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Number of closed-channel molecules in the BEC-BCS crossover

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Abstract. Using a two-channel model, we show that the number of closed-channel molecules in a two-component Fermi gas close to a Feshbach resonance is directly related to the derivative of the energy of the gas with respect to the inverse scattering length. We extract this quantity from the fixed-node Monte Carlo equation of state and we compare to the number of closed-channel molecules measured in the Rice experiment with lithium [Partridge et al., Phys. Rev. Lett. 95, 020404 (2005)]. We also discuss the effect of a difference between the trapping potentials seen by a closed-channel molecule and by an open-channel pair of atoms in terms of an effective position-dependent scattering length.

PACS. 03.75.Ss Degenerate Fermi gases - 67.90.+z Other topics in quantum fluids and solids

1 Introduction

It is now experimentally possible to prepare two-component atomic Fermi gases at low temperature with a fully controllable interaction strength, in a regime where the interaction range is negligible and the atomic interactions are characterized by a single parameter, the s -wave scattering length a between two opposite “spin” atoms. The value of a can be adjusted at will thanks to a magnetically induced Feshbach resonance. The weakly interacting limits $k_F a \rightarrow 0^+$ and $k_F a \rightarrow 0^-$, where k_F is the Fermi wavevector of the gas, correspond respectively to the BEC limit (a Bose-Einstein condensate of dimers, observed in [1, 2, 3, 4, 5]) and the BCS limit (a “condensate” of Cooper pairs approximately described by the BCS theory). Furthermore, the experiments can access the so-called crossover regime between BEC and BCS, where the gas is strongly interacting ($k_F |a| \gtrsim 1$), which includes the celebrated unitary limit $k_F |a| = \infty$, where the gas acquires fully universal properties [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17].

In this context, early theoretical studies [18, 19, 20] put forward a many-body Hamiltonian which accurately models the microscopic two-body physics of the Feshbach resonance. The interaction potential is described by two channels, an open channel and a closed channel. The atoms exist in the form of fermionic particles in the open channel and in the form of bosonic short range molecules in the closed channel. Two atoms may be converted into a short range closed-channel molecule and *vice versa* due to the

interchannel coupling. The corresponding Hamiltonian is

$$\begin{aligned}
 H_2 = \int d^3r \left\{ \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \Delta + U(\mathbf{r}) \right] \psi_\sigma(\mathbf{r}) \right. \\
 \left. + \psi_b^\dagger(\mathbf{r}) \left[E_b(B) - \frac{\hbar^2}{4m} \Delta + U_b(\mathbf{r}) \right] \psi_b(\mathbf{r}) \right\} \\
 + \Lambda \int d^3r_1 d^3r_2 \chi(\mathbf{r}_1 - \mathbf{r}_2) \left\{ \psi_b^\dagger[(\mathbf{r}_1 + \mathbf{r}_2)/2] \psi_\downarrow(\mathbf{r}_1) \psi_\uparrow(\mathbf{r}_2) + \text{h.c.} \right\} \\
 + g_0 \int d^3r_1 d^3r_2 d^3r_3 d^3r_4 \chi(\mathbf{r}_1 - \mathbf{r}_2) \chi(\mathbf{r}_3 - \mathbf{r}_4) \\
 \delta \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} - \frac{\mathbf{r}_3 + \mathbf{r}_4}{2} \right) \psi_\uparrow^\dagger(\mathbf{r}_1) \psi_\downarrow^\dagger(\mathbf{r}_2) \psi_\downarrow(\mathbf{r}_3) \psi_\uparrow(\mathbf{r}_4) \quad (1)
 \end{aligned}$$

where the atomic fields $\psi_\sigma(\mathbf{r})$ obey the usual fermionic anticommutation relations and the field $\psi_b(\mathbf{r})$ describing the closed-channel molecules obeys the usual bosonic commutation relations. Λ gives the coupling between the closed and open channels, with a short range cut-off function $\chi(\mathbf{r})$, of range b , and such that $\int d^3r \chi(\mathbf{r}) = 1$. A typical value for b is in the nanometer range¹. The coupling constant g_0 represents the background atomic interaction in the open channel, which is conveniently modeled by a separable potential with the same cut-off function χ . The energy E_b is the energy of a closed-channel molecule, in the absence of the coupling Λ , counted with respect to the dissociation limit of the open channel. This energy is adjusted with a magnetic field B , using the fact that the different magnetic moments in the open and closed channels lead to a differential Zeeman shift. The resulting

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¹ b can be estimated by the van der Waals length, that is the length that one forms with \hbar , m and the C_6 coefficient of the van der Waals interaction [21].

effective magnetic moment is

$$\mu_b \equiv \frac{dE_b}{dB}. \quad (2)$$

$U(\mathbf{r})$ and $U_b(\mathbf{r})$ are the trapping potentials experienced by the atoms and the closed-channel molecules respectively.

On the contrary, recent Monte Carlo simulations of the many-body problem in the BEC-BCS crossover simply use single channel model Hamiltonians [22, 23, 24, 25, 26, 27, 28]. In most unbiased Quantum Monte Carlo simulations, a lattice model is used:

$$H_1 = \sum_{\mathbf{r}} b^3 \left\{ \sum_{\sigma=\uparrow,\downarrow} \psi_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \Delta + U(\mathbf{r}) \right] \psi_{\sigma}(\mathbf{r}) + g_0 \psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}) \right\}. \quad (3)$$

Here b is the lattice spacing (which coincides with the “range” of the discrete delta interaction potential), Δ is a discrete representation of the Laplacian, and g_0 is a coupling constant adjusted to have the desired scattering length: As was shown e.g. in [24, 25, 29, 30],

$$\frac{1}{g} - \frac{1}{g_0} = \int_{[-\pi/b, \pi/b]^3} \frac{d^3k}{(2\pi)^3} \frac{1}{2\epsilon_{\mathbf{k}}} \quad (4)$$

where $g = 4\pi\hbar^2 a/m$ is the effective coupling constant and $\epsilon_{\mathbf{k}}$ the energy of a single particle with wavevector \mathbf{k} on the lattice. In fixed-node Monte Carlo calculations, one rather uses an interaction potential in continuous real space, e.g. a square well potential [31, 32, 33, 34, 35, 36].

There is now a consensus about the fact that, in the zero-range limit, there is a convergence of predictions for the two models H_1 and H_2 , in particular for the equation of state of the gas. The zero-range limit means, for single channel models, that $k_F b \ll 1$, $b \ll \lambda$, and $b \ll |a|$, where k_F is the Fermi wavevector and λ is the thermal de Broglie wavelength.² For two-channel models, one has to impose the same conditions, not only for the interaction range b but also for the effective range r_e (one indeed has $|r_e| \gg b$ on narrow Feshbach resonances [37, 38]); we shall see in appendix A that one also needs to impose a condition on the background scattering length, and that all conditions are satisfied in the experiment [5].³

One can however consider observables which exist in reality and are included in the two-channel model, but which are absent in a single channel model. The most natural example is the number of closed-channel molecules,

² The assumption $b \ll |a|$ is not necessary on the BCS side if one restricts to macroscopic observables such as the total energy, but it is necessary for microscopic observables such as the ones considered in section 3.

³ A simple formal definition of the zero-range limit for the homogeneous gas is to take the limit of vanishing density $k_F \rightarrow 0$ while tuning the magnetic field B in such a way that $1/(k_F a)$ remains constant, and keeping constant all parameters of the Hamiltonian other than B ; one then also has to take the limit $T \rightarrow 0$ so that T/T_F remains constant.

which was recently measured at Rice using laser molecular excitation techniques [5].

In this paper, we show that the equilibrium number of closed-channel molecules N_b is directly related to the equation of state of the gas, more precisely to the derivative of the gas energy (or free energy at non-zero temperature) with respect to $1/a$. Paradoxically, we can thus use the equation of state calculated in [32] within a single channel model, in order to predict N_b in the crossover and compare to Rice measurements, see section 2. Since the derivative of the energy with respect to $1/a$ is related to other observables involving atomic properties only [39, 40], it is also possible in principle to access N_b by a pure atomic measurement, see section 3. We conclude in section 4.

2 Prediction for the number of closed-channel molecules

2.1 General result

We first suppose that the system is in an arbitrary eigenstate $|\psi\rangle$ of the two-channel Hamiltonian H_2 , with eigenenergy E . From Hellmann-Feynman theorem we have

$$\frac{dE}{dB} = \langle \psi | \frac{dH_2}{dB} | \psi \rangle. \quad (5)$$

The only magnetic field dependent part of the Hamiltonian H_2 is the bare closed-channel molecule energy $E_b(B)$ so that

$$\frac{dE}{dB} = \mu_b N_b \quad (6)$$

where

$$N_b = \int d^3r \langle \psi_b^{\dagger}(\mathbf{r}) \psi_b(\mathbf{r}) \rangle \quad (7)$$

is the mean number of closed-channel molecules.

We then eliminate the magnetic field by using as a parameter the scattering length a experienced by the trapped atoms rather than B . In the general case where the trapping potential $U_b(\mathbf{r})$ for the closed-channel molecule differs from the twice the trapping potential $U(\mathbf{r})$ experienced by an open-channel atom, the scattering length of two atoms around point \mathbf{r} depends on \mathbf{r} , see appendix B. To lift the ambiguity we thus take for a the scattering length in the trap center taken as the origin of coordinates, $\mathbf{r} = \mathbf{0}$. We then rewrite (6) as

$$N_b = \frac{dE}{d(1/a)} \frac{d(1/a)}{dB} \frac{1}{\mu_b}. \quad (8)$$

Assuming that μ_b is magnetic field independent, a as a function of B can be calculated explicitly for H_2 by solving the zero-energy two-body scattering problem in free space (see appendix A), and by including the energy shifts due to the trapping potentials $U_b(\mathbf{0})$ and $U(\mathbf{0})$, as explained in the appendix B. The function takes the form

$$a = a_{\text{fs}}(B - \delta B_0) \quad (9)$$

where we have introduced the function giving the free space scattering length as a function of B ,

$$a_{\text{fs}}(B) = a_{\text{bg}} \left(1 - \frac{\Delta B}{B - B_0} \right). \quad (10)$$

Here a_{bg} is the background scattering length, B_0 is the location of the Feshbach resonance in the absence of trapping potential, $\delta B_0 = [2U(\mathbf{0}) - U_b(\mathbf{0})]/\mu_b$ the shift of the resonance location due to the trapping potential, and ΔB the resonance width.

Equation (8) is directly applicable at zero temperature. At non-zero temperature, one has to take a thermal average of (8), keeping in mind that the mean value of a derivative is not necessarily equal to the derivative of the mean value. In the canonical ensemble one can check the exact relation [41]

$$\left\langle \frac{dE}{d(1/a)} \right\rangle = \left(\frac{dF}{d(1/a)} \right)_T = \left(\frac{d\langle E \rangle}{d(1/a)} \right)_S \quad (11)$$

where $\langle \dots \rangle$ is the thermal average, the derivative of the free energy F is taken for a fixed temperature T , and the derivative of $\langle E \rangle$ is taken for a fixed entropy S . We thus have in the canonical ensemble

$$\langle N_b \rangle = \left(\frac{d\langle E \rangle}{d(1/a)} \right)_S \frac{d(1/a)}{dB} \frac{1}{\mu_b}. \quad (12)$$

2.2 Analytical results in a trap in limiting cases

We now restrict to a spin balanced gas where the number of particles is equal to $N/2$ in each spin component. We also assume that the gas is at zero temperature (or at temperatures much smaller than the Fermi temperature T_F), in a harmonic trap

$$U(\mathbf{r}) = U(\mathbf{0}) + \frac{1}{2}m \sum_{\alpha=x,y,z} \omega_\alpha^2 r_\alpha^2, \quad (13)$$

in the macroscopic regime where $k_B T_F$ is much larger than the oscillation quanta $\hbar\omega_\alpha$. The usual definition of the Fermi temperature T_F and of the Fermi wavevector k_F is then

$$k_B T_F = \frac{\hbar^2 k_F^2}{2m} = (3N)^{1/3} \hbar \bar{\omega} \quad (14)$$

where $\bar{\omega}$ is the geometric mean of the three oscillation frequencies ω_α . In this macroscopic regime, we rely on the local density approximation to calculate $dE/d(1/a)$ for the trapped gas: This is expected to be exact in the large N limit, and to already hold for the Rice experiment [5] since $k_B T_F / (\hbar\omega_\alpha) \gtrsim 9$.

The key ingredient of the local density approximation is the equation of state of the interacting homogeneous gas. At zero temperature, and in the zero-range limit detailed in the introduction, the equation of state is expected to be a universal function of the gas density and of the scattering length, independent of the microscopic details of the interaction. Furthermore, the spatial dependence of

the scattering length in presence of the trapping potential, due to $U_b(\mathbf{r}) \neq 2U(\mathbf{r})$, is expected to be negligible in the zero-range limit, as argued in the appendix B. Under these assumptions, the local-density approximation for the trapped gas leads to the universal form

$$-\frac{dE}{d(1/a)} = \frac{\hbar^2 k_F}{m} N \mathcal{F} \left(\frac{1}{k_F a} \right), \quad (15)$$

where \mathcal{F} is a dimensionless function, expressed in the appendix C in terms of the dimensionless universal function f giving the energy per particle ϵ^{hom} of the homogeneous interacting gas:

$$\epsilon^{\text{hom}} = \epsilon_0^{\text{hom}} f \left(\frac{1}{k_F^{\text{hom}} a} \right). \quad (16)$$

Here ϵ_0^{hom} and k_F^{hom} are the energy per particle and the Fermi wavevector of the ideal Fermi gas with the same total density n as the interacting gas:

$$k_F^{\text{hom}} = (3\pi^2 n)^{1/3} \quad (17)$$

$$\epsilon_0^{\text{hom}} = \frac{3}{10} \frac{\hbar^2 (k_F^{\text{hom}})^2}{m}. \quad (18)$$

In the BEC regime $0 < k_F a \ll 1$ we have [42, 43, 44]

$$f \left(\frac{1}{k_F^{\text{hom}} a} \right) = -\frac{5}{3(k_F^{\text{hom}} a)^2} + \frac{5}{18\pi} k_F^{\text{hom}} a_d \left[1 + \frac{128}{15\sqrt{6}\pi^3} (k_F^{\text{hom}} a_d)^{3/2} \right] + \dots \quad (19)$$

where the first term comes from the dimer binding energy $\hbar^2/(ma^2)$, the second term is the mean field interaction energy among the dimers, proportional to the dimer-dimer scattering length a_d , and the last term is the (bosonic) Lee-Huang-Yang correction. The solution of the 4-fermion problem gives [45, 46]

$$a_d \simeq 0.60a. \quad (20)$$

The local-density approximation then leads to

$$\mathcal{F} \left(\frac{1}{k_F a} \right) = \frac{1}{k_F a} + \frac{5^{2/5}}{2^{12/5} \cdot 7} \left(\frac{a_d}{a} \right)^{2/5} (k_F a)^{7/5} + \dots \quad (21)$$

where we have omitted the Lee-Huang-Yang correction.

In the BCS limit $0 < -k_F a \ll 1$, we have [43, 44, 47, 48]

$$f \left(\frac{1}{k_F^{\text{hom}} a} \right) = 1 + \frac{10}{9\pi} k_F^{\text{hom}} a + \frac{4(11 - 2 \ln 2)}{21\pi^2} (k_F^{\text{hom}} a)^2 + \dots \quad (22)$$

where the first term is the ideal gas result, the second term is the Hartree-Fock mean field term, and the last

term is the (fermionic) Lee-Huang-Yang correction. This leads to ⁴

$$\mathcal{F}\left(\frac{1}{k_F a}\right) = \frac{512}{945\pi^2} (k_F a)^2 \left[1 + \left(\frac{256}{35\pi^2} - \frac{63 + 189 \ln 2}{1024} \right) k_F a + \dots \right]. \quad (23)$$

Around the unitary limit $1/(k_F a) \rightarrow 0$ we use the expansion

$$f\left(\frac{1}{k_F^{\text{hom}} a}\right) = \xi - \frac{\zeta}{k_F^{\text{hom}} a} + \dots, \quad (24)$$

which gives for the trapped gas:

$$\mathcal{F}(0) = \frac{2^7}{5^2 \cdot 7 \cdot \pi} \frac{\zeta}{\xi^{1/4}} \simeq 0.28 \quad (25)$$

where we took the estimates

$$\xi \simeq 0.41 \quad (26)$$

$$\zeta \simeq 0.95. \quad (27)$$

The estimate for ξ is obtained by averaging the predictions of [32] ($\xi = 0.42(1)$), of [26] ($\xi = 0.449(9)$), of [33] ($\xi = 0.42(1)$) and of [27] ($\xi = 0.37(5)$). The estimate for ζ is obtained from the calculation of the short range pair correlation of [34], see subsection 3.1, and is close to the value $\zeta \simeq 1.0$ that may be extracted directly from the values of f in [32] by approximating the derivative by a two-point formula. ⁵

2.3 Comparison to Rice experiment

At Rice [5] the quantity $Z = N_b/(N/2)$ was measured for a lithium gas, by resonantly exciting the closed-channel molecules with a laser that transfers them to another, short-lived molecular state; the molecule depletion reflects into a reduction of the atom number that can be measured.

We now compare the Rice results to our prediction (8). We first insert (9,10) into (8) which gives

$$N_b = N k_F R_* \mathcal{F}\left(\frac{1}{k_F a}\right) \left(1 - \frac{a_{\text{bg}}}{a}\right)^2 \quad (28)$$

⁴ For a small *positive* scattering length $0 < k_F a \ll 1$, Eqs.(22,23) also apply to the *atomic* gas state; since the interaction potentials considered here have a two-body bound state for $a > 0$, this atomic gas state is only metastable [49], the ground state being the BEC of dimers considered previously [cf. Eq.(21)].

⁵ The values (26,27) of ξ and ζ can be inserted into the expressions [50,51] for the derivatives of the frequencies of the hydrodynamic collective modes with respect to $1/(k_F a)$ taken at unitarity. The resulting slope is compatible with the experimental data for the radial mode [12,52], while the agreement with the data for the axial mode [53] is only marginal. The data from [12] agree very well for all positive values of a with the theoretical result [54] obtained from the fixed-node Monte Carlo equation of state [32], while in [52,53] finite-temperature effects may play a role [12,54,55].

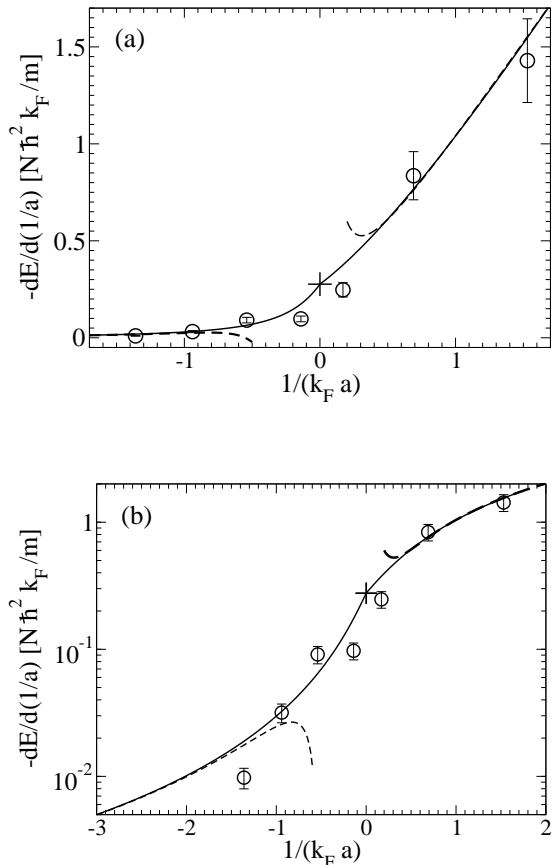


Fig. 1. Derivative $-dE/d(1/a)$ of the energy E of a trapped two-component Fermi gas, where a is the s -wave scattering length. Solid line: Theoretical prediction combining the Lee-Huang-Yang formulas (19,22) in the weakly interacting regimes with an interpolation of the fixed-node Monte Carlo results of [32,34] in the strongly interacting regime (see appendix D). Dashed lines: Analytical predictions in the weakly interacting regimes, on the BEC side (21) and on the BCS side (23). Cross: Result (25) at unitarity. Circles (with error bars): Experimental measurement of the number N_b of closed-channel molecules in a lithium gas at Rice [5], combined with the present theory linking $dE/d(1/a)$ to N_b , see (28). (a): Linear scale on the vertical axis. (b): Logarithmic scale. $-dE/d(1/a)$ is expressed in units of $N \hbar^2 k_F / m$. All the theoretical predictions are obtained in the local-density approximation.

where the function \mathcal{F} is defined in (15). The length R_* depends on the interchannel coupling and is related to the width of the Feshbach resonance as:

$$R_* = \frac{\hbar^2}{m a_{\text{bg}} \mu_b \Delta B}. \quad (29)$$

For the $B_0 \simeq 834\text{G}$ Feshbach resonance in ${}^6\text{Li}$, we have $\mu_b \simeq 2\mu_B$ where μ_B is the Bohr magneton [21], $\Delta B = -300\text{G}$, $a_{\text{bg}} = -1405a_0$ where $a_0 = 0.0529177\text{ nm}$ is the Bohr radius [56]; this gives $R_* = 0.0269\text{ nm}$. From the Rice data for N_b/N , using (28), we thus get values of \mathcal{F} ,

i.e. of $dE/d(1/a)$, that we compare in Fig.1 to theoretical predictions, given in the local-density approximation either by the expansions (21,23) in the weakly interacting regime, or by (25) at the unitary limit, or by an interpolation of the Monte Carlo results of [32,34] in the strongly interacting regime (see appendix D for details)⁶. The agreement is satisfactory, the experimental points being scattered around the theoretical prediction. In particular, a possible shift δB_0 of the resonance location due to the fact that $U_b(\mathbf{r}) \neq 2U(\mathbf{r})$, see (9), an effect not explicitly included in [5] for the calculation of $1/(k_F a)$ as a function of B , and which would manifest itself in horizontal shifts of the experimental data with respect to theory, does not show up in Fig.1. For the considered broad resonance of lithium, this is not surprising, see appendix B.

Our approach even allows to predict the time evolution of the particle number, in presence of the depleting laser, under the assumption that the molecular depletion rate is so weak that the equilibrium relation (28) holds at all times. Neglecting the slow off-resonant free-bound photoassociation process [5], we have

$$\frac{dN}{dt} = -2N_b(t) \frac{\Omega^2}{\gamma} \quad (30)$$

where Ω^2/γ is the effective decay rate of the closed-channel molecule, the Rabi frequency Ω and the spontaneous emission rate γ being defined in [5].⁷

Simple expressions can be obtained in limiting cases: In the BEC limit, the dominant term of the expansion (21) gives

$$N(t) = N(0) e^{-\Gamma_0 t}, \quad (31)$$

in the unitary limit, (25) gives

$$N(t) = \frac{N(0)}{(1 + \Gamma_0 t/6)^6}; \quad (32)$$

and in the BCS limit the dominant term of (23) gives

$$N(t) = \frac{N(0)}{(1 + \Gamma_0 t/2)^2}. \quad (33)$$

Here, $\Gamma_0 = -[dN(0)/dt]/N(0)$ is the initial atom loss rate, which can be expressed in terms of the initial atom number $N(0)$ using Eqs. (28,30). We see that in general $N(t)$ is

⁶ The error bars in Fig. 1 include the systematic theoretical uncertainty resulting from the leading order correction to (10) given in [56], but are largely dominated by the experimental error bars from [5] because we did not include the three experimental points from [5] which are deep in the BEC regime [$1/(k_F a) > 5$]; in this regime, two-body theories which go beyond our two-channel model give good agreement with the Rice measurements [5,21,57].

⁷ Eq. (30) can be obtained from the following master equation for the density matrix $\hat{\rho}$ of the gas: $d\hat{\rho}/dt = (\Omega^2/\gamma) \int d^3r [\psi_b(\mathbf{r})\hat{\rho}\psi_b^\dagger(\mathbf{r}) - \frac{1}{2}\{\psi_b^\dagger(\mathbf{r})\psi_b(\mathbf{r}), \hat{\rho}\}] + [H_2, \hat{\rho}]/(i\hbar)$. N in (30) stands for $N_f + 2N_b$, where N_f is the number of fermions; thus $N \simeq N_f$ in the regime considered in this paper.

not an exponential function of time. For the last point on the BCS side in [5], the (unpublished) data for $N(t)$ are better fitted by Eq.(33) than by an exponential; however the value of Γ_0 resulting from this new fitting procedure does not differ significantly from the published value [58].

3 Related observables

In this section, contrarily to subsections 2.2 and 2.3, we return to the general case and we do not assume that the temperature is $\ll T_F$ and that the numbers of atoms in each spin component are equal. For concreteness we take the lattice model (3), even if the reasonings may be generalized to a continuous space model and to a two-channel model.

3.1 Short range pair correlations

As was shown in [39] and recently rederived in [59], in the zero interaction range limit, the derivative of the gas energy with respect to the inverse scattering length can be expressed in terms of the short range behavior of the pair distribution function of opposite spin particles:

$$-\left(\frac{dE}{d(1/a)}\right)_S = \frac{4\pi\hbar^2}{m} \int d^3\mathbf{R} \lim_{r \rightarrow 0} r^2 g_{\uparrow\downarrow}(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2) \quad (34)$$

where the pair distribution function is given by

$$g_{\uparrow\downarrow}(\mathbf{r}_1, \mathbf{r}_2) = \langle \psi_{\uparrow}^\dagger(\mathbf{r}_1) \psi_{\downarrow}^\dagger(\mathbf{r}_2) \psi_{\downarrow}(\mathbf{r}_2) \psi_{\uparrow}(\mathbf{r}_1) \rangle. \quad (35)$$

Since we are dealing here with a finite range interaction model, we have taken a zero-range limit in (34), introducing the notation

$$\lim_{r \rightarrow 0} \tilde{} = \lim_{r \rightarrow 0} \lim_{b \rightarrow 0}. \quad (36)$$

Note that the order of the limits is important. In a degenerate regime, the limit in (34) is reached for a distance r much smaller than $|a|$, the mean distance between particles, and the thermal de Broglie wavelength λ , but still much larger than the interaction range b .

We thus see that a measurement of the pair distribution function of the atoms gives access, using (8), to the number of closed-channel molecules. Experimentally, the pair distribution function was measured via the photoassociation rate in a 1D Bose gas [60,61], or simply by dropping the gas on a detector with high enough spatio-temporal resolution [62,63,64]. The possibility of measuring the pair distribution function in the BEC-BCS crossover was studied in [34,65]. In the unitary limit, by inserting into Eq.(34) the value of $\lim_{r \rightarrow 0} r^2 g_{\uparrow\downarrow}$ calculated in [34] with the fixed-node Monte Carlo technique, we get the value (27) for the parameter ζ defined in (24).

The relation (34) is the three-dimensional version of the relation obtained in [66] for a one-dimensional Bose gas with contact interaction, using the Hellmann-Feynman

theorem. We now show that the Hellmann-Feynman technique also provides a simple derivation of (34). Taking the derivative of the gas eigenergy E with respect to the effective coupling constant $g = 4\pi\hbar^2 a/m$, for a fixed lattice spacing b , the Hellmann-Feynman theorem gives

$$\left(\frac{dE}{dg}\right)_S = \frac{dg_0}{dg} \left\langle \sum_{\mathbf{r}} b^3 \psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \psi_{\uparrow} \right\rangle \quad (37)$$

$$= \frac{dg_0}{dg} \sum_{\mathbf{r}} b^3 g_{\uparrow\downarrow}(\mathbf{r}, \mathbf{r}), \quad (38)$$

where g_0 is a function of g as given in (4), and where we used the relation $\langle dE/dg \rangle = (dE/dg)_S$ [cp. (11)]. In a gas, with an interaction range much smaller than the mean distance $\sim 1/k_F$ between particles and than the thermal de Broglie wavelength λ , the pair distribution function is dominated by two-body physics if $|\mathbf{r}_1 - \mathbf{r}_2|$ is much smaller than $1/k_F$ and λ (and also much smaller than a in the BEC regime), a property contained in the Yvon [67] and Waldmann-Snyder [68] ansatz of kinetic theory, which also appeared in the context of quantum gases [34, 69, 70, 71]:

$$g_{\uparrow\downarrow}(\mathbf{r}_1, \mathbf{r}_2) \simeq C \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right) |\phi(\mathbf{r}_1 - \mathbf{r}_2)|^2 \quad (39)$$

where ϕ is the two-body zero-energy free space scattering state for two atoms, here in the spin singlet state. With the lattice model we find ⁸

$$|\phi(\mathbf{0})|^2 = \frac{dg}{dg_0}, \quad (40)$$

so that Eq.(38) simplifies to

$$\left(\frac{dE}{dg}\right)_S \simeq \sum_{\mathbf{r}} b^3 C(\mathbf{r}). \quad (41)$$

On the other hand, at interparticle distances much larger than b , the zero-energy scattering wavefunction ϕ behaves as $1 - a/|\mathbf{r}_1 - \mathbf{r}_2|$ so that

$$\lim_{r \rightarrow 0} r^2 g_{\uparrow\downarrow}(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2) = a^2 C(\mathbf{R}). \quad (42)$$

Eq.(41) thus leads to (34).

3.2 Tail of the momentum distribution

As was shown in [40] and recently rederived in [59], in the zero-range limit, the momentum distribution of the

⁸ An elegant derivation is to enclose two atoms in a fictitious cubic box with periodic boundary conditions of volume L^3 , with $L \gg |a|, b$. To leading order in a/L , the wavefunction is $\phi_{\text{box}}(\mathbf{r}_1 - \mathbf{r}_2) = \phi(\mathbf{r}_1 - \mathbf{r}_2)/L^{3/2}$ with an energy given by the ‘‘mean-field’’ shift $E_{\text{box}} = g/L^3$. The Hellmann-Feynman theorem (37) then gives the result (40). An alternative derivation is to directly calculate ϕ in Fourier space [see (47)] which gives $\phi(\mathbf{r}) = 1 - g_0 \phi(\mathbf{0}) \int_{[-\pi/b, \pi/b]^3} [d^3\mathbf{k}/(2\pi)^3] \exp(i\mathbf{k} \cdot \mathbf{r}) / (2\epsilon_{\mathbf{k}})$; this, combined with (4), gives (40).

gas has a large momentum tail scaling as $1/k^4$, with a coefficient common to the two spin states and proportional to $-dE/d(1/a)$:

$$\lim_{k \rightarrow +\infty} k^4 n_{\sigma}(k) = -\frac{4\pi m}{\hbar^2} \frac{dE}{d(1/a)} \quad (43)$$

where

$$\lim_{k \rightarrow +\infty} = \lim_{k \rightarrow +\infty} \lim_{b \rightarrow 0}, \quad (44)$$

$\sigma = \uparrow$ or \downarrow and the momentum distribution is normalized as

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3} n_{\sigma}(\mathbf{k}) = N_{\sigma}, \quad (45)$$

where N_{σ} is the mean number of particle in the spin state σ . When combined with (8), this relation reveals that the number of closed-channel molecules may be deduced from a measurement of the momentum distribution of the atoms.

The momentum distribution in a two-component Fermi gas was actually already measured [72, 73, 74], simply by switching off the interaction and measuring the cloud density after a ballistic expansion. Two practical problems however arise, the effect of the non-zero switch-off time of the interaction [72, 75] and the signal to noise ratio in the far tails of the distribution; we have therefore not been able to extract the value of $dE/d(1/a)$ from the published data for $n_{\sigma}(k)$. The value of $dE/d(1/a)$ has not been extracted either from the fixed-node Monte Carlo calculations of $n_{\sigma}(k)$ performed in [76].

The relation (43) is a three-dimensional version of the relation derived for a one-dimensional Bose gas in [77]. We now present a very simple rederivation of (43).

In a gas with short range interactions, i.e. $b \ll 1/k_F$ and $b \ll \lambda$ (and $b \ll a$ on the BEC side), the tail of the momentum distribution is dominated by binary collisions in the spin singlet channel between a particle with a large momentum \mathbf{k} and a particle with a momentum $\simeq -\mathbf{k}$, so that

$$n_{\sigma}(\mathbf{k}) \simeq \mathcal{B} |\tilde{\phi}(\mathbf{k})|^2 \quad (46)$$

where \mathcal{B} is momentum-independent and $\tilde{\phi}(\mathbf{k})$ is the Fourier transform $\sum_{\mathbf{r}} b^3 e^{-i\mathbf{k} \cdot \mathbf{r}} \phi(\mathbf{r})$ of the zero-energy two-body free space scattering state $\phi(\mathbf{r})$. For the contact interaction in the lattice model the two-particle Schrödinger’s equation takes the form [30]

$$2\epsilon_{\mathbf{k}} \tilde{\phi}(\mathbf{k}) + g_0 \phi(\mathbf{r} = \mathbf{0}) = 0, \quad (47)$$

where $\epsilon_{\mathbf{k}}$ is the free wave dispersion relation in the lattice model, so that $\tilde{\phi}(\mathbf{k})$ drops as $1/\epsilon_{\mathbf{k}}$ for large k , and the associated kinetic energy diverges for $b \rightarrow 0$. Eq.(46) implies that the kinetic energy of the gas is proportional to the kinetic energy of the zero-energy two-body scattering state in the zero-range limit:

$$E_{\text{kin}}[\text{gas}] \simeq \mathcal{B} \cdot E_{\text{kin}}[\phi]. \quad (48)$$

Since the total energies have a finite limit for $b \rightarrow 0$, we can replace the kinetic energies by the opposite of the interaction energies in the above formula:

$$E_{\text{int}}[\text{gas}] \simeq \mathcal{B} \cdot E_{\text{int}}[\phi]. \quad (49)$$

The interaction energy of the gas is $g_0 \left\langle \sum_{\mathbf{r}} b^3 \psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \psi_{\uparrow} \right\rangle$, equal to $(dE/dg)_S g_0 (dg/dg_0)$ according to (37). The interaction energy of ϕ is simply $g_0 |\phi(\mathbf{0})|^2$, equal to $g_0 (dg/dg_0)$ according to (40). The common factor $g_0 (dg/dg_0)$ simplifies and

$$\left(\frac{dE}{dg} \right)_S = \mathcal{B}. \quad (50)$$

It remains to relate the coefficient \mathcal{B} to $\lim_{k \rightarrow +\infty} k^4 n_{\sigma}(k)$, using (46). In the zero-range limit, the scattering state $\phi(\mathbf{r})$ tends to $1 - a/r$, so that, by Fourier transform, $\tilde{\phi}(\mathbf{k})$ tends to $(2\pi)^3 \delta(\mathbf{k}) - 4\pi a/k^2$. We then get (43).

4 Conclusion

We have calculated the number N_b of closed-channel molecules in the whole BEC-BCS crossover for a two-component Fermi gas. Our result is in satisfactory agreement with the experimental results from Rice [5]. The expression (8) for N_b is proportional to the quantity $-dE/d(1/a)$ where E is the energy of the gas; this quantity is universal in the zero interaction range limit. At unitarity we find $N_b/N = k_F R_* \mathcal{F}(0)$ where $\mathcal{F}(0)$ is a universal constant given in (25) and the length R_* is related to the resonance parameters by (29); in the zero range and zero effective range limit where $k_F b \ll 1$ and $k_F |r_e| \ll 1$ we have $k_F R_* \ll 1$ [see Eq.(65)], we thus confirm that $N_b \ll N$ i.e. the gas mainly populates the open channel. In the BCS limit, $-dE/d(1/a)$ and thus N_b are determined by the Hartree-Fock mean field energy, and do not tend exponentially to zero with $1/(k_F |a|)$, contrarily to the prediction of usual BCS theory [5]. This is also related to the fact that the BCS theory does not predict the correct short-distance pair correlations [78].

The quantity $-dE/d(1/a)$ is related to the short-distance behavior of the pair correlation function and to the large- k tail of the momentum distribution, as discovered by Tan [39,40] and rederived in [59] and in this paper. The quantity $-dE/d(1/a)$ is also proportional to the average radiofrequency shift [79,80]. The general idea that various short-range two-body quantities such as the number of closed-channel molecules, the interaction energy of the gas and the average radiofrequency shift are the product of the value of the considered observable in the zero-energy two-body scattering state and a single universal many-body quantity was given by Leggett [71]. Our work shows that the Rice experiment [5] is the first direct measurement of this fundamental quantity in the BEC-BCS crossover.

It would be interesting to study the effect of a finite temperature. Experimentally, this could be achieved by measuring the number of closed-channel molecules together with the density profile of the trapped gas, the released energy [6,4], or the entropy [14,15]. Theoretically, Eq.(12) can be used when more Monte Carlo results at finite temperature will become available. A useful tool in this context is the virial theorem: at unitarity it directly gives the total energy in terms of the density profile [11,15,81,82] while for a finite a it also involves $[dE/d(1/a)]_S$ [83,84].

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Note: We became aware of the related work [85] while completing this paper, and of [86] while revising it.

A Two-body analysis of the two-channel model in free space

A.1 Scattering amplitude

In this appendix we briefly discuss the two-body scattering properties for our model Hamiltonian H_2 in free space, that is in the absence of trapping potential ($U_b(\mathbf{r}) \equiv 0, U(\mathbf{r}) \equiv 0$). The scattering problem may be considered in the center of mass frame so that we take the two-body scattering state

$$|\psi\rangle = \beta b_{\mathbf{0}}^{\dagger} |0\rangle + \int \frac{d^3 k}{(2\pi)^3} A(\mathbf{k}) a_{\mathbf{k}\uparrow}^{\dagger} a_{\mathbf{k}\downarrow}^{\dagger} |0\rangle, \quad (51)$$

with the unknown amplitude β in the closed channel and the unknown momentum dependent amplitude $A(\mathbf{k})$ in the open channel. The annihilation operators for the bosonic molecules, $b_{\mathbf{k}}$, and for the fermionic atoms $a_{\mathbf{k}\sigma}$, $\sigma = \uparrow$ or \downarrow , are the Fourier transforms of the corresponding field operators $\psi_b(\mathbf{r})$ and $\psi_{\sigma}(\mathbf{r})$, where the Fourier transform of a function $f(\mathbf{r})$ is $\tilde{f}(\mathbf{k}) = \int d^3 r \exp(-i\mathbf{k} \cdot \mathbf{r}) f(\mathbf{r})$. Inserting the state (51) in Schrödinger's equation $(H_2 - E)|\psi\rangle = 0$ and projecting respectively on the molecular subspace and the atomic subspace leads to

$$(E_b - E)\beta + A\gamma = 0 \quad (52)$$

$$\left(\frac{\hbar^2 k^2}{m} - E \right) A(\mathbf{k}) + \tilde{\chi}(\mathbf{k})(\beta A + g_0 \gamma) = 0 \quad (53)$$

where we used the fact that the function $\chi(\mathbf{r})$ is real and even, and where we introduced the amplitude

$$\gamma = \int \frac{d^3 k}{(2\pi)^3} \tilde{\chi}(\mathbf{k}) A(\mathbf{k}). \quad (54)$$

We now specialize to a state corresponding to the scattering of a spin \uparrow atom with incoming wavevector \mathbf{k}_0 onto a spin \downarrow atom with incoming wavevector $-\mathbf{k}_0$, so that $E = \hbar^2 k_0^2/m$ is the energy of the incoming state. Eliminating β in terms of γ with (52) and using (53) leads to

$$A(\mathbf{k}) = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}_0) + \frac{\gamma \tilde{\chi}(\mathbf{k}) [g_0 + \Lambda^2 / (E - E_b)]}{E + i0^+ - \hbar^2 k^2 / m} \quad (55)$$

where we have singled out the incoming state, and the scattered component is guaranteed to correspond to a pure outgoing wave in real space by the introduction of $+i0^+$ in

the denominator. Injecting (55) in (54) gives a closed linear equation for γ . From the known large r expression for the kinetic energy Green's function we extract the scattering amplitude

$$f_{k_0} = \frac{-m\tilde{\chi}(\mathbf{k}_0)^2/(4\pi\hbar^2)}{\left[g_0 + \frac{\Lambda^2}{\frac{\hbar^2 k_0^2}{m} - E_b}\right]^{-1} - \int \frac{d^3k}{(2\pi)^3} \frac{\tilde{\chi}^2(\mathbf{k})}{\frac{\hbar^2 k^2}{m} + i0^+ - \frac{\hbar^2 k^2}{m}}}. \quad (56)$$

Since we are considering a s -wave Feshbach resonance, the function $\chi(\mathbf{r})$ is rotationally invariant, a property that we have used in (56).

We now perform explicit calculations of various quantities characterizing the low energy scattering, such as the scattering length and the effective range. To this end, it is convenient as in [38] to perform the specific choice

$$\tilde{\chi}(\mathbf{k}) = \exp(-k^2 b^2/2) \quad (57)$$

and to extend (56) to negative energies, setting $k_0 = iq$, $q > 0$ and $E = -\hbar^2 q^2/m$. One then obtains an explicit expression

$$-\frac{1}{f_{iq}} = e^{-q^2 b^2} \left[\frac{4\pi\hbar^2/m}{g_0 - \frac{\Lambda^2}{E_b + \hbar^2 q^2/m}} + \frac{1}{b\sqrt{\pi}} \right] + q \operatorname{erf}(qb) - q \quad (58)$$

where the last term $-q$ is imposed by the optical theorem and erf is the error function.

The inverse of the scattering length is obtained by taking $q \rightarrow 0$ in (58):

$$\frac{1}{a} = \frac{4\pi\hbar^2/m}{g_0 - \Lambda^2/E_b} + \frac{1}{b\sqrt{\pi}}. \quad (59)$$

The large E_b limit of this expression is the inverse of the background scattering length:

$$\frac{1}{a_{\text{bg}}} = \frac{4\pi\hbar^2/m}{g_0} + \frac{1}{b\sqrt{\pi}}. \quad (60)$$

The location of the Feshbach resonance corresponds to an energy E_b^0 of the closed-channel molecule such that $1/a = 0$, so that

$$E_b^0 = \frac{\Lambda^2}{g_0 + 4\pi^3/2\hbar^2 b/m}. \quad (61)$$

Supposing that the energy E_b of the closed-channel molecule varies linearly with the magnetic field B ,

$$E_b(B) = E_b^0 + \mu_b(B - B_0), \quad (62)$$

and introducing the (possibly negative) resonance width ΔB such that

$$\mu_b \Delta B = \frac{\Lambda^2}{g_0} - E_b^0, \quad (63)$$

we get from (59) exactly the B -field dependence (10) for the scattering length a in free space.

We now consider the effective range r_e defined by the low- q expansion $-1/f_{iq} = a^{-1} - q + \frac{1}{2}q^2 r_e + O(q^4)$. Its general expression for our model is

$$r_e = \frac{-8\pi\hbar^4 \Lambda^2/m^2}{(g_0 E_b - \Lambda^2)^2} + \frac{4b}{\sqrt{\pi}} - \frac{2b^2}{a}. \quad (64)$$

Of particular interest is the value of the effective range right on resonance,

$$r_e^{\text{res}} = -2R_* + \frac{4b}{\sqrt{\pi}}, \quad (65)$$

where the length R_* is always non-negative,

$$R_* = \left(\frac{\Lambda}{2\pi b E_b^0} \right)^2. \quad (66)$$

This definition of R_* agrees with Eq. (29).

A very convenient rewriting of the scattering amplitude f_{iq} is obtained by taking as independent parameters, in addition to the van der Waals length b , the two lengths a_{bg} , R_* rather than the bare parameters g_0 , Λ of the Hamiltonian. The quantity $E_b - \Lambda^2/g_0$ appearing in (58) is conveniently rewritten using the quantity

$$Q^2 \equiv \frac{m}{\hbar^2 g_0} (g_0 E_b - \Lambda^2) \quad (67)$$

$$= \frac{-1}{a_{\text{bg}} R_*} \frac{1}{1 - a_{\text{bg}}/a} \quad (68)$$

which can be positive or negative. The ratio g_0/Λ is also easily eliminated with the identity

$$\frac{g_0^2}{4\pi\Lambda^2} = R_* a_{\text{bg}}^2. \quad (69)$$

Our final expression for the scattering amplitude is thus

$$-\frac{1}{f_{iq}} = \frac{e^{-q^2 b^2}}{a} \left[1 - (1 - a/a_{\text{bg}}) \frac{q^2}{q^2 + Q^2} \right] + q \operatorname{erf}(qb) - q \quad (70)$$

i.e.

$$-\frac{1}{f_k} = \frac{e^{k^2 b^2}}{a} \left[1 - (1 - a/a_{\text{bg}}) \frac{k^2}{k^2 - Q^2} \right] - ik \operatorname{erf}(-ikb) + ik. \quad (71)$$

We deduce the effective range in terms of a , a_{bg} , R_* and b :

$$r_e = -2R_*(1 - a_{\text{bg}}/a)^2 + \frac{4b}{\sqrt{\pi}} - \frac{2b^2}{a}. \quad (72)$$

A.2 Conditions for reaching the zero-range limit

In a degenerate gas, we expect that the zero-range limit is reached and the equation of state $E(1/a)$ becomes model independent provided the conditions

$$kb \ll 1 \quad (73)$$

$$-\frac{1}{f_k} \simeq \frac{1}{a} + ik \quad (74)$$

hold for $k \sim k_F$ and for $k \sim 1/a$ on the BEC side [38].

We now assume that (73) holds, and we derive validity conditions for (74) in the case of our two-channel model. Following the usual procedure, we use the second order expansion

$$-\frac{1}{f_k} = \frac{1}{a} + ik - \frac{1}{2}r_e k^2 + \dots, \quad (75)$$

which reduces to (74) if the effective range is small enough to have

$$\frac{1}{2}|r_e|k^2 \ll \left| \frac{1}{a} + ik \right|. \quad (76)$$

Taking into account the condition (73) as well as the expression (72) of r_e for the two-channel model, and using $|i + 1/(ka)| \geq 1$ and $|1 + ika| \geq 1$, we find that the condition (76) becomes equivalent to

$$k^2 R_* \left(1 - \frac{a_{\text{bg}}}{a}\right)^2 \left| \frac{1}{a} + ik \right|^{-1} \ll 1. \quad (77)$$

A second condition is obtained by imposing that the higher order terms \dots in (75) are indeed negligible compared to $k^2|r_e|/2$. For this to hold we need not only (73), but also $k^2 \ll |Q^2|$ i.e.

$$k^2 |a_{\text{bg}}| R_* \left| 1 - \frac{a_{\text{bg}}}{a} \right| \ll 1. \quad (78)$$

We conclude that to reach the universal zero-range limit, it is sufficient to fulfill the three conditions (73,77,78). All three conditions are satisfied for the experimental data on ${}^6\text{Li}$ from [5] reproduced in Fig.1, where $1/k_F > 250$ nm and $|a| > 200$ nm: using the values $|a_{\text{bg}}| = 74$ nm and $R_* = 0.027$ nm (see section 2.3) and taking the estimate $b \simeq 2.1$ nm obtained by imposing that the effective range on resonance (65) should be equal to the value 4.7 nm obtained in the multi-channel calculation of [87], we find that the left hand sides of Eqs.(73,77,78) are respectively smaller than 10^{-2} , $3 \cdot 10^{-4}$ and $7 \cdot 10^{-5}$.

To be complete, let us point out that the conditions (77,78) are not strictly necessary since it is possible that the \dots in (75) are not negligible compared to $k^2|r_e|/2$ and (74) nevertheless holds. We have chosen these conditions because they simplify the discussion, in particular they automatically ensure that the analytic continuation f_{iq} has a pole at $q \simeq 1/a$ so that the dimer energy is $\simeq -\hbar^2/(ma^2)$. For this last property, in the regime $b \ll a$, one directly gets from (70) the truly necessary condition

$$\left| (1 - a/a_{\text{bg}})^{-1} + (1 - a_{\text{bg}}/a)^{-2} a/R_* \right| \gg 1. \quad (79)$$

Close to the Feshbach resonance, $a \gg |a_{\text{bg}}|$, this reduces to the simpler condition

$$a \gg R_*. \quad (80)$$

B Effect of a difference between the trapping potentials seen by a closed-channel molecule and by an open-channel pair of atoms

In this appendix, we consider the physical consequences of the fact that, in general, the trapping potential $U_b(\mathbf{r})$ seen

by a closed-channel molecule is not simply the trapping potential $2U(\mathbf{r})$ seen by two separated atoms in the open channel:

$$U_b(\mathbf{r}) \neq 2U(\mathbf{r}), \quad (81)$$

and we derive conditions for the gas to behave approximately as if we had $U_b(\mathbf{r}) = 2U(\mathbf{r})$. Note that a significant deviation in (81) is not *a priori* excluded for the laser traps used e.g. in [5,56] for lithium, with a laser wavelength $\lambda_L \simeq 1 \mu\text{m}$: Contrarily to the atomic lightshift, the lightshift of the closed-channel molecule may be sensitive to the laser detuning from transitions to bound states of the $1^1\Sigma_u^+(A)$ Born-Oppenheimer interaction potential between a ground-state atom and an excited atom, considering the fact that the minimum of this excited-ground interaction potential is separated from the dissociation limit of the ground-ground interaction potential by only $\simeq 0.6 \mu\text{m}^{-1} \simeq 1/\lambda_L$ in spectroscopic units [88].

B.1 Position dependent scattering length and effective magnetic field

At the two-body level, (81) leads to an effective position dependent scattering length for two opposite spin atoms. To define such a local scattering length around point \mathbf{r}_0 , we consider the ‘‘tangential’’ free space problem where the trapping potentials are replaced by the constant values $U_b(\mathbf{r}_0)$ and $U(\mathbf{r}_0)$ and we call $a(\mathbf{r}_0)$ the resulting scattering length. We simply have to revisit the calculations of appendix A: In (52) one has to replace E_b by $E_b + U_b(\mathbf{r}_0)$ to include the trapping energy shift of the closed-channel molecule; similarly in (53) one has to replace $\frac{\hbar^2 k^2}{m}$ by $\frac{\hbar^2 k^2}{m} + 2U(\mathbf{r}_0)$ to include the trapping energy shift of the two atoms; finally, for atoms with incoming wavevectors $\pm \mathbf{k}_0$, the scattering state eigenenergy is now $E = \frac{\hbar^2 k_0^2}{m} + 2U(\mathbf{r}_0)$. The net effect on the scattering amplitude f_{k_0} in (56) is to apply the substitution

$$E_b \longrightarrow E_b + U_b(\mathbf{r}_0) - 2U(\mathbf{r}_0), \quad (82)$$

so that $a(\mathbf{r}_0)$ is simply obtained by applying (82) to (59).

A powerful interpretation of this substitution procedure may be given for a magnetic field independent μ_b : We can rewrite the term $E_b(B) + U_b(\mathbf{r})$ appearing in (1) as $E_b[B_{\text{eff}}(\mathbf{r})] + 2U(\mathbf{r})$ provided we set

$$B_{\text{eff}}(\mathbf{r}) = B + \frac{U_b(\mathbf{r}) - 2U(\mathbf{r})}{\mu_b}. \quad (83)$$

Thus we can replace $U_b(\mathbf{r})$ by $2U(\mathbf{r})$ in (1) provided we also replace the homogeneous magnetic field B in (1) by the inhomogeneous effective magnetic field $B_{\text{eff}}(\mathbf{r})$. One then immediately obtains the position dependence of the scattering length,

$$a(\mathbf{r}) = a_{\text{fs}}[B_{\text{eff}}(\mathbf{r})], \quad (84)$$

the function $a_{\text{fs}}(B)$ being given in (10).

This effective magnetic field picture is also very efficient at the many-body level. In the grand canonical point

of view, one adds the term $-\mu\hat{N}$ to the Hamiltonian H_2 , where μ is the chemical potential, and the particle number operator \hat{N} is defined as $\hat{N} = \hat{N}_f + 2\hat{N}_b$, \hat{N}_f giving the number of fermions and \hat{N}_b the number of bosons, since this is the quantity which commutes with H_2 . In the local density approximation, in the general case $U_b \neq 2U$, we thus see that the gas behaves locally like a free space, homogeneous gas of chemical potential $\mu - U(\mathbf{r})$, in presence of the locally homogeneous magnetic field $B_{\text{eff}}(\mathbf{r})$.

B.2 Shift of the resonance location

We now consider the case of an optical trap such as the one at Rice [5]: $U(\mathbf{r})$ and $U_b(\mathbf{r})$ are the lightshift potentials experienced by an atom and by a closed-channel molecule. Being both proportional to the laser intensity, they are mutually proportional:

$$U_b(\mathbf{r}) = 2(1 + \eta)U(\mathbf{r}) \quad (85)$$

where the dimensionless parameter η is a convenient measure of the relative deviation between U_b and $2U$. At large \mathbf{r} the laser intensity vanishes, so do U_b and U .

In practice, the gas is trapped around the intensity maximum of the laser field, located in $\mathbf{r} = \mathbf{0}$, and the extension of the cloud along the axial (resp. radial) direction is small compared to the Rayleigh length (resp. the waist) of the laser beam; thus, to leading order, $U(\mathbf{r}) \simeq U(\mathbf{0})$, we can temporarily forget about the spatial variation of B_{eff} and take $B_{\text{eff}} \simeq B - \delta B_0$, where

$$\delta B_0 = \frac{-U_b(\mathbf{0}) + 2U(\mathbf{0})}{\mu_b} = -\frac{2\eta U(\mathbf{0})}{\mu_b}. \quad (86)$$

Since the free space scattering length $a_{\text{fs}}(B)$ only depends on the difference $B - B_0$, replacing B by B_{eff} is equivalent to shifting the position B_0 of the Feshbach resonance by the quantity δB_0 . Introducing the length R_* defined in (29), the ratio of this shift to the width ΔB of the Feshbach resonance may be written as

$$\frac{\delta B_0}{\Delta B} = -\frac{2mU(\mathbf{0})}{\hbar^2} a_{\text{bg}} R_* \eta. \quad (87)$$

In the Rice experiment, the trap depth $-U(\mathbf{0})$ is at most $k_B \times 2.71 \mu\text{K}$ [89], so that we have

$$\frac{|\delta B_0|}{\Delta B} < \frac{|\eta|}{7500} \quad (88)$$

where we have used the values of a_{bg} and R_* given below (29) and the mass of lithium. Except if η takes truly large values for the laser wavelength $\lambda_L = 1064 \text{ nm}$ used in [5], we expect only a small shift of the resonance location due to the laser trap, relative to the resonance width.

In [5] the value of the scattering length as a function of B was calculated essentially from the free space formula $a_{\text{fs}}(B)$ ignoring the shift δB_0 due to the trap, and taking for the resonance location B_0 the value measured in [56] in a laser trap with different laser wavelength $\lambda_L = 1030 \text{ nm}$

and intensity. On the contrary, our definition of a as a function of B includes the shift δB_0 , $a = a_{\text{fs}}(B - \delta B_0)$, as already defined in (9). This may introduce a systematic discrepancy between our theory curves and the experimental data in Fig.1, in the form of shifts of the abscissas of the experimental points. We thus define the horizontal shift

$$\delta \left(\frac{1}{k_F a} \right) \equiv \frac{1}{k_F a_{\text{fs}}(B - \delta B_0)} - \frac{1}{k_F a_{\text{fs}}(B)} \quad (89)$$

$$= \frac{\delta B_0}{\Delta B} \frac{1}{k_F a_{\text{bg}}} \frac{(1 - a_{\text{bg}}/a)^2}{1 - (1 - a_{\text{bg}}/a)\delta B_0/\Delta B}. \quad (90)$$

To leading order in η (that is for $|\delta B_0/\Delta B| \ll 1$), and using the fact that the data from [5] reproduced in Fig. 1 is sufficiently close to resonance to have $|1 - a_{\text{bg}}/a| < 1.4$, this simplifies to:

$$\delta \left(\frac{1}{k_F a} \right) \simeq \frac{\delta B_0}{\Delta B} \frac{1}{k_F a_{\text{bg}}} (1 - a_{\text{bg}}/a)^2. \quad (91)$$

Using the parameters of the Rice experiment [89] and Eq.(87) this gives

$$\left| \delta \left(\frac{1}{k_F a} \right) \right| < \frac{|\eta|}{1000}. \quad (92)$$

Even without knowing η , we can thus reasonably expect that this shift is negligible on the scale of Fig. 1, i.e. that

$$\left| \delta \left(\frac{1}{k_F a} \right) \right| \ll 1. \quad (93)$$

This is also consistent with the fact that no systematic horizontal shift is apparent in Fig.1 between the experimental data and the theory curves.

B.3 Effect of the position dependence of $B_{\text{eff}}(\mathbf{r})$

We now discuss the effect on the many-body properties of the gas of the inhomogeneity of $B_{\text{eff}}(\mathbf{r})$, that is of a spatial dependence of the scattering length $a(\mathbf{r})$, see (84), now taking into account the \mathbf{r} dependence of $U(\mathbf{r})$. We rewrite (83) as

$$B_{\text{eff}}(\mathbf{r}) = B + \frac{2\eta U(\mathbf{r})}{\mu_b} = B - \delta B_0 + \frac{2\eta[U(\mathbf{r}) - U(\mathbf{0})]}{\mu_b}. \quad (94)$$

When inserted in (84) this leads to the following position dependence for the scattering length:

$$\frac{1}{a(\mathbf{r}) - a_{\text{bg}}} = \frac{1}{a - a_{\text{bg}}} - \eta \frac{2mR_*}{\hbar^2} [U(\mathbf{r}) - U(\mathbf{0})], \quad (95)$$

where we recall that a is the scattering length in the trap center. Right on resonance, $|a| = +\infty$, R_* is one of the contributions to the interaction effective range, see (65), so that the zero-range limit implies $k_F |R_*| \ll 1$. Since the typical value of $U(\mathbf{r}) - U(\mathbf{0})$ over the cloud size is of the order of $\hbar^2 k_F^2 / 2m$, we see that the small parameter $k_F R_*$

appears in (95) so that we may expect that the position dependence of $a(\mathbf{r})$ is negligible in the zero-range limit (for a fixed value of η).

Let us investigate this expectation more quantitatively and beyond the unitary limit, however still in a limiting case with simplifying assumptions. First, we assume that we are sufficiently close to resonance to have $|a(\mathbf{r})| \gg |a_{\text{bg}}|$ over the atomic cloud size. This implies that the excursion of $B_{\text{eff}}(\mathbf{r})$ over the cloud size is small as compared to $|\Delta B|$; since the excursion of $U(\mathbf{r})$ over the laser trap size is at most $|U(\mathbf{0})|$, we note that this condition is automatically satisfied for $|\delta B_0| \ll |\Delta B|$. Second, we shall assume that the gas may be treated in the zero temperature local density approximation. Third, we use the quadratic approximation (13) for $U(\mathbf{r})$, further supposing for simplicity that the harmonic trap is isotropic, a case to which one can always reduce within the local density approximation by a rescaling of the coordinates, see appendix C. Equation (95) then reduces to

$$\frac{1}{a(r)} \simeq \frac{1}{a} - \eta \frac{mR_*}{\hbar^2} m\omega^2 r^2, \quad (96)$$

and the gas density profile $n(\mathbf{r})$ is given by

$$\mu - U(\mathbf{0}) = \frac{1}{2} m\omega^2 r^2 + \mu^{\text{hom}}[n(\mathbf{r}), \frac{1}{a(r)}] \quad (97)$$

where $\mu^{\text{hom}}[n, 1/a]$ is the chemical potential of a free space homogeneous gas of density n and scattering length a .

Let us derive simple conditions to have a weak effect of the scattering length inhomogeneity on the density profile. Some of these conditions will be expressed in terms of k_F defined by (14).

In the BCS regime, $a < 0$ and $k_F|a| < 1$, we have $\mu - U(\mathbf{0}) \simeq k_B T_F = \hbar^2 k_F^2 / 2m$. Over the Thomas-Fermi radius R of the cloud, such that $\frac{1}{2} m\omega^2 R^2 \simeq k_B T_F$, we see that the relative change of $1/a(r)$ is negligible if

$$|1 - a/a(R)| \simeq (k_F|a|)(|\eta|k_F R_*) \ll 1. \quad (98)$$

This is satisfied in the zero-range limit, for fixed η , according to the condition (77) written for $k = k_F$.

In the unitary limit $k_F|a| \gg 1$, the previous reasoning fails, because requiring that the relative change of $a(r)$ is small is too stringent. Taking for simplicity the limiting case $|a| = +\infty$, it is sufficient to check that the gas remains locally unitary except in a small region near the edge of the cloud. First, to zeroth order in η , we calculate the local Fermi wavevector $k_F^{\text{hom}}(\mathbf{r})$ using the unitary equation of state $\mu^{\text{hom}}[n, 1/a = 0] = \xi \hbar^2 (k_F^{\text{hom}})^2 / 2m$, where k_F^{hom} is defined in (17), and using the value of the chemical potential $\mu - U(\mathbf{0}) = \sqrt{\xi} k_B T_F$. We obtain

$$k_F^{\text{hom}}(r) = \frac{k_F}{\xi^{1/4}} \left(1 - \frac{r^2}{R^2}\right)^{1/2} \quad (99)$$

where R is the unperturbed Thomas-Fermi radius such that $m\omega^2 R^2 / 2 = \sqrt{\xi} k_B T_F$. Then, we include the η position dependent term in $1/a(r)$ to calculate at which distance l from the edge of the cloud the gas starts leaving

the unitary regime, that is

$$k_F^{\text{hom}}(R-l)|a(R-l)| = 1. \quad (100)$$

Assuming *a priori* $l \ll R$ we obtain from (99)

$$\frac{l}{R} \simeq \frac{\xi^{3/2}}{2} (\eta k_F R_*)^2. \quad (101)$$

We conclude *a posteriori* that $l/R \ll 1$ and that the spatial dependence of $a(r)$ is negligible when

$$|\eta|k_F R_* \ll 1. \quad (102)$$

As in the BCS case, this is equivalent for a fixed $|\eta|$ to the zero range condition (77) written here with $k = k_F$ and $|a| = +\infty$.

Finally we turn to the BEC regime $a > 0$ and $k_F|a| < 1$. We then use the approximate equation of state

$$\mu^{\text{hom}}[n(r), 1/a(r)] \simeq -\frac{\hbar^2}{2ma^2(r)} + \frac{\pi\hbar^2}{2m} \alpha a(r)n(r) \quad (103)$$

where $\alpha \simeq 0.60$ is the proportionality factor in (20) between the dimer-dimer scattering length a_d and a . In particular, this requires $a \gg R_*$, see (80). Replacing $1/a(r)$ by (96) in the above expression, we find that the leading term in $1/a^2(r)$ gives rise to an external potential that sums up with the trapping potential to give

$$\begin{aligned} U_{\text{eff}}(r) &\equiv U(r) - \frac{\hbar^2}{2ma^2(r)} \\ &= U_{\text{eff}}(0) + \frac{1}{2} \omega_{\text{eff}}^2 r^2 - \frac{m(\eta R_*)^2}{2\hbar^2} (m\omega^2 r^2)^2 \end{aligned} \quad (104)$$

We see that the atomic oscillation frequency is renormalized into

$$\omega_{\text{eff}} = \left(1 + \frac{2\eta R_*}{a}\right)^{1/2} \omega. \quad (106)$$

To have a small effect of the scattering length inhomogeneity on the trapped gas, we first require $\omega_{\text{eff}} \simeq \omega$ so that

$$|\eta|R_*/a \ll 1, \quad (107)$$

a condition with no counterpart in the BCS regime and more stringent than (102) since $k_F a < 1$ here. Again, we find that we recover, for a fixed $|\eta|$, the zero range condition (77) written here for $k = 1/a$. Second we require that the r^4 term in $U_{\text{eff}}(r)$ remains small as compared to the r^2 one over the Thomas-Fermi radius R of the condensate of dimers, calculated here to zeroth order in η ; we reach the second condition

$$\frac{m(\eta R_*)^2}{\hbar^2} m\omega^2 R^2 \simeq (\eta k_F R_*)^2 \left(\frac{5}{64} k_F a_d\right)^{2/5} \ll 1. \quad (108)$$

Since $k_F a < 1$ here, this second condition is automatically ensured by the first condition (107). Third, we require that the relative variation of $1/a(r)$ is small over the Thomas-Fermi radius R of the condensate, to ensure that the spatial inhomogeneity of $a(r)$ in the mean field term

$[\pi\hbar^2/(2m)]\alpha a(r)n(r)$ has a small impact on the density profile:

$$|1-a/a(R)| \simeq (k_F a)(|\eta|k_F R_*) \left(\frac{5}{64}k_F a_d\right)^{2/5} \ll 1, \quad (109)$$

which is also implied by (107).

To summarize, discussing perturbatively the effect of the position dependence of $B_{\text{eff}}(\mathbf{r})$ on the gas density profile in the local density approximation, we find close to the Feshbach resonance ($|a| \gg |a_{\text{bg}}|$, and also $a \gg R_*$ in the BEC regime) that the effect is small under the condition (98) in the BCS regime, under the condition (102) in the unitary regime, and under the condition (107) in the BEC regime: In all three cases, this is the zero range condition (77), written respectively for $k = k_F$, $k = k_F$ and $k = 1/a$, and *multiplied* by the parameter $|\eta|$. If $|\eta|$ is not too large, neglecting the r dependence of the scattering length is thus automatically justified in the zero-range limit.

Interestingly, in the unitary limit, it is possible to relate $\eta k_F R_*$ to the quantity $\delta(1/k_F a)$ introduced in the previous subsection:

$$|\eta|k_F R_* \xi^{1/2} \simeq \left| \delta \left(\frac{1}{k_F a} \right) \frac{\mu - U(\mathbf{0})}{U(\mathbf{0})} \right|. \quad (110)$$

Experimentally, the gas is confined at the bottom of the laser trap so that $[\mu - U(\mathbf{0})]/|U(\mathbf{0})| \ll 1$ (its value near unitarity at Rice is 0.15 [89]). Together with the assumption (93) this implies that the right-hand-side of (110) is $\ll 1$, and that the position dependence of $a(\mathbf{r})$ has a negligible effect on the gas density.

A quantitative extension of the present qualitative discussion is to evaluate the density change $\delta n(r)$ of the gas to first order in η . To this end, one simply expands (97) to first order in η around the solution $n_0(r)$ with $\eta = 0$, writing to first order $n(r) = n_0(r) + \delta n(r)$ and $\mu = \mu_0 + \delta\mu$:

$$\delta n(\mathbf{r}) = \frac{\delta\mu - \delta \left(\frac{1}{a} \right) (r) \partial_{1/a} \mu^{\text{hom}}[n_0(r), 1/a]}{\partial_n \mu^{\text{hom}}[n_0(r), 1/a]} \quad (111)$$

where we have introduced the variation of $1/a(r)$ around $\eta = 0$ to first order in η , not supposing $|a(r)| \gg |a_{\text{bg}}|$ in (95):

$$\delta \left(\frac{1}{a} \right) (r) = - \left(1 - \frac{a_{\text{bg}}}{a} \right)^2 \eta \frac{m R_*}{\hbar^2} m \omega^2 r^2. \quad (112)$$

$\delta\mu$ is then determined by the condition of a fixed number of particles $\int_{r < R_0} d^3r \delta n(r) = 0$, where R_0 is the Thomas-Fermi radius of the gas for $\eta = 0$. In this way, taking the variation of (130) to first order in η around $\eta = 0$, one can calculate the effect of a non-uniformity of $a(r)$ on $dE/d(1/a)$ to first order in η . We give here the result for the unitary gas:

$$\frac{\delta [dE/d(1/a)]}{dE/d(1/a)|_{\eta=0}} = \eta k_F R_* \left[\left(\frac{64}{25\pi} - \frac{63\pi}{256} \right) \xi^{-1/4} \zeta + \frac{315\pi}{2048} \xi^{3/4} \zeta^{-1} f^{(2)}(0) + \frac{2}{3} \xi^{1/2} k_F a_{\text{bg}} \right], \quad (113)$$

where we recall that $\xi = f(0)$, $\zeta = -f'(0)$, see (24), and $f^{(2)}(0)$ is the second order derivative of $f(x)$ with respect to x in $x = 0$. Note that, in this first order variation with respect to η , the trapping potential $U(\mathbf{r})$ is kept fixed so that k_F is also fixed.

The calculation (113) shows that, at unitarity, a measurement of the variation of the number of closed-channel molecules N_b as a function of $U_b(\mathbf{r})/U(\mathbf{r})$ may give access to $f^{(2)}(0)$. It also shows that, in the unitary limit, the condition to neglect a_{bg} with respect to $a(\mathbf{r})$ as done in the qualitative reasoning around (102), is $k_F |a_{\text{bg}}| \ll 1$.

B.4 Metastability issues for a position dependent scattering length

We now discuss whether it is energetically possible for a pair of atoms to form a dimer which could escape from the trap by tunneling. The energy variation in such a process is

$$\Delta E = -\frac{\hbar^2}{ma^2(\infty)} - 2\mu \quad (114)$$

where μ is the chemical potential of the trapped gas and $a(\infty)$ is the effective scattering length at infinity, which we assume to be positive. We discuss under which conditions this process is energetically forbidden, i.e. $\Delta E > 0$.

We assume that the gas has the usual Thomas-Fermi density profile and is weakly affected by the position dependence of $B_{\text{eff}}(\mathbf{r})$, see subsection B.3. We distinguish between two regimes for the scattering length a in the trap center: the negative- a regime where $1/a \leq 0$, and the BEC regime where $0 < k_F a < 1$. Under the usual assumption that the gas is confined in a small region around the bottom of the laser trap we have $\mu \simeq U(\mathbf{0})$ in the negative- a regime and $\mu \simeq U(\mathbf{0}) - \hbar^2/(2ma^2)$ in the BEC regime. We also make the simplifying assumption $a(\infty) \gg |a_{\text{bg}}|$ so that (95) reduces to

$$\frac{1}{a(\infty)} \simeq \frac{1}{a} + 2\eta \frac{m}{\hbar^2} R_* U(\mathbf{0}). \quad (115)$$

In the BEC regime one easily deduces

$$\frac{\Delta E}{2|U(\mathbf{0})|} \simeq 1 + \mathcal{A} - \mathcal{B} \quad (116)$$

where

$$\mathcal{A} \equiv 2\eta \frac{R_*}{a} \quad (117)$$

$$\mathcal{B} \equiv 2\eta^2 \frac{m R_*^2}{\hbar^2} |U(\mathbf{0})|; \quad (118)$$

since we already assumed (107) we automatically have $|\mathcal{A}| \ll 1$. In the negative- a regime, Eq.(115) immediately gives an upper bound on $1/a(\infty)$, from which we get

$$\frac{\Delta E}{2|U(\mathbf{0})|} \gtrsim 1 - \mathcal{B}. \quad (119)$$

In both regimes we conclude that under the condition

$$|\mathcal{B}| \ll 1 \quad (120)$$

we have $\Delta E \gtrsim 2|U(\mathbf{0})|$ so that the process is energetically forbidden.

Finally we note that under the assumption $|a| \gg |a_{\text{bg}}|$ we have from (90,87)

$$\delta \left(\frac{1}{k_F a} \right) \simeq \eta k_F R_* \frac{|U(\mathbf{0})|}{k_B T_F} \quad (121)$$

so that

$$\mathcal{B} \simeq \left| \delta \left(\frac{1}{k_F a} \right) \right|^2 \frac{k_B T_F}{|U(\mathbf{0})|}. \quad (122)$$

In a typical experiment such as the one at Rice we have $k_B T_F < |U(\mathbf{0})|$; thus the condition $|\mathcal{B}| \ll 1$ is satisfied as soon as $|\delta(1/k_F a)| \ll 1$, which is likely to hold at Rice, see (92).

C Calculation of $dE/d(1/a)$ in the local density approximation

Restricting to a spin balanced gas, we first consider the general case of the two-channel model (1), in which $U_b(\mathbf{r}) \neq 2U(\mathbf{r})$. As explained in the appendix B, where an effective position dependent magnetic field $B_{\text{eff}}(\mathbf{r})$ is introduced, this leads to a position dependent scattering length $a(\mathbf{r})$. As a consequence, in the local density approximation, here at zero temperature, the gas density $n(\mathbf{r})$ is given by

$$\mu = U(\mathbf{r}) + \mu^{\text{hom}}[n(\mathbf{r}), 1/a(\mathbf{r})] \quad (123)$$

where $\mu^{\text{hom}}[n, 1/a]$ is the chemical potential of the free space homogeneous gas of density n and scattering length a . The mean energy and particle numbers in the gas are given in the same approximation by

$$E = \int d^3r \{U(\mathbf{r}) + \epsilon^{\text{hom}}[n(\mathbf{r}), 1/a(\mathbf{r})]\} n(\mathbf{r}) \quad (124)$$

$$N = \int d^3r n(\mathbf{r}) \quad (125)$$

where $\epsilon^{\text{hom}}[n, 1/a]$ is the mean energy per particle of the free space gas. We wish to calculate the derivative of E with respect to $1/a$, where a is the scattering length in the trap center $\mathbf{r} = \mathbf{0}$, with the constraint that N should be fixed.

Let us perform an infinitesimal variation $\delta \left(\frac{1}{a} \right)$ of $1/a$. This leads to a variation $\delta\mu$ of the chemical potential and $\delta n(\mathbf{r})$ of the density, that may be calculated from (123) but this is not required here. This also leads to a variation of $1/a(\mathbf{r})$, according to (95):

$$\delta \left(\frac{1}{a(\mathbf{r})} \right) = \left(\frac{1 - a_{\text{bg}}/a(\mathbf{r})}{1 - a_{\text{bg}}/a} \right)^2 \delta \left(\frac{1}{a} \right). \quad (126)$$

The variation of the gas energy is then

$$\begin{aligned} \delta E = \int d^3r \delta n(\mathbf{r}) \left[U(\mathbf{r}) + \epsilon^{\text{hom}}[n(\mathbf{r}), 1/a(\mathbf{r})] \right. \\ \left. + n(\mathbf{r}) \frac{\partial \epsilon^{\text{hom}}}{\partial n}[n(\mathbf{r}), 1/a(\mathbf{r})] \right] \\ + \delta \left(\frac{1}{a(\mathbf{r})} \right) n(\mathbf{r}) \frac{\partial \epsilon^{\text{hom}}}{\partial (1/a)}[n(\mathbf{r}), 1/a(\mathbf{r})]. \end{aligned} \quad (127)$$

Writing $\epsilon^{\text{hom}}[n, 1/a] = E^{\text{hom}}[N, V, 1/a]/N$, where V is the volume and N the particle number of the homogeneous gas, we find the relation

$$n \frac{\partial \epsilon^{\text{hom}}}{\partial n}[n, 1/a] = \mu^{\text{hom}}[n, 1/a] - \epsilon^{\text{hom}}[n, 1/a]. \quad (128)$$

Using this expression and (123) one finds that a simplification occurs in (127). Furthermore, the fact that the particle number is fixed imposes

$$\int d^3r \delta n(\mathbf{r}) = 0 \quad (129)$$

so that (127) leads to

$$\begin{aligned} \left(\frac{dE}{d(1/a)} \right)_N = \int d^3r n(\mathbf{r}) \left(\frac{1 - a_{\text{bg}}/a(\mathbf{r})}{1 - a_{\text{bg}}/a} \right)^2 \\ \times \frac{\partial \epsilon^{\text{hom}}}{\partial (1/a)}[n(\mathbf{r}), 1/a(\mathbf{r})]. \end{aligned} \quad (130)$$

We note that an alternative derivation of this result is possible: One can introduce the density of closed-channel molecules $n_b^{\text{hom}}[n, 1/a]$ for a free space gas of density n and scattering length a , a quantity that can be related to the derivative of $\epsilon^{\text{hom}}[n, 1/a]$ with respect to $1/a$ simply by applying the general formula (8) to a free space system. Then setting for the trapped system in the local density approximation $N_b = \int d^3r n_b^{\text{hom}}[n(\mathbf{r}), 1/a(\mathbf{r})]$ and using (8) for the trapped system leads to (130).

In practice, in the present paper, we perform explicit calculations in the limiting cases presented in §2.2: One takes the zero-range limit, which also allows to neglect the spatial variation of $a(\mathbf{r})$ under conditions discussed in the appendix B. Then ϵ^{hom} is given by the relation (16) involving some universal function $f(x)$. For the free space chemical potential we then introduce the convenient parametrization

$$\mu^{\text{hom}}[n, 1/a] = \frac{\hbar^2}{2ma^2} u \left(\frac{1}{k_F^{\text{hom}} a} \right) \quad (131)$$

where $k_F^{\text{hom}} = (3\pi^2 n)^{1/3}$ is the ideal gas Fermi wvector, and the function u is

$$u(x) = \frac{f(x) - \frac{1}{5}x f'(x)}{x^2}. \quad (132)$$

One also restricts to a harmonic trap for $U(\mathbf{r})$, see (13). The surface $n(\mathbf{r}) = 0$ is then an ellipsoid with Thomas-Fermi radii R_α along the directions α .

For $a < 0$ we set

$$\mu = \frac{\hbar^2 q^2}{2m} \quad (133)$$

with $q > 0$. Then $\omega_\alpha R_\alpha = \hbar q/m$, and the density depends only on $X \geq 0$ such that $X^2 = \sum_\alpha r_\alpha^2/R_\alpha^2$. Equation (123) then reduces to the implicit equation

$$q^2 a^2 (1 - X^2) = u \left[\frac{1}{k_F^{\text{hom}}(X)a} \right] \quad (134)$$

that one can solve numerically, using the interpolation for $f(x)$ given in appendix D.

For $a > 0$, $\mu^{\text{hom}}[n, 1/a]$ tends to $-\hbar^2/(2ma^2)$ for $n \rightarrow 0$ so that we set

$$\mu = \frac{\hbar^2 q^2}{2m} - \frac{\hbar^2}{2ma^2} \quad (135)$$

with $q > 0$. Then again $\omega_\alpha R_\alpha = \hbar q/m$, and (123) reduces to

$$q^2 a^2 (1 - X^2) = 1 + u \left[\frac{1}{k_F^{\text{hom}}(X)a} \right] \quad (136)$$

to be solved numerically in general.

One can then calculate $dE/d(1/a)$ and k_F defined in (14) from the expressions valid on both sides of the resonance:

$$\frac{dE}{d(1/a)} = \frac{3N\hbar^2}{10m} \frac{\int_0^1 dX X^2 k_F^{\text{hom}}(X)^4 f' \left[\frac{1}{k_F^{\text{hom}}(X)a} \right]}{\int_0^1 dX X^2 k_F^{\text{hom}}(X)^3} \quad (137)$$

$$k_F = \frac{\sqrt{2q}}{\pi^{1/3}} \left[4\pi \int_0^1 dX X^2 k_F^{\text{hom}}(X)^3 \right]^{1/6} \quad (138)$$

The analytical calculations performed in the weakly interacting regimes are also obtained from the above formulas.

D Interpolation formula for the homogeneous gas energy

We explain how an interpolation formula was constructed for the function f defined in (16), which was then used to produce the solid line in Fig.1a and Fig.1b.

On the BEC side of the resonance, we applied a cubic spline interpolation to the points in Table I of [32] with values of $x = 1/(k_F^{\text{hom}}a)$ equal to 0, 1, 2, 4 and 6, using the last column of Table I (the one said to give $E/N - \epsilon_b/2$) and adding to the corresponding data the quantity $-\hbar^2/(2ma^2)$. We added a home made point at $x = 8$ where the value of $f(x)$ and its first order derivative $f'(x)$ are obtained from the bosonic Lee-Huang-Yang expansion (19).

On the BCS side of the resonance we used the empirical interpolation formula of [90],

$$f_S(x) = \alpha_1 - \alpha_2 \arctan[\alpha_3 x(\beta_1 - x)/(\beta_2 - x)]. \quad (139)$$

Constraints on $\alpha_1, \alpha_2, \alpha_3$ and β_1, β_2 are obtained from the values $f(0), f'(0)$ and from the large $|x|$ expansion

$f(x) = 1 + c_1/x + c_2/x^2 + O(1/x^3)$, where the coefficients c_1 and c_2 are given in (22). This differs from [90] where the coefficient c_2 was not used and β_2 was deduced from a fit to the Monte Carlo data of [32] on the BCS side. Another difference with [90] is that we took the value $f'(0) = -0.95$, that we extracted from [34] using the relation (34). Also, we set the value of $f(0)$ to 0.41, which is within the error bars of [32], in order to reduce the spurious discontinuity of the second order derivative of $f(x)$ in $x = 0$ between the interpolation formula for $x < 0$ and the spline for $x > 0$. All this leads to $\alpha_1 \simeq 0.41, \alpha_2 \simeq 0.3756, \alpha_3 \simeq 1.062, \beta_1 \simeq 0.9043, \beta_2 \simeq 0.3797$.

A test of this interpolation formulation is to compare its prediction for $f'(-1)$ with the value $\simeq -0.13$ that one can extract from [34] using (34); one gets the satisfactory result $f'_S(-1) \simeq -0.14$.

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