

One particle in a box: the simplest model for a Fermi gas in the unitary limit

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We consider a single quantum particle in a spherical box interacting with a fixed scatterer at the center, to construct a model of a degenerate atomic Fermi gas close to a Feshbach resonance. One of the key predictions of the model is the existence of two branches for the macroscopic state of the gas, as a function of the magnetic field controlling the value of the scattering length. This model is able to draw a qualitative picture of all the different features recently observed in a degenerate atomic Fermi gas close to the resonance, even in the unitary limit.

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Recently several experiments have produced two spin-component degenerate Fermi gases in the unitary limit, that is in a limit where the scattering length a of two atoms with different spin components is much larger than the mean interparticle separation [1, 2, 3, 4, 5]. Similar experiments have also been performed with bosonic atoms [6, 7, 8, 9]. This was made possible by a tuning of the scattering length virtually from $-\infty$ to $+\infty$ using a Feshbach resonance driven by an external uniform magnetic field, as first demonstrated on bosonic atoms [10, 11].

This regime constitutes a theoretical challenge. Some theories, based on the Hartree-Fock mean field approximation for the normal gas or on the BCS mean field calculation for the superfluid phase, rely on the small parameter $k_F a$, where the Fermi momentum of the gas is conventionally related to the mean total density ρ by the non-interacting case formula:

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

Such approaches are not quantitative in the limit $k_F|a| \rightarrow +\infty$. More sophisticated approaches have been developed to extend the accuracy of the theory to the unitary regime [12, 13, 14, 15, 16]. The difficulty comes from the fact that there exists no obvious small parameter for the theory in the unitary limit, at least in the degenerate regime of a temperature T much smaller than the Fermi temperature T_F , which is the regime considered here and also the present experimental situation. Note that, in the classical regime $T \gg T_F$, one recovers a small parameter $\rho^{1/3}|f| \ll 1$ since the typical scattering amplitude f for $|a| \rightarrow +\infty$, is on the order of λ , where λ is the thermal de Broglie wavelength [17, 18].

The scope of the present work is to give the simplest possible physical picture of a two spin-component Fermi gas for arbitrary values of the scattering length a , essentially at zero temperature. The model is not made to give quantitative predictions, but, as we shall see, it qualitatively reproduces the experimental observations, and it will provide, we hope, useful guidelines for experiments to come.

The model: We consider a spatially homogeneous gas of $N/2$ fermions of spin $+1/2$ and $N/2$ fermions of spin $-1/2$, each particle having a mass m . The interaction of a given spin $+1/2$ particle with the $N/2$ spin $-1/2$ particles is modeled (i) by the interaction of a fictitious particle of mass equal to the reduced mass $m/2$, with a fixed scatterer at the center of a spherical box of radius R , and (ii) with the boundary conditions that the wavefunction $\phi(\vec{r})$ of the fictitious particle vanishes on the surface of the box. (i): The interaction of the fictitious particle with the scatterer represents the interaction of the given spin $+1/2$ particle with its nearest spin $-1/2$ neighbour: in the model, these two opposite spin particles are considered in their center of mass frame and in the singlet spin state. (ii): The boundary condition mimics the interaction effect of the $N/2 - 1$ other spin $-1/2$ particles and the Fermi statistical effect of the remaining $N/2 - 1$ spin $+1/2$ particles, see Figure 1. A similar model was very recently put forward for bosons, with the difference that the box is replaced by a harmonic potential [19].

In the absence of interactions between the fermions, the total energy of the gas is given by the known ideal Fermi gas formula in the thermodynamic limit:

$$E = \frac{3}{5}N\epsilon_F , \quad (2)$$

where the Fermi energy $\epsilon_F = \hbar^2 k_F^2 / 2m$ is related to the mean density through (1). The gas energy E is also related to the energy ϵ of the fictitious particle in the spherical box by

$$E = \frac{1}{2}N\epsilon . \quad (3)$$

For the ideal Fermi gas, there is no scatterer in the box so that the ground state value of ϵ is

$$\epsilon_0 = \frac{\hbar^2}{m} \left(\frac{\pi}{R} \right)^2 . \quad (4)$$

This establishes the link between the radius R and the

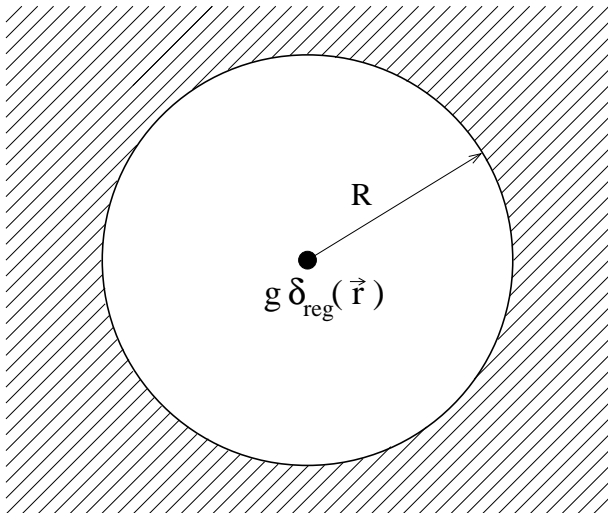


FIG. 1: Model used: a fictitious particle corresponding to the relative motion of a fermion with spin $+1/2$ and the nearest fermion with spin $-1/2$ is scattered by the fixed delta Fermi pseudo-potential [22] in the center of a spherical box of radius R with absorbing boundary conditions. The box mimics the interaction effect of the $N/2 - 1$ remaining spin $-1/2$ atoms and the Fermi statistical effect of the remaining $N/2 - 1$ spin $+1/2$ fermions. The coupling constant g is $4\pi\hbar^2 a/m$, where a is the scattering length of two fermions with opposite spin, $g\delta_{\text{reg}}(\vec{r}) = g\delta(\vec{r})\partial_r(r)$ is the Fermi pseudo-potential which imposes the contact condition (9) on the two-body wave function [21, 22, 23, 24].

mean density of the gas [20] :

$$k_F R = \left(\frac{5}{3}\right)^{1/2} \pi . \quad (5)$$

In presence of interactions, the scatterer in the model is the Fermi delta pseudo-potential with a coupling constant $g = 4\pi\hbar^2 a/m$ where a is the s -wave scattering length of two fermions with opposite spin components [21, 22, 23, 24]. The choice of such a zero-range potential is allowed in the regime

$$\rho r_e^3 \ll 1 , \quad (6)$$

where r_e is the effective range of the true interaction potential, and which allows to consider these systems as gases rather than liquids even in the unitary limit. The two-body scattering amplitude derived from the pseudo-potential,

$$f_k = -\frac{1}{a^{-1} + ik} \quad (7)$$

is indeed a good approximation of the scattering amplitude in simple models of a Feshbach resonance:

$$f_k^{\text{Fesh}} = -\frac{1}{a^{-1} + ik - k^2 r_e/2}, \quad (8)$$

when $k_F r_e \ll 1$ since k is at most on the order of k_F at $T \ll T_F$. r_e was calculated in [25] and one finds that condition (6) is very well satisfied in present experiments on Li^6 [15].

We will use the fact that the pseudo-potential is equivalent to replacing the interaction potential by the contact condition [21, 23, 24]

$$\lim_{r \rightarrow 0} \frac{\partial_r(r\phi)}{r\phi} = -\frac{1}{a} , \quad (9)$$

where r is the distance to the origin. Out of the origin in the box, the wavefunction then solves the free Schrödinger equation:

$$-\frac{\hbar^2}{m}\Delta\phi = \epsilon\phi . \quad (10)$$

Restricting to the s -wave, which is the only partial wave in which the pseudo-potential scatters, ϕ is rotationally symmetric and we set $\phi(r) = u(r)/r$. For positive energies $\epsilon = \hbar^2 k^2/m$, where $k > 0$, one then finds

$$u(r) \propto \sin[k(r - R)] , \quad (11)$$

and the contact condition Eq.(9) imposes:

$$\tan kR = ka . \quad (12)$$

For negative energies $\epsilon = -\hbar^2 \kappa^2/m$, where $\kappa > 0$, one finds

$$u(r) \propto \sinh[k(r - R)] , \quad (13)$$

where Eq.(9) imposes:

$$\tanh \kappa R = \kappa a . \quad (14)$$

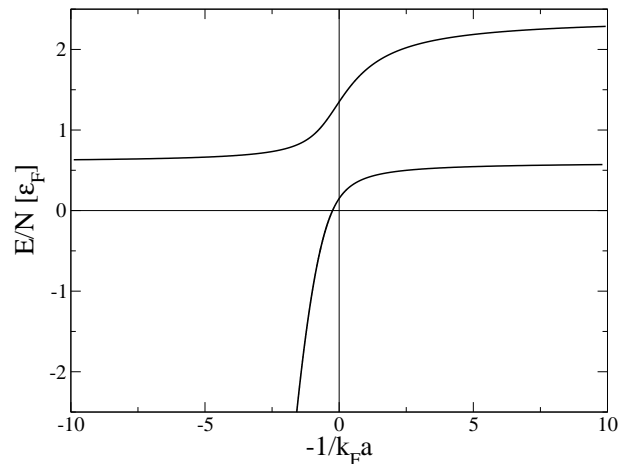


FIG. 2: Total energy of the gas in units of the Fermi energy, as function of $-1/k_F a$. Only the first two branches of the model are represented.

Discussion: The energy spectrum of the previous model allows to calculate the energy of the gas according to

Eq.(3). The result is shown in Figure 2 as function of $-1/k_F a$, restricting to the two lowest energy branches. The choice of the parameter $-1/k_F a$ is inspired by the way the experimental results on ${}^6\text{Li}$ are usually presented: in this way, the right part of the Figure 2 corresponds to magnetic fields above the Feshbach resonance, and the left part to magnetic fields below the resonance. The existence of several energy branches for the macroscopic state of the gas is a first crucial prediction of the model. The ground branch connects two clearly identified regimes:

- the first regime $k_F a \rightarrow 0^-$ (on the right hand side of Figure 2) is a weakly attractive Fermi gas which corresponds at zero temperature to the BCS phase in a more complete treatment.
- the second regime $k_F a \rightarrow 0^+$ (on the left hand side of Figure 2) corresponds to a dilute gas of dimers; each dimer corresponds to the bound state of the two-body problem in free space since the size of the box R , on the order of the mean interatomic distance, is here much larger than the spatial extension $\sim a$ of the dimer. The energy of a dimer is $-\hbar^2/ma^2$ which explains the quadratic drop of the ground energy on the left part of the resonance. In a more complete treatment, one would find at $T = 0$ that these dimers form a Bose-Einstein condensate since they are bosons in the limit $\rho^{1/3}a \ll 1$.

The upper branch in Figure 2 is also easy to identify in the weakly interacting limit $k_F a \rightarrow 0^+$, where it corresponds to a weakly repulsive Fermi gas. It clearly corresponds to a metastable state of the gas: a three body collision between atoms will form a dimer plus an extra atom carrying away the binding energy, a mechanism that will depopulate the upper branch and populate the ground branch. This constitutes a first experimental way to produce dimers from an atomic gas, already proposed in the case of bosons in [33], with the disadvantage that the resulting molecules have a high center of mass kinetic energy, on the order of \hbar^2/ma^2 . These strong three-body losses prevent in present experiments to follow adiabatically the upper branch in Figure 2 from the left part of the Figure ($a > 0$) to the right part of the Figure ($a < 0$). In the unitary regime, our model predicts in the upper branch an energy per particle scaling as $\hbar^2 \rho^{2/3}/m$ larger than the ideal Fermi gas case, that is corresponding to an effective repulsion. A similar behavior was predicted for bosons by A. Leggett [34].

Inspection of Figure 2 immediately inspires another way to produce a gas of ultracold molecules than the one relying on three-body inelastic collisions: one starts with a weakly attractive atomic Fermi gas, on the right of the Feshbach resonance, and one slowly crosses the resonance from right to left in order to follow adiabatically the ground branch. Note that a similar mechanism has been developed in the case of an atomic Bose gas [26].

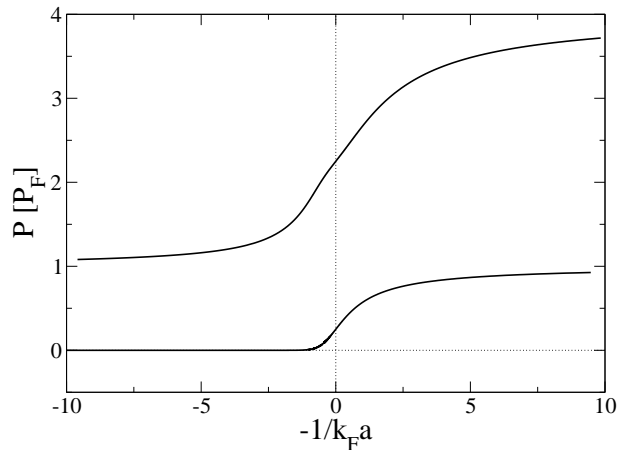


FIG. 3: Pressure P of the gas in units of the Fermi pressure $P_F = \hbar^2 k_F^5 / 15\pi^2 m$, as function of $-1/k_F a$. Only the first two branches of the model are represented.

Another important feature of the model is that nothing dramatic happens right on the Feshbach resonance, the mean energy per particle being simply proportional to the Fermi energy with some numerical factor (here $3/40$). As this mean energy is less than the ideal gas value (2), the gas experiences an effective attraction due to the atomic interactions. This universality and this effective attraction appeared already in several approaches [14, 15, 17, 18], and are confirmed by the experimental results [2, 4]. As the total energy remains positive, so will be the pressure and the compressibility of the gas at the Feshbach resonance: the Fermi gas will not experience a collapse when $k_F a$ becomes large in absolute value and negative, in agreement with the recent experiments [1, 2, 3, 4, 5] and contrarily to what was feared a few years ago based on the calculation of the compressibility in the mean field approximation [27].

To check in a systematic way the stability of the gas in our model, we have calculated the pressure (see Figure 3) and the compressibility (not shown) of the gas for the lowest two branches for an arbitrary value of a . The compressibility and the pressure are positive everywhere. Moreover, the pressure on the ground branch is lower than the ideal Fermi gas pressure and tends exponentially to zero from above in the molecular limit $a \rightarrow 0^+$, revealing the absence of a non-zero scattering length of dimers in our model [28]. The decrease of the pressure across the Feshbach resonance from the $a < 0$ part to the $a > 0$ part is observable in a trap through a shrinking of the size of the cloud.

In conclusion, the heuristic model that we have presented contains all the essential features of a two spin-component Fermi gas for s -wave interactions with an arbitrary scattering length, such as the existence of a metastable atomic phase (upper branch) and a molecular phase (lower branch) for $a \rightarrow 0^+$ and the continuous connection between the molecular regime and the weakly attractive regime when a is varied from 0^+ to 0^- across

the Feshbach resonance.

Note: after the submission of this paper, both scenarios for the production of a molecular condensate have been realized experimentally: the adiabatic scenario [29, 30] and the scenario assisted by three-body inelastic collisions [31, 32].

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