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Universal phase diagram of a strongly interacting Fermi gas with unbalanced spin populations.

F. Chevy

Laboratoire Kastler Brossel, École normale supérieure, Paris, France

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We present a theoretical interpretation of a recent experiment presented in ref. [1] on the density profile of Fermi gases with unbalanced spin populations. We show that in the regime of strong interaction, the boundaries of the three phases observed in [1] can be characterized by two dimensionless numbers η_α and η_β . Using a combination of a variational treatment and a study of the experimental results, we infer rather precise bounds for these two parameters.

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In fermionic systems, superfluidity arises from the pairing of two particles with opposite spin states, a scenario first pointed out by Bardeen Cooper and Schrieffer (BCS) to explain the onset of superconductivity in metals. For this mechanism to be efficient, the Fermi surfaces associated with each spin component need be matched, and soon after the seminal BCS work the question of the effect of a population imbalance between the two states was raised. At the time, it was understood that pairing and superfluidity could sustain a certain amount of mismatch, above which the system would undergo a quantum phase transition towards a normal state [2]. The original work of Fulde, Ferrel, Larkin and Ovshinnikov, who proposed the existence of Cooper pairing at finite momentum, was later generalized to trapped systems [3, 4, 5]. Alternative scenarios were also proposed, including deformed Fermi surfaces [6], interior gap superfluidity [7], phase separation between a normal and a superfluid state through a first order phase transition [8, 9, 10, 11], or BCS quasi-particle interactions [12]. When the strength of the interactions is varied, a complicated phase diagram mixing several of these scenarios is expected [13, 14, 15].

However, due to the absence of experimental evidence, these scenarios could never be tested experimentally until the subject was revived by the possibility of reaching superfluidity in ultra-cold fermionic gaseous systems [16, 17, 18, 19, 20, 21]. Contrarily to usual condensed matter systems, spin relaxation is very weak in cold atoms, and this allows one to keep spin polarized samples for long times. This unique possibility led to the first experimental studies of imbalanced Fermi gases at MIT and Rice University [1, 22, 23]. These results triggered a host of theoretical work aiming at explaining the various results observed by the two groups [24, 25, 26, 27, 28].

One interesting feature of ref. [1] is the observation of three different phases in the cloud. At the center, the authors observe a superfluid core, where the densities of the two spin states are equal, then an intermediate normal shell where the two states coexist and finally an outer rim of the majority component. In the present paper, we show that, though performed in a trap, the observations of MIT can offer valuable information on the phase

diagram of a strongly interacting Fermi gas with unbalanced populations. In a first part we will present a brief overview of the simplest free space scenario for transition from a paired superfluid to a pure normal state, through a mixed phase. Focusing on the disappearance of the minority component, we will present a variational study of the problem of a single minority particle embedded in the Fermi sea of majority atoms. Finally, we will show that the comparison with experiments allows for a rather precise determination of the transition thresholds. One of the key point is that, contrarily to previous works, we mostly rely on “exact” experimental or Monte Carlo results, without the need of the BCS ansatz often used in other publications.

Before addressing the case of trapped fermions, let us first discuss the zero temperature phase diagram of an ensemble in free space. We consider fermions of mass m with two internal states labelled 1 and 2. Within a quantization volume V and in the limit of short range interactions, we can write the hamiltonian of the system as

$$\hat{H} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{a}_{\mathbf{k}, \sigma}^\dagger \hat{a}_{\mathbf{k}, \sigma} + \frac{g_b}{V} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \hat{a}_{\mathbf{k}+\mathbf{q}, 1}^\dagger \hat{a}_{\mathbf{k}'-\mathbf{q}, 2}^\dagger \hat{a}_{\mathbf{k}', 2} \hat{a}_{\mathbf{k}, 1}. \quad (1)$$

Here, $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$, $\hat{a}_{\mathbf{k}, \sigma}$ is the annihilation operator of a species σ particle with momentum \mathbf{k} , and g_b is the bare coupling constant characterizing inter-particle interactions. It is related to the s-wave scattering length of the system a by the Lippmann-Schwinger equation

$$\frac{1}{g_b} = \frac{m}{4\pi\hbar^2 a} - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2\epsilon_{\mathbf{k}}}. \quad (2)$$

In this paper, we assume we are working at the unitary limit where $|a| = \infty$ and, using the grand canonical ensemble, we wish to find the ground state of the grand-potential $\hat{\Xi} = \hat{H} - \mu_1 \hat{N}_1 - \mu_2 \hat{N}_2$. Here \hat{N}_i is the particle number operator for species i and μ_i is the associated chemical potential (we take species 1 as majority hence $\mu_1 > \mu_2$). The grand potential can be expressed as the

function of the volume V and pressure P of the ensemble according to $\langle \widehat{\Xi} \rangle = -PV$. In other words, searching the ground state of the system is equivalent to searching the phase with the highest pressure P . To start our analysis, we note first that two exact eigenstates of $\widehat{\Xi}$ can be found quite easily.

1. First, a fully polarized gas, constituted only of particles 1. Due to the Pauli principle, there are no interactions and we just need to find the ground state of an ideal Fermi gas, for which we know that

$$P_N = \frac{1}{15\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \mu_1^{5/2}.$$

2. Let us now consider the exact ground state $|\text{SF}\rangle_\mu$ of the balanced grand potential $\widehat{\Xi}' = \widehat{H} - \mu(\widehat{N}_1 + \widehat{N}_2)$, describing a superfluid with chemical potential μ . This potential commutes with the number operators, hence the ground state can be searched as an eigenstate for both \widehat{N}_1 and \widehat{N}_2 , with $\widehat{N}_1|\text{SF}\rangle_\mu = \widehat{N}_2|\text{SF}\rangle_\mu$. We check readily that $|\text{SF}\rangle_{\bar{\mu}}$, with $\bar{\mu} = (\mu_1 + \mu_2)/2$, is still an eigenstate of the unbalanced $\widehat{\Xi}$, by noting that $\widehat{\Xi} = \widehat{\Xi}' + (\mu_1 - \mu_2)(\widehat{N}_1 - \widehat{N}_2)/2$. At unitarity the pressure of a balanced Fermi gas reads $P_S = 2(2m/\xi\hbar^2)^{3/2} \mu^{5/2}/15\pi^2$, where $\xi \sim 0.45$ is a universal parameter whose determination has attracted interest of both theoreticians [10, 29, 30, 31] and experimentalists [19, 23, 32, 33, 34]. In the case of mismatched chemical potentials, the pressure of this fully paired superfluid state is therefore

$$P_S = \frac{1}{15\pi^2} \left(\frac{m}{\xi\hbar^2} \right)^{3/2} (\mu_1 + \mu_2)^{5/2}.$$

The evolution of P_N and P_S is presented in Fig. 1 as a function of $\eta = \mu_2/\mu_1$. We see that they cross for $\eta_c = (2\xi)^{3/5} - 1 \sim -0.061$, marking the instability of the superfluid against large population imbalances [28]. However, since we only compare the energy of the fully paired state to the one of the fully polarized ideal gas, the real breakdown of superfluidity could very well happen for some η larger than η_c . We know this is actually the case, since in ref. [1], the authors observed an intermediate normal phase, containing atoms of both species. From universality at unitarity, the phase transition from the fully paired to the intermediate phase, and then from the intermediate to the fully polarized normal phase are given by conditions $\mu_1/\mu_2 = \eta_\alpha$, and $\mu_1/\mu_2 = \eta_\beta$, where η_α and η_β are two universal parameters we would like to determine as precisely as possible.

Noting that the transition from the fully paired state to the intermediate one must happen before the transition

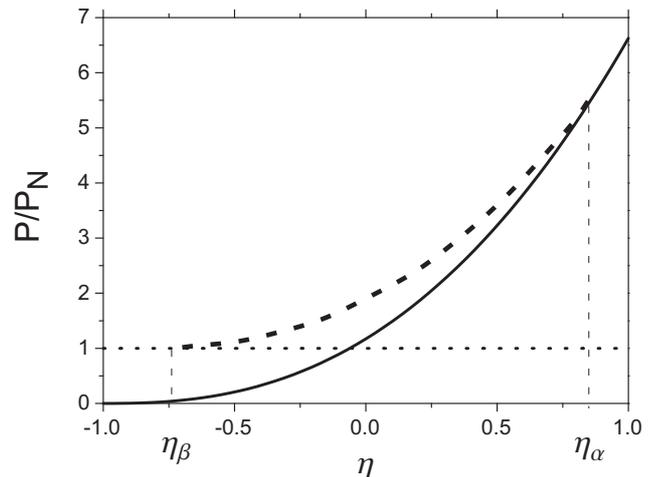


FIG. 1: Comparison of the pressure of the various phases, normalized by the pressure P_N of the fully polarized ideal Fermi gas, as a function of the chemical potential mismatch $\eta = \mu_2/\mu_1$. Dotted line: fully polarized phase. Full line: fully paired superfluid phase. The fully paired and fully polarized states meet for $\eta \sim -0.06$. Dashed line: sketch of the intermediate normal phase. η_α and η_β designate the universal chemical potential thresholds for this phase.

to the fully polarized phase, we see graphically that we have necessarily $\eta_\alpha > \eta_c$, and, similarly, $\eta_\beta < \eta_c$. The upper bound on η_β can be further improved by noting that at the threshold between the normal mixture and the fully polarized ideal gas, there are only a few atoms of the majority species. In principle, the value of η_β should then be found by studying the $N+1$ body problem of a Fermi sea of N particles 1, in presence of a single minority atom. To address this problem, we use here a variational method. Let us start with a Fermi sea of particles 1, characterized by a Fermi wave-vector k_F , and then let us add a particle of 2, and because we know some pairing will occur, let us also add one particle of 1. By definition of the chemical potential, the energy of the system is increased by $\mu_1 + \mu_2$. We can try to find the state of the system using a variational ansatz in which the two additional particles are paired according to a slightly modified Cooper scenario. If the 2 particle has a momentum \mathbf{k} with $k > k_F$, then the particle 1 is placed in a state with wave vector $\bar{\mathbf{k}} = -\mathbf{k}$. Because of the presence of the majority Fermi sea, this cannot be done anymore when $k < k_F$. In this case, we simply place the particle 1 at the surface of the Fermi sea with a momentum $\bar{\mathbf{k}} = -k_F \mathbf{k}/k$. In other words, the trial wave function of the many-body system is

$$|\psi\rangle = \left(\sum_{\mathbf{k}} \varphi_{\mathbf{k}} \hat{a}_{\mathbf{k},2}^\dagger \hat{a}_{\bar{\mathbf{k}},1}^\dagger \right) \prod_{k' < k_F} \hat{a}_{\mathbf{k}',1}^\dagger |0\rangle, \quad (3)$$

where $|0\rangle$ is the vacuum and $\varphi_{\mathbf{k}}$ satisfy the normalization condition $\sum_{\mathbf{k}} |\varphi_{\mathbf{k}}|^2 = 1$. The energy $E[\varphi_{\mathbf{k}}] = \langle \psi | \hat{H} | \psi \rangle$ associated with this state reads

$$E[\varphi_{\mathbf{k}}] = E_{\text{FS}} + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} + \epsilon_{\bar{\mathbf{k}}} + g_{\text{b}} n_1) |\varphi_{\mathbf{k}}|^2 + \frac{g_{\text{b}}}{V} \sum_{\mathbf{k}, \mathbf{k}'} \varphi_{\mathbf{k}} \varphi_{\mathbf{k}'}^*, \quad (4)$$

where E_{FS} is the energy of the Fermi sea and n_1 is the density of species 1. After a straightforward calculation, the minimization of E with respect to $\varphi_{\mathbf{k}}$ yields an optimum wave function $\varphi_{\mathbf{k}}^{(0)}$ given by

$$\varphi_{\mathbf{k}}^{(0)} = \frac{-\Delta}{\epsilon_{\mathbf{k}} + \epsilon_{\bar{\mathbf{k}}} + g_{\text{b}} n_1 - \lambda}, \quad (5)$$

where $\Delta = g_{\text{b}} V^{-1} \sum_{\mathbf{k}} \varphi_{\mathbf{k}}^{(0)}$ and λ is the Lagrange coefficient associated with the normalization constraint. λ has actually a very simple physical interpretation, since, after plugging $\varphi_{\mathbf{k}}^{(0)}$ in eq. (4) one obtains $\lambda = E[\varphi_{\mathbf{k}}^{(0)}] - E_{\text{FS}}$. In other words, λ is the energy of the trial state. It can be calculated by summing eq. 5 over \mathbf{k} , which permits us to eliminate Δ and $\varphi_{\mathbf{k}}$ and finally leads to the following implicit equation for λ

$$\sum_{\mathbf{k}} \left(\frac{1}{\lambda - \epsilon_{\mathbf{k}} - \epsilon_{\bar{\mathbf{k}}}} + \frac{1}{2\epsilon_{\mathbf{k}}} \right) = 0.$$

Here we have also regularized the coupling constant according to eq. (2), implying in particular that $g_{\text{b}} n_1 \rightarrow 0$. This equation can be solved numerically and yields $\lambda \sim 0.56\mu_1$. Since λ is the energy of the trial state, it constitutes an upper bound of the true energy $\mu_1 + \mu_2$ of the system, from which we conclude that the minority component disappears at a ratio $\eta_{\beta} = \mu_2/\mu_1 < -0.44$

Up to now, we have proposed some boundaries for the values η_{α} and η_{β} at which the two quantum phase transitions occur. We would now like to show how experimental data from ref. [1] permits to improve this determination. In this pursuit, we use the Local Density Approximation (LDA) to calculate the density profile of the cloud in a harmonic trap, which for simplicity we assume is isotropic. In this case, the chemical potentials $\mu_{1,2}$ of each species depends on position according to the law $\mu_{1,2}(\mathbf{r}) = \mu_{1,2}^0 - m\omega^2 r^2/2$, where ω is the trap frequency.

Using this assumption, the transition between the various phases will happen at radii R_{α} and R_{β} given by $\mu_2(R_{\alpha,\beta})/\mu_1(R_{\alpha,\beta}) = \eta_{\alpha,\beta}$. When these two equations are associated with the condition giving the radius R_1 of the majority component, $\mu_1(R_1) = 0$, we can eliminate both μ_1^0 and μ_2^0 from the equations, yielding the following close formula relating the radii R_{α} , R_{β} and R_1

$$\frac{R_{\alpha}}{R_1} = \sqrt{\frac{(R_{\beta}/R_1)^2 - q}{1 - q}}. \quad (6)$$

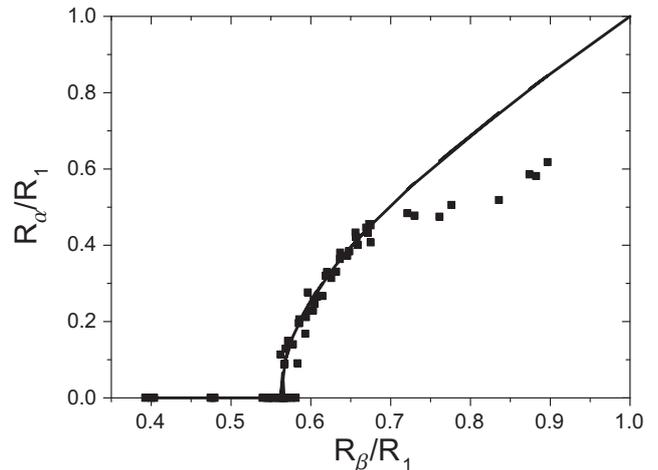


FIG. 2: Comparison between experimental data of ref. [1] (squares) and eq. (6) (full line). R_{α} , R_{β} and R_1 are respectively the radii of the superfluid, minority and majority components. The condensate vanishes for $R_{\alpha} = 0$ at $q = R_{\beta}^2/R_1^2 \sim 0.32$.

Here, $q = (\eta_{\alpha} - \eta_{\beta})/(1 - \eta_{\beta})$ corresponds to the value of the R_{β}^2/R_1^2 at which R_{α} vanishes, *i.e.* at which the superfluid fraction disappears. In Fig. 2, we compare the prediction of eq. 6 with the experimental finding of ref. [1], taking $q = 0.32$ to match the superfluidity thresholds. We see that close to the threshold, the agreement between the two graphs is quite good. However, they depart from each other for $R_{\beta}/R_1 \gtrsim 0.7$, corresponding to low population imbalance. One explanation for this discrepancy might involve finite temperature effects. Indeed, it was already noted in Fig. 4 of ref. [22] that, although the superfluid fraction was very sensitive to temperature at small imbalances, the value of the critical population imbalance was more robust.

The superfluid phase disappears when R_{α} vanishes. From eq. 6, we see this happens for a ratio $R_{\beta}^2/R_1^2 = q$. As seen in Fig. 2, q can be extracted from the experimental data of ref. [1], which yield $q \sim 0.32$ and therefore constrain the possible values of η_{α} and η_{β} . Indeed, using this determination of q , as well as the rough upper and lower values for $\eta_{\alpha,\beta}$, one obtains

$$-0.06 < \eta_{\alpha} < 0.02 \quad (7)$$

$$-0.55 < \eta_{\beta} < -0.44 \quad (8)$$

These bounds can be compared to the values deduced by BCS theory, predicting $\eta_{\alpha} \sim 0.1$ and $\eta_{\beta} = 0$. Our calculation excludes these values and explains why the width of the mixed normal state predicted by BCS theory is much narrower than observed in experiments [27].

In conclusion, we have presented an analysis of the experimental data of ref. [1] providing stringent bounds

on the values of the thresholds for quantum phase transitions in uniform unbalanced fermi gases. Since they were obtained using minimal assumptions (mainly LDA), these bounds are fairly robust. In particular, they do not depend precisely on the superfluid nature of the intermediate phase. Our results suggest interesting follow-ups. First, the threshold to the normal polarized phase was obtained by a variational study of the problem of a single atom in presence of a non-interacting Fermi sea. This problem is considerably simpler than the BCS problem (two Fermi seas), since a small parameter (N_2/N_1) is now available and should permit a perturbative analysis leading to the exact value of η_β . Second, the full understanding of the system, and in particular of the density profile of the cloud, requires the knowledge of the state equation of the intermediate phase, whose exact nature then needs to be clarified. Second, the comparison with the data of ref. [23] suggests an intriguing issue. Indeed, although the superfluidity threshold was not directly measured in this paper, the parameter q can be inferred from the critical imbalance 0.7 measured by MIT. Rice's experimental data yield at this value $q \sim 0.16$. Not only is this value very far from the one obtained here from the analysis of MIT's experiments, but it also contradicts the theoretical bounds $\eta_\alpha > -0.06$ and $\eta_\beta < -0.44$ which imply $q > 0.26$. As suggested in ref. [35], this discrepancy may arise from surface tension effects provoked by the strong anisotropy of Rice's trap. Finally, the $\eta_{\alpha,\beta}$ parameters can be evaluated experimentally using the value of q associated with the measurement of the density discontinuity $\Delta n_{1,2}$ at $r = R_\alpha$, given by $\Delta n_1/\Delta n_2 = -\eta_\alpha$ [36]. The preliminary data presented in fig. 2.b of ref. [37] suggest that the discontinuity Δn_1 is very weak, hence indicating a small value of η_α , in agreement with the bounds obtained here.

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