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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 \cite{1} and \cite{2}) 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 \( k_F|a| = \infty \); where the gas acquires fully universal properties \cite{3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20}.

In this context, early theoretical studies \cite{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

\[
H_2 = \int d^3r \left\{ \sum_{\sigma = \uparrow, \downarrow} \psi_\sigma^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right] \psi_\sigma(r) + \psi_3^\dagger(r) \left[ E_0(B) - \frac{\hbar^2}{4m} \nabla^2 + U_0(r) \right] \psi_3(r) \right\} + A \int d^3r_1 d^3r_2 \chi(r_1 - r_2) \left\{ \psi_1^\dagger(r_1) \psi_1(r_2) / 2 \psi_\uparrow(r_1) \psi_\uparrow(r_2) + h.c. \right\} + g_0 \int d^3r_1 d^3r_2 d^3r_3 d^3r_4 \chi(r_1 - r_2) \chi(r_3 - r_4) \left\{ \delta \left( \frac{r_1 + r_2}{2} - \frac{r_3 + r_4}{2} \right) \psi_1^\dagger(r_1) \psi_1(r_2) \psi_1(r_3) \psi_1(r_4) \right\} \tag{1}
\]

where the atomic fields \( \psi_\sigma(r) \) obey the usual fermionic anticommutation relations and the field \( \psi_3(r) \) describing the closed-channel molecules obeys the usual bosonic commutation relations. \( A \) gives the coupling between the closed and open channels, with a short range cut-off function \( \chi(r) \), of range \( b \), and such that \( \int d^3r \chi(r) = 1 \). A typical value for \( b \) is in the nanometer range.\footnote{\( b \) can be estimated by the van der Waals length, that is the length that one forms with \( \ell_b \) and \( m \) and the \( C_6 \) coefficient of the van der Waals interaction.\cite{21}} 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 \( \chi \). The energy \( E_0 \) is the energy of a closed-channel molecule, in the absence of the coupling \( A \), 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
effective magnetic moment is

\[ \mu_b = \frac{dE_b}{dB}. \]  

(2)

\( U(r) \) and \( U_b(r) \) 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 2, 23, 24, 25, 26, 27, 28. In most unbiased Quantum Monte Carlo simulations, a lattice model is used:

\[ H_1 = \sum_r b^3 \left\{ \sum_{\sigma=1,\downarrow} \psi^\dagger_\sigma(r) \left[ -\frac{\hbar^2}{2m} \Delta + U(r) \right] \psi_\sigma(r) 
+ g_0 \psi^\dagger_\uparrow(r) \psi^\dagger_\downarrow(r) \psi_\downarrow(r) \psi_\uparrow(r) \right\}. \]

(3)

Here \( b \) is the lattice spacing (which coincides with the “range” of the discrete delta interaction potential), \( \Delta \) 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, the only magnetic field dependent part of the Hamiltonian can be calculated explicitly for the two-channel Hamiltonian \( H_2 \). For two-channel models, one has to impose the same conditions, not only for the interaction range \( b \) but also for the effective range \( \epsilon_k \) of a single particle with wavevector \( k \) 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 particles, a lattice model is used:

\[ \frac{1}{g} - 1 = \frac{\int_{-\pi/b,\pi/b} d^3k (2\pi)^3 1}{2\epsilon_k} \]

(4)

where \( g = 4\pi\hbar^2a/m \) is the effective coupling constant and \( \epsilon_k \) the energy of a single particle with wavevector \( k \) 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.

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where we have introduced the function giving the free space
scattering length as a function of \( B \),
\[
a_{hs}(B) = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right). \tag{10}
\]

Here \( a_{bg} \) is the background scattering length, \( B_0 \) is the
location of the Feshbach resonance in the absence of trap-
ing potential, \( \delta B_0 = |2U(0) - \nu_0(0)|/\mu_0 \) the shift of the
resonance location due to the trapping potential, and \( \Delta B \) the
resonance width.

Equation (8) is directly applicable at zero tempera-
ture. 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
\[
\frac{d\langle E \rangle}{d(1/a)} = \frac{dF}{d(1/a)} \left( \frac{dE}{d(1/a)} \right)_S \tag{11}
\]
where \( \langle \ldots \rangle \) 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
\[
\langle N_h \rangle = \frac{d\langle E \rangle}{d(1/a)} \frac{d(1/a)}{dB} \frac{1}{\rho_b}. \tag{12}
\]

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
\[
U(r) = U(0) + \frac{1}{2} m \sum_{\alpha=x,y,z} \omega_{\alpha}^2 r_{\alpha}^2, \tag{13}
\]
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
\[
k_B T_F = \frac{\hbar^2 k_F^2}{2m} = (3N)^{1/3} \bar{\hbar} \tag{14}
\]
where \( \bar{\omega} \) is the geometric mean of the three oscillation
frequencies \( \omega_\alpha \). 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 \cite{14} 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 de-
tailed 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 poten-
tial, due to \( U_b(r) \neq 2U(r) \), is expected to be negligible in the
zero-range limit, as argued in the appendix \cite{43}. Under
these assumptions, the local-density approximation for the
trapped gas leads to the universal form
\[
- \frac{dE}{d(1/a)} = \frac{\hbar^2 k_F}{m} N F \left( \frac{1}{k_F a} \right), \tag{15}
\]
where \( F \) is a dimensionless function, expressed in the
appendix \cite{43} in terms of the dimensionless universal function
\( f \) giving the energy per particle \( \epsilon_{hom} \) of the homogeneous
interacting gas:
\[
\epsilon_{hom} = \epsilon_0 f \left( \frac{1}{k_F \alpha a} \right), \tag{16}
\]
Here \( \epsilon_0 \) and \( k_F \) are the energy per particle and the
Fermi wavevector of the ideal Fermi gas with the same
total density \( n \) as the interacting gas:
\[
k_F = \frac{3}{2} \pi n \frac{\hbar}{m}, \tag{17}
\]
\[
\epsilon_0 = \frac{3}{10} \frac{\hbar^2 (k_F)^2}{m}. \tag{18}
\]
In the BEC regime \( 0 < k_F a \ll 1 \) we have
\[
f \left( \frac{1}{k_F \alpha a} \right) = - \frac{5}{3} \frac{1}{(k_F \alpha a)^2} \tag{19}
\]
\[
+ \frac{5}{18 \pi} k_F \alpha a \left[ 1 + \frac{128}{15 \sqrt{6} a^3} (k_F \alpha a)^3/2 \right] + \ldots
\]
where the first term comes from the dimer binding energy
\( h^2/(ma^2) \), 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
\[
a_d \simeq 0.60a. \tag{20}
\]
The local-density approximation then leads to
\[
F \left( \frac{1}{k_F a} \right) = \frac{1}{k_F a} + \frac{5^{2/5}}{2^{12/5}} \cdot \frac{1}{7} \frac{1}{a} (k_F a)^{2/5} + \ldots \tag{21}
\]
where we have omitted the Lee-Huang-Yang correction.
In the BCS limit \( 0 < -k_F a \ll 1 \), we have
\[
f \left( \frac{1}{k_F \alpha a} \right) = 1 + \frac{10}{9 \pi} (k_F \alpha a)^2
\]
\[
+ \frac{4(11 - 2 \ln 2)}{21 \pi^2} (k_F \alpha a)^2 + \ldots \tag{22}
\]
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
\[
\mathcal{F} \left( \frac{1}{k_F a} \right) = \frac{512}{945 \pi^2} (k_F a)^2 \left[ 1 + \frac{256}{35 \pi^2} - \frac{63 + 189 \ln 2}{1024} k_F a + \ldots \right].
\] (23)

Around the unitary limit \(1/(k_F a) \to 0\) we use the expansion
\[
f \left( \frac{1}{k_F a} \right) = \xi - \frac{\zeta}{k_F a} + \ldots,
\] (24)
which gives for the trapped gas:
\[
\mathcal{F}(0) = \frac{2 \pi}{27} \frac{\zeta}{\pi} \xi^{1/4} \simeq 0.28
\] (25)
where we took the estimates
\[
\xi \simeq 0.41 \quad \text{(26)}
\]
\[
\zeta \simeq 0.95 \quad \text{(27)}
\]
The estimate for \(\xi\) is obtained by averaging the predictions of \[32\] \((\xi = 0.42(1))\), of \[20\] \((\xi = 0.449(9))\), of \[33\] \((\xi = 0.42(1))\) and of \[27\] \((\xi = 0.37(5))\). The estimate for \(\zeta\) is obtained from the calculation of the short range pair correlation of \[34\], see subsection 5.1, 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. \[4\]

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 \[6\]. We first insert \[27\] into \[8\] which gives
\[
N_b = N k_F R_s \mathcal{F} \left( \frac{1}{k_F a} \right) \left( 1 - \frac{a a_F}{a} \right)^2 \] (28)
where the function \(\mathcal{F}\) is defined in \[15\]. The length \(R_s\) depends on the interchannel coupling and is related to the width of the Feshbach resonance as:
\[
R_s = \frac{\hbar^2}{m a_{bg} \mu_B \Delta B}.
\] (29)

For the \(B_0 \simeq 834\) G Feshbach resonance in \(^6\)Li, we have \(\mu_B \simeq 2 \mu_B\) where \(\mu_B\) is the Bohr magneton \[24\], \(\Delta B = -300\) G, \(a_{bg} = -1405 a_0\) where \(a_0 = 0.0529177\) nm is the Bohr radius \[56\]; this gives \(R_s \simeq 0.0269\) nm. From the Rice data for \(N_b/N\), using \[28\], we thus get values of \(\mathcal{F},\)

\[\text{Fig. 1. Derivative } -dE/d(1/a) \text{ of the energy } E \text{ of a trapped two-component Fermi gas, where } a \text{ is the } s\text{-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 24, 34 in the strongly interacting regime (see appendix D). Dashed lines: Analytical predictions in the weakly interacting regimes, on the BEC side 23 and on the BCS side 24. Cross: Result 29 at unitarity. Circles (with error bars): Experimental measurement of the number } N_b \text{ of closed-channel molecules in a lithium gas at Rice 5, combined with the present theory linking } dE/d(1/a) \text{ to } N_b \text{, see (28). (a): Linear scale on the vertical axis, (b): Logarithmic scale. } -dE/d(1/a) \text{ is expressed in units of } N_b^2 k_F/m\).\]
i.e. of $dE/d(1/a)$, that we compare in Fig.
6 to theoretical
predictions, given in the local-density approximation
either by the expansions of \( \rho \) in the weakly
interacting regime, or by \( \mathcal{H}_2 \) at the unitary limit, or by an interpolation
of the Monte Carlo results of \( \mathcal{H}_2 \) in the strongly
interacting regime (see appendix \( \mathcal{H} \) for details \( \mathcal{H} \)). The agreement is satisfactory, the experimental points being
scattered around the theoretical prediction. In particular, a possible shift \( \delta B_0 \) of the resonance location due to the
fact that \( U_0(r) \neq 2U(r) \), an effect not explicitly included in \( \mathcal{H} \) 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.\( \mathcal{H} \). For the considered broad resonance
of lithium, this is not surprising, see appendix \( \mathcal{H} \).

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 \( \mathcal{H} \) holds
at all times. Neglecting the slow off-resonant free-bound
photoassociation process \( \mathcal{H} \), we have

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

where \( \Omega^2/\gamma \) is the effective decay rate of the closed-channel
molecule, the Rabi frequency \( \Omega \) and the spontaneous emission
rate \( \gamma \) being defined in \( \mathcal{H} \).

Simple expressions can be obtained in limiting cases:
In the BEC limit, the dominant term of \( \mathcal{H} \) gives

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

in the unitary limit, \( \mathcal{H} \) gives

$$ N(t) = \frac{N(0)}{(1 + \Gamma_0 t/6)^2} ; \quad (32) $$

and in the BCS limit the dominant term of \( \mathcal{H} \) 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. \( \mathcal{H} \). We see that in general \( N(t) \) is

not an exponential function of time. For the last point on
the BCS side in \( \mathcal{H} \), the (unpublished) data for \( N(t) \) are
better fitted by Eq. \( \mathcal{H} \) than by an exponential; however
the value of \( \Gamma_0 \) resulting from this new fitting procedure
does not differ significantly from the published value \( \mathcal{H} \).

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 \( \mathcal{H} \), 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 \( \mathcal{H} \) and recently rederived in \( \mathcal{H} \), 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:

$$ - \left( \frac{d(E)}{d(1/a)} \right)_S = \frac{4\pi h^2}{m} \int d^3R \lim_{r \to 0} r^2 g_{11}(R + r/2, R - r/2) \quad (34) $$

where the pair distribution function is given by

$$ g_{11}(r_1, r_2) = \langle \psi_1^\dagger(r_1) \psi_1^\dagger(r_2) \psi_1(r_2) \psi_1(r_1) \rangle . \quad (35) $$

Since we are dealing here with a finite range interaction model,
we have taken a zero-range limit in \( \mathcal{H} \), introducing
the notation

$$ \lim_{r \to 0} \lim_{b \to 0} \quad (36) $$

Note that the order of the limits is important. The limit in \( \mathcal{H} \) is
reached for a distance \( r \) much smaller than \( |a| \), the mean distance between particles, and the thermal de Broglie wavelength \( \lambda \), 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 \( \mathcal{H} \), to the number of closed-channel molecules. Experimentally, the pair distribution function was measured \( \mathcal{H} \) via the photoassociation rate in a 1D Bose gas \( \mathcal{H} \), or simply by dropping the gas on a detector with high enough spatio-temporal resolution \( \mathcal{H} \). The possibility of measuring the pair distribution function in the BECS crossover was studied in \( \mathcal{H} \). In the unitary limit, by inserting into Eq. \( \mathcal{H} \) the value of \( \lim_{r \to 0} \lim_{b \to 0} \) calculated in \( \mathcal{H} \) with the fixed-node Monte Carlo technique, we get the value \( \mathcal{H} \) for the parameter \( \zeta \) defined in \( \mathcal{H} \).

The relation \( \mathcal{H} \) is the three-dimensional version of the relation
obtained in \( \mathcal{H} \) 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 \( \mathcal{H} \). Taking the
derivative of the gas eigenenergy $E$ with respect to the effective coupling constant $g = 4\pi\hbar^2a/m$, for a fixed lattice spacing $b$, the Hellmann-Feynman theorem gives
\[
\frac{d(E)}{dg} = \frac{dg_0}{dg} \left\{ \sum b^2\psi^{\dagger}_1\psi^{\dagger}_1\psi_1\psi_1 \right\} (37)
\]
where $g_0$ is a function of $g$ as given in (4), and where we used the relation $\langle dE/dg \rangle = \langle d(E)/dg \rangle S$ [cp. (1)]. 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 $\lambda$, the pair distribution function is dominated by two-body physics if $|r_1 - r_2| > \lambda$ (and also much smaller than $a$ in the BEC regime), a property contained in the Yvon-El [17] and Waldmann-Snider [18] ansatz of kinetic theory, which also appeared in the context of quantum gases [19, 20, 21, 22].

where $\phi$ 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 [4]
\[
|\phi(0)|^2 = \frac{d g}{d g_0},
\]
so that Eq. (38) simplifies to
\[
\frac{d(E)}{dg} \approx \sum b^2 C(r).
\]
On the other hand, at interparticle distances much larger than $b$, the zero-energy scattering wavefunction $\phi$ behaves as $1 - a/|r_1 - r_2| \leq b$, so that
\[
\lim_{r \to 0} r^2 g(r) = 0,
\]
so Eq. (39) thus leads to (40).

3.2 Tail of the momentum distribution

As was shown in [4] and recently rederived in [23], in the zero-range limit, the momentum distribution of the gas has a large momentum tail scaling as $1/k^4$, with a coefficient common to the two spin states and proportional to $-dE/d(1/a)$:
\[
\lim_{k \to +\infty} k^4 n_\sigma(k) = \frac{4\pi m}{\hbar^2} \left( \frac{d(E)}{d(1/a)} \right)_{S}
\]
where
\[
\lim_{k \to +\infty} = \lim_{k \to -\infty} \lim_{b \to 0}
\]
$\sigma = \uparrow $ or $\downarrow$ and the momentum distribution is normalized as
\[
\int d^3k k^4 n_\sigma(k) = \langle N_\sigma \rangle,
\]
where $\langle N_\sigma \rangle$ is the mean number of particle in the spin state $\sigma$. When combined with (6), 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 [22, 23, 24, 25], 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 [26, 27] and the signal to noise ratio for a fixed-node Monte Carlo calculations of $n_\sigma(k)$ performed in [26].

The relation (43) is a three-dimensional version of the relation derived for a one-dimensional Bose gas in [28]. 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 $k$ and a particle with a momentum $\sim -k$, so that at large $k$
\[
n_\sigma(k) \sim B |\tilde{\phi}(k)|^2
\]
where $B$ is momentum-independent and $\tilde{\phi}(k)$ is the Fourier transform $\sum r e^{-i k \cdot r} \phi(r)$ of the zero-energy two-body free space scattering state $\phi(r)$. For the contact interaction in the lattice model the two-particle Schrödinger’s equation takes the form [30]
\[
2\epsilon_k \tilde{\phi}(k) + g \phi(r = 0) = 0,
\]
where $\epsilon_k$ is the free wave dispersion relation in the lattice model, so that $\tilde{\phi}(k)$ drops as $1/\epsilon_k$ for large $k$, and the associated kinetic energy diverges for $b \to 0$. 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:
\[
E_{\text{kin}}[\text{gas}] \simeq B \cdot E_{\text{kin}}[\phi].
\]
Since the total energies have a finite limit for $b \to 0$, we can replace the kinetic energies by the opposite of the interaction energies in the above formula:
\[
E_{\text{int}}[\text{gas}] \simeq B \cdot E_{\text{int}}[\phi].
\]
The interaction energy of the gas is $g_0 \left( \sum_r b^\dagger_\sigma \psi^* \sigma \psi^* \right)$, equal to $(dE/d g) g_0 (d g/dg_0)$ according to (37). The interaction energy of a Fermi gas is simply $g_0 \phi(0)^2$, equal to $g_0 (d g/dg_0)$ according to (40). The common factor $g_0 (d g/dg_0)$ simplifies and

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

It remains to relate the coefficient $B$ to $\lim_{r \to +\infty} k^4 n_\sigma(k)$, using (44). In the zero-range limit, the scattering state $\phi(r)$ tends to $1 - a/r$, so that, by Fourier transform, $\phi(k)$ tends to $(2\pi)^4 \delta(k) - 4\pi a/k^2$. We then get (43).

4 Conclusion

We have calculated the number $N_\beta$ of closed-channel molecules in the whole BEC-BCS crossover for a two-component Fermi gas. Our work is in satisfactory agreement with the experimental results from Rice [5]. The expression (3) for $N_\beta$ 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 $N_\beta/N = k_F R, F(0)$ where $F(0)$ is a universal constant given in (45) and the length $R_*$ is related to the resonance parameters by (49); in the zero range and zero effective range limit where $k_F b \ll 1$ and $k_F r_0 \ll 1$ we have $k_F R_* \ll 1$ [see Eq. (45)], we thus confirm that $N_\beta \ll N$ i.e. the gas mainly populates the open channel. In the BCS limit, $-dE/d(1/a)$ and thus $N_\beta$ 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 [3]. This is also related to the fact that the BCS theory does not predict the correct short-distance pair correlations [75].

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 [3]. We thank A. Bulgac, F. Chevy, M. Colomé-Tatché, R. Hulet, M. Jona-Lasinio, F. Laloe, P. Naidon, S. Nascimbene, G. Partridge, L. Pricoupenko and C. Salomon for very useful discussions and comments, and G. Partridge et al. for providing us with the data of $\overline{\psi}$ in numerical form. Our group is a member of IFRAF.

Note: We became aware of the related work [57] while completing this paper, and of [80] 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 ($U_0(r) \equiv 0, U(r) \equiv 0$). The scattering problem may be considered in the center of mass frame so that we take the two-body scattering state

$$|\psi\rangle = \beta b^\dagger_0 |0\rangle + \int \frac{d^3k}{(2\pi)^3} A(k) a^\dagger_k |a^\dagger_k |0\rangle, \quad (51)$$

with the unknown amplitude $\beta$ in the closed channel and the unknown momentum dependent amplitude $A(k)$ in the open channel. The annihilation operators for the bosonic molecules, $b_\sigma$, and for the fermionic atoms $a_\sigma$, $\sigma = \uparrow$ or $\downarrow$, are the Fourier transforms of the corresponding field operators $\psi^\dagger_{\sigma}(r)$ and $\psi_{\sigma}(r)$, where the Fourier transform of a function $f(r)$ is $f(k) = \int d^3r \exp(-i k \cdot r) f(r)$. 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

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

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

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

We now specialize to a state corresponding to the scattering of a spin $\uparrow$ atom with incoming wavevector $k_0$ onto a spin $\downarrow$ atom with incoming wavevector $-k_0$, so that $E = \hbar^2 k_0^2/m$ is the energy of the incoming state. Eliminating $\beta$ in terms of $\gamma$ with (42) and using (53) leads to

$$A(k) = (2\pi)^3 \delta(k - k_0) + \frac{\gamma \tilde{\chi}(k)(g_0 + A^2/(E - E_0))}{E + i\delta + \hbar^2 k^2/m} \quad (55)$$

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 $+i\delta$ in
the denominator. Injecting (57) in (56) 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

\[ f_{k0} = \frac{-m\chi(k_0)^2/(4\pi\hbar^2)}{[g_0 + A^2/(\pi\hbar^2 - E_k)]^{-1} + \int \frac{d^3k}{(2\pi)^3} \frac{\chi^2(k)}{\pi^2 + \epsilon^2 + \epsilon f_{k0}}}. \]  

(56)

Since we are considering a s-wave Feshbach resonance, the function \( \chi(r) \) 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

\[ \chi(k) = \exp(-k^2b^2/2) \]  

(57)

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

\[ -\frac{1}{f_{iq}} = e^{-q^2b^2} \left[ \frac{4\pi\hbar^2/m}{g_0} + \frac{1}{b\sqrt{\pi}} \right] + q \text{erf}(gb) - q \]  

(58)

where the last term \(-q\) is imposed by the optical theorem and \text{erf} is the error function.

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

\[ \frac{1}{a} = \frac{4\pi\hbar^2/m}{g_0} - \frac{1}{b\sqrt{\pi}}. \]  

(59)

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

\[ \frac{1}{a_{bg}} = \frac{4\pi\hbar^2/m}{g_0} + \frac{1}{b\sqrt{\pi}}. \]  

(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

\[ E_b^0 = \frac{A^2}{g_0 + 4\pi\hbar^2b^2/2m}. \]  

(61)

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

\[ E_b(B) = E_b^0 + \mu_b(B - B_0), \]  

(62)

and introducing the (possibly negative) resonance width \( \Delta B \) such that

\[ \mu_b \Delta B = A^2 - E_b^0, \]  

(63)

we get from (59) exactly the B-field dependence (14) for the scattering length \( a \) in free space.

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

\[ r_e = -\frac{8\pi\hbar^4A^2/m^2}{(g_0E_b - A^2)^2} + \frac{4b}{\sqrt{\pi}} - \frac{2b^2}{a}. \]  

(64)

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

\[ r_e^{res} = -2R_e + \frac{4b}{\sqrt{\pi}}, \]  

(65)

where the length \( R_e \) is always non-negative,

\[ R_e = \left( \frac{A}{2\pi\hbar E_b^0} \right)^2. \]  

(66)

This definition of \( R_e \) agrees with Eq. (24).

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 \( a_{bg}, R_e \) rather than the bare parameters \( g_0, \Lambda \) of the Hamiltonian. The quantity \( E_b - A^2/g_0 \) appearing in [68] is conveniently rewritten using the quantity

\[ Q^2 \equiv \frac{m}{\hbar^2g_0} (g_0E_b - A^2) \]  

(67)

\[ = -\frac{1}{a_{bg}}R_e - 1 - a_{bg}/a \]  

(68)

which can be positive or negative. The ratio \( g_0/\Lambda \) is also easily eliminated with the identity

\[ \frac{g_0^2}{4\pi\Lambda^2} = R_e a_{bg}^2. \]  

(69)

Our final expression for the scattering amplitude is thus

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

(70)

i.e.

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

(71)

We deduce the effective range in terms of \( a, a_{bg}, R_e \) and \( b \):

\[ r_e = -2R_e(1 - a_{bg}/a)^2 + \frac{4b}{\sqrt{\pi}} - \frac{2b^2}{a}. \]  

(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

\[ kb \ll 1 \]  

(73)

\[ -\frac{1}{f_k} \simeq \frac{1}{a} + ik \]  

(74)
hold for $k \sim k_F$ and for $k \sim 1/a$ on the BEC side.  

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

$$- \frac{1}{f_k} = \frac{1}{a} + ik - \frac{1}{2} r_e k^2 + \ldots, \tag{75}$$

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

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

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 $|1 + ik| \geq 1$, we find that the condition (76) becomes equivalent to

$$k^2 R_e \left(1 - \frac{a \text{bg}}{a}\right)^2 \left| \frac{1}{a} + ik \right|^{-1} \ll 1. \tag{77}$$

A second condition is obtained by imposing that the higher order terms $\ldots$ in (74) 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.

$$k^2 |a_{\text{bg}}|/R_e \left|1 - \frac{a \text{bg}}{a}\right| \ll 1. \tag{78}$$

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 $^6$Li from $[\text{4}]$ reproduced in Fig.4 where $|k| > 250$ nm and $|a| > 200$ nm: using the values $|a_{\text{bg}}| = 74$ nm and $R_e = 0.027$ nm we find $|1 + ik| \geq 1$, $|1 + ik| \geq 1$, and $k^2 r_e/2 < 1/a$.

To be complete, let us point out that the conditions (73,77,78) are not strictly necessary since it is possible that the $\ldots$ in (73) 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 $q \approx 1/a$ so that the dimer energy is $\approx -\hbar^2/(2ma^2)$. For this last property, in the regime $b \ll a$, one directly gets from (74) the truly necessary condition

$$\left|1 - a_{\text{bg}}/a_{\text{bg}}\right|^{-1} + \left|1 - a_{\text{bg}}/a\right|^{-2}/R_e \gg 1. \tag{79}$$

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

$$a \gg R_e. \tag{80}$$

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

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

and we derive conditions for the gas to behave approximately as if we had $U_b(r) = 2U(r)$. Note that a significant deviation in (81) is not a priori excluded for the laser traps used e.g. in $[\text{23}]$ for lithium, with a laser wavelength $\lambda_L \approx 1 \mu$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 $\approx 0.6 \text{nm} - 1/\lambda_L$ in spectroscopic units $[\text{8}]$.

B.1 Position dependent scattering length and effective magnetic field

At the two-body level, $[\text{8}]$ leads to an effective position dependent scattering length for two opposite spin atoms. To define such a local scattering length around point $r_0$, we consider the “tangential” free space problem where the trapping potentials are replaced by the constant values $U_b(r_0)$ and $U(r_0)$ and we call $a(r_0)$ the resulting scattering length. We simply have to revisit the calculations of appendix A. In (72) one has to replace $E_b$ by $E_b + U_b(r_0)$ to include the trapping energy shift of the closed-channel molecule; similarly in (81) one has to replace $\hbar^2 k^2/m$ by $\hbar^2 k^2/m + 2U(r_0)$ to include the trapping energy shift of the two atoms; finally, for atoms with incoming wavevectors $\pm k_0$, the scattering state eigenenergy is now $E = \hbar^2 k^2/m + 2U(r_0)$. The net effect on the scattering amplitude $f_{b0}$ in (74) is to apply the substitution

$$E_b \longrightarrow E_b + U_b(r_0) - 2U(r_0), \tag{82}$$

so that $a(r_0)$ is simply obtained by applying (82) to (83).

A powerful interpretation of this substitution procedure may be given for a magnetic field independent $\mu_b$: We can rewrite the term $E_b(B) + U_b(r)$ appearing in (82) as $E_b[B_{\text{eff}}(r)] + 2U(r)$ provided we set

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

Thus we can replace $U_b(r)$ by $2U(r)$ in (82) provided we also replace the homogeneous magnetic field $B$ in (82) by the inhomogeneous effective magnetic field $B_{\text{eff}}(r)$. One then immediately obtains the position dependence of the scattering length,

$$a(r) = a_{b0}[B_{\text{eff}}(r)], \quad (84)$$

the function $a_{b0}(B)$ being given in (83).

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 \(-\mu N\) to the Hamiltonian \(H_2\), where \(\mu\) 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 \(\mu - U(r)\), in presence of the locally homogeneous magnetic field \(B_{\text{eff}}(r)\).

**B.2 Shift of the resonance location**

We now consider the case of an optical trap such as the one at Rice \([3]\): \(U(r)\) and \(U_b(r)\) 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:

\[
U_b(r) = 2(1 + \eta)U(r)
\]

(85)

where the dimensionless parameter \(\eta\) is a convenient measure of the relative deviation between \(U_b\) and 2\(U\). At large \(r\) 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 \(r = 0\), 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, \(U(r) \simeq U(0)\), we can temporarily forget about the spatial variation of \(B_{\text{eff}}\) and take \(B_{\text{eff}} \simeq B - \delta B_0\), where

\[
\delta B_0 = \frac{-U_b(0) + 2U(0)}{\mu_b} = -\frac{2\eta U(0)}{\mu_b}.
\]

(86)

Since the free space scattering length \(a_{bg}(B)\) only depends on the difference \(B - B_0\), replacing \(B\) by \(B_{\text{eff}}\) is equivalent to shifting the position \(B_0\) of the Feshbach resonance by the quantity \(\delta B_0\). Introducing the length \(R_s\) defined in \([24]\), the ratio of this shift to the width \(\Delta B\) of the Feshbach resonance may be written as

\[
\frac{\delta B_0}{\Delta B} = -\frac{2mU(0)}{\hbar^2}a_{bg}R_s\eta.
\]

(87)

In the Rice experiment, the trap depth \(-U(0)\) is at most \(k_B \times 2.71 \mu K\) \([39]\), so that we have

\[
\frac{\left|\frac{\delta B_0}{\Delta B}\right|}{\left|\eta\right|} < \frac{1}{7000}
\]

(88)

where we have used the values of \(a_{bg}\) and \(R_s\) given below \([24]\) and the mass of lithium. Except if \(\eta\) takes truly large values for the laser wavelength \(\lambda_L = 1064\) nm used in \([3]\), we expect only a small shift of the resonance location due to the laser trap, relative to the resonance width.

In \([3]\) the value of the scattering length as a function of \(B\) was calculated essentially from the free space formula \(a_{bg}(B)\) ignoring the shift \(\delta B_0\) due to the trap, and taking for the resonance location \(B_0\) the value measured in \([4]\) in a laser trap with different laser wavelength \(\lambda_L = 1030\) nm and intensity. On the contrary, our definition of \(a\) as a function of \(B\) includes the shift \(\delta B_0\), \(a = a_{bg}(B - \delta B_0)\), as already defined in \([4]\). This may introduce a systematic discrepancy between our theory curves and the experimental data in Fig. \([4]\), in the form of shifts of the abscissas of the experimental points. We thus define the horizontal shift

\[
\delta \left(\frac{1}{k_Fa}\right) = \frac{1}{k_Fa_{bg}(B - \delta B_0)} - \frac{1}{k_Fa_{bg}(B)} = \frac{\delta B_0}{\Delta B} \left(\frac{1}{k_Fa_{bg}} \frac{1}{1 - (1 - a_{bg}/a)^2}\right)
\]

(89)

To leading order in \(\eta\) (that is for \(\frac{\delta B_0}{\Delta B} \ll 1\), and using the fact that the data from \([4]\) reproduced in Fig. \([4]\) is sufficiently close to resonance to have \(1 - a_{bg}/a < 1\), this simplifies to:

\[
\delta \left(\frac{1}{k_Fa}\right) \simeq \frac{\delta B_0}{\Delta B} \frac{1}{k_Fa_{bg}}(1 - a_{bg}/a)^2.
\]

(90)

Using the parameters of the Rice experiment \([89]\) and Eq.\((77)\) this gives

\[
\left|\delta \left(\frac{1}{k_Fa}\right)\right| < \frac{|\eta|}{1000}.
\]

(91)

Even without knowing \(\eta\), we can thus reasonably expect that this shift is negligible on the scale of Fig. \([4]\), i.e. that

\[
\left|\delta \left(\frac{1}{k_Fa}\right)\right| \ll 1.
\]

(92)

This is also consistent with the fact that no systematic horizontal shift is apparent in Fig. \([4]\) between the experimental data and the theory curves.

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

We now discuss the effect on the many-body properties of the gas of the inhomogeneity of \(B_{\text{eff}}(r)\), that is of a spatial dependence of the scattering length \(a(r)\), see \([54]\), now taking into account the \(r\) dependence of \(U(r)\). We rewrite \((83)\) as

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

(93)

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

\[
\frac{1}{a(r) - a_{bg}} = \frac{1}{a - a_{bg}} - \frac{2mR_s}{\hbar^2} \left(U(r) - U(0)\right).
\]

(94)

where we recall that \(a\) is the scattering length in the trap center. Right on resonance, \(|a| = +\infty\), \(R_s\) is one of the contributions to the interaction effective range, see \([55]\), so that the zero-range limit implies \(k_F R_s \ll 1\). Since the typical value of \(U(r) - U(0)\) over the cloud size is of the order of \(\hbar^2 k_F^2 / 2m\), we see that the small parameter \(k_F R_s\)
appears in (23) so that we may expect that the position dependence of \( a(r) \) is negligible in the zero-range limit (for a fixed value of \( \eta \)).

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 \( |a(r)| \gg |a_{bg}| \) over the atomic cloud size. This implies that the excursion of \( B_\text{eff}(r) \) over the cloud size is small as compared to \( |\Delta B| \); since the excursion of \( U(r) \) over the laser trap size is at most \( |U(0)| \), 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 \( U(r) \), 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 (13) then reduces to

\[
\frac{1}{a(r)} \approx \frac{1}{a} - \frac{m R_a}{\hbar^2} m \omega^2 r^2,
\]

and the gas density profile \( n(r) \) is given by

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

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

\[
\mu - U(0) \approx k_B T_F = \hbar^2 k_F^2 / 2 m.
\]

Over the Thomas-Fermi radius \( R \), such that \( \frac{1}{2} m \omega^2 R^2 \approx k_B T_F \), we see that the relative change of \( 1/a(r) \) is negligible if

\[
|1 - a/a(R)| \approx (k_F |a|)/|\eta| k_F R_a \ll 1.
\]

This is satisfied in the zero-range limit, for fixed \( \eta \), according to the condition (72) written for \( k_F = k_F^* \).

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 \( \eta \), we define the local Fermi wavevector \( k_F^{\text{hom}}(r) \) using the unitary equation of state \( \mu^{\text{hom}}[n, 1/a] = \xi \hbar^2 (k_F^{\text{hom}})^2 / 2 m \), where \( k_F^{\text{hom}} \) is defined in (72), and using the value of the chemical potential \( \mu - U(0) = \sqrt{\xi} k_B T_F \). We obtain

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

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 \( \eta \) 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

\[
k_F^{\text{hom}}(R - l)|a(R - l)| = 1.
\]

Assuming \textit{a priori} \( l \ll R \) we obtain from (100)

\[
\frac{l}{R} \approx \frac{\xi^{3/2}}{2}(\eta k_F R_a)^2.
\]

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

\[
|\eta| k_F R_a \ll 1.
\]

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

\[
\mu^{\text{hom}}[n(r), 1/a(r)] \approx -\frac{\hbar^2}{2 m \omega^2(r)} + \frac{\pi n^2}{3 m a(r)}
\]

where \( \alpha \approx 0.60 \) is the proportionality factor in (24) between the dimer-dimer scattering length \( a_d \) and \( a \). In particular, this requires \( a \gg R_a \), see (83). Replacing \( 1/a(r) \) by (80) 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

\[
U_{\text{eff}}(r) \equiv U(r) - \frac{\hbar^2}{2 m a^2(r)}
\]

\[
= U_{\text{eff}}(0) + \frac{1}{2} \omega_{\text{eff}}^2 r^2 - \frac{m (\eta R_a)^2}{4 \hbar^2} \left( m \omega^2 r^2 \right)^2
\]

We see that the atomic oscillation frequency is renormalized into

\[
\omega_{\text{eff}} = \left( 1 + \frac{2 \eta R_a}{a} \right)^{1/2} \omega.
\]

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

\[
|\eta| R_a/a \ll 1,
\]

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 \( k = k_F \). Second we require that the \( r^2 \)-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 \( \eta \); we reach the second condition

\[
\frac{m (\eta R_a)^2}{4 \hbar^2} \left( m \omega^2 r^2 \right)^2 \left( \frac{5}{64} k_F a_d \right)^{2/5} \ll 1.
\]

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 spatially inhomogeneity of \( a(r) \) in the mean field term
\[ \frac{\pi \hbar^2}{(2m)} \alpha a(r) n(r) \text{ has a small impact on the density profile:} \]
\[ |1 - a/a(R)| \simeq (k_F a)(|\eta| k_F R_c) \left( \frac{5}{64} k_F a_d \right)^{2/5} \ll 1, \tag{109} \]
which is also implied by (107).

To summarize, discussing perturbatively the effect of the position dependence of \( B_{\text{eff}}(r) \) on the gas density profile in the local density approximation, we find close to the Feshbach resonance \(|a| \gg |a_{bg}|\), and also \( a \gg R_c \) in the BEC regime) that the effect is small under the condition (108) 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 \( \eta k_F R_c \xi^{1/2} \) to the quantity \( \delta(1/k_F a) \) introduced in the previous subsection:
\[ |\eta| k_F R_c \xi^{1/2} \simeq \delta \left( \frac{1}{k_F a} \right) \left( \frac{\mu - U(0)}{U(0)} \right). \tag{110} \]

Experimentally, the gas is confined at the bottom of the laser trap so that \(|\mu - U(0)|/|U(0)| \ll 1 \) (its value near unitarity at Rice is 0.15 \( \xi \)). Together with the assumption (103) this implies that the right-hand-side of (110) is \( \ll 1 \), and that the position dependence of \( a(r) \) 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 \( \eta \). To this end, one simply expands (97) to first order in \( \eta \) around the solution \( n_0(r) \) with \( \eta = 0 \), writing to first order \( n(r) = n_0(r) + \delta n(r) \) and \( \mu = \mu_0 + \delta \mu \):
\[ \delta n(r) = \frac{\delta \mu}{\partial \mu_{\text{hom}}[n_0(r), 1/a]} |\partial_{\mu_{\text{hom}}}[n_0(r), 1/a]| \]
where we have introduced the variation of \( 1/a(r) \) around \( \eta = 0 \) to first order in \( \eta \), not supposing \( |a(r)| \gg |a_{bg}| \) in (10):
\[ \delta \left( \frac{1}{a} \right) (r) = - \left( 1 - \frac{a_{bg}}{a} \right)^2 \frac{m R_c}{\hbar^2} m \omega^2, \tag{111} \]
where \( \delta \mu \) is then determined by the condition of a fixed number of particles \( \int_{r < R_0} d^3 r \delta n(r) = 0 \), where \( R_0 \) is the Thomas-Fermi radius of the gas for \( \eta = 0 \). In this way, taking the variation of (103) to first order in \( \eta \) around \( \eta = 0 \), one can calculate the effect of a non-uniformity of \( a(r) \) on \( dE/d(1/a) \) to first order in \( \eta \). We give here the result for the unitary gas:
\[ \frac{\delta [dE/d(1/a)]}{dE/d(1/a)} \bigg|_{\eta = 0} = \eta k_F R_c \left[ \frac{64}{25 \pi} - \frac{63 \pi}{256} \right] \xi^{-1/2} \xi \]
\[ + \frac{315 \pi}{2048} \xi^{3/4} \xi^{-1} f(0) + \frac{2}{3} \xi^{1/2} k_F a_{bg} \], \tag{113} \]
where we recall that \( \xi = f(0), \xi = -f'(0), \text{ see (24)}, \) and \( f(0) \) is the second order derivative of \( f(x) \) with respect to \( x = 0 \). Note that, in this first order variation with respect to \( \eta \), the trapping potential \( U(r) \) 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 \( U_b(r)/U(r) \) may give access to \( f(0) \). It also shows that, in the unitary limit, the condition to neglect \( a_{bg} \) with respect to \( a(r) \) as done in the qualitative reasoning around (102), is \( k_F |a_{bg}| \ll 1 \).

### 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
\[ \Delta E = - \frac{\hbar^2}{m a_0^2 \xi} - 2\mu \tag{114} \]
where \( \mu \) 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 the gas has the usual Thomas-Fermi density profile and is weakly affected by the position dependence of \( B_{\text{eff}}(r) \), 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 \( \mu \simeq U(0) \) in the negative-\( a \) regime and \( \mu \simeq U(0) - \hbar^2/(2ma^2) \) in the BEC regime. We also make the simplifying assumption \( a(\infty) \gg |a_{bg}| \)
so that (13) reduces to
\[ \frac{1}{a(\infty)} \simeq \frac{1}{a} + 2 \pi \frac{m R_c}{\hbar^2} U(0). \tag{115} \]

In the BEC regime one easily deduces
\[ \frac{\Delta E}{2|U(0)|} \simeq 1 + A - B \tag{116} \]
where
\[ A \equiv 2 \pi \frac{R_c}{a} \tag{117} \]
\[ B \equiv 2 \pi^2 \frac{m R_c^2}{\hbar^2} |U(0)|; \tag{118} \]

since we already assumed (103) we automatically have \( |A| \ll 1 \). In the negative-\( a \) regime, Eq. (115) immediately gives an upper bound on \( 1/a(\infty) \), from which we get
\[ \frac{\Delta E}{2|U(0)|} \gtrsim 1 - B. \tag{119} \]
In both regimes we conclude that under the condition
\[ |\mathcal{B}| \ll 1 \]  
(120)
we have \( \Delta E \gtrsim 2|U(0)| \) so that the process is energetically forbidden.

Finally we note that under the assumption \( |a| \gg |a_b| \) we have from (23)
\[ \delta \left( \frac{1}{k_F a} \right) \simeq \eta k_F R_a \frac{|U(0)|}{k_B T_F} \]  
(121)
so that
\[ \mathcal{B} \simeq \left| \delta \left( \frac{1}{k_F a} \right) \right|^2 \frac{k_B T_F}{|U(0)|} \]  
(122)
In a typical experiment such as the one at Rice we have \( k_B T_F < |U(0)| \); 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 (22).

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 \( U_b(r) \neq 2U(r) \). As explained in the appendix B, where an effective position dependent magnetic field \( B_{\text{eff}}(r) \) is introduced, this leads to a position dependent scattering length \( a(r) \).

As a consequence, in the local density approximation, here at zero temperature, the gas density \( n(r) \) is given by
\[ \mu = U(r) + \mu_{\text{hom}}[n(r), 1/a(r)] \]  
(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
\[ E = \int d^3r \left\{ U(r) + \epsilon_{\text{hom}}[n(r), 1/a(r)] \right\} n(r) \]  
(124)
\[ N = \int d^3r n(r) \]  
(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 \( r = 0 \), 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 \( \delta n(r) \) of the density, that may be calculated from (123) but this is not required here. This also leads to a variation of \( 1/a(r) \), according to (23):
\[ \delta \left( \frac{1}{a(r)} \right) = \left( \frac{1 - a_{bg}/a(r)}{1 - a_{bg}/a} \right)^2 \delta \left( \frac{1}{a} \right). \]  
(126)
The variation of the gas energy is then
\[ \delta E = \int d^3r \delta n(r) \left[ U(r) + \epsilon_{\text{hom}}[n(r), 1/a(r)] \right] + n(r) \frac{\partial \mu_{\text{hom}}}{\partial n} \frac{1}{a(r)} \]  
(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
\[ n \frac{\partial \mu_{\text{hom}}}{\partial n} [n, 1/a] = \mu_{\text{hom}}[n, 1/a] - \epsilon_{\text{hom}}[n, 1/a]. \]  
(128)
Using this expression and (124), one finds that a simplification occurs in (127). Furthermore, the fact that the particle number is fixed imposes
\[ \int d^3r \delta n(r) = 0 \]  
(129)
so that (127) leads to
\[ \left( \frac{dE}{d(1/a)} \right)_N = \int d^3r n(r) \left( \frac{1 - a_{bg}/a}{1 - a_{bg}/a} \right)^2 \times \frac{\partial \mu_{\text{hom}}}{\partial (1/a)} [n(r), 1/a(r)]. \]  
(130)
We note that an alternative derivation of this result is possible: One can introduce the density of closed-channel molecules \( n_{bg} \) of 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 (6) to a free space system. Then setting for the trapped system in the local density approximation \( N_b = \int d^3r n_{bg}(r, 1/a(r)) \) and using (6) 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 \( a(r) \) under conditions discussed in the appendix B. Then \( \epsilon_{\text{hom}} \) is given by the relation (6) involving some universal function \( f(x) \). For the free space chemical potential we then introduce the convenient parametrization
\[ \mu_{\text{hom}}[n, 1/a] = \frac{\hbar^2}{2ma^2} u \left( \frac{1}{k_F^{\text{hom}} a} \right) \]  
(131)
where \( k_F^{\text{hom}} = (3\pi^2 n)^{1/3} \) is the ideal gas Fermi wavenumber, and the function \( u \) is
\[ u(x) = \frac{f(x) + \frac{1}{2} x f'(x)}{x^2} \]  
(132)
One also restricts to a harmonic trap for \( U(r) \), see (6). The surface \( n(r) = 0 \) is then an ellipsoid with Thomas-Fermi radii \( R_\alpha \) along the directions \( \alpha \).
For $a < 0$ we set
\[ \mu = \frac{\hbar^2 q^2}{2m} \] (133)
with $q > 0$. Then $\omega_n R_n = \hbar q/m$, and the density depends only on $X \geq 0$ such that $X^2 = \sum \omega_n^2 R_n^2$. Equation (132) then reduces to the implicit equation
\[ q^2 a^2 (1 - X^2) = u \left[ \frac{1}{k_{F\text{hom}}(X)/a} \right] \] (134)
that one can solve numerically, using the interpolation for $f(x)$ given in appendix [3].

For $a > 0$, $\mu_{\text{hom}}[n, 1/a]$ tends to $-\hbar^2/(2ma^2)$ for $n \to 0$ so that we set
\[ \mu = \frac{\hbar^2 q^2}{2ma^2} - \frac{\hbar^2}{2ma^2} \] (135)
with $q > 0$. Then again $\omega_n R_n = \hbar q/m$, and (123) reduces to
\[ q^2 a^2 (1 - X^2) = 1 + u \left[ \frac{1}{k_{F\text{hom}}(X)/a} \right] \] (136)
to be solved numerically in general.

One can then calculate $dE/d(1/a)$ and $k_F$ defined in (4) from the expressions valid on both sides of the resonance:
\[ \frac{dE}{d(1/a)} \left( \frac{1}{k_{F\text{hom}}} \right) = \frac{3\pi \hbar^4}{10m} \int_0^1 dX X^2 k_{F\text{hom}}(X)^4 f' \left( \frac{\mu}{k_{F\text{hom}}(X)/a} \right) \] (137)
\[ k_F = \frac{\sqrt{2\pi}}{\pi^{1/3}} \left[ 4\pi \int_0^1 dX X^2 k_{F\text{hom}}(X)^3 \right]^{1/6} \] (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 [22] with values of $x = 1/(k_F a)$ equal to 0, 1, 2, 4, and 6, using the last column of Table I (the one said to give $E/N - c_0/2$) 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 (14).

On the BCS side of the resonance we used the empirical interpolation formula of [20].
\[ f_S(x) = \alpha_1 - \alpha_2 \arctan[\alpha_3 x (\beta_1 - x)/(\beta_2 - x)]. \] (139)

Constraints on $\alpha_1, \alpha_2, \alpha_3$ and $\beta_1, \beta_2$ 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 [20] where the coefficient $c_2$ was not used and $\beta_2$ was deduced from a fit to the Monte Carlo data of [32] on the BCS side. Another difference with [20] is that we took the value $f'(0) = -0.95$, that we extracted from [32] using the relation (14). Also, we set the value of $f(0)$ to 0.41, which is within the error bars of [22] 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 $\alpha_1 \approx 0.41, \alpha_2 \approx 0.3756, \alpha_3 \approx 1.062, \beta_1 \approx 0.9043, \beta_2 \approx 0.3707$.

A test of this interpolation formulation is to compare its prediction for $f_S'(1)$ with the value $z = -0.13$ that one can extract from [20] using (14); one gets the satisfactory result $f_S'(1) = -0.14$.

### References

89. R. Hulet, private communication