, the second order density correlation function defined in terms of the fermionic field operators as

$$g^{(2)}_{\sigma\sigma'}(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_\sigma^\dagger(\mathbf{r})\psi_{\sigma'}^\dagger(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r})\rangle, \tag{5.117}$$

evolves in time according to the scaling

$$g^{(2)}_{\sigma\sigma'}(\mathbf{r}, \mathbf{r}', t) = \frac{1}{\lambda^6(t)}g^{(2)}_{\sigma\sigma'}(\mathbf{r}/\lambda(t), \mathbf{r}'/\lambda(t), 0). \tag{5.118}$$

As a consequence, if one abruptly switches off the trapping potential at $t = 0^+$, the gas experiences a ballistic expansion with a scaling factor

$$\lambda(t) = [1 + \omega^2 t^2]^{1/2}, \tag{5.119}$$

which acts as a perfect magnifying lens on the density distribution.

For non-diagonal observables in position space, some information is also obtained, with the gauge transform now contributing. For example the first order coherence function

$$g_{\sigma\sigma}^{(1)}(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_\sigma^\dagger(\mathbf{r}')\psi_\sigma(\mathbf{r})\rangle, \tag{5.120}$$

which is simply the matrix element of the one-body density operator between $\langle \mathbf{r}, \sigma|$ and $|\mathbf{r}', \sigma\rangle$, evolves according to

$$g_{\sigma\sigma}^{(1)}(\mathbf{r}, \mathbf{r}', t) = \frac{1}{\lambda^3(t)} \exp\left[\frac{im\dot{\lambda}(t)}{2\hbar\lambda(t)}(r^2 - r'^2)\right] g_{\sigma\sigma}^{(1)}(\mathbf{r}/\lambda(t), \mathbf{r}'/\lambda(t), 0). \tag{5.121}$$

The momentum distribution $n_\sigma(\mathbf{k})$ in the spin component σ is the Fourier transform over $\mathbf{r} - \mathbf{r}'$ and the integral over $(\mathbf{r} + \mathbf{r}')/2$ of the first order coherence function. For a ballistic expansion, directly transposing to three dimensions the result obtained in [87] from a time dependent scaling solution for the one-dimensional gas of impenetrable bosons, one has that the momentum distribution of the ballistically expanding unitary gas is asymptotically homothetic to the gas initial spatial density profile:

$$\lim_{t\to+\infty} n_\sigma(\mathbf{k}, t) = \left(\frac{2\pi\hbar}{m\omega}\right)^3 \rho_\sigma\left(\mathbf{r} = \frac{\hbar\mathbf{k}}{m\omega}, 0\right). \tag{5.122}$$

We emphasize that the above results hold for an arbitrary gas polarization, that is for arbitrary numbers of particles in each of the two spin states $\sigma = \uparrow, \downarrow$. If the initial state is thermal, they hold whatever the value of the temperature, larger or smaller than the critical temperature T_c. These results however require the unitary limit (in particular $|a| = +\infty$) and a perfect isotropy of the harmonic trap. If the experimental goal is simply to have the ballistic expansion as a perfect magnifying lens, these two requirements remarkably may be removed, as shown in [88], if one is ready to impose an appropriate time dependence to the scattering length $a(t)$ and to the trap aspect ratio, in which case the ansatz (5.109) holds at all times. In the particular case of an isotropic trap, the procedure of [88] is straightforward to explain: If $\psi(t = 0)$ obeys the contact conditions with a finite scattering length a, the ansatz (5.109) obeys the contact conditions for a scattering length $\lambda(t)a$ so one simply has to adjust the actual scattering length in a time dependent way:

$$a(t) = \lambda(t)a \tag{5.123}$$

where λ evolves according to Eq. 5.111. As shown in the next section, the time dependent solution in the unitary case, apart from providing convenient scaling relations

on the density, is connected to several interesting intrinsic properties of the system, whereas the procedure of [88] does not imply such properties.

To be complete, we finally address the general case where the initial wavefunction of the unitary gas is not necessarily a stationary state but is arbitrary [89]. Then the observables of the gas have in general a non-trivial time dependence, even for a fixed trap curvature. If the trap curvature is time dependent, we modify the gauge plus scaling ansatz as follows:

$$\psi(\mathbf{X}, t) = \frac{1}{\lambda^{3N/2}(t)} \exp\left[\frac{im\dot{\lambda}(t)}{2\hbar\lambda(t)} X^2\right] \tilde{\psi}(\mathbf{X}/\lambda(t), \tau(t)), \qquad (5.124)$$

where $\tau(t)$ is the modified time introduced in Eq. 5.112, $\lambda(t)$ evolves according to Eq. 5.111 with the initial conditions (5.110), and the time-dependent wavefunction $\tilde{\psi}$ coincides with ψ at time $t = \tau = 0$ and obeys the unitary gas contact conditions. Then this ansatz obeys the contact conditions. When inserted in the time dependent Schrödinger equation (5.107), it leads to a Schrödinger equation for $\tilde{\psi}$ in the time independent external potential fixed to the $t = 0$ trap:

$$i\hbar\partial_\tau \tilde{\psi}(\mathbf{X}, \tau) = \left[-\frac{\hbar^2}{2m}\Delta_\mathbf{X} + \frac{1}{2}m\omega^2 X^2\right] \tilde{\psi}(\mathbf{X}, \tau). \qquad (5.125)$$

The gauge plus scaling transform, and the redefinition of time, have then totally cancelled the time dependence of the trap. If the initial wavefunction is an eigenstate of energy E, as was previously the case, one simple has $\tilde{\psi}(\tau) = \exp(-iE\tau/\hbar)\psi(t = 0)$ and one recovers the global phase factor in Eq. 5.109.

5.3.2 SO(2,1) Dynamical Symmetry and the Decoupled Breathing Mode

As shown in [90] for a two-dimensional Bose gas with $1/r^2$ interactions, the existence of a scaling solution such as Eq. 5.109 reflects a hidden symmetry of the Hamiltonian, the SO(2,1) dynamical symmetry. Following [89], we construct explicitly this dynamical symmetry for the unitary gas and we show that it has interesting consequences for the energy spectrum in a static isotropic harmonic trap.

Let us consider a gedankenexperiment: starting from the unitary gas is an energy eigenstate ψ, we modify in an infinitesimal way the trap curvature during the time interval $[0, t_f]$, and for $t > t_f$ we restore the initial trap curvature, $\omega(t) = \omega(0) = \omega$. Linearizing Eq. 5.111 around $\lambda = 1$ for $t > t_f$, we see that the resulting change in the scaling parameter λ is

$$\lambda(t) - 1 = \varepsilon e^{-2i\omega t} + \varepsilon^* e^{2i\omega t} + O(\varepsilon^2) \qquad (5.126)$$

where ε is proportional to the infinitesimal curvature change. Since λ oscillates indefinitely at frequency 2ω, this shows the existence of an undamped mode of frequency

2ω. This conclusion actually extends to excitations during $[0, t_f]$ of arbitrarily large amplitudes, as noted below Eq. 5.111 [90].

We calculate the resulting change in the N-body wavefunction, expanding Eq. 5.109 to first order in ε, putting in evidence the components that oscillate with Bohr frequencies $\pm 2\omega$:

$$\psi(\mathbf{X}, t) = e^{i\alpha} \left[e^{-iEt/\hbar} - \varepsilon e^{-i(E+2\hbar\omega)t/\hbar} L_+ + \varepsilon^* e^{-i(E-2\hbar\omega)t/\hbar} L_- \right]$$
$$\psi(\mathbf{X}, 0) + O(\varepsilon^2). \tag{5.127}$$

The time independent phase α depends on the details of the excitation procedure. We have introduced the operators

$$L_\pm = \pm i D + \frac{H}{\hbar\omega} - \frac{m\omega}{\hbar} X^2 \tag{5.128}$$

where D is the generator of the scaling transforms, as defined in Eq. 5.83, and $L_+ = L_-^\dagger$. We then read on Eq. 5.127 the remarkable property that the action of L_+ on an energy eigenstate ψ of energy E produces an energy eigenstate of energy $E + 2\hbar\omega$.[13] Similarly, the action of L_- on ψ produces an energy eigenstate of energy $E - 2\hbar\omega$, or eventually gives zero since the spectrum is bounded from below by $E \geq 0$ according to the virial theorem (5.88) applied to $U(\mathbf{r}) = \frac{1}{2} m\omega^2 r^2$. We see that the spectrum has thus a very simple structure, it is a collection of semi-infinite ladders, each ladder being made of equidistant energy levels separated by $2\hbar\omega$, see Fig. 5.9 , and $L_\pm$ acting respectively as a raising/lowering operator in that structure. Within each ladder, we call ψ_g the wavefunction corresponding to the ground step of that ladder, such that

$$L_- \psi_g = 0. \tag{5.129}$$

As shown in [90], this structure implies a dynamical SO(2,1) symmetry, meaning that the Hamiltonian H is part of the SO(2,1) Lie algebra. One starts with the commutation relations:
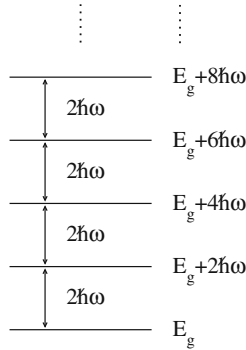
$$[H, L_\pm] = \pm 2\hbar\omega L_\pm \tag{5.130}$$

$$[L_+, L_-] = -4H/(\hbar\omega). \tag{5.131}$$

The first relation was expected from the raising/lowering nature of $L_\pm$. Both relations can be checked from the commutation relations Eqs. 5.85, 5.86 and from

$$\left[\frac{1}{2} X^2, -\frac{1}{2} \Delta_\mathbf{X} \right] = i D. \tag{5.132}$$

---

[13] As shown in [89], $L_+ \psi$ cannot be zero.

Fig. 5.9 The energy spectrum of the unitary gas in an isotropic harmonic trap is a collection of semi-infinite ladders such as the one depicted in the figure, with various ground step energies E_g. This structure is related to the existence of a decoupled bosonic mode, and holds whatever the numbers of fermions in each of the two spin components

We emphasize again the crucial point that the operators $L_\pm$ preserve the domain of the Hamiltonian in the present unitary case, since D and X^2 do. Obtaining the canonical commutation relations among the generators T_1, T_2 and T_3 of the SO(2,1) Lie algebra,

$$[T_1, T_2] \equiv -iT_3, \quad [T_2, T_3] \equiv iT_1, \quad [T_3, T_1] \equiv iT_2, \qquad (5.133)$$

is then only a matter of rewriting:

$$T_1 \pm iT_2 \equiv \frac{1}{2}L_\pm \quad \text{and} \quad T_3 = \frac{H}{2\hbar\omega}. \qquad (5.134)$$

Note the sign difference in the first commutator of Eq. 5.133 with respect to the other two commutators, and with respect to the more usual SO(3) or SU(2) Lie algebra.

Have we gained something in introducing the SO(2,1) Lie algebra, or is it simply a formal rewriting of the ladder structure already apparent in the simple minded approach Eq. 5.127, may ask a reader unfamiliar with dynamical symmetries. Well, an advantage is that we can immediately exhibit the so-called Casimir operator C,

$$C \equiv -4[T_1^2 + T_2^2 - T_3^2] = H^2 - \frac{1}{2}(\hbar\omega)^2(L_+L_- + L_-L_+), \qquad (5.135)$$

guaranteed to commute with all the elements T_1, T_2 and T_3 of the algebra, so that C is necessarily a scalar within each ladder. Taking as a particularly simple case the expectation value of C within the ground step ψ_g of the ladder of energy E_g, and using Eq. 5.131 to evaluate $\langle \psi_g | L_-L_+ | \psi_g \rangle$, we obtain $C | \psi_g \rangle = E_g(E_g - 2\hbar\omega) | \psi_g \rangle$. Inverting this relation thanks to the property $E_g \geq 3\hbar\omega/2$,[14] we can define the ground energy step operator H_g:

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[14] To obtain this inequality, one uses a virial theorem after separation of the center of mass motion [89].

$$H_g = \hbar\omega + [C + (\hbar\omega)^2]^{1/2}, \tag{5.136}$$

which is scalar and equal to E_g within each ladder. A useful application of H_g is to rescale the raising and lowering operator $L_\pm$ to obtain simpler commutation relations: It appears that

$$b = [2(H + H_g)/(\hbar\omega)]^{-1/2} L_- \tag{5.137}$$

is a bosonic annihilation operator, which obeys the usual bosonic commutation relations, in particular with its hermitian conjugate

$$[b, b^\dagger] = 1. \tag{5.138}$$

$b^\dagger$ and b have the same raising/lowering properties as $L_\pm$, and commute with H_g. They have the usual simple matrix elements, e.g. $b^\dagger|n\rangle = (n + 1)^{1/2}|n + 1\rangle$ where $|n\rangle$ is the step number n of a ladder, n starting from 0. They allow an illuminating rewriting of the Hamiltonian:

$$H = H_g + 2\hbar\omega b^\dagger b \tag{5.139}$$

revealing that the unitary gas in a harmonic isotropic trap has a fully decoupled bosonic degree of freedom. This bosonic degree of freedom, physically, is simply the undamped breathing mode of the gas of frequency 2ω, identified for a different system in [90].

We now give two simple applications of the above formalism [89]. First, one can calculate the various moments of the trapping Hamiltonian $H_{\text{trap}} = \frac{1}{2}m\omega^2 X^2$, from the identity

$$H_{\text{trap}} = \frac{1}{2}H - \frac{\hbar\omega}{4}(L_+ + L_-) = \frac{\hbar\omega}{2}A^\dagger A \tag{5.140}$$

where $A = [b^\dagger b + H_g/(\hbar\omega)]^{1/2} - b$. Taking the expectation value of Eq. 5.140 within a given eigenstate of energy E, or within a statistical mixture of eigenstates, immediately gives

$$\langle H_{\text{trap}}\rangle = \frac{1}{2}\langle H\rangle, \tag{5.141}$$

a particular case of the virial theorem Eq. 5.88. Taking the expectation value of H_{trap}^2 for the thermal equilibrium density operator gives

$$4\langle H_{\text{trap}}^2\rangle = \langle H^2\rangle + \langle H\rangle\hbar\omega[2\langle b^\dagger b\rangle + 1] \tag{5.142}$$

where we used $\langle H_g b^\dagger b\rangle = \langle H_g\rangle\langle b^\dagger b\rangle$ for the thermal equilibrium. From the Bose formula, one has also $\langle b^\dagger b\rangle = [\exp(2\beta\hbar\omega) - 1]^{-1}$, with $\beta = 1/(k_B T)$ and T is the temperature.

The second, more impressive, application is to uncover a very interesting structure of the N-body wavefunction $\psi_g(\mathbf{X})$ of the ground energy step of an arbitrary ladder. We introduce hyperspherical coordinates $(X, \mathbf{n} = \mathbf{X}/X)$, where $\mathbf{n}$ is a unit vector is the space of $3N$ real coordinates. The innocent equation (5.129) becomes

$$\left[-\frac{3N}{2} - X\partial_X + \frac{E_g}{\hbar\omega} - \frac{m\omega}{\hbar}X^2 \right] \psi_g(\mathbf{X}) = 0. \qquad (5.143)$$

This is readily integrated for a fixed hyperdirection $\mathbf{n}$:

$$\psi_g(\mathbf{X}) = e^{-m\omega X^2/(2\hbar)} X^{\frac{E_g}{\hbar\omega} - \frac{3N}{2}} f(\mathbf{n}) \qquad (5.144)$$

where $f(\mathbf{n})$ is an unknown function of the hyperdirection. Eq. 5.144 has fascinating consequences.

First, it shows that ψ_g, being the product of a function of the modulus X and of a function of the hyperdirection, is *separable* in hyperspherical coordinates. The physical consequences of this separability, in particular for the few-body problem, are investigated in Sect. 5.3.4. Note that this separability holds for all the other steps of the ladder, since L_+ only acts on the hyperradius.

Second, we take the limit $\omega \to 0$ in Eq. 5.144: according to Eq. 5.12, $E_g/(\hbar\omega)$ is a constant, and $E_g \to 0$, whereas the Gaussian factor tends to unity. $\mathbf{n}$ is dimensionless, and we can take $f(\mathbf{n})$ to be ω independent if we do not normalize ψ_g to unity. We thus obtain in this limit a zero energy eigenstate of the free space problem,

$$\psi^{\text{free}}(\mathbf{X}) = X^{\frac{E_g}{\hbar\omega} - \frac{3N}{2}} f(\mathbf{n}) \qquad (5.145)$$

which is independent of ω. This zero energy eigenstate is scaling invariant, in the sense that

$$\psi_\lambda^{\text{free}}(\mathbf{X}) = \frac{1}{\lambda^v} \psi^{\text{free}}(\mathbf{X}) \quad \forall \lambda > 0, \qquad (5.146)$$

where ψ_λ is defined in Eq. 5.81 and

$$v = \frac{E_g}{\hbar\omega}. \qquad (5.147)$$

In summary, starting from the wavefunction ψ_g of any ladder ground state of the trapped gas spectrum, one gets a scaling-invariant zero-energy free-space eigenstate $\psi_\lambda^{\text{free}}$, simply by removing the gaussian factor $e^{-m\omega X^2/(2\hbar)}$ in the expression (5.144) of ψ_g.

Remarkably, the reverse property is true. Let us imagine that we know a zero energy eigenstate ψ^{free} of the free space problem $H_{\text{free}} = -\frac{\hbar^2}{2m}\Delta_{\mathbf{X}}$,

$$\Delta_{\mathbf{X}} \psi^{\text{free}}(\mathbf{X}) = 0, \qquad (5.148)$$

that of course also obeys the Wigner-Bethe-Peierls contact conditions for the unitary gas. Since H_{free} commutes with the generator D of the scaling transforms, we generally expect ψ^{free} to obey Eq. 5.146 with some exponent v, so that

$$i D\psi^{\text{free}} = v\psi^{\text{free}}. \tag{5.149}$$

Since ψ^{free} is not square integrable, the hermiticity of D does not imply that $v \in i\mathbb{R}$; on the contrary, we will see that $v \in \mathbb{R}$. Let us multiply ψ^{free} with a Gaussian factor:

$$\psi(\mathbf{X}) \equiv e^{-m\omega X^2/(2\hbar)}\psi^{\text{free}}(\mathbf{X}). \tag{5.150}$$

As we did for the gauge transform, see Eq. 5.115, we can show that ψ so defined obeys the Wigner-Bethe-Peierls contact conditions. Calculating the action on ψ of the Hamiltonian H of the trapped gas, and using Eq. 5.149, we directly obtain

$$H\psi = v\hbar\omega\psi, \tag{5.151}$$

i.e. ψ is indeed an eigenstate of the trapped gas with the eigenenergy $v\hbar\omega$. This ψ corresponds to the ground energy step of a ladder. Repeated action of L_+ will generate the other states of the ladder.

We have thus constructed a mapping between the trapped case and the zero energy free space case, for the unitary gas in an isotropic harmonic trap. A similar mapping (restricting to the ground state) was constructed by Tan in an unpublished work [91].

5.3.3 Separability in Internal Hyperspherical Coordinates

As shown in Sect. 5.3.2, the SO(2,1) dynamical symmetry of the unitary gas in an isotropic harmonic trap implies that the eigenstate wavefunctions $\psi(\mathbf{X})$ may be written as the product of a function of the modulus X and of a function of the direction $\mathbf{X}/X$. Here, following [89], we directly use this property at the level of the N-body Schrödinger equation, for $N > 2$, and we derive an effective Schrödinger equation for a hyperradial wavefunction, with interesting consequences discussed in Sect. 5.3.4. The derivation is restricted here to the case of particles of identical masses, as in the previous sections, but the separability in internal spherical coordinates may also hold for particles of different masses, as detailed in Appendix 3.

First, we introduce a refinement to the separability of Sect. 5.3.2: in a harmonic trap, the center of mass of the system is totally decoupled from the internal variables, that is from the relative coordinates $\mathbf{r}_i - \mathbf{r}_j$ of the particles. This is quite straightforward in Heisenberg picture, for an interaction modeled by a potential $V(|\mathbf{r}_i - \mathbf{r}_j|)$. The Heisenberg equations of motion for the center of mass position

$$\mathbf{C} \equiv \frac{1}{N}\sum_{i=1}^{N}\mathbf{r}_i \tag{5.152}$$

and the center of mass momentum $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$ are indeed coupled only among themselves, due in particular to the fact that the interaction potential cannot change the total momentum $\mathbf{P}$ of the system:

$$\frac{d}{dt}\hat{\mathbf{P}}(t) = -Nm\omega^2 \hat{\mathbf{C}}(t) \tag{5.153}$$

$$\frac{d}{dt}\hat{\mathbf{C}}(t) = \frac{\hat{\mathbf{P}}(t)}{Nm}. \tag{5.154}$$

The center of mass of the system thus behaves as a fictitious particle of mass Nm trapped in the harmonic potential $Nm\omega^2 \mathbf{C}^2/2$, with a Hamiltonian

$$H_{\text{CM}} = -\frac{\hbar^2}{2Nm}\Delta_{\mathbf{C}} + \frac{1}{2}Nm\omega^2 C^2. \tag{5.155}$$

The center of mass has of course the same angular oscillation frequency as the individual particles. This center of mass decoupling property clearly holds in the general harmonic *anisotropic* case. It persists in the zero range limit so it holds also for the zero-range model.

We can thus split the Hamiltonian Eq. 5.74 as the sum of the center of mass Hamiltonian H_{CM} and the internal Hamiltonian $H_{\text{internal}} \equiv H - H_{\text{CM}}$. As a consequence, we introduce as new spatial coordinates the center of mass position $\mathbf{C}$ and the set of internal coordinates

$$\mathbf{R} \equiv (\mathbf{r}_1 - \mathbf{C}, \ldots, \mathbf{r}_N - \mathbf{C}), \tag{5.156}$$

and we can seek eigenstates in the factorized form $\psi(\mathbf{X}) = \psi_{\text{CM}}(\mathbf{C})\psi_{\text{internal}}(\mathbf{R})$.

The crucial step is then to define *internal* hyperspherical coordinates, consisting in the hyperradius

$$R = \left[\sum_{i=1}^{N}(\mathbf{r}_i - \mathbf{C})^2\right]^{1/2} \tag{5.157}$$

and a convenient parameterization of the set of dimensionless internal coordinates $\mathbf{R}/R$. There is a technical subtlety due to the fact that the coordinates of $\mathbf{R}$ are not independent variables: Since the sum of the components of $\mathbf{R}$ along each spatial direction x, y and z is exactly zero, and since $\mathbf{R}/R$ is a unit vector, the vector $\mathbf{R}/R$ contains actually only $3N - 4$ independent dimensionless real variables. We then use the following result, that may be obtained with the appropriate Jacobi coordinates[15] [92]: There exists a parameterization of $\mathbf{R}/R$ by a set of $3N - 4$ internal hyperangles that we call Ω, such that the internal Hamiltonian takes the form

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[15] For particles of equal masses one introduces the Jacobi coordinates $\mathbf{u}_i = (\frac{N-i}{N+1-i})^{1/2} \left[\mathbf{r}_i - (N-i)^{-1}\sum_{j=i+1}^{N} \mathbf{r}_j\right]$ for $1 \leq i \leq N - 1$. Then $\Delta_{\mathbf{X}} = N^{-1}\Delta_{\mathbf{C}} + \sum_{i=1}^{N-1} \Delta_{\mathbf{u}_i}$ and $R^2 = X^2 - NC^2 = \sum_{i=1}^{N-1} \mathbf{u}_i^2$. The general case of arbitrary masses is detailed in the Appendix 3.

$$H_{\text{internal}} = -\frac{\hbar^2}{2m}\left[\partial_R^2 + \frac{3N-4}{R}\partial_R + \frac{1}{R^2}\Delta_\Omega\right] + \frac{1}{2}m\omega^2 R^2, \qquad (5.158)$$

where Δ_Ω is the Laplacian on the unit sphere of dimension $3N-4$. The expression between square brackets is the standard form for the usual Laplacian in dimension $d = 3N - 3$, written in hyperspherical coordinates, which justifies the name of "internal hyperspherical coordinates".

The separability in internal spherical coordinates means that the internal eigenstates in a trap can be written as products of a function of R and a function of Ω. This basically results from the reasoning below Eq. 5.148, with the little twist that one can further assume that the zero-energy free space eigenstate $\psi^{\text{free}}(\mathbf{X})$ has a zero total momentum, i. e. it is independent of the center of mass position.[16] The scale invariance Eq. 5.146 or equivalently Eq. 5.149 then implies

$$\psi^{\text{free}}(\mathbf{X}) = R^{s-(3N-5)/2}\phi(\Omega) \qquad (5.159)$$

with some exponent s shifted for convenience by $(3N - 5)/2$. The challenge is of course to determine the unknown function $\phi(\Omega)$ and the corresponding value of s. From Schrödinger's equation $\Delta_\mathbf{X}\psi^{\text{free}} = 0$ and the expression of the internal Laplacian in hyperspherical coordinates, see Eq. 5.158, one finds that s^2 solves the eigenvalue problem

$$\left[-\Delta_\Omega + \left(\frac{3N-5}{2}\right)^2\right]\phi(\Omega) = s^2\phi(\Omega), \qquad (5.160)$$

where $\phi(\Omega)$ has to obey the Wigner-Bethe-Peierls contact conditions Eq. 5.108 reformulated in hyperangular coordinates.[17] The merit of the shift $(3N - 5)/2$ is thus to reveal a symmetry $s \leftrightarrow -s$.

The generalization of the zero energy free space solution Eq. 5.159 to the finite energy trapped problem is simply provided by the ansatz:

$$\psi(\mathbf{X}) = \psi_{\text{CM}}(\mathbf{C})\phi(\Omega)R^{-(3N-5)/2}F(R). \qquad (5.161)$$

Here $\psi_{\text{CM}}(\mathbf{C})$ is any center of mass eigenstate wavefunction of energy E_{CM}, $\phi(\Omega)$ is any solution of the eigenvalue problem Eq. 5.160. Injecting the ansatz into Schrödinger's equation of eigenenergy E and using Eq. 5.158, one finds that

$$E = E_{\text{CM}} + E_{\text{internal}}, \qquad (5.162)$$

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[16] The reasoning below Eq. 5.143 can also be adapted by putting the center of mass in its ground state $\psi_{\text{CM}}(\mathbf{C}) \propto \exp[-Nm\omega C^2/(2\hbar)]$ and by constructing purely internal raising and lowering operators of an internal SO(2,1) dynamical symmetry, that do not excite the center of mass motion contrarily to L_+ and L_- [89].

[17] These reformulated contact conditions are given explicitly in [55], Eq. 1.38.

where the hyperradial wavefunction $F(R)$ and the internal eigenenergy E_{internal} solve the eigenvalue problem:

$$-\frac{\hbar^2}{2m}\left[F''(R) + \frac{1}{R}F'(R)\right] + \left(\frac{\hbar^2 s^2}{2mR^2} + \frac{1}{2}m\omega^2 R^2\right)F(R) = E_{\text{internal}}F(R).$$
(5.163)

We note that, as detailed in the Appendix 3, this separability remarkably also holds in the case where the N particles have different masses [89], provided that they all have the same angular oscillation frequency ω in the trap, and that the Wigner-Bethe-Peierls model still defines a self-adjoint Hamiltonian for the considered mass ratios. The separability even holds when the Wigner-Bethe-Peierls model *supplemented with an additional boundary condition for $R \to 0$ and fixed Ω is self-adjoint*, as is the case e.g. for $N = 3$ bosons, see below; indeed such a boundary condition only affects the hyperradial problem.

In practice the explicit calculation of s is possible for the few-body problem. The most natural approach in general is to try to calculate the functions A_{ij} in Eq. 5.108 in momentum space. From Eq. 5.108 it appears that A_{ij} is scaling invariant with an exponent $s + 1 - (3N - 5)/2$. Its Fourier transform[18] is then also scaling invariant, with an exponent given by a simple power-counting argument: Since A_{ij} is a function of $3(N - 2)$ variables, if one takes into account the fact that it does not depend on the center of mass position $\mathbf{C}$, and since one has $[s + 1 - (3N - 5)/2] + 3(N - 2) = s + (3N - 5)/2$, its Fourier transform $\tilde{A}_{ij}$ scales as

$$\tilde{A}_{ij}(\mathbf{K}) = K^{-[s+(3N-5)/2]} f_{ij}(\mathbf{K}/K)$$
(5.164)

where $\mathbf{K}$ collects all the $3(N - 2)$ variables of $\tilde{A}_{ij}$ and f_{ij} denotes some functions to be determined. Remarkably it is the same quantity $(3N - 5)/2$ which appears in both Eqs. 5.159, 5.164.

This momentum space approach leads to integral equations. For $N = 3$, this integral equation was obtained in [93]; it was solved analytically in [94], the allowed values of s being the solutions of a transcendental equation. This transcendental equation was rederived from a direct analytical solution of (5.160) in position space in [4, 5], and generalised to arbitrary angular momenta, masses and statistics in [5]; for equal masses it is conveniently written in the form ([95] and refs. therein):

$$\frac{\Gamma\left(l + \frac{3}{2}\right)}{\Gamma\left(\frac{l+1+s}{2}\right)\Gamma\left(\frac{l+1-s}{2}\right)} = \frac{\eta}{\sqrt{3\pi}(-2)^l}\,_2F_1\left(\frac{l+1+s}{2}, \frac{l+1-s}{2}; l + \frac{3}{2}; \frac{1}{4}\right)$$
(5.165)

or alternatively [32]

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[18] Since the Fourier transform $\tilde{A}_{ij}(\mathbf{K}) = \int d^{3(N-2)}Y e^{-i\mathbf{K}\cdot\mathbf{Y}} A_{ij}(\mathbf{Y})$ may lead to non-absolutely converging integrals at infinity, the calculation has to be performed using the language of distributions, with a regularizing factor $e^{-\eta Y}$, $\eta \to 0^+$.

$$\left[i^l \sum_{k=0}^{l} \frac{(-l)_k (l+1)_k}{k!} \frac{(1-s)_l}{(1-s)_k} \left(2^{-k} i(k-s) e^{is\frac{\pi}{2}} + \eta(-1)^l \frac{4}{\sqrt{3}} e^{i\frac{\pi}{6}(2k+s)} \right) \right]$$

$$- \left[(-i)^l \sum_{k=0}^{l} \frac{(-l)_k (l+1)_k}{k!} \frac{(1-s)_l}{(1-s)_k} \left(2^{-k} (-i)(k-s) e^{-is\frac{\pi}{2}} + \eta(-1)^l \frac{4}{\sqrt{3}} e^{-i\frac{\pi}{6}(2k+s)} \right) \right] = 0$$

$$(5.166)$$

where l is the total internal angular momentum quantum number, η is -1 for fermions ($N_\uparrow = 2$, $N_\downarrow = 1$) or $+2$ for spinless bosons, $_2F_1$ is a hypergeometric function, and $(x)_n \equiv x(x+1)\ldots(x+n-1)$ with $(x)_0 \equiv 1$. The Eq. 5.165 has some spurious integer solutions ($l = 0$, $s = 2$ for fermions; $l = 0$, $s = 4$ and $l = 1$, $s = 3$ for bosons) which must be eliminated. For $N = 4$ there is no known analytical solution of the integral equation. Using the scale invariance of $\tilde{A}_{ij}(\mathbf{K})$ as in Eq. 5.164 and rotational symmetry however brings it to a numerically tractable integral equation involving the exponent s, that allowed to predict a four-body Efimov effect for three same-spin state fermions interacting with a lighter particle [7].

5.3.4 Physical Consequences of the Separability

As seen in the previous Sect. 5.3.3, the solution of the N-body problem ($N > 2$) for the unitary gas in a harmonic isotropic trap boils down to (i) the calculation of exponents s from zero-energy free space solutions, and (ii) the solution of the hyperradial eigenvalue problem Eq. 5.163. Whereas (i) is the most challenging part on a practical point of view, the step (ii) contains a rich physics that we now discuss.

Formally, the hyperradial problem Eq. 5.163 is Schrödinger's equation for one (fictitious) particle moving in two dimensions with zero angular momentum in the (effective) potential

$$U_{\text{eff}}(R) = \frac{\hbar^2}{2m} \frac{s^2}{R^2} + \frac{1}{2} m \omega^2 R^2. \qquad (5.167)$$

We will see that the nature of this problem is very different depending on the sign of s^2. The case $s^2 \geq 0$, i.e. s real, happens for $N = 3$ fermions ($N_\uparrow = 2$, $N_\downarrow = 1$), not only for equal masses, as can be tested numerically from (5.166) and even demonstrated analytically from the corresponding hyperangular eigenvalue problem [32] but also for unequal masses provided $m_\uparrow / m_\downarrow$ is below the critical value $13.60\ldots$ where one of the s (in the angular momentum $l = 1$ channel) becomes imaginary [5]. For $N = 4$ fermions with ($N_\uparrow = 3$, $N_\downarrow = 1$,) the critical mass ratio above which one of the s (in the angular momentum $l = 1$ channel) becomes imaginary is slightly smaller, $m_\uparrow / m_\downarrow \simeq 13.384$ [7]. In the physics literature, s is believed to be real for fermions for any ($N_\uparrow$, $N_\downarrow$) for equal masses, this belief being supported by numerical and experimental evidence. For 3 identical bosons, it is well-known that one of the values of s (in the $l = 0$ channel) is imaginary [4], all other values being real.

5.3.4.1 Universal Case

In this section we assume that s is real and we can take the sign convention $s \geq 0$. We impose that the hyperradial wavefunction $F(R)$ is bounded for $R \to 0$; indeed, allowing $F(R)$ to diverge would physically correspond to a N-body resonance (see Appendix 6). The spectrum and the corresponding hyperradial wavefunctions then are [89]

$$E_{\text{internal}} = (s + 1 + 2q)\hbar\omega, \quad q \in \mathbb{N} \tag{5.168}$$

$$F(R) = \sqrt{\frac{2q!}{\Gamma(s+1+q)}} \frac{R^s}{(a_{ho})^{s+1}} e^{-\left(\frac{R}{2a_{ho}}\right)^2} L_q^{(s)}\left(\left(\frac{R}{a_{ho}}\right)^2\right) \tag{5.169}$$

where $L_q^{(s)}$ is a generalised Laguerre polynomial of order q, $a_{ho} \equiv \sqrt{\frac{\hbar}{m\omega}}$ is the harmonic oscillator length, and the normalisation is such that $\int_0^\infty dR\, R F(R)^2 = 1$. Eq. 5.168 generalises to excited states the result obtained for the ground state in [91].

We thus recover the $2\hbar\omega$ spacing of the spectrum discussed in Sect. 5.3.2. We can also reinterpret the scaling solution of Sect. 5.3.1 as a time-evolution of the hyperradial wavefunction with a time-independent hyperangular wavefunction; in particular, the undamped breathing mode corresponds to an oscillation of the fictitious particle in the effective potential (5.167).[19]

The expression (5.169) of $F(R)$ immediately yields the probability distribution $P(R)$ of the hyperradius via $P(R) = F(R)^2 R$. This analytical prediction is in good agreement with the numerical results obtained in [96] for up to 17 fermions.

In the large N limit (more precisely if $N_\uparrow$ and $N_\downarrow$ tend to infinity and their ratio goes to a constant), the ground state energy of the trapped unitary gas is expected to be given in an asymptotically exact way by hydrostatics (also called local density approximation). Amusingly, this allows to predict the large-N asymptotics of the smallest possible value of s. For $N_\uparrow = N_\downarrow = N/2 \to \infty$ this gives [91, 96]

$$s \sim \sqrt{\xi} \frac{(3N)^{4/3}}{4} \tag{5.170}$$

where ξ appears in the expression Eq. 5.14 for the ground state energy of the homogeneous unitary gas.

For spin-1/2 fermions, Eqs. 5.168, 5.169, combined with the transcendental equation (5.165) and the expression of the hyperangular wavefunctions [5], provide the complete solution of the unitary three-body problem in an isotropic harmonic trap

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[19] Strictly speaking, such a time evolution of the wavefunction in *internal* hyperspherical coordinates corresponds to an internal scaling solution where the center of mass wavefunction is constant, whereas the scaling solution of Sect. 5.3.1 corresponds to a hyperradial motion in the hyperspherical coordinates $(X, \mathbf{n})$.

[32] (for completeness, one also has to include the eigenstates which are common to the unitary and the non-interacting problem [32], mentioned at the end of Sect. 5.2.2.1). This was first realised for the ground state in [91]. Remarkably, this 3-body spectrum in a trap allows to compute the third virial coefficient of the homogeneous unitary gas [97], whose value was confirmed experimentally (see [45] and the contribution of F. Chevy and C. Salomon in Chap. 11 of this volume).

For spinless bosons, the unitary three-body problem in an isotropic harmonic trap has two families of eigenstates (apart from the aforementioned common eigenstates with the non-interacting problem) [31, 32]: the states corresponding to real solutions s of the transcendental Equation 5.165, which we call universal states; and the states corresponding to the imaginary solution for s, which we call efimovian. Equations. 5.168, 5.169 apply to universal states. The efimovian states are discussed in the next section.

5.3.4.2 Efimovian Case

In this section we consider the case $s^2 < 0$, i.e. s is purely imaginary. In this case, all solutions of the Schrödinger-like equation 5.163 are bounded and oscillate more and more rapidly when $R \to 0$. In order to obtain a hermitian problem with a discrete spectrum, one has to impose the boundary condition [94, 55]:

$$\exists A/ \ F(R) \sim A \ \text{Im} \left[\left(\frac{R}{R_t} \right)^s \right] \quad \text{for } R \to 0, \tag{5.171}$$

where R_t is an additional three-body parameter. An equivalent form is:

$$\exists A'/F(R) \sim A'\sin \left[|s|\ln \left(\frac{R}{R_t} \right) \right] \quad \text{for } R \to 0. \tag{5.172}$$

The corresponding hyperradial wavefunctions are

$$F(R) = R^{-1}W_{E/2,s/2}(R^2/a_{ho}^2) \tag{5.173}$$

where W is a Whittaker function, and the spectrum is given by the implicit equation

$$\text{arg}\Gamma \left[\frac{1 + s - E/(\hbar\omega)}{2} \right] = -|s|\ln(R_t/a_{ho}) + \text{arg } \Gamma(1 + s) \text{mod } \pi \tag{5.174}$$

obtained in [31], whose solutions form a discrete series, which is unbounded from below, and can be labeled by a quantum number $q \in \mathbb{Z}$.

In free space ($\omega = 0$,) there is a geometric series of bound states

$$E_q = -\frac{2\hbar^2}{mR_t^2}\exp \left(-q\frac{2\pi}{|s|} + \frac{2}{|s|}\text{arg}\Gamma(1 + s) \right), \quad q \in \mathbb{Z} \tag{5.175}$$

$$F(R) = K_s \left(R\sqrt{2m|E|/\hbar^2} \right) \tag{5.176}$$

where K is a Bessel function. For three particles this corresponds to the well-known series of Efimov three-body bound states [4, 5]. This also applies to the four-body bound states in the aforementioned case of $(3 + 1)$ fermions with $m_\uparrow/m_\downarrow$ between $\simeq 13.384$ and $13.607\ldots$ [7]. As expected, in the limit $E \to -\infty$, the spectrum of the efimovian states in the trap (5.174) approaches the free space spectrum (5.175). The unboundedness of the spectrum in the zero-range limit is a natural consequence of the Thomas effect and of the limit cycle behavior [55].

5.3.5 Vanishing Bulk Viscosity

In this section, we give a simple rederivation of the fact that the bulk viscosity of the unitary gas in the normal phase is zero. This result was obtained in [98] (see also [99]). It helps analysing e.g. the ongoing experimental studies of the shear viscosity, whose value is of fundamental importance ([100] and refs. therein). Although the superfluid regime was also treated in [98], we omit it here for simplicity. In our rederivation we shall use the scaling solution and the existence of the undamped breathing mode.[20]

In the hydrodynamic theory for a normal compressible viscous fluid [101, 98], the (coarse-grained) evolution of the gas in a trapping potential $U(\mathbf{r}, t)$ is described by the atom number density $\rho(\mathbf{r}, t)$, the velocity vector field $\mathbf{v}(\mathbf{r}, t)$, and the entropy per particle (in units of k_B) $s(\mathbf{r}, t)$. These 5 scalar functions solve five equations which are given for completeness in Appendix 4 although we will not directly use them here. We will only need the equation for the increase of the total entropy $S = \int \rho s\, d^3r$ of the gas

$$\frac{dS}{dt} = \int \frac{\kappa \|\nabla T\|^2}{T^2} d^3r + \int \frac{\eta}{2T} \sum_{ik} \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3}\delta_{ik}\nabla \cdot \mathbf{v} \right)^2 d^3r + \int \frac{\zeta}{T} \|\nabla \cdot \mathbf{v}\|^2 d^3r \tag{5.177}$$

which follows from the hydrodynamic equations (5.217, 5.215); note that the thermal conductivity κ, the shear viscosity η and the bulk viscosity ζ have to be ≥ 0 so that $dS/dt \geq 0$ [101]. The hydrodynamic theory is expected to become exact in the limit where the length (resp. time) scales on which the above functions vary are much larger than microscopic length (resp. time) scales such as $1/k_F$ (resp. $\hbar/E_F$).

We consider the following gedankenexperiment: starting with the gas at thermal equilibrium in a trap of frequency ω, we suddenly switch the trapping frequency at

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[20] In article [98], the vanishing of the bulk viscosity was deduced from the so-called general coordinate and conformal invariance, the scaling solution being unknown to its author at the time of writing (although it had been obtained in [58]). The scaling solution was recently rederived using this general coordinate and conformal invariance [99]. Several other results presented in Sects. 5.3.2–5.3.4 were also rederived using this field theoretical formalism ([99] and refs. therein).

$t = 0$ to a different value ω_+. As we have seen in Sect. 5.3.1 and at the beginning
of Sect. 5.3.2, this excites an *undamped* breathing mode: For $t > 0$, the size of the
gas oscillates *indefinitely*. This rigorously periodic evolution of the system implies
that the total entropy $S(t)$ is periodic, and since it cannot decrease, it has to be
constant. Thus each of the terms in the right-hand-side of (5.177), and in particular the
last term, has to vanish. Thus $\zeta(\mathbf{r}, t) \|\nabla \cdot \mathbf{v}(\mathbf{r}, t)\|^2 \equiv 0$. This implies that ζ is
identically zero, as we now check. From the scaling evolution (5.109) of each many-
body eigenstate, one can deduce (using the quantum-mechanical expression for the
particle flux) that

$$\mathbf{v}(\mathbf{r}, t) = \frac{\dot{\lambda}}{\lambda}\mathbf{r}, \tag{5.178}$$

so that $\nabla \cdot \mathbf{v} = 3\dot{\lambda}/\lambda$. For t approaching 0 from above, we have $\dot{\lambda}(t) \neq 0$, as is
intuitively clear and can be checked from Eqs. 5.110, 5.111; thus $\zeta(\mathbf{r}, t) = 0$ and by
continuity $\zeta(\mathbf{r}, t = 0) = 0$. Since the central density and temperature in the initial
equilibrium state of the gas are arbitrary, we conclude that $\zeta(\rho, T) = 0$ for all ρ and
T. An alternative derivation of this result is presented in Appendix 5.

5.3.6 Short-Range Scaling Laws

As opposed to the previous sections, we now consider an arbitrary scattering length
and an arbitrary external potential, possibly with periodic boundary conditions. Of
all the particles $1, \ldots, N$, let us consider a subset $J \subset \{1, \ldots, N\}$ containing $n_\uparrow$
particles of spin $\uparrow$ and $n_\downarrow$ particles of spin $\downarrow$. From the particle positions $(\mathbf{r}_i)_{i \in J}$, we
can define a hyperradius R_J and hyperangles Ω_J, and a center of mass position $\mathbf{C}_J$.
The positions of all particles that do not belong to J are denoted by $\mathscr{R}_J = (\mathbf{r}_i)_{i \notin J}$.
In the absence of a $(n_\uparrow + n_\downarrow)$-body resonance (see Appendix 6), one expects that,
for any eigenstate, in the limit $R_J \to 0$ where all particles belonging to the subset
J approach each other while $(\Omega_J, \mathbf{C}_J, \mathscr{R}_J)$ remain fixed, there exists a function A_J
such that

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = R_J^\nu \phi(\mathbf{\Omega}_J) A_J(\mathbf{C}_j, \mathscr{R}_J) + o(R_J^\nu). \tag{5.179}$$

Here, $\nu = s_{\min}(n_\uparrow, n_\downarrow) - \frac{3(n_\uparrow + n_\downarrow) - 5}{2}$ with $s_{\min}(n_\uparrow, n_\downarrow)$ the smallest possible value of
s for the problem of $n_\uparrow$ particles of spin $\uparrow$ and $n_\downarrow$ particles of spin $\downarrow$ (s being defined
in Sect. 5.3.3) and $\phi(\Omega_J)$ is the corresponding hyperangular wavefunction (also
defined in Sect. 5.3.3). This statement is essentially contained in [17, 91]. It comes
from the intuition that, in the limit where the $n_\uparrow + n_\downarrow$ particles approach each other, the
N-body wavefunction should be proportional to the $(n_\uparrow + n_\downarrow)$-body zero-energy free
space wavefunction Eq. 5.159. This was used in [17] to predict that the formation rate
of deeply bound molecules by three-body recombination, $\Gamma \equiv -\dot{N}/N$, behaves as
$\hbar\Gamma/E_F \sim K \cdot (k_F b)^{2s_{\min}(2,1)}$ in the low-density limit, with b on the order of the van
der Waals range and K a numerical prefactor which depends on short-range physics.

The analytical solution of the hyperangular three-body problem [Eq. 5.166] yields $s_{\min}(2, 1) = 1.772724\ldots$ (this value is reached in the angular momentum $l = 1$ channel). Experimentally, this scaling has not been checked, but the smallness of $\hbar\Gamma/E_F$ is one of the crucial in-gredients which allow to realise the unitary gas.

Appendix 1: Effective Range in a Lattice Model

To calculate the effective range r_e [defined by Eq. 5.5] for the lattice model of Sect. 5.2.1, it is convenient to perform in the expression (5.46) of the scattering amplitude an analytic continuation to purely imaginary incoming wavevectors k_0, setting $k_0 = iq_0$ with q_0 real and positive. Eliminating $1/g_0$ thanks to Eq. 5.47 we obtain the useful expression:

$$-\frac{1}{f_{k_0}} = \frac{1}{a} + 4\pi \int_{\mathscr{D}} \frac{d^3k}{(2\pi)^3} \left[\frac{1}{q_0^2 + 2m\varepsilon_{\mathbf{k}}/\hbar^2} - \frac{1}{2m\varepsilon_{\mathbf{k}}/\hbar^2} \right]. \tag{5.180}$$

We first treat the case of the parabolic dispersion relation Eq. 5.48. A direct expansion of Eq. 5.180 in powers of q_0 leads to an infrared divergence. The trick is to use the fact that the integral over $\mathscr{D}$ in Eq. 5.180 can be written as the integral of the same integrand over the whole space minus the integral over the supplementary space $\mathbb{R}^3 \setminus \mathscr{D}$. The integral over the whole space may be performed exactly using

$$\int_{\mathbb{R}^3} \frac{d^3k}{(2\pi)^3} \left[\frac{1}{q_0^2 + k^2} - \frac{1}{k^2} \right] = -\frac{q_0}{4\pi}. \tag{5.181}$$

This leads to the transparent expression, where the term corresponding to ik in Eq. 5.3, and which is non-analytic in the energy E, is now singled out:

$$-\frac{1}{f_{k_0}^{\text{parab}}} = \frac{1}{a} - q_0 - 4\pi \int_{\mathbb{R}^3 \setminus \mathscr{D}} \frac{d^3k}{(2\pi)^3} \left[\frac{1}{q_0^2 + k^2} - \frac{1}{k^2} \right]. \tag{5.182}$$

This is now expandable in powers of q_0^2, leading to the effective range for the parabolic dispersion relation:

$$r_e^{\text{parab}} = \frac{1}{\pi^2} \int_{\mathbb{R}^3 \setminus \mathscr{D}} \frac{d^3k}{k^4}. \tag{5.183}$$

We now turn back to the general case. The trick is to consider the difference between the inverse scattering amplitudes of the general case and the parabolic case with a common value of the scattering length:

$$\frac{1}{f_{k_0}^{\text{parab}}} - \frac{1}{f_{k_0}} = 4\pi \int_{\mathscr{D}} \frac{d^3k}{(2\pi)^3} \left[\frac{1}{q_0^2 + 2m\varepsilon_{\mathbf{k}}/\hbar^2} - \frac{1}{q_0^2 + k^2} - \frac{1}{2m\varepsilon_{\mathbf{k}}/\hbar^2} + \frac{1}{k^2} \right]. \tag{5.184}$$

This is directly expandable to second order in q_0, leading to:

$$r_e - r_e^{\text{parab}} = 8\pi \int_{\mathscr{D}} \frac{d^3k}{(2\pi)^3} \left[\frac{1}{k^4} - \left(\frac{\hbar^2}{2m\varepsilon_{\mathbf{k}}} \right)^2 \right]. \tag{5.185}$$

The numerical evaluation of this integral for the Hubbard dispersion relation Eq. 5.59 leads to the Hubbard model effective range Eq. 5.60.

Finally, we specialize the general formula to the parabolic plus quartic form Eq. 5.61. Setting $\mathbf{k} = (\pi/b)\mathbf{q}$ and using Eq. 5.183, we obtain

$$\frac{\pi^3 r_e^{\text{mix}}}{b} = \int_{\mathbb{R}^3 \setminus [-1,1]^3} \frac{d^3q}{q^4} + \int_{[-1,1]^3} \frac{d^3q}{q^4} \left[1 - \frac{1}{(1 - Cq^2)^2} \right]. \tag{5.186}$$

The trick is to split the cube $[-1, 1]^3$ as the union of $B(0, 1)$, the sphere of center 0 and unit radius, and of the set $X = [-1, 1]^3 \setminus B(0, 1)$. One has also $\left(\mathbb{R}^3 \setminus [-1, 1]^3 \right) \cup X = \mathbb{R}^3 \setminus B(0, 1)$ so that

$$\frac{\pi^3 r_e^{\text{mix}}}{b} = \int_{\mathbb{R}^3 \setminus B(0,1)} \frac{d^3q}{q^4} + \int_{B(0,1)} \frac{d^3q}{q^4} \left[1 - \frac{1}{(1 - Cq^2)^2} \right] - \int_X \frac{d^3q}{q^4} \frac{1}{(1 - Cq^2)^2}. \tag{5.187}$$

One then moves to spherical coordinates of axis z. The first two terms in the right hand side may be calculated exactly. In particular, one introduces a primitive of $q^{-2}(1 - Cq^2)^{-2}$, given by $C^{1/2}\Phi(C^{1/2}q)$ with

$$\Phi(x) = \frac{x}{2(1 - x^2)} + \frac{3}{2}\text{arctanh}\, x - \frac{1}{x}. \tag{5.188}$$

In the last term of Eq. 5.187 one integrates over the modulus q of $\mathbf{q}$ for a fixed direction (θ, ϕ) where θ is the polar angle and ϕ the azimuthal angle. One then finds that q ranges from 1 to some maximal value $Q(\theta, \phi)$, and the integral over q provides the difference $\Phi(C^{1/2}Q) - \Phi(C^{1/2})$. Remarkably, the term $-\Phi(C^{1/2})$ cancels the contribution of the first two integrals in the right hand side of Eq. 5.187, so that

$$\frac{r_e^{\text{mix}}}{b} = -\frac{C^{1/2}}{\pi^3} \int_0^{2\pi} d\phi \int_{-1}^{1} du\, \Phi[C^{1/2}Q(\theta, \phi)] \tag{5.189}$$

where as usual we have set $u = \cos\theta$. Using the symmetry under parity along each Cartesian axis, which adds a factor 8, and restricting to the face $q_x = 1$ of the cube, which adds a factor 3, the expression of $Q(\theta, \phi)$ is readily obtained, leading to

$$\frac{r_e^{\text{mix}}}{b} = -\frac{24C^{1/2}}{\pi^3} \int_0^{\pi/4} d\phi \int_0^{\frac{\cos\phi}{\sqrt{1 + \cos^2\phi}}} du\, \Phi \left(\frac{C^{1/2}}{\cos\phi\sqrt{1 - u^2}} \right). \tag{5.190}$$

In the limit $C \to 0$, $r_e^{\text{mix}} \to r_e^{\text{parab}}$, and Eq. 5.190 may be calculated analytically with $\Phi(x) \sim -1/x$ and with an exchange of the order of integration: This leads to Eq. 5.58. For a general value of $C \in [0, 1/3]$ we have calculated Eq. 5.190 numerically, and we have identified the magic value of C leading to a zero effective range, see Eq. 5.62. With the same technique, we can calculate the value of K appearing in Eq. 5.49 from the expression

$$K = \frac{12}{\pi C^{1/2}} \int_0^{\pi/4} d\phi \int_0^{\frac{\cos\phi}{\sqrt{1+\cos^2\phi}}} du \ \text{arctanh} \ \frac{C^{1/2}}{\cos\phi\sqrt{1-u^2}}. \tag{5.191}$$

Appendix 2: What is the Domain of a Hamiltonian?

Let us consider a Hamiltonian H represented by a differential operator also called H. A naive and practical definition of the domain $D(H)$ of H is that it is the set of wavefunctions over which the action of the Hamiltonian is indeed represented by the considered differential operator. In other words, if a wavefunction ψ_{bad} does not belong to $D(H)$, one should not calculate the action of H on ψ_{bad} directly using the differential operator H. If H if self-adjoint, one should rather expand ψ_{bad} on the Hilbert basis of eigenstates of H and calculate the action of H in this basis.

For example, for a single particle in one dimension in a box with infinite walls in $x = 0$ and $x = 1$, so that $0 \le x \le 1$, one has the Hamiltonian

$$H = -\frac{1}{2}\frac{d^2}{dx^2}, \tag{5.192}$$

with the boundary conditions on the wavefunction

$$\psi(0) = \psi(1) = 0 \tag{5.193}$$

representing the effect of the box. To be in the domain, a wavefunction $\psi(x)$ should be twice differentiable for $0 < x < 1$ and should obey the boundary conditions (5.193). An example of a wavefunction which is not in the domain is the constant wavefunction $\psi(x) = 1$. An example of wavefunction in the domain is

$$\psi(x) = 30^{1/2}x(1-x). \tag{5.194}$$

If one is not careful, one may obtain wrong results. Let us calculate the mean energy and the second moment of the energy for ψ given by (5.194). By repeated action of H onto ψ, and calculation of elementary integrals, one obtains

$$\langle H \rangle_\psi = 5 \tag{5.195}$$

$$\langle H^2 \rangle_\psi = 0?! \tag{5.196}$$

Eq. 5.195 is correct, but Eq. 5.196 is wrong (it would lead to a negative variance of the energy) because $H\psi$ is not in $D(H)$ and the subsequent illicit action of H as the differential operator (5.192) gives zero.

How to calculate the right value of $\langle H^2 \rangle_\psi$? One introduces the orthonormal Hilbert basis of eigenstates of H,

$$\psi_n(x) = 2^{1/2}\sin[\pi(n+1)x], \quad n \in \mathbb{N}, \tag{5.197}$$

with the eigenenergy $\varepsilon_n = \frac{\pi^2}{2}(n+1)^2$. Then ψ of Eq. 5.194 may be expanded as $\sum_n c_n \psi_n(x)$, and the kth moment of the energy may be defined as

$$\langle H^k \rangle_\psi = \sum_{n \in \mathbb{N}} (\varepsilon_n)^k |c_n|^2. \tag{5.198}$$

Since $c_n = 4\sqrt{15}[1+(-1)^n]/[\pi(n+1)]^3$, one recovers $\langle H \rangle_\psi = 5$ and one obtains the correct value $\langle H^2 \rangle_\psi = 30$, that leads to a positive energy variance as it should be. Also $\langle H^k \rangle_\psi = +\infty$ for $k \geq 3$.

The trick of expanding ψ in the eigenbasis of H is thus quite powerful, it allows to define the action of H on any wavefunction ψ in the Hilbert space (not belonging to the domain). It may be applied of course only if H is self-adjoint, as it is the case in our simple example.

Appendix 3: Separability and Jacobi Coordinates for Arbitrary Masses

We here consider $N \geq 2$ harmonically trapped particles interacting in the unitary limit, with possibly different masses m_i but with the same isotropic angular oscillation frequency ω. The Hamiltonian reads

$$H = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m_i}\Delta_{\mathbf{r}_i} + \frac{1}{2}m_i\omega^2 r_i^2\right] \tag{5.199}$$

and the unitary interaction is described by the Wigner-Bethe-Peierls contact conditions on the N-body wavefunction: For all pairs of particles (i,j), in the limit $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \to 0$ with a *fixed* value of the centroid of the particles i and j, $\mathbf{R}_{ij} \equiv (m_i\mathbf{r}_i + m_j\mathbf{r}_j)/(m_i + m_j)$, that differs from the positions $\mathbf{r}_k$ of the other particles, $k \neq i, j$, there exists a function A_{ij} such that

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{A_{ij}(\mathbf{R}_{ij}; (\mathbf{r}_k)_{k\neq i,j})}{r_{ij}} + O(r_{ij}). \tag{5.200}$$

As is well known and as we will explain below, the internal Hamiltonian $H_{\text{internal}} = H - H_{\text{CM}}$, where $H_{\text{CM}} = -\frac{\hbar^2}{2M}\Delta_{\mathbf{C}} + \frac{1}{2}M\omega^2 C^2$, takes the form

$$H_{\text{internal}} = \sum_{i=1}^{N-1}\left[-\frac{\hbar^2}{2\bar{m}}\Delta_{\mathbf{u}_i} + \frac{1}{2}\bar{m}\omega^2 u_i^2\right] \tag{5.201}$$

in suitably defined Jacobi coordinates [see Eqs. 5.205, 5.214]. Here $\mathbf{C} = \sum_{i=1}^{N} m_i\mathbf{r}_i/M$ is the center of mass position, $M = \sum_{i=1}^{N} m_i$ is the total mass, and $\bar{m}$ is some arbitray mass reference, for example the mean mass M/N. Then it is straightforward to express Eq. 5.201 in hyperspherical coordinates, the vector $(\mathbf{u}_1, \ldots, \mathbf{u}_{N-1})$ with $3N - 3$ coordinates being expressed in terms of its modulus R and a set of $3N - 4$ hyperangles Ω, so that

$$H_{\text{internal}} = -\frac{\hbar^2}{2\bar{m}}\left[\partial_R^2 + \frac{3N-4}{R}\partial_R + \frac{1}{R^2}\Delta_\Omega\right] + \frac{1}{2}\bar{m}\omega^2 R^2 \tag{5.202}$$

where Δ_Ω is the Laplacian over the unit sphere of dimension $3N - 4$. As we shall see, the expression for the hyperradius is simply

$$R^2 \equiv \sum_{i=1}^{N-1} u_i^2 = \frac{1}{\bar{m}}\sum_{i=1}^{N} m_i(\mathbf{r}_i - \mathbf{C})^2. \tag{5.203}$$

This form of the Hamiltonian is then useful to show the separability of Schrödinger's equation for the unitary gas in hyperspherical coordinates [55, 89] for $N \geq 3$ and arbitrary masses. The separability Eq. 5.161 that was described for simplicity in the case of equal mass particles in Sect. 5.3.3 indeed still holds in the case of different masses, if the Wigner-Bethe-Peierls model defines a self-adjoint Hamiltonian.[21] We recall here the various arguments. First, for zero energy free space eigenstates, the form Eq. 5.159 is expected from scale invariance, if the Hamiltonian is self-adjoint [89]. Second, the form Eq. 5.161 for the general case, including non-zero energy and an isotropic harmonic trap, is expected because (i) the Hamiltonian (5.199), after separation of the center of mass, has the separable form (5.202) in hyperspherical coordinates, and (ii) Eq. 5.161 obeys the Wigner-Bethe-Peierls contact conditions if Eq. 5.159 does. This point (ii) results from the fact that the Wigner-Bethe-Peierls conditions are imposed, for each pair of particles *(i,j)*, for $r_{ij} \to 0$ with a *fixed* value of $\mathbf{R}_{ij}$ that differs from the positions $\mathbf{r}_k$ of the other particles, $k \neq i, j$. Using $\mathbf{r}_i = \mathbf{R}_{ij} + [m_j/(m_i + m_j)]\mathbf{r}_{ij}$ and $\mathbf{r}_j = \mathbf{R}_{ij} - [m_i/(m_i + m_j)]\mathbf{r}_{ij}$, with $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$, we indeed find that

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[21] Strictly speaking, it is sufficient that the Laplacian on the unit sphere together with the Wigner-Bethe-Peierls boundary conditions reexpressed in terms of hyperangles is self-adjoint, as extensively used in [7]. This is less restrictive than having the full Hamiltonian self-adjoint, since it allows for example to have a N-body Efimov effect while the $N - 1$ zero-range model is perfectly well-defined and does not experience any Efimov effect.

$$\bar{m}R^2 = \frac{m_i m_j}{m_i + m_j} r_{ij}^2 + (m_i + m_j)(\mathbf{R}_{ij} - \mathbf{C})^2 + \sum_{k \neq i, j} m_k (\mathbf{r}_k - \mathbf{C})^2. \quad (5.204)$$

For $N \geq 3$, we see that $\lim_{r_{ij} \to 0} R^2 > 0$, so that R varies only to second order in r_{ij} in that limit. Provided that the function $F(R)$ in Eq. 5.161 has no singularity at nonzero R, the Wigner-Bethe-Peierls contact conditions are preserved [similarly to the argument Eq. 5.115]. Third, bosonic or fermionic exchange symmetries imposed on the N-body wavefunction cannot break the separability in hyperspherical coordinates: Exchanging the positions of particles of same mass does not change the value of the hyperradius R, it only affects the hyperangles and thus the eigenvalues $[(3N - 5) /2]^2 - s^2$ of the Laplacian on the unit sphere.

To derive the form Eq. 5.201 of the internal Hamiltonian, we introduce the usual Jacobi coordinates given for example in [102]:

$$\mathbf{y}_i \equiv \mathbf{r}_i - \frac{\sum_{j=i+1}^{N} m_j \mathbf{r}_j}{\sum_{j=i+1}^{N} m_j} \quad \text{for } 1 \leq i \leq N - 1. \quad (5.205)$$

We note that $\mathbf{y}_i$ simply gives the relative coordinates of particle i with respect to the center of mass of the particles from $i + 1$ to N. To simplify notations, we also set $\mathbf{y}_N \equiv \mathbf{C}$. Here we derive Eq. 5.201 in a pedestrian way. Note that a more elegant derivation by recursion is given in page 63 of [55]. In compact form, the Jacobi change of variables corresponds to setting $\mathbf{y}_i = \sum_{j=1}^{N} M_{ij} \mathbf{r}_j$ for $1 \leq i \leq N$, where the non-symmetric matrix M is such that:

- In the case $1 \leq i < N$, one has: $M_{ij} = 0$ for $1 \leq j < i$, $M_{ij} = 1$ for $j = i$, and $M_{ij} = -m_j / \left(\sum_{k=i+1}^{N} m_k \right)$ for $i < j \leq N$.
- $M_{Nj} = m_j / \left(\sum_{k=1}^{N} m_k \right)$ for $1 \leq j \leq N$.

From the formula giving the derivative of a composite function, the kinetic energy operator writes

$$H_{\text{kin}} \equiv \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i} \Delta_{\mathbf{r}_i} = -\frac{\hbar^2}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} S_{jk} \text{grad}_{\mathbf{y}_j} \cdot \text{grad}_{\mathbf{y}_k}, \quad (5.206)$$

where the *symmetric* matrix S is defined as $S_{jk} = \sum_{i=1}^{N} M_{ji} M_{ki} / m_i$. The explicit calculation of the matrix elements S_{jk} is quite simple. Taking advantage of the fact that S is symmetric, one has to distinguish three cases, (i) $1 \leq j, k \leq N - 1$, with $j = k$ and $j < k$ as subcases, (ii) $j = k = N$, and (iii) $j < N, k = N$. One then finds that S is purely diagonal, with $S_{ii} = 1/\mu_i$ for $1 \leq i \leq N - 1$ and $S_{NN} = 1/M$. Here μ_i is the reduced mass for the particle i and for a fictitious particle of mass equal to the sum of the masses of the particles from $i + 1$ to N:

$$\frac{1}{\mu_i} = \frac{1}{m_i} + \frac{1}{\sum_{j=i+1}^{N} m_j} \quad \text{for } 1 \leq i \leq N - 1. \quad (5.207)$$

This results in the following form

$$H_{\text{kin}} = -\frac{\hbar^2}{2M}\Delta_{\mathbf{C}} - \sum_{i=1}^{N-1}\frac{\hbar^2}{2\mu_i}\Delta_{\mathbf{y}_i}. \tag{5.208}$$

The next step is to consider the trapping potential energy term. Inspired by Eq. 5.208 one may consider the guess

$$H_{\text{trap}} \equiv \sum_{i=1}^{N}\frac{1}{2}m_i\omega^2 r_i^2 \overset{?}{=} \frac{1}{2}M\omega^2 C^2 + \sum_{i=1}^{N-1}\frac{1}{2}\mu_i\omega^2 y_i^2. \tag{5.209}$$

Replacing each $\mathbf{y}_i$ by their expression in the guess gives

$$MC^2 + \sum_{i=1}^{N-1}\mu_i y_i^2 = \sum_{j=1}^{N}\sum_{k=1}^{N}Q_{jk}\mathbf{r}_j \cdot \mathbf{r}_k \tag{5.210}$$

where Q is uniquely defined once it is imposed to be a *symmetric* matrix. Setting $M_i = \sum_{j=i+1}^{N}m_j$ for $0 \leq i \leq N-1$, and $M_N = 0$, we find for the off-diagonal matrix elements

$$Q_{jk} = -\frac{\mu_{\min(j,k)}m_{\max(j,k)}}{M_{\min(j,k)}} + \frac{m_j m_k}{M} + m_j m_k \sum_{i=1}^{\min(j,k)-1}\frac{\mu_i}{M_i^2} \tag{5.211}$$

where $1 \leq j, k \leq N$, $\min(j,k)$ and $\max(j,k)$ respectively stand for the smallest and for the largest of the two indices j and k. The key relation is then that

$$\frac{\mu_i}{M_i^2} = \frac{1}{M_i} - \frac{1}{m_i + M_i} = \frac{1}{M_i} - \frac{1}{M_{i-1}} \tag{5.212}$$

since $M_i + m_i = M_{i-1}$ for $1 \leq i \leq N$. This allows to calculate the sum over i of μ_i/M_i^2, as all except the border terms compensate by pairs. E.g. for $j < k$:

$$\sum_{i=1}^{j-1}\frac{\mu_i}{M_i^2} = \frac{1}{M_{j-1}} - \frac{1}{M} \tag{5.213}$$

since $M_0 = M$. One then finds that the off-diagonal elements of the matrix Q vanish. The diagonal elements of Q may be calculated using the same tricks (5.212, 5.213), one finds $Q_{ii} = m_i$ for $1 \leq i \leq N$. As a consequence, the guess was correct and the question mark can be removed from Eq. 5.209.

The last step to obtain Eq. 5.201 is to appropriately rescale the usual Jacobi coordinates, setting

$$\mathbf{u}_i \equiv (\mu_i/\bar{m})^{1/2}\mathbf{y}_i \tag{5.214}$$

where $\bar{m}$ is an arbitrarily chosen mass. A useful identity is the expression for the square of the hyperradius, Eq. 5.203. Starting from the definition [first identity in Eq. 5.203] we see that $R^2 = \sum_{i=1}^{N-1}\frac{\mu_i}{\bar{m}}y_i^2$. Then the second identity in Eq. 5.203 results from the fact that the guess in Eq. 5.209 is correct.

Appendix 4: Hydrodynamic Equations

The hydrodynamic equations for a normal compressible viscous fluid are (see [98],[22] or Sect. 15 and Sect. 49 in [101]):

• the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{5.215}$$

• the equation of motion

$$m\rho \left(\frac{\partial v_i}{\partial t} + \mathbf{v} \cdot \nabla v_i \right) = -\frac{\partial p}{\partial x_i} - \rho \frac{\partial U}{\partial x_i} + \sum_k \frac{\partial}{\partial x_k} \left[\eta \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3} \delta_{ik} \nabla \cdot \mathbf{v} \right) \right]$$
$$+ \frac{\partial}{\partial x_i} \left(\zeta \, \nabla \cdot \mathbf{v} \right) \tag{5.216}$$

where m is the atomic mass, η is the shear viscosity, ζ is the bulk viscosity, and the pressure $p(\mathbf{r}, t)$ [as well as the temperature $T(\mathbf{r}, t)$ appearing in the next equation] is as always expressible in terms of $\rho(\mathbf{r}, t)$ and $s(\mathbf{r}, t)$ *via* the equation of state,[23]

• the entropy-production equation

$$\rho T \left(\frac{\partial s}{\partial t} + \mathbf{v} \cdot \nabla s \right) = \nabla \cdot (\kappa \nabla T) + \frac{\eta}{2} \sum_{i,k} \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3} \delta_{ik} \nabla \cdot \mathbf{v} \right)^2 + \zeta \| \nabla \cdot \mathbf{v} \|^2 \tag{5.217}$$

where κ is the thermal conductivity.

Appendix 5: Alternative Derivation of the Vanishing Bulk Viscosity

Consider the particular case of a unitary gas initially prepared at thermal equilibrium in an isotropic harmonic trap at a temperature T above the critical temperature. When the harmonic trap becomes time dependent, $U(\mathbf{r}, t) = \frac{1}{2} m\omega^2(t) r^2$, each many-body eigenstate of the statistical mixture evolves under the combination Eq. 5.109 of a time dependent gauge transform and a time dependent scaling transform of scaling factor $\lambda(t)$. The effect of the gauge transform is to shift the momentum operator $\mathbf{p}_i$ of each particle i by the spatially slowly varying operator $m\mathbf{r}_i \dot{\lambda}/\lambda$. In

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[22] There is a typo in Eq. 5.10 of [98]: $\nabla_i(\rho v^i \partial_i s)$ should be replaced by $\nabla_i(\rho v^i s)$.

[23] If we would neglect the position-dependence of η and ζ, (5.216) would reduce to the Navier-Stokes equation.

the hydrodynamic framework, this is fully included by the velocity field Eq. 5.178.[24]
Using the macroscopic consequences of a spatial scaling Eqs. 5.19–5.22, one *a priori*
obtains a time dependent solution of the hydrodynamic equations:

$$T(\mathbf{r}, t) = T(t = 0)/\lambda^2(t) \tag{5.218}$$

$$\rho(\mathbf{r}, t) = \rho(\mathbf{r}/\lambda, 0)/\lambda^3(t) \tag{5.219}$$

$$s(\mathbf{r}, t) = s(\mathbf{r}/\lambda, 0) \tag{5.220}$$

$$p(\mathbf{r}, t) = p(\mathbf{r}/\lambda, 0)/\lambda^5(t) \tag{5.221}$$

$$v_i(\mathbf{r}, t) = x_i \dot{\lambda}(t)/\lambda(t). \tag{5.222}$$

One then may *a posteriori* check that Eq. 5.215 is inconditionally satisfied, and that
Eq. 5.217 is satisfied if $\zeta \equiv 0$. Setting $\zeta \equiv 0$ in Eq. 5.216, and using the hydrostatic
condition $\nabla p = -\rho \nabla U$ at time $t = 0$, one finds that Eq. 5.216 holds provided that
$\lambda(t)$ solves Eq. 5.111 as it should be.

Appendix 6: *n*-Body Resonances

Usually in quantum mechanics one takes the boundary condition that the wavefunc-
tion is bounded when two particles approach each other; in contrast, the Wigner-
Bethe-Peierls boundary condition (5.75) expresses the existence of a two-body res-
onance. If the interaction potential is fine-tuned not only to be close to a two-body
resonance (i.e. to have $|a| \gg b$) but also to be close to a n-body resonance (mean-
ing that a real or virtual n-body bound state consisting of $n_\uparrow$ particles of spin $\uparrow$
and $n_\downarrow$ particles of spin $\downarrow$ is close to threshold), then one similarly expects that, in

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[24] To formalize this statement, we consider a small but still macroscopic element of the equilib-
rium gas of volume dV around point $\bar{\mathbf{r}}$, with $k_F^{-1} \ll dV^{1/3} \ll R$ where k_F is the Fermi momen-
tum and R the Thomas-Fermi radius of the gas. We can define the density operator $\hat{\rho}_{\text{elem}}$ of this
element by taking the trace of the full N-body density operator over the spatial modes outside
the element. Since the gauge transform in Eq. 5.109 is local in position space, $\hat{\rho}_{\text{elem}}$ experiences
the same unitary gauge transform. It would be tempting to conclude from the general formula
$dS = -k_B \text{Tr}[\hat{\rho}_{\text{elem}} \ln \hat{\rho}_{\text{elem}}]$ that the entropy dS of the element is not changed by the gauge trans-
form. This is a valid conclusion however only if the gauge transform does not bring $\hat{\rho}_{\text{elem}}$ too far
from local thermal equilibrium. To check this, we split the gauge transform for a single particle
of position $\mathbf{r}$ as $mr^2\dot{\lambda}/(2\hbar\lambda) = m\dot{\lambda}/(2\hbar\lambda)[\bar{r}^2 + 2\bar{\mathbf{r}} \cdot (\mathbf{r} - \bar{\mathbf{r}}) + (\mathbf{r} - \bar{\mathbf{r}})^2]$. The first term is an
innocuous uniform phase shift. The second term performs a uniform shift in momentum space by
the announced value $m\mathbf{v}(\bar{\mathbf{r}}, t)$. Due to Galilean invariance, this has no effect on the thermodynamic
quantities of the small element, such as its temperature, its pressure, its density, its entropy. With the
estimate $\dot{\lambda}/\lambda \sim \omega, \bar{r} \sim R, m\omega R \sim \hbar k_F$, this second term is of order $k_F dV^{1/3} \gg 1$, not negligible.
The third term is of order $m\omega dV^{2/3}/\hbar \sim N^{-1/3} k_F^2 dV^{2/3}$, negligible in the thermodynamic limit.

the zero-range limit, the interaction potential can be replaced by the Wigner-Bethe-Peierls boundary condition, *together with an additional boundary condition in the limit where any subset of $n_\uparrow$ particles of spin $\uparrow$ and $n_\downarrow$ particles of spin $\downarrow$ particles approach each other*. Using the notations of Sect. 5.3.6, this additional boundary condition reads [55, 70, 89, 103]:

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \left(R_J^{-s} - \frac{\varepsilon}{l^{2s}} R_J^s\right) R_J^{-\frac{3n-5}{2}} \phi(\Omega_J) A_J(\mathbf{C}_j, \mathscr{R}_J) + o(R_J^v) \quad (5.223)$$

where $s = s_{\min}(n_\uparrow, n_\downarrow)$, while $l > 0$ and $\varepsilon = \pm 1$ are parameters of the model playing a role analogous to the absolute value and the sign of the two-body scattering length. This approach is only possible if the wavefunction remains square integrable, i.e. if $0 \le s < 1$, which we assume in what follows. This condition is satisfied e.g. for $n_\uparrow = 2, n_\downarrow = 1$ for a mass ratio $m_\uparrow/m_\downarrow \in [8.62\ldots; 13.6\ldots]$ [5]. Moreover we are assuming for simplicity that $s \ne 0$.

Let us now consider the particular case where the two-body scattering length is infinite, and the external potential is either harmonic isotropic, or absent. Then the separability in internal hyperspherical coordinates of Sect. 5.3.3 still holds for $n = N$. Indeed, Eq. 5.223 then translates into the boundary condition on the hyperradial wavefunction

$$\exists A \in \mathbb{R}/\ F(R) \underset{R\to 0}{=} A \cdot \left(R^{-s} - \frac{\varepsilon}{l^{2s}} R^s\right) + O\left(R^{s+2}\right) \quad (5.224)$$

and does not affect the hyperangular problem. Consequently [55],

- For the n-body bound state, which exists if $\varepsilon = +1$:

$$E = -\frac{2\hbar^2}{m\,l^2} \left[\frac{\Gamma(1+s)}{\Gamma(1-s)}\right]^{\frac{1}{s}}, \quad (5.225)$$

$$F(R) = K_s \left(R\sqrt{-2E\frac{m}{\hbar^2}}\right). \quad (5.226)$$

- For the eigenstates in a trap:

$$E\text{ solves: } -\varepsilon \cdot \left(\frac{\hbar}{m\omega l^2}\right)^s = \frac{\Gamma\left(\frac{1+s-E/(\hbar\omega)}{2}\right)\Gamma(-s)}{\Gamma\left(\frac{1-s-E/(\hbar\omega)}{2}\right)\Gamma(s)}, \quad (5.227)$$

$$F(R) = \frac{1}{R} W_{\frac{E}{2\hbar\omega}, \frac{s}{2}}\left(R^2\frac{m\omega}{\hbar}\right). \quad (5.228)$$

In particular, for $l = \infty$, we are exactly at the n-body resonance, since the energy of the n-body bound state vanishes. The spectrum in a trap then is $E = (-s+1+2q)\hbar\omega$ with $q \in \mathbb{N}$.

Note that, most often, $s \ge 1$, in which case one would have to use an approach similar to the one developed by Pricoupenko for the case of two-body resonances in non-zero angular momentum channels, and to introduce a modified scalar product [22, 104].

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