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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)].

**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]) 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 [5,6,7,8,9,10,11,12,13,14].

In this context, early theoretical studies [15,16] 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

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

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.  $U(\mathbf{r})$  and  $U_b(\mathbf{r})$  are the trapping potentials experienced by the atoms and the closed channel molecules respectively.  $\Lambda$  gives the coupling between the closed and open channels, with a short range cut-off function  $\chi(\mathbf{r})$ , of range  $b$ . A typical value for  $b$  is in the nanometer range<sup>1</sup>. The coupling constant  $g_0^{(\text{bg})}$  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  $E_b$  is the energy of a closed channel molecule, in the absence of the coupling  $\Lambda$ , 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

<sup>1</sup>  $b$  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 [17].

moment is

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

On the contrary, recent Monte-Carlo simulations of the many-body problem in the BEC-BCS crossover simply use single channel model Hamiltonians. In unbiased Quantum Monte-Carlo simulations a lattice model is used [18, 19, 20, 21, 22]

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

where  $\Delta$  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 [20, 21, 23, 24],

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

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  $\mathbf{k}$ . In fixed node Monte-Carlo calculations, one rather uses an interaction potential in continuous real space, e.g. a square well potential [25, 26, 27, 28, 29, 30].

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  $k_F b \ll 1$  and  $b \ll \lambda$ , where  $k_F$  is the Fermi wavevector and  $\lambda$  is the thermal de Broglie wavelength; for  $a > 0$  one adds the assumption  $b \ll a$ . For two channel models, the zero range limit is defined by the same assumptions, 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 [31, 32]).

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, which was recently measured at Rice using laser molecular excitation techniques [33].

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 [26] within a single channel model, in order to predict  $N_b$  in the cross-over 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 [34, 35], 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  $a$  rather than  $B$ :

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

The function  $a(B)$  can be calculated explicitly for  $H_2$ , solving the zero energy two-body scattering problem in free space, and takes the form

$$a(B) = a_{\text{bg}} \left( 1 - \frac{\Delta B}{B - B_0} \right) \quad (9)$$

with  $a_{\text{bg}}$  the background scattering length,  $B_0$  the location of the Feshbach resonance and  $\Delta B$  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 [36]

$$\left\langle \frac{dE}{d(1/a)} \right\rangle = \left( \frac{dF}{d(1/a)} \right)_T = \left( \frac{d\langle E \rangle}{d(1/a)} \right)_S \quad (10)$$

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

$$\langle N_b \rangle = \left( \frac{d\langle E \rangle}{d(1/a)} \right)_S \frac{d(1/a)}{dB} \frac{1}{\mu_b}. \quad (11)$$

Under the assumptions of the zero range limit detailed in the introduction, the function  $E(1/a)$  is universal, i.e. model independent, and one can use a single channel Hamiltonian such as  $H_1$  to calculate it and to access the mean number of closed channel molecules.<sup>2</sup>

<sup>2</sup> In particular, on the BEC side, we shall stay sufficiently close to the resonance to have  $a$  much larger than the van der

## 2.2 Analytical results in a trap in limiting cases

We now restrict to a gas at zero temperature (or at temperatures much smaller than the Fermi temperature  $T_F$ ), in a harmonic trap

$$U(\mathbf{r}) = \frac{1}{2}m \sum_{\alpha=x,y,z} \omega_\alpha^2 r_\alpha^2, \quad (12)$$

in the macroscopic regime where  $k_B T_F$  is much larger than the oscillation quanta  $\hbar\omega_\alpha$ . We thus use the local density approximation, which is expected to be asymptotically exact in the large  $N$  limit. We also restrict to the balanced case where the number of atoms is equal to  $N/2$  in each spin component. The Fermi energy is then defined as the zero temperature chemical potential of the trapped ideal gas in the large  $N$  limit,

$$k_B T_F = \frac{\hbar^2 k_F^2}{2m} = (3N)^{1/6} \hbar \bar{\omega} \quad (13)$$

where  $\bar{\omega}$  is the geometric mean of the three oscillation frequencies  $\omega_\alpha$ . Within the local density approximation we have the general form

$$-\frac{dE}{d(1/a)} = \frac{\hbar^2 k_F^2}{m} N \mathcal{F} \left( \frac{1}{k_F a} \right), \quad (14)$$

where  $\mathcal{F}$  is a dimensionless function.

In the BEC regime  $0 < k_F a \ll 1$ , a mean field calculation of  $E$  is possible: Apart from the dimer binding energy  $\hbar^2/(ma^2)$ , the chemical potential of the homogeneous gas contains a mean field interaction energy among the dimers, proportional to the dimer-dimer scattering length  $a_d$  [38, 39, 40, 41, 42]. The solution of the 4-fermion problem gives [43, 44]

$$a_d \simeq 0.60a. \quad (15)$$

The local density approximation then leads to

$$\mathcal{F} \left( \frac{1}{k_F a} \right) = \frac{1}{k_F a} + \frac{5^{2/5}}{2^{12/5} \cdot 7} \left( \frac{a_d}{a} \right)^{2/5} (k_F a)^{7/5} + \dots \quad (16)$$

In the BCS limit  $0 < -k_F a \ll 1$ , the chemical potential of the homogeneous gas contains, in addition to the ideal gas Fermi energy, the Hartree-Fock mean field term proportional to  $a$ , so that

$$\mathcal{F} \left( \frac{1}{k_F a} \right) = \frac{2^9}{3^3 \cdot 5 \cdot 7 \cdot \pi^2} (k_F a)^2 + \dots \quad (17)$$

In the unitary limit one needs an expansion of the energy per particle  $\epsilon^{\text{hom}}$  of the homogeneous gas in powers of  $1/a$ . We set

$$\epsilon^{\text{hom}} = \epsilon_0^{\text{hom}} f \left( \frac{1}{k_F^{\text{hom}} a} \right) \quad (18)$$

where  $\epsilon_0^{\text{hom}}$  is the energy per particle of the homogeneous gas with the same density  $n$  and than the effective range  $r_e$ , so that the binding energy of the dimer is given by the universal expression  $\hbar^2/(ma^2)$ . Further away from resonance in the weakly interacting BEC regime, more detailed theories for the dimer wavefunction give good agreement with the Rice measurements [17, 33, 37].

where  $\epsilon_0^{\text{hom}}$  and  $k_F^{\text{hom}}$  are the energy per particle and the Fermi wavevector of the ideal Fermi gas with the same density  $n$ :

$$k_F^{\text{hom}} = (3\pi^2 n)^{1/3} \quad (19)$$

$$\epsilon_0^{\text{hom}} = \frac{3}{10} \frac{\hbar^2 (k_F^{\text{hom}})^2}{m}. \quad (20)$$

Introducing the expansion

$$f \left( \frac{1}{k_F^{\text{hom}} a} \right) = \xi - \frac{\zeta}{k_F^{\text{hom}} a} + \dots, \quad (21)$$

we obtain for the trapped gas:

$$\mathcal{F}(0) = \frac{2^7}{5^2 \cdot 7 \cdot \pi} \frac{\zeta}{\xi^{1/4}} \simeq 0.27 \quad (22)$$

where we took the estimates

$$\xi \simeq 0.43 \quad (23)$$

$$\zeta \simeq 0.95. \quad (24)$$

The estimate for  $\xi$  is obtained by averaging the predictions of [26] ( $\xi = 0.42(1)$ ), of [22] ( $\xi = 0.449(9)$ ) and of [27] ( $\xi = 0.42(1)$ ). The estimate for  $\zeta$  is obtained from the calculation of the short range pair correlation of [28], 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 [26] by approximating the derivative by a two-point formula.

## 2.3 Comparison to Rice experiment

At Rice [33] 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.

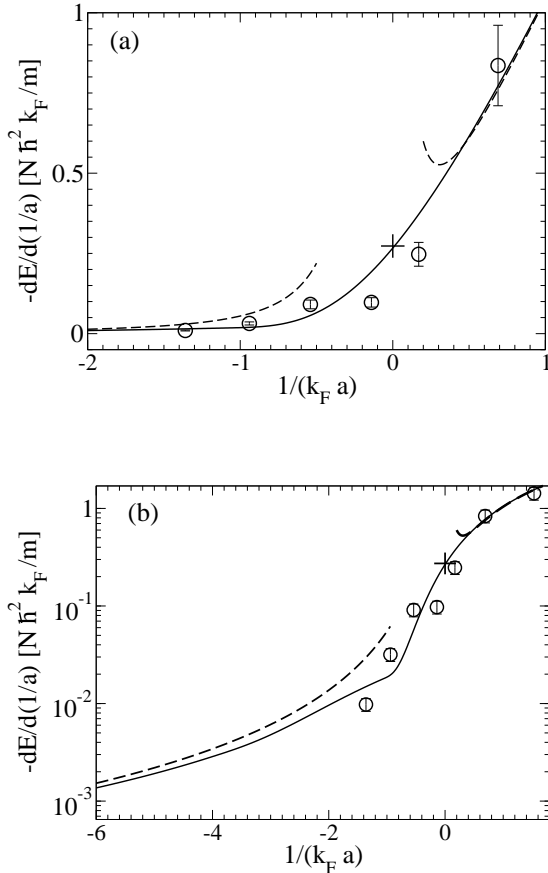
We now compare the Rice results to our prediction (8). We first insert (9) into (8) which gives

$$N_b = N k_F R_* \mathcal{F} \left( \frac{1}{k_F a} \right) \left( 1 - \frac{a_{\text{bg}}}{a} \right)^2 \quad (25)$$

where the function  $\mathcal{F}$  is defined in (14). The length  $R_*$  depends on the interchannel coupling and is related to the width of the Feshbach resonance as:

$$R_* = \frac{\hbar^2}{m a_{\text{bg}} \mu_b \Delta B}. \quad (26)$$

For the  $B_0 \simeq 83.4\text{mT}$  Feshbach resonance in  ${}^6\text{Li}$ , we have  $\mu_b \simeq 2\mu_B$  where  $\mu_B$  is the Bohr magneton [17],  $\Delta B = -30\text{mT}$ ,  $a_{\text{bg}} = -1405$  Bohr radii [45]. From the Rice data for  $N_b/N$ , using (25), 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 (16,17) in the weakly interacting regime, or by (22) at the unitary limit, or by an interpolation of



**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 Galitskii and Lee-Huang-Yang [38, 39, 40, 41] formulas in the weakly interacting regimes with a spline interpolation of the fixed node Monte-Carlo results of [26] in the strongly interacting regime. Dashed lines: Analytical predictions in the weakly interacting regimes, on the BEC side (16) and on the BCS side (17). Cross: Result (22) at unitarity. Circles (with error bars): Experimental measurement of the number  $N_b$  of closed channel molecules in a lithium gas at Rice [33], combined with the present theory linking  $dE/d(1/a)$  to  $N_b$ , see (25). (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.

the Monte-Carlo results of [26] in the strongly interacting regime<sup>3</sup>. The agreement is satisfactory, the experimental points being scattered around the theoretical prediction.

<sup>3</sup> We applied a cubic spline interpolation to the points of [26] with integer values of  $x = 1/k_F^{\text{hom}} a$  in between  $-2$  and  $6$ , adding home made points of abscissa  $-4$  and  $8$  where the values of the function  $f$  and its first order derivatives are obtained from the weakly interacting Galitskii and Lee-Huang-Yang expansions. These expansions are also used for  $x < -4$  and  $x > 8$ . The values of  $f$  in  $x = -1$  and  $x = 0$  were shifted

Our approach even allows to predict the time evolution of the atom number, in presence of the depleting laser, under the assumption that the molecular depletion rate is so weak that the equilibrium relation (25) holds at all times. Neglecting the slow off-resonant free-bound photoassociation process [33], we have

$$\frac{dN}{dt} = -2N_b(t) \frac{\Omega^2}{\gamma} \quad (27)$$

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 [33]. Simple expressions can be obtained in limiting cases: In the BEC limit, the dominant term of the expansion (16) gives

$$N(t) = N(0) e^{-\Gamma_0 t}; \quad (28)$$

in the unitary limit, (22) gives

$$N(t) = \frac{N(0)}{(1 + \Gamma_0 t/6)^6}; \quad (29)$$

and in the BCS limit (17) gives

$$N(t) = \frac{N(0)}{(1 + \Gamma_0 t/2)^2}. \quad (30)$$

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. (25,27). We see that in general  $N(t)$  is not an exponential function of time. We thus propose to reanalyze the data for  $N(t)$  obtained at Rice: E.g. at unitarity, the data should be fitted by (29), rather than by an exponential as was done in [33].

## 3 Related observables

### 3.1 Short range pair correlations

As was shown in [34] and recently rederived in [46], 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:

$$-\frac{dE}{d(1/a)} = \frac{4\pi\hbar^2}{m} \int d^3\mathbf{R} \lim_{r \rightarrow 0} r^2 g_{\uparrow\downarrow}(\mathbf{R}+\mathbf{r}/2, \mathbf{R}-\mathbf{r}/2) \quad (31)$$

where the pair distribution function is given by

$$g_{\uparrow\downarrow}(\mathbf{r}_1, \mathbf{r}_2) = \langle \psi_{\uparrow}^{\dagger}(\mathbf{r}_1) \psi_{\downarrow}^{\dagger}(\mathbf{r}_2) \psi_{\downarrow}(\mathbf{r}_2) \psi_{\uparrow}(\mathbf{r}_1) \rangle. \quad (32)$$

upwards by 0.01 (within the error bars given in [26]) to improve the agreement between the spline and the values of  $f$  in the non-integer  $x$  values of [26]. The resulting spline is then almost within all error bars of [26]. To eliminate a spurious cusp in  $f'(x)$  in  $x = -4$ , we shift  $f(-2)$  by  $-0.005$ , which is within the error bars of [26]. The rapid variation of the slope of our result on Fig. 1(b) near  $1/(k_F a) = -1$  may be due to residual imperfections of our interpolation.

Since we are dealing here with finite range interaction models, we have taken a zero range limit in (31), introducing the notation

$$\tilde{\lim}_{r \rightarrow 0} = \lim_{r \rightarrow 0} \lim_{b \rightarrow 0}. \quad (33)$$

Note that the order of the limits is important. In a real gas, in a degenerate regime, the limit in (31) is reached for a distance  $r$  much smaller than  $|a|$  and the mean distance between particles, 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 [47, 48], or simply by dropping the gas on a detector with high enough spatio-temporal resolution [49, 50, 51]. The possibility of measuring the pair distribution function in the BEC-BCS crossover was studied in [28, 52]. In the unitary limit, by inserting into Eq.(31) the value of  $\tilde{\lim}_{r \rightarrow 0} r^2 g_{\uparrow\downarrow}$  calculated in [28] with the fixed node Monte-Carlo technique, we get the value (24) for the parameter  $\zeta$  defined in (21).

The relation (31) is the three-dimensional version of the relation obtained in [53] 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 (31). For concreteness we take the lattice model (3), even if the reasoning also applies for a continuous space model. Taking the derivative of the gas eigenenergy  $E$  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

$$\frac{dE}{dg} = \frac{dg_0}{dg} \left\langle \sum_{\mathbf{r}} b^3 \psi_{\uparrow}^{\dagger} \psi_{\downarrow}^{\dagger} \psi_{\downarrow} \psi_{\uparrow} \right\rangle \quad (34)$$

$$= \frac{dg_0}{dg} \sum_{\mathbf{r}} b^3 g_{\uparrow\downarrow}(\mathbf{r}, \mathbf{r}), \quad (35)$$

where  $g_0$  is a function of  $g$  as given in (4). In a gas, with an interaction range much smaller than the mean distance  $\sim 1/k_F$  between particles, 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 also much smaller than  $a$  in the BEC regime), a property contained in the Yvon [54] and Waldmann-Snyder [55] ansatz of kinetic theory, and also apparent in the context of quantum gases [28, 56, 57, 58]:

$$g_{\uparrow\downarrow}(\mathbf{r}_1, \mathbf{r}_2) \simeq C \left( \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right) |\phi(\mathbf{r}_1 - \mathbf{r}_2)|^2 \quad (36)$$

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 <sup>4</sup>

$$|\phi(\mathbf{0})|^2 = \frac{dg}{dg_0}, \quad (37)$$

<sup>4</sup> 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

so that Eq.(35) simplifies to

$$\frac{dE}{dg} \simeq \sum_{\mathbf{r}} b^3 C(\mathbf{r}). \quad (38)$$

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

$$\tilde{\lim}_{r \rightarrow 0} r^2 g_{\uparrow\downarrow}(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2) = a^2 C(\mathbf{R}). \quad (39)$$

Eq.(38) thus leads to (31).

### 3.2 Tail of the momentum distribution

As was shown in [35] and recently rederived in [46], 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  $-dE/d(1/a)$ :

$$\tilde{\lim}_{k \rightarrow +\infty} k^4 n_{\sigma}(k) = -\frac{4\pi m}{\hbar^2} \frac{dE}{d(1/a)} \quad (40)$$

where

$$\tilde{\lim}_{k \rightarrow +\infty} = \lim_{k \rightarrow +\infty} \lim_{b \rightarrow 0}, \quad (41)$$

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

$$\int \frac{d^3 k}{(2\pi)^3} n_{\sigma}(\mathbf{k}) = N_{\sigma}, \quad (42)$$

where  $N_{\sigma}$  is the mean number of particles in the spin state  $\sigma$ . In practice, the limit in (40) is reached in a degenerate gas for  $k \gg k_F$  (and also  $k \gg a$  on the BEC side) while keeping  $k \ll 1/b$ . 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 [59, 60, 61], 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 [59, 62] 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 relation (40) is a three-dimensional version of the relation derived for a one-dimensional Bose gas in [63]. We now present a very simple rederivation of (40).

In a gas with short range interactions, i.e.  $b \ll 1/k_F$  in the degenerate regime (and  $b \ll a$  on the BEC side), the tail of the momentum distribution is dominated by binary

“mean-field” shift  $E_{\text{box}} = g/L^3$ . The Hellmann-Feynman theorem (34) then gives the result (37). An alternative derivation is to directly calculate  $\phi$  in Fourier space [see (44)] 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 (37).

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

$$n_\sigma(\mathbf{k}) \simeq \mathcal{B} |\tilde{\phi}(\mathbf{k})|^2 \quad (43)$$

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 [24]

$$2\epsilon_{\mathbf{k}} \tilde{\phi}(\mathbf{k}) + g_0 \phi(\mathbf{r} = \mathbf{0}) = 0, \quad (44)$$

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.(43) 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:

$$E_{\text{kin}}[\text{gas}] \simeq \mathcal{B} \cdot E_{\text{kin}}[\phi]. \quad (45)$$

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:

$$E_{\text{int}}[\text{gas}] \simeq \mathcal{B} \cdot E_{\text{int}}[\phi]. \quad (46)$$

The interaction energy of  $\phi$  is simply  $g_0 |\phi(\mathbf{0})|^2$ , equal to  $g_0 (dg/dg_0)$  according to (37). The interaction energy of the gas is equal to the right hand side of (34) times  $g_0 (dg/dg_0)$ . The common factor  $g_0 (dg/dg_0)$  simplifies and

$$\frac{dE}{dg} = \mathcal{B}. \quad (47)$$

It remains to relate the coefficient  $\mathcal{B}$  to  $\lim_{k \rightarrow +\infty} k^4 n_\sigma(k)$ , using (43). 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 (40).

## 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 [33]. 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 (22) and the length  $R_*$  is related to the resonance parameters by (26); since  $R_* \lesssim |r_e|/2$  where  $r_e$  is the effective range [31,32] our result confirms that in the zero effective range limit  $k_F |r_e| \ll 1$ , one has  $N_b \ll N$  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 [33]. This is also related to the fact that the BCS theory does not predict the correct short-distance pair correlations [64].

According to the finite- $a$  virial theorem, in a harmonic trap, the quantity  $-dE/d(1/a)$  is also related to the difference between the total energy and twice the trapping potential energy [46,65,66]. The quantity  $-dE/d(1/a)$  is also 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 [34,35] and rederived in [46] and in this paper. The quantity  $-dE/d(1/a)$  is also proportional to the average radiofrequency shift [67,68]. 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 with a single universal many-body quantity was given by Leggett [58]. Our work shows that the Rice experiment [33] is the first direct measurement of this fundamental quantity.

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**Note:** During completion of this paper, we became aware of a related work [69].

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