Fermi gases, BEC-BCS crossover and strongly interacting regime

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1 The ideal Fermi gas

In a non-interacting Fermi gas at thermal equilibrium at temperature T in the grand canonical ensemble, the mean occupation number of an eigenmode of energy ϵ is given by the Fermi-Dirac formula:

$$n(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1} \tag{1}$$

where $\beta = 1/k_B T$ and μ is the chemical potential.

We are concerned by the strongly degenerate regime, where the chemical potential is positive and much larger than the thermal energy $k_B T$. In this case, the Fermi-Dirac distribution has the shape shown in figure 1: it is almost a step function, with a rounded part of width $\sim k_B T$, a feature that can be used to perform low temperature expansion of thermodynamic quantities [1].

Here we shall need only the expression of the Fermi energy ϵ_F of a zero temperature homogeneous Fermi gas, defined as the zero temperature value of the chemical potential:

$$\epsilon_F \equiv \mu(T=0) \equiv \frac{\hbar^2 k_F^2}{2m} \tag{2}$$

where k_F is called the Fermi wavevector. In the thermodynamic limit the mean density of particles in a given spin component σ is

$$\rho_\sigma = \int \frac{d^3k}{(2\pi)^3}\, \theta(\epsilon_F - \hbar^2 k^2/2m) = \frac{k_F^3}{6\pi^2} \tag{3}$$

where $\theta(x)$ is the Heaviside step function, equal to zero for $x < 0$ and to unity for $x > 1$.

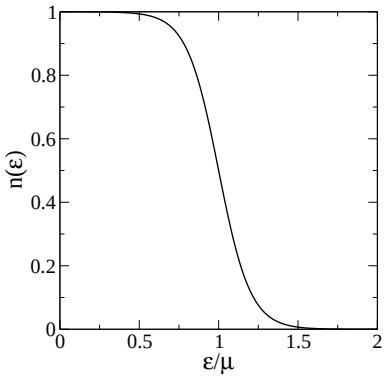

Figure 1: The Fermi-Dirac distribution for the strongly degenerate ideal Fermi gas (here $k_B T = \mu/10$).

2 Controlling the interaction strength

We assume that the Fermi gas has only two populated spin components, $\sigma = \uparrow$ and $\sigma = \downarrow$. We shall characterize the interaction between these two spin components only by a, the s-wave scattering length: the effective range of the potential is supposed to be much smaller than a and than $1/k_F$ so that a zero-range model interaction potential can be used.

Particles in the same spin state cannot interact in the s-wave channel, because of the anti-symmetry of their relative wavefunction, but can interact in the p-wave channel. We will assume here that this p-wave interaction is negligible. Note that some experiments are investigating Feshbach resonances in the p-wave, in which case the assumption no longer holds [2].

We assume that a Feshbach resonance in the s-wave channel is used to adjust the value of the scattering length a almost at will, by applying a uniform magnetic field B on the optically trapped fermions, based on a mechanism sketched in figure 2. Inspired by the case of the lithium 6 fermionic isotope, see figure 3, we assume that the scattering length tends to $+\infty$ on the left

side of the resonance ($B \to B_0^-$) and tends to $-\infty$ on the right side of the resonance ($B \to B_0^+$).

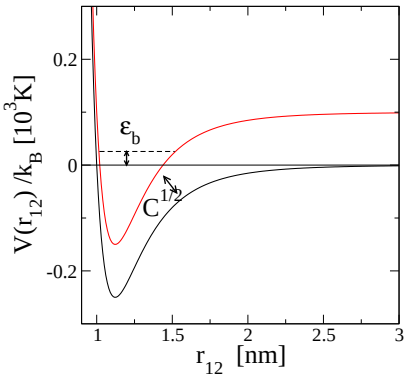

Figure 2: Principle of the Feshbach resonance: at short interatomic separation the potential curves mainly consist of the electronic spin triplet and electronic spin singlet curves, with a coupling between the two curves due to the hyperfine interaction. By shifting the two curves one with respect to the other by an external magnetic field of well chosen value, one can arrange that the energy of a quasi-bound state in the upper potential curve matches the dissociation limit of the lower curve ($\epsilon_b = 0$). A zero energy resonance then occurs in the lower input channel, corresponding to an infinite scattering length.

In this way, the strongly interacting regime $k_F|a| > 1$ is accessible. We show experimental results on the interaction energy in figure 4, taken from [3]. Crosses are obtained by ramping the B field from the left to the right, starting with a weakly repulsive Fermi gas ($0 < k_F a < 1$), and squares are obtained by ramping the B field from the right to the left, starting with a weakly attractive Fermi gas ($-1 < k_F a < 0$). In the left to right scan, the interaction energy increases, as expected for an increasing positive a, until at some value of B strictly less than the Feshbach resonance location B_0, something rather dramatic happens: there is a loss in the number of atoms,

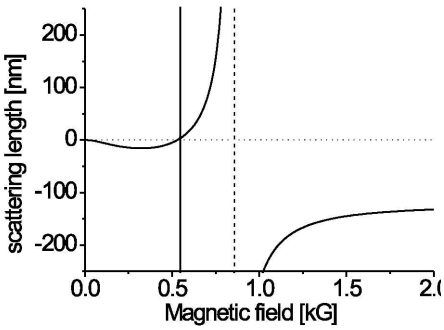

Figure 3: Expected variation of the scattering length between two lithium 6 atoms in the two lowest internal atomic states as a function of the applied magnetic field. The location of the Feshbach resonance is close to 820 Gauss (figure taken from [3]).

and the interacting energy changes sign, even if $a > 0$. In the right to left scan, the interaction energy remains negative, even on the $a > 0$ side of the resonance, and nothing dramatic happens right on the resonance. Note that the crosses with negative interaction energy and the squares do not exactly overlap, probably due to the change in the number of atoms due to the loss [3].

As we will show in the next section, these at first sight surprising experimental results can be interpreted easily if one admits that they correspond to the exploration of two distinct branches for the macroscopic state of the gas as a function of $-1/k_F a$, a stable ground branch and a metastable excited branch [4].

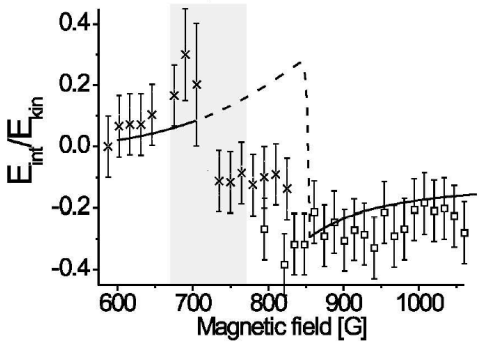

Figure 4: Measured interaction energy of a two component lithium 6 gas (in units of the kinetic energy of the gas) as a function of the external magnetic field B close to a Feshbach resonance. Crosses: the B field is ramped from the left ($a > 0$) of the resonance to the right ($a < 0$). Squares: the B field is ramped from the right to the left. The solid and dashed line corresponds to a simple extrapolation of mean field theory from the weakly to the strongly interacting regime (figure taken from [3]).

3 A purely qualitative toy model

Consider a matter wave of isotropic wavefunction $\phi(r)$ in a hard wall spherical cavity of radius R, in presence of a point-like scatterer of fixed position in the center of the cavity. The effect of the point-like scatterer is treated by imposing the following boundary conditions on ϕ in $r = 0$:

$$\phi(r) \stackrel{r\to 0}{=} A\left(\frac{1}{r} - \frac{1}{a}\right) + o(1) \tag{4}$$

where A is a constant. This is equivalent to the use of the regularised delta pseudo-potential introduced by Fermi [5] with a coupling constant

$$g = \frac{4\pi\hbar^2 a}{m}. \tag{5}$$

The effect of the cavity is represented by the boundary condition

$$\phi(R) = 0 \tag{6}$$

where R is the radius of the cavity.

What is the link between this model and the many-body problem of N interacting fermions ? The wavefunction $\phi(r)$ describes the relative motion of a, let us say, spin $\uparrow$ atom, with respect to the nearest spin $\downarrow$ atom modelized by the point-like scatterer. The cavity represents (i) the interaction effect of the other $N/2-1$ spin $\downarrow$ atoms and (ii) the Pauli blocking effect of the other $N/2-1$ spin $\uparrow$ atoms. Interaction effect (i): the radius of the cavity should then be of the order of the mean interparticle separation in the gas,

$$R \sim \frac{1}{k_F}. \tag{7}$$

Pauli blocking effect (ii): in the case $g = 0$, the zero point energy of ϕ should be on the order of the Fermi energy so that one has also the choice (7). This explains also the choice of hard walls for the cavity; in the case of bosons, a cubic cavity with periodic boundary conditions would be more appropriate. Finally, the total energy of the gas is related to ϵ by

$$E = N\epsilon/2 \tag{8}$$

since ϵ is the energy of one of the $N/2$ spin $\uparrow$ particle including the interaction energy with all the spin $\downarrow$ particles.

Let us proceed with the calculation of the eigenenergies of the matter wave in the cavity. An eigenmode of the cavity with energy ϵ solves Schrödinger's equation for $0 < r < R$

$$-\frac{\hbar^2}{m}\Delta\phi(r) = \epsilon\phi(r) \tag{9}$$

with the above mentioned boundary conditions. If $\epsilon > 0$, we set $\epsilon = \hbar^2k^2/m$ and k solves

$$\tan kr = ka. \tag{10}$$

If $\epsilon < 0$, we set $\epsilon = -\hbar^2\kappa^2/m$ and κ solves

$$\tanh \kappa R = \kappa a. \tag{11}$$

An important remark is to realize that, in the free space limit $R \to +\infty$, the matter wave has a bound state corresponding to $\kappa a = 1$, as is easily checked on Eq.(11). The energy of this bound state and its wavefunction are given by

$$\epsilon_0 = -\frac{\hbar^2}{ma^2} \qquad \phi_0(r) = \frac{1}{\sqrt{2\pi a}}\frac{e^{-r/a}}{r}. \tag{12}$$

This means that two atoms interacting via a short range potential and with a positive scattering length have a molecular bound state. This dimer has a radius of the order of a, so it can be in the 100 nm rang : it is much more extended and weakly bound that ordinary dimer molecules! In the case of $a < 0$, there is no such bound state for two atoms in free space.

In the cavity, there is an infinite number of discrete modes. We have plotted the energy of the first two of them as a function of $-1/k_F a$ on figure 5. We have taken $-1/k_F a$ as the abscissa because it allows a direct mapping with the B field axis of figure 4: the left part corresponds to $a > 0$, the right part to $a < 0$ and the precise location of the resonance to $-1/k_F a = 0$.

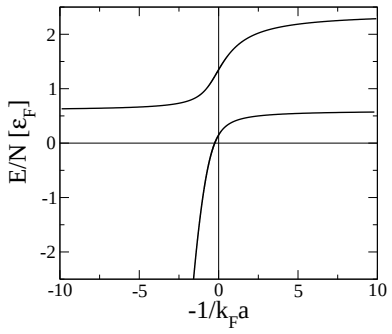

Figure 5: In the qualitative model of a matter wave with a scatterer in a cavity, energy per particle of a $T = 0$ two-component Fermi gas (in units of the Fermi energy of the ideal gas with the same density) as a function of $-1/(k_F a)$.

The first excited branch is metastable. It starts with a weakly repulsive Fermi gas on the extreme left and has a larger energy than the ideal Fermi gas, indicating effective repulsion. When a gets too large, three-body collisions (not included in the toy model) become frequent and lead to the formation of a dimer ϕ_0: the system starts populating the ground branch. This is the dramatic change seen in the experiment.

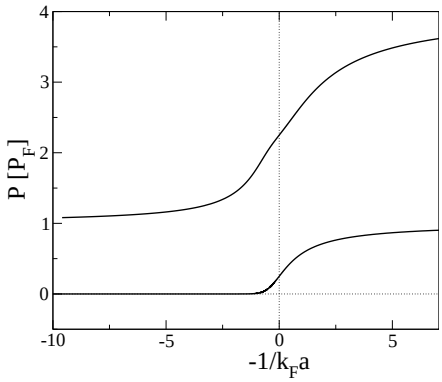

Figure 6: In the qualitative model of a matter wave with a scatterer in a cavity, pressure of a $T = 0$ two-component Fermi gas (in units of the pressure of an ideal Fermi gas with the same density) as a function of $-1/(k_F a)$.

The ground branch continuously connects the weakly attractive Fermi gas (on the right) to a gas of dimers (on the left). The sharp decrease of the total energy on the left part reflects the $1/a^2$ dependence of the dimer binding energy ϵ_0. This sharp decrease does not show up in the experimental results of figure 4. This is due to the fact that the interaction energy extracted from the experiment comes from an analysis of the ballistic expansion of the cloud (once the optical trap is switched off), where the center of mass energy rather than the internal energy of the molecules is relevant. We therefore calculated the pressure of the gas, from the relation $P = -\partial_V E$, where $V = N/\rho$ is the total volume of the gas, see figure 6. One see that on the ground branch, the pressure is always less than the Fermi pressure of the ideal Fermi gas, indicating effective attraction with respect to the ideal Fermi gas. Note that P drops very rapidly on the left side, due to the absence of interaction between the molecules in the toy model.

The regime of infinite scattering length $|a| = +\infty$, the so-called unitary regime, is interesting as it is universal: for a bulk system, the only energy

scale left is the Fermi energy so that the ground state energy of the corresponding unitary gas has to be proportional to the ground state energy of the ideal Fermi gas:

$$E_0^{\text{unitary}} = \eta E_0^{\text{ideal}} \tag{13}$$

where $E_0^{\text{ideal}} = 3N\epsilon_F/5$ and η is a numerical constant.

4 More quantitative study of the ground branch at $T = 0$

4.1 Two known limiting cases

At zero temperature, the two extreme cases $k_F a \to 0^{\pm}$ are well understood theoretically, see figure 7:

- The case $k_F a \to 0^+$ corresponds to a Bose-Einstein condensate of dimers: as the radius of the dimers $\sim a$ is much smaller than the mean inter-dimer separation $\sim 1/k_F$, the dimers can be considered as bosons and can Bose condense. The scattering length between two dimers was calculated recently to be $a_{\text{mol}} = 0.6a$ [6]. Molecular condensates have been produced experimentally, for example by ramping B from the right to the left of the resonance, so as to adiabatically convert a weakly attractive Fermi gas into a BEC of molecules [7, 8, 9, 10].

- The case $k_F a \to 0^-$ corresponds to a BCS state, that is to a condensate of pairs (called Cooper pairs in the case of electrons in a superconducting system). The size of a pair is much larger than the mean interparticle separation so that the pairs cannot be considered as bosons, and the condensate that they form is not strictly speaking a Bose-Einstein condensate.

These two extreme cases present long-range order on the first order coherence function of pairs:

$$g_1^{\text{pair}}(\mathbf{r}) \equiv \langle \hat{\psi}_\uparrow^\dagger(\mathbf{r}) \hat{\psi}_\downarrow^\dagger(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{0}) \hat{\psi}_\uparrow(\mathbf{0}) \rangle \tag{14}$$

has a non-zero limit when $r \to +\infty$. In this expression, $\hat{\psi}_\sigma(\mathbf{r})$ is the atomic field operator in spin component σ, and $\hat{\psi}_\uparrow^\dagger(\mathbf{r})\hat{\psi}_\downarrow^\dagger(\mathbf{r})$ creates a pair of particles with opposite spin in $\mathbf{r}$. It is natural to assume that this long range order

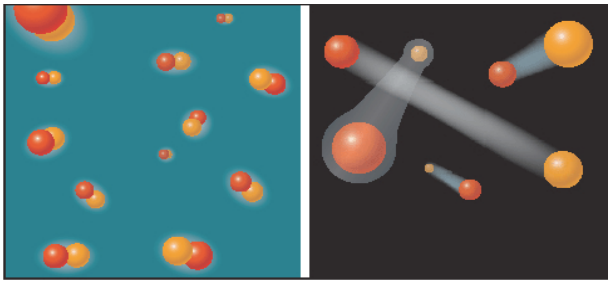

Figure 7: Schematic view of the ground state of a two spin component Fermi gas in the weakly interacting limit. Left panel: when $k_F a \to 0^+$, a Bose-Einstein condensate of quasi-bosonic dimers is expected. Right panels: when $k_F a \to 0^-$, a condensate of extended Cooper pairs is expected.

will persist for any value of $-1/k_F a$, so that the ground branch constitutes an interesting cross-over between the BEC regime and the BCS regime [11, 12, 13]. Evidence of condensation of pairs on the $a < 0$ of the resonance was actually obtained recently in the strongly interacting regime $k_F|a| > 1$, but not yet in the strict BCS regime $k_F|a| < 1$ [14, 15]. On the theoretical side, one may also hope that the BCS variational wavefunction gives a reasonably good description of the many-body state even in the strongly interacting regime $k_F|a| > 1$.

4.2 The BCS variational state

The BCS trial wavefunction corresponds to a condensate of pairs, with $N/2$ particles in each spin component. The first step is therefore to introduce the operator creating a pair. As the interactions are here in the s-wave channel, we assume that each pair is in the spin singlet state with an even and real orbital wavefunction $\phi(\mathbf{r_1} - \mathbf{r_2})$ function of the relative coordinates of the two atoms [16]. The pair creation operator then reads

$$C^\dagger = \int d^3 r_1 \int d^3 r_2 \; \phi(\mathbf{r_1} - \mathbf{r_2}) \hat{\psi}^\dagger_\uparrow(\mathbf{r_1}) \hat{\psi}^\dagger_\downarrow(\mathbf{r_2}). \tag{15}$$

Even if we call it a creation operator, note that $C^\dagger$ and C do not have bosonic commutation relations.

A more operational writing can be obtained by introducing the Fourier

decomposition of ϕ:

$$\phi(\mathbf{r_1} - \mathbf{r_2}) = \frac{1}{L^3} \sum_{\mathbf{k}} \phi_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r_1}-\mathbf{r_2})} \tag{16}$$

where L is the size of the cubic box with periodic boundary conditions used as a quantization volume. As ϕ is a real and even function of the coordinates, each Fourier coefficient $\phi_{\mathbf{k}}$ is real. As ϕ is a two-body wavefunction normalized to unity, one has

$$\sum_{\mathbf{k}} \phi_{\mathbf{k}}^2 = 1. \tag{17}$$

This leads to

$$C^\dagger = \sum_{\mathbf{k}} \phi_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}, \tag{18}$$

where $a_{\mathbf{k}\uparrow}$ is the annihilation operator of one particle of momentum $\mathbf{k}$ and spin component σ, with the usual fermionic anticommutation relations. This writing makes apparent the pairing in $\mathbf{k}$ space.

A natural form for the state of a condensate of pairs would be

$$|\psi\rangle \propto C^{\dagger N/2}|0\rangle \tag{19}$$

where $|0\rangle$ is the vacuum. This form is actually rather difficult to use, as the calculation of the corresponding mean energy does not lead to a really simple result.

As Bardeen, Cooper and Schrieffer did, it is much more convenient to represent the condensate by a coherent state rather than by a Fock state:

$$|\psi_{\rm BCS}\rangle \propto e^{\gamma C^\dagger}|0\rangle \tag{20}$$

where γ is taken here for simplicity to be real. One can show that the variance of the number of particles in this state is less that its mean number, so that fluctuations in N do not degrade the accuracy of the ansatz in the large N limit. One can check that the various $\mathbf{k}$ terms in Eq.(18) commute, so that $e^{\gamma C^\dagger}$ may be written as a product over $\mathbf{k}$ of factors of the form

$$e^{\Gamma_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}} \tag{21}$$

where we set $\Gamma_{\mathbf{k}} \equiv \gamma\phi_k$. One then expands this exponential in powers of $\Gamma_{\mathbf{k}}$ and one realizes that the expansion terminates at order one, since the square of a creation operator vanishes for fermions. This leads to the canonical form

$$|\psi_{\rm BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow})|0\rangle \tag{22}$$

where the coefficients of the standard BCS notation

$$u_{\mathbf{k}} = \frac{1}{\sqrt{1+\Gamma_{\mathbf{k}}^2}} \tag{23}$$

$$v_{\mathbf{k}} = \frac{\Gamma_{\mathbf{k}}}{\sqrt{1+\Gamma_{\mathbf{k}}^2}} \tag{24}$$

$$\tag{25}$$

are normalized to $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$.

Calculation of expectation values in the BCS state is rather simple. First Wick theorem can be applied, as we show in the Appendix, so that one is left with the expectation values of quadratic forms, best performed in the momentum space representation. One can indeed use the fact that each pair of modes $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is decoupled from the others, so that one is left in calculation of expectation values in states

$$|\psi_{\mathbf{k}}^{\text{pair}}\rangle = u_{\mathbf{k}}|0\rangle + v_{\mathbf{k}}|\mathbf{k}\uparrow, -\mathbf{k}\downarrow\rangle. \tag{26}$$

4.3 The model Hamiltonian

We use the lattice model detailed in [17]: the spatial coordinates of the particles are discretized on a grid of step l in each direction. The length L of the quantization box is an integer multiple of l. Plane waves exist on the lattice, with wave vector components $\mathbf{k}$ having a meaning modulo $2\pi/l$ so that we restrict $\mathbf{k}$ to the fundamental domain

$$D = \left[\frac{-\pi}{l}, \frac{\pi}{l}\right[^3. \tag{27}$$

This provides automatically an energy cut-off $\propto \hbar^2/ml^2$. The kinetic energy of a plane wave with wavevector $\mathbf{k}$ is taken to be $\hbar^2k^2/2m$. The interaction between the particles is represented by a discrete delta potential,

$$V_{12} = \frac{g_0}{l^3}\delta_{\mathbf{r_1},\mathbf{r_2}} \tag{28}$$

with a bare coupling constant g_0 determined by the condition that the s-wave scattering length of the discrete delta potential is exactly the same as the one, a, of the true interaction potential. As shown in [17] this leads to

$$\frac{1}{g_0} = \frac{1}{g} - \int_D \frac{d^3k}{(2\pi)^3}\frac{m}{\hbar^2k^2} \tag{29}$$

where g is defined in Eq.(5). The dependence of g_0 on the grid spacing l is reminiscent of the technique of renormalisation of the coupling constant [13]. Note that g_0 tends to 0^- linearly with l in the $l \to 0$ limit. Here we assume that l is much smaller than both $|a|$ and $1/k_F$ (to avoid unphysical effects due to the cut-off) so that $g_0 < 0$.

To summarize, the lattice model is defined by the grand canonical Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + g_0 \sum_{\mathbf{r}} l^3 \; \hat{\psi}^\dagger_\uparrow \hat{\psi}^\dagger_\downarrow \hat{\psi}_\downarrow \hat{\psi}_\uparrow \tag{30}$$

where the field operator is

$$\hat{\psi}_\sigma(\mathbf{r}) = \frac{1}{L^{3/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}\sigma}. \tag{31}$$

4.4 Key quantities in the thermodynamic limit

A first quantity is the mean density per spin component in the BCS trial state. We find the following expression in the thermodynamic limit:

$$\rho_\uparrow \equiv \langle \hat{\psi}^\dagger_\uparrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \rangle = \int_D \frac{d^3k}{(2\pi)^3} \frac{\Gamma^2_{\mathbf{k}}}{1+\Gamma^2_{\mathbf{k}}}, \tag{32}$$

which is useful to relate the chemical potential to the mean density.

A second, crucial quantity is the so-called gap parameter Δ:

$$\Delta \equiv g_0 \langle \hat{\psi}_\uparrow(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) \rangle = -g_0 \int_D \frac{d^3k}{(2\pi)^3} \frac{\Gamma_{\mathbf{k}}}{1+\Gamma^2_{\mathbf{k}}}. \tag{33}$$

We assume here that $\Delta > 0$. In the limit of a vanishing grid spacing, g_0 tends to zero and the anomalous average $\langle \hat{\psi}_\uparrow \hat{\psi}_\downarrow \rangle$ tends to infinity, in a way such that Δ has a finite limit. Dividing Eq.(33) by g_0 and eliminating $1/g_0$ thanks to Eq.(29) leads indeed to an equation eliminating infinities in the $l \to 0$ limit:

$$\frac{\Delta}{g} = -\int_D \frac{d^3k}{(2\pi)^3} \left[\frac{\Gamma_{\mathbf{k}}}{1+\Gamma^2_{\mathbf{k}}} - \frac{m\Delta}{\hbar^2 k^2} \right]. \tag{34}$$

The expectation value of the model Hamiltonian in the BCS state can be calculated explicitly:

$$L^{-3} \langle \psi_{\rm BCS} | H | \psi_{\rm BCS} \rangle = \left[\int \frac{d^3k}{(2\pi)^3} \frac{2\Gamma^2_{\mathbf{k}}}{1+\Gamma^2_{\mathbf{k}}} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \right] + g_0 \rho_\uparrow \rho_\downarrow + \frac{\Delta^2}{g_0}. \tag{35}$$

Each Γ_k is a variational parameter, so that the first order derivative of this expression with respect to Γ_k has to vanish. This leads to the second order equation:

$$\Gamma_{\mathbf{k}}^2 + \frac{2}{\Delta}\left(\frac{\hbar^2 k^2}{2m} + g_0\rho_\uparrow - \mu\right)\Gamma_{\mathbf{k}} - 1 = 0. \tag{36}$$

To minimize the energy, one sees that all the $\Gamma_{\mathbf{k}}$ should have the same sign, which is positive to give a positive Δ. This determines Γ_k in a unique way, as the two roots of Eq.(36) have opposite signs. One can then rewrite the gap equation in a more explicit form:

$$\frac{1}{g} = -\int_D \frac{d^3k}{(2\pi)^3}\left[\frac{1}{2}\frac{1}{\sqrt{\Delta^2 + (\hbar^2k^2/(2m) + g_0\rho_\uparrow - \mu)^2}} - \frac{m}{\hbar^2 k^2}\right]. \tag{37}$$

In the limit $l \to 0$ this gives the so-called BCS gap equation. When $\Gamma_{\mathbf{k}} \ll 1$, which always happens in the large k limit, one can neglect the quadratic term in Eq.(36) to get

$$\Gamma_{\mathbf{k}} \simeq \frac{\Delta}{2g_0\rho_\uparrow - 2\mu + \hbar^2k^2/m}. \tag{38}$$

Finally, one takes the $l \to 0$ limit. The mean field terms $g_0\rho_\uparrow$ disappear in this limit [18], and the domain D can be replaced by the whole three-dimensional real space without inducing any divergence in Eq.(32), Eq.(34), as can be checked from the large k behavior of $\Gamma_{\mathbf{k}}$ in Eq.(38).

4.5 Main results of the BCS ansatz

Limit $k_F a \to 0^-$: the gap parameter Δ tends to zero in this limit, as

$$\Delta \propto \epsilon_F e^{-\frac{\pi}{2k_F|a|}}, \tag{39}$$

whereas the chemical potential is $\mu \simeq \epsilon_F$. Note the non-analytic dependence of the gap with the small parameter $k_F|a|$, which indicates that the BCS state in the thermodynamic limit cannot be obtained by a perturbative treatment of the interaction potential. This non-analytic dependence can be readily seen from Eq.(37), whose integrand diverges in $k = \sqrt{2m\mu}/\hbar$, in the limit $\Delta \to 0$. Replacing the k integration variable by the energy ϵ, and

approximating the density of states by a constant in the energy interval of half-width $\delta \ll \mu$ around μ, one gets a contribution

$$\int_{\mu-\delta}^{\mu+\delta} \frac{d\epsilon}{\sqrt{\Delta^2+(\epsilon-\mu)^2}} \overset{\Delta\to 0}{\propto} \log\frac{\Delta}{\delta}. \tag{40}$$

One can show from BCS theory that 2Δ is the energy required to break a pair, that is to get from a condensate of $N/2$ pairs a condensate of $N/2-1$ pairs and two unpaired atoms [19]. This justifies the name of Δ.

Limit $k_F a \to 0^+$: the coefficients $\Gamma_{\mathbf{k}}$ tend uniformly to zero in this limit, so that the pair creation operator $C^\dagger$ obeys approximately bosonic commutation relations, in the sense that

$$\langle\psi_{\rm BCS}|[C,C^\dagger]|\psi_{\rm BCS}\rangle = 1 - 2\sum_{\mathbf{k}} \phi_{\mathbf{k}}^2 \frac{\Gamma_{\mathbf{k}}^2}{1+\Gamma_{\mathbf{k}}^2} \simeq 1. \tag{41}$$

This was expected physically, since the ground state of the gas is a condensate of almost bosonic dimers. Let us check that the BCS theory correctly reproduces that. We first simplify the gap equation Eq.(34) by using the approximation Eq.(38): after division by Δ, we get an equation for the chemical potential

$$\frac{1}{g} \simeq -\int \frac{d^3\mathbf{k}}{(2\pi)^3}\left[\frac{1}{\frac{\hbar^2k^2}{m}-2\mu} - \frac{m}{\hbar^2k^2}\right] \tag{42}$$

which leads to

$$\mu \simeq -\frac{\hbar^2}{2ma^2}. \tag{43}$$

This is minus half the binding energy of a dimer, exactly what was expected (keep in mind that $\mu N = \mu_{\rm mol} N_{\rm mol}$ where $N_{\rm mol}$ is the total number of dimers and is equal to $N/2$, so that the molecular chemical potential $\mu_{\rm mol}$ is twice the atomic one). The next step is to use the low $\Gamma_{\mathbf{k}}$ approximation to Eq.(32) to calculate the gap parameter:

$$\Delta \simeq \frac{2}{\sqrt{3\pi}}(k_F a)^{3/2}\frac{\hbar^2}{ma^2} \ll \frac{\hbar^2}{ma^2}. \tag{44}$$

Note that in this molecular BEC regime, Δ is **not** proportional to the energy required to break a pair. Finally, by performing the Fourier transform of Eq.(38), one obtains the pair wavefunction

$$\phi(\mathbf{r_1}-\mathbf{r_2}) = \frac{1}{L^{3/2}}\phi_0(|\mathbf{r_1}-\mathbf{r_2}|) \tag{45}$$

where ϕ_0 is the bound state of two atoms given by Eq.(12).

Limit $k_F|a| = +\infty$: the numerical solution of the gap equation Eq.(34) and of the density equation Eq.(32) gives the BCS estimate of the numerical coefficient η of Eq.(13). This estimate is an upper bound [20]:

$$\eta \leq \eta_{\rm BCS} = 0.5906\ldots \tag{46}$$

A better upper bound was obtained recently by fixed node Monte Carlo calculations [21]:

$$\eta \leq \eta_{\rm FNMC} = 0.44. \tag{47}$$

Early measurements of η were in contradiction with these upper bounds [22], but a more precise measurement performed in Innsbruck [23]:

$$\eta = 0.32^{+0.13}_{-0.10}, \tag{48}$$

is compatible with the upper bounds, and so is the recent measurement of η performed in [10].

A The BCS state as a fermionic squeezed vacuum

An interesting rewriting of the BCS state Eq.(22) can be obtained from the identity

$$e^{\theta\left(b^\dagger c^\dagger - cb\right)}|0\rangle = \cos\theta|0\rangle + \sin\theta\ b^\dagger c^\dagger|0\rangle \tag{49}$$

where θ is a real number, b and c are two fermionic annihilation operators with standard anticommutation relations [24]. Then $|\psi_{\rm BCS}\rangle = U|0\rangle$ where the unitary operator is

$$U = \prod_{\mathbf{k}} e^{\theta_{\mathbf{k}}\left(a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow} - \text{h.c.}\right)} \tag{50}$$

and the angles $\theta_{\mathbf{k}}$ are such that

$$u_{\mathbf{k}} = \cos\theta_{\mathbf{k}} \qquad v_{\mathbf{k}} = \sin\theta_{\mathbf{k}}. \tag{51}$$

The BCS state is therefore the equivalent for fermions of the squeezed vacuum for bosons.

Calculating the expectation value in the BCS state of a product of operators a and $a^\dagger$ is therefore equivalent to calculating the expectation value in the vacuum state of the product of the transformed operators $U^\dagger a U$ and $U^\dagger a^\dagger U$. These transformed operators have a linear expression in terms of the original a and $a^\dagger$:

$$U^\dagger a_{\mathbf{k}\uparrow} U = u_{\mathbf{k}} a_{\mathbf{k}\uparrow} + v_{\mathbf{k}} a^\dagger_{-\mathbf{k}\downarrow} \quad (52)$$

$$U^\dagger a^\dagger_{-\mathbf{k}\downarrow} U = -v_{\mathbf{k}} a_{\mathbf{k}\uparrow} + u_{\mathbf{k}} a^\dagger_{-\mathbf{k}\downarrow}. \quad (53)$$

As a consequence, Wick theorem can be applied to calculate expectation values in the BCS state, since it applies for the vacuum.

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