Boundstates and the BEC-BCS Crossover

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This report presents a basic overview of the crossover from the Bardeen–Cooper–Schrieffer (BCS) state of weakly-correlated pairs of fermions to the Bose–Einstein condensation (BEC) of diatomic molecules in the atomic Fermi gas. We discuss how this crossover (called the BEC-BCS Crossover) is achieved without any phase transition by tuning the interaction strength via Feshbach resonances. This is supplemented by a discussion on boundstates and the contingencies of their appearence in an atomic gas.

I. INTRODUCTION

The BEC paradigm, first developed for non-interacting bosons and later generalized to take into account repulsive interactions, describes bosonic fluids like ^{4}He or ultracold Bose gases like ^{87}Rb. The condensate is a macroscopic occupation of a single quantum state that occurs below a transition temperature T_c, which, even in strongly interacting Bose systems like ^{4}He, is of the same order of magnitude as the quantum degeneracy temperature at [1] which the inter-particle spacing becomes of the order of the thermal de-Broglie wavelength.

Even though the BCS theory became successfully and widely applicable to many phenomena, it is basically a weak attraction theory. A generalization of the BCS theory has been developed to include the strong attraction regime in which fermion pairs become tightly bound diatomic Bose molecules and undergo Bose–Einstein condensation. The BEC state is on the the strong attraction side of the phase space, and is formed by the condensation of bound fermions in real space. There is now a clear recognition that the BCS and BEC paradigms are not as distinct as they were once thought to be, but rather are the two extrema of a continuum. The difference between the pairs and the molecules is that the molecules are localized in the real (position) space, whereas the BCS pairs are made of two particles with opposite momenta. Thus, the BCS pairs are large (much larger than the inter-particle spacing), whereas the BEC molecules are small (Figure 1).

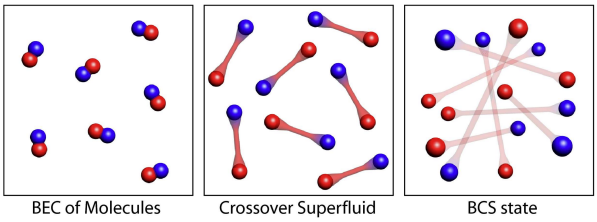

FIG. 1: BEC-BCS crossover. By tuning the interaction strength between the two fermionic spin states, one can smoothly cross over from a regime of tightly bound molecules to a regime of long-range Cooper pairs, whose characteristic size is much larger than the inter-particle spacing. In between these two extremes, one encounters an intermediate regime where the pair size is comparable to the inter-particle spacing [2]

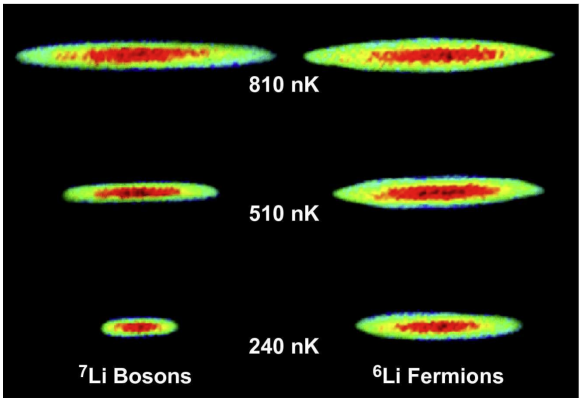

FIG. 2: Simultaneous cooling of a bosonic and fermionic quantum gas of ^{7}Li and ^{6}Li to quantum degeneracy. In the case of the Fermi gas, the Fermi pressure prohibits the atom cloud to shrink in space as quantum degeneracy is approached. [3]

This report goes over a basic description of the BEC-BCS crossover, and discusses its realization in terms of a simple account of Feshbach resonances which are used to tune the interaction between the system's constituents. We also present a discussion on bound-state formation in quantum systems, and how results from the same describe Cooper Pairing.

II. THEORY

A. Bound States

In contrast to bosons, the non-interacting Fermi gas does not show any phase transition down to zero temperature

figure(2). One might assume that this qualitative fact should not change as interactions are introduced, at least as long as they are weak. This is essentially true in the case of repulsive interactions [4]. For attractive interactions, the situation is, however, dramatically different. Even for very weak attraction, the fermions form pairs and become superfluid, due to a generalized form of pair condensation. The idea of pairing might be natural, as tightly bound pairs of fermions can be regarded as point-like bosons, which should form a Bose-Einstein condensate. However, for weak attractive interaction – as is the case for the residual, phonon-induced electron-electron interaction in metals – it is not evident that a paired state exists. Indeed, we will see in the following that in three dimensions there is no bound state for two isolated particles and arbitrarily weak interaction. However, by discussing exact solutions in 1D and 2D, where bound states exist for weak interactions, we gain insight into how a modified density of states will lead to bound states even in 3D – this is the famous Cooper instability. What physical quantity decides whether there are bound states or not? To answer this question, we formulate the problem of two interacting particles of mass m in momentum space [2]. This identifies the density of states in the different dimensions as the decisive factor for the existence of bound states.

We start our search for a bound-state state of energy $E = -\frac{\hbar^2 k^2}{m}$ (as $m/2$ is the reduced mass) and write the Schrodinger equation:

$$\frac{\hbar^2}{m}\left(\nabla^2 - k^2\right)\psi = V\psi \tag{1}$$

A Fourier-transform takes us to the equivalent momentum-space relation:

$$\psi_{\mathbf{k}}(\mathbf{q}) = -\frac{m}{\hbar^2}\frac{1}{q^2+k^2}\int \frac{d^n q'}{(2\pi)^n} V\left(\mathbf{q}-\mathbf{q}'\right)\psi_{\mathbf{k}}\left(\mathbf{q}'\right) \tag{2}$$

Assuming a short-range potential, we can introduce a cut-off $|\mathbf{q}| < R$ in the integral. For a short-range potential of range $R \ll \frac{1}{k}, V(q)$ is practically constant as $V(q) \approx V_0$, for all relevant q, and falls off to zero on a large q-scale of $\approx \frac{1}{R}$. For example, for a potential well of depth V and size R, we have $V_0 \approx VR^n$.

We integrate over q, and divide by the common factor on either side of the equation to get:

$$-\frac{1}{V_0} = \frac{m}{\hbar^2}\int_{q<\frac{1}{R}} \frac{d^n q}{(2\pi)^n}\frac{1}{q^2+k^2} = \frac{1}{\Omega}\int_{\epsilon<E_R} d\epsilon \frac{\rho_n(\epsilon)}{2\epsilon+|E|} \tag{3}$$

with the bound-state energy E, the density of states $\rho_n(\epsilon)$ in n dimensions, the energy cut-off $E_R = \hbar^2/mR^2$ and the volume Ω of the system (note that V_0 has units of energy times volume). The second equality in (3) is because $\frac{\hbar^2}{m\Omega}\rho_{3D}(\epsilon) = \frac{1}{2\pi^2}\sqrt{\frac{2mE}{\hbar^2}}$. This equation has a solution for small $|V_0|$ only if the right hand side also diverges for vanishing bound state energy $|E| \to 0$ and this involves an integral over the density of states. The calculations of ρ_n shows that in 1D, the integral diverges as $\sqrt{E}$, and for 2D (where $\rho(\epsilon)$ is constant) it does so logarithmically [2]. Hence, we infer that boundstate solutions exist in 1D and 2D for arbitrarily shallow potentials. However, in 3D the integral is finite for vanishing $|E|$, and there is a threshold for the interaction potential to create a boundstate.

These results indicate why there might be a paired state for two fermions in attendance of a Fermi sea, even for arbitrarily weak interactions: the density of available states to the two fermions is maybe modified. This is precisely what happens, as will be discussed in the next section.

B. Fermionic Pairing

Consider now two weakly interacting spin 1/2 fermions not in vacuum, but on top of a (non-interacting) filled Fermi sea. We can write the Schrodinger equation for the two interacting particles as before, but now we need to search for a small binding energy $E_B = E - 2E_F < 0$ on top of the large Fermi energy $2E_F$ of the two particles:

$$-\frac{1}{V_0} = \frac{1}{\Omega}\int_{E_F<\epsilon<E_F+E_R} d\epsilon \frac{\rho_{3D}(\epsilon)}{2(\epsilon-E_F)+|E_B|} \tag{4}$$

In conventional superconductors, the natural cut-off energy E_R is given by the Debye frequency $\omega_D, E_R = \hbar\omega_D$, corresponding to the highest frequency at which ions in the crystal lattice can respond to a bypassing electron. Since we have $\hbar\omega_D \ll E_F$, we can approximate $\rho_{3D}(\epsilon) \approx \rho_{3D}(E_F)$ and find:

$$E_B = -2\hbar\omega_D e^{-2\Omega/\rho_{3D}(E_F)|V_0|} \tag{5}$$

This result, applicable to a gas of electrons can be easily modified to deal with our system of interest: an atomic Fermi gas. We replace V_0 by the physically relevant scattering length $a < 0$ as follows:

$$\frac{1}{V_0} = \frac{m}{4\pi\hbar^2 a} - \frac{m}{\hbar^2}\int \frac{d^3 q}{(2\pi)^3}\frac{1}{q^2} \tag{6}$$

The origin for this expression can be seen from the usual definition of a [5]:

$$a = -\lim_{k \ll 1/r_0} \frac{\tan \delta_s}{k} \tag{7}$$

where δ_s is the s-wave phase shift. Here, it is assumed that the gas is sufficiently dilute and that the behavior is insensitive to the microscopic details of the potential. For ultracold collisions, we are interested in describing the scattering process at low momenta $k \ll \frac{1}{r_0}$, where r_0 is the range of the interatomic potential. In the absence of resonance phenomena for $l \neq 0$, s-wave scattering $l = 0$ is dominant over all other partial waves (if allowed by the Pauli principle). The integral in (6) will usually have a natural cut-off at $k = \frac{\hbar}{r_0}$.

Repeating the calculations as previous for $|E_B|$, we get:

$$E_B = -\frac{8}{e^2} E_F e^{-\frac{\pi}{k_F |a|}} \tag{8}$$

Hence, the essence of Cooper pairing in this language is that our density of states becomes constant, just like it does in 2D, and allows a small attractive potential to bind two fermions. An interesting extension of this result shows that this is true even in N-dimensions: all we require is the $\rho_N(\epsilon)$ be constant, irrespective of in how many dimensions the "motion" is taking place. [6]

These calculations were made assuming that we have non-interacting Fermi Sea, and indicates that the ground state should be a Bose-Einstein Condensate of these weakly bound pairs. However, as we increase the density of particles in the system, the Pauli pressure of the fermionic constituents becomes important. The origin for this can be traced to the Pauli limitation of unity occupation per momentum space: only when the fermions are tightly bound (Figure 3) are they spread out in momentum space. We can then treat the bound fermion-pairs as bosons, as indicated by the bosonic commutation relations in eq(12). This indicates that the fermionic nature of the constituents of the system becomes irrelevant only when the size of the molecules is much smaller than the interparticle spacing i.e when the binding energy exceeds the E_F. Relevant details for these inferences will be discussed in the next section.

We have explicitly calculated the conditions for the appearance of the bound state, with the critical parameter being the density of states. Because of the restriction to a "small" manifold of energy above the Fermi sea, the system can be approximated as having a constant $\rho(\epsilon)$. This endows it with the properties reminiscent of a $2D$ system, namely the ability to support bound-states for arbitrarily low binding energy.

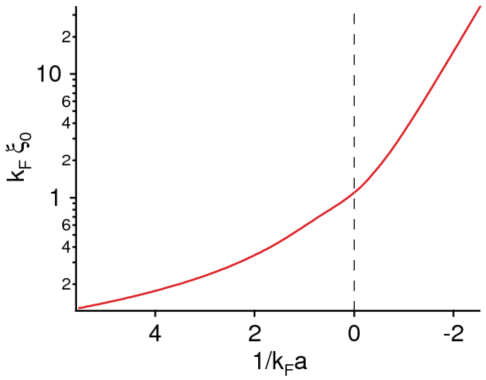

FIG. 3: From tightly bound molecules to long-range Cooper pairs [2]. Evolution of the pair size $\xi_0 = \sqrt{\frac{\langle \psi(\mathbf{r}) | r^2 | \psi(\mathbf{r}) \rangle}{\langle \psi(\mathbf{r}) | \psi(\mathbf{r}) \rangle}}$ as a function of the interaction parameter $\frac{1}{k_F a}$. The dashed line indicates resonance.

C. The BEC-BCS Wavefunction

Leggett [7] realized that the crossover from BCS to the BEC regime is smooth. This is somewhat surprising since just focusing on the two-body physics shows a threshold behavior at a critical interaction strength, below which there is no bound state for two particles. In the presence of the Fermi sea, however, we simply cross over from a regime of tightly bound molecules to a regime where the pairs are of much larger size than the interparticle spacing.

For s-wave interactions, the orbital part of the pair wave function $\varphi(r_1, r_2)$ will be symmetric under exchange of the paired particles' coordinates. In a uniform system, it will also only depend on their distance $|r_1 - r_2|$. We hence analyze the many-body wavefunction:

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = A\{\varphi(|\mathbf{r}_1 - \mathbf{r}_2|)\chi_{12}...\varphi(|\mathbf{r}_{N-1} - \mathbf{r}_N|)\chi_{N-1,N-2}\} \tag{9}$$

that describes a condensate of such fermion pairs, with the operator A denoting the correct antusymmetrization of all coordinates, and the spin singlet $\chi_{ij} = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i |\downarrow\rangle_j - |\downarrow\rangle_i |\uparrow\rangle_j$. In second quantization, we write:

$$\begin{aligned} |\Psi\rangle_N = \int \textstyle\prod_i d^3 r_i \varphi(\mathbf{r}_1 - \mathbf{r}_2) \Psi_\uparrow^\dagger(\mathbf{r}_1) \Psi_\downarrow^\dagger(\mathbf{r}_2) \dots \\ \varphi(\mathbf{r}_{N-1} - \mathbf{r}_N) \Psi_\uparrow^\dagger(\mathbf{r}_{N-1}) \Psi_\downarrow^\dagger(\mathbf{r}_N) |0\rangle \end{aligned} \tag{10}$$

where the fields $\Psi_\sigma^\dagger(\mathbf{r}) = \sum_k c_{k\sigma}^\dagger \frac{e^{-i\mathbf{k}.\mathbf{r}}}{\sqrt{\Omega}}$. Using the fourier transform of the wavefunction $\varphi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_k \varphi_k \frac{e^{-i\mathbf{k}.(\mathbf{r_1} - \mathbf{r_2})}}{\sqrt{\Omega}}$, we introduce the pair creation operator $b^\dagger = \sum_k \varphi_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$, finding:

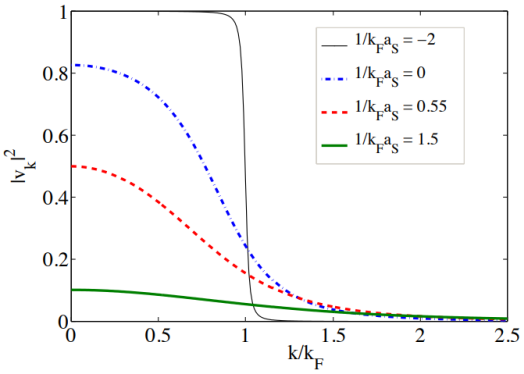

FIG. 4: Evolution of the momentum distribution v_k^2 with interaction $\frac{1}{k_F a}$ across the BCS–BEC crossover. [4]

$$|\Psi\rangle_N = b^{\dagger\frac{N}{2}}|0\rangle \tag{11}$$

This expression for $|\Psi\rangle_N$ is formally identical to the Gross-Pitaevskii ground state [8] of a condensate of bosonic particles. In order to treat fermionic pairs on the same footing as bosons, we need to establish that the correct bosonic commutation relations are satisfied :

$$\begin{aligned}
\left[b^\dagger, b^\dagger\right]_- &= \sum_{kk'} \varphi_k \varphi_{k'} \left[c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}, c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\right]_- = 0 \\
[b, b]_- &= \sum_{kk'} \varphi^*_k \varphi_{k'} \left[c_{-k\downarrow} c_{k\uparrow}, c_{-k'\downarrow} c_{k'\uparrow}\right]_- = 0 \\
\left[b, b^\dagger\right]_- &= \sum_{kk'} \varphi^*_k \varphi_{k'} \left[c_{-k\downarrow} c_{k\uparrow}, c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\right]_- \\
&= \sum_k |\varphi_k|^2 \left(1 - n_{k\uparrow} - n_{k\downarrow}\right)
\end{aligned} \tag{12}$$

The third commutator is equal to one only in the limit where the pairs are tightly bound and occupy a wide region in momentum space. In this case, the occupation numbers n_k of any momentum state k are very small (Figure 4), and $\left[b, b^\dagger\right]_- = \sum_k |\varphi_k|^2 = 1$.

The ground-state wave function can be written as a coherent state of these bosons:

$$\begin{aligned}
\mathcal{N}|\Psi\rangle &= \sum_{J_{\text{even}}} \frac{N_p^{J/4}}{(J/2)!} |\Psi\rangle_J = \sum_M \frac{1}{M!} N_p^{M/2} b^{\dagger M} |0\rangle = e^{\sqrt{N_p} b^\dagger} |0\rangle \\
&= \prod_k e^{\sqrt{N_p}\varphi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}} |0\rangle = \prod_k \left(1 + \sqrt{N_p}\varphi_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right) |0\rangle
\end{aligned} \tag{13}$$

where $N_p = \frac{N}{2}$ is the number of pairs. It can be argued [9] that the coherent state is energetically favored over the number state $|\Psi\rangle_N = b^{\dagger\frac{N}{2}}|0\rangle$ in the presence of weak repulsive interactions. However, in practice they both yield equivalent results for thermodynamic quantities and thus we can use whichever is most convenient. If we choose the constant $\mathcal{N} = \prod_k \frac{1}{u_k} = \prod_k \sqrt{1 + N_p|\varphi|^2}$, then $|\Psi\rangle$ becomes a properly normalized state:

$$|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}) |0\rangle \tag{14}$$

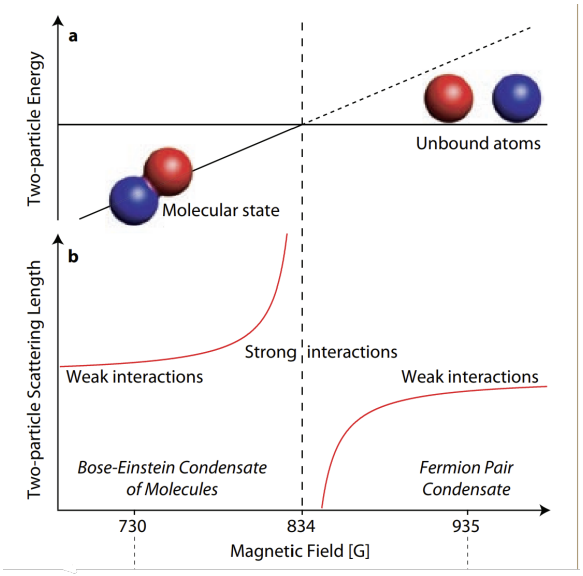

FIG. 5: Illustration of the Feshbach Resonance [12]

with $v_k = \sqrt{N_p}\varphi_k u_k$ and $|u_k|^2 + |v_k|^2 = 1$. This is the familiar BCS wavefunction [10]. The above derivation makes it clear that this wave function encompasses the entire regime of pairing, from point bosons (small molecules) to weakly and non-interacting fermions.

III. FESHBACH RESONANCES AND INTERACTION TUNING

We now explore the tuning of the interaction strength a, which determines the BEC-BCS crossover. The BCS and BEC regimes then correspond, respectively, to the limits $\frac{1}{k_F a} \ll 1$ and $\frac{1}{k_F a} \gg 1$. This can be intuitively understood from the following qualitative discussion of Feshbach resonances.

Feshbach resonances [11] are a unique tool for the study of ultracold atoms. By the simple change of a magnetic field, the interactions between atoms can be controlled over an enormous range. This tunability arises from the coupling (say, by a hyperfine interaction) of free unbound atoms to a molecular state in which the atoms are tightly bound (Figure 5). The closer this molecular level lays with respect to the energy of two free atoms, the stronger the interaction between them. Indeed, right on resonance the scattering length describing this interaction diverges (Figure 5).

As a simple example [13] consider a two channel Hamiltonian $\mathcal{H}$ with one open and one closed channel. This means that H has one inaccessible (bound) eigenstate $|C\rangle = \psi(r)|c\rangle$ with energy E_c. The state $|c\rangle$ labels the channel, which is closed in this case. In addition to this bound state, there is a continuum of eigenstates $|E\rangle = \phi(r, E)|bg\rangle$, where $|bg\rangle$ is the open background scattering channel. The wave functions

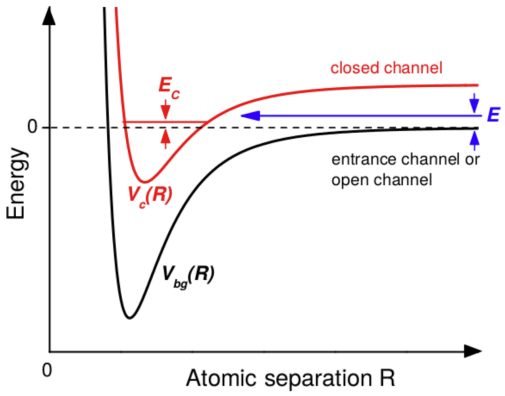

FIG. 6: The two channels of a Feshbach resonance. The red curve corresponds to the closed channel $|c\rangle$, while the black curve corresponds to the open channel $|bg\rangle$. The potential curves are given in the center of mass frame. [11]

$\psi(r)$ and $\phi(r, E)$ are eigenfunctions of the Hamiltonian with the potentials V_c and V_{bg} given in figure 6. If the Hamiltonian contains a small mixing term $\propto |c\rangle \langle bg| + h.c.$ true eigenstates are mixtures of the ones given above. If the atoms in the trap have different magnetic moments, an external magnetic field can be used to tune E_c to lie above or below E. If E is close to E_c the two channels strongly mix. This changes the scattering length. For these magnetically tuned Feshbach resonances, the scattering length is given as a function of an external magnetic field B as [14]

$$a = a_{bg}\left(1 - \frac{\Delta}{B - B_0}\right) \tag{15}$$

where a_{bg} is the scattering length associated with V_{bg}, Δ is called scattering-width and B_0 is called the resonance position. On the left-hand limit of the lower branch in Figure 5, we have strongly bound pairs that form Bose-Einstein condensates, whereas to the right we have weakly bound pairs which can form Cooper pairs in the presence of a Fermi sea.

IV. CONCLUSION

We have given a basic overview of the BEC-BCS crossover, and there are many interesting details that we omitted that can be explored in the literature. In particular, the calculations of the single-particle excitation spectrum in the BCS $\frac{1}{k_F a} \ll -1$ limit and BEC $\frac{1}{k_F a} \gg 1$ limit show the the existence of a superfluid gap, which results in phase separation in imbalanced Fermi mixtures[15]. Another notable omission was the discussion of the cross-over regime. Here, the pair size becomes of order the interparticle spacing and thus the system can no longer be regarded as either a weakly interacting Bose or Fermi gas. The unitarity limit $\frac{1}{k_F a} = 0$ gives rise to a universal strongly interacting Fermi gas [16] that is independent of any interaction length scale.

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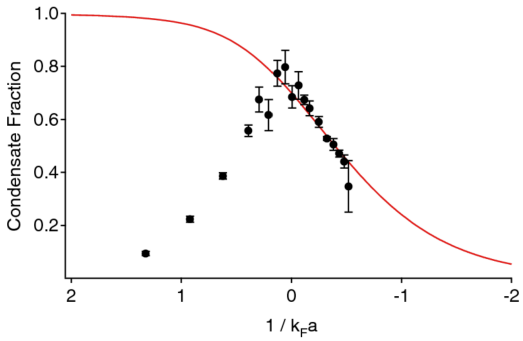

FIG. 7: Condensate fraction as a function of interaction strength. Comparison of theory and experiments.[2]. On the BEC side heating due to vibrational relaxation leads to the rapid decay of the condensate.[2]

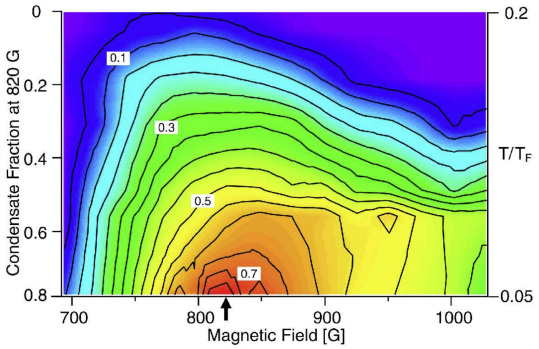

FIG. 8: Condensate fraction as a function of magnetic field and temperature in experiments on ^{6}Li. Arrow marks the position of the Feshbach resonance.[2]

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V. APPENDIX: EXPERIMENTAL OBSERVATION OF SUPERFLUIDITY IN FERMIONIC SYSTEMS

On the BEC side of the Feshbach resonance the superfluid state of tightly bound molecules should be very similar to a condensate of Bosonic atoms. Hence one can look for standard signatures of superfluidity: bimodal density distributions both inside the trap and after some expansion. Observation of vortex lattice is another important signature of superfluidity.

On the BCS side of the Feshbach resonance Cooper pairs exist only as a manybody effect. To demonstrate pairing in this regime one should convert Cooper pairs into molecules first and expand after that. This can be achieved by quickly sweeping the magnetic field to the BEC side of the resonance [17] [2]. We will discuss only the simplest model of such experiments, in which we assume that the sweep rate is very large, and we can treat these experiments as a projection of the many-body wavefunction. In analyzing real experiments there may be important corrections due to finite rate of the magnetic field sweep [18].

We can express the operator that creates a molecule in the final point of the projection experiment as

$$b_q^\dagger = \int dk \phi_f(k) c^\dagger_{\frac{q}{2}+k\uparrow} c^\dagger_{\frac{q}{2}-k\downarrow} \tag{16}$$

Here q is the momentum of the molecule and $\phi_f(k)$ is the molecular wavefunction. The number of molecules with momentum q is $n_m(q) = b_q^\dagger b_q$. For a projection type experiment we can calculate the number of molecules by taking the expectation value of $n_m(q)$ in the initial state

$$n_m(q) = \int dk dk' \phi_f^*(k)\phi_f\left(k'\right) \left\langle c^\dagger_{\frac{q}{2}+k\uparrow} c^\dagger_{\frac{q}{2}-k\downarrow} c_{\frac{q}{2}-k'} \downarrow c_{\frac{q}{2}+k'\uparrow} \right\rangle \tag{17}$$

We take the initial state to be of the type (14). Direct calculation gives

$$\begin{aligned} n_m(q) =& \delta(q) \left| \int dk \phi(k) \left\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right\rangle \right|^2 \\ &+ \int dk |\phi(k)|^2 \left\langle n_{\frac{q}{2}+k\uparrow} \right\rangle \left\langle n_{\frac{q}{2}-k\downarrow} \right\rangle \end{aligned} \tag{18}$$

The first term in (18) measures the number of molecules created in the condensate, i.e. in the $q = 0$ state. This contribution is present only when there is coherent pairing in the initial state and $\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle \neq 0$. Not surprisingly this term is proportional to the overlap of the wavefunctions for Cooper pairs and the final state molecules. The second term in (18) gives the number of non-condensate molecules produced after the sweep. This contribution is present even when the initial state is not paired. It reflects a finite probability of atoms to be close to each other in the initial state, so that the magnetic field sweep can turn them into molecules. In the simplest approximation one can take the wavefunction of the final state molecules to be constant for $k < \frac{1}{a_*}$ and zero otherwise. Here a_* is the size of the molecule. Note that this is not the size of the closed channel bound state but the size of the Feshbach molecules including the open channel, which should be of the order of the scattering length. For the coherent part we find

$$\frac{N_0}{V} = \frac{6a_*^3}{(2\pi)^3} \int_0^{a_*^{-1}} \frac{dk k^2 \Delta/2}{\sqrt{\Delta^2 + \xi_k^2}} = \frac{9n}{8} \left(\frac{\Delta}{E_f}\right)^2 k_f a_* \tag{19}$$

Here n is the density of atoms. It is easy to understand why the final result is proportional to $|\Delta|^2$ and a_*. The Cooper pair wavefunction goes as $\phi_c(r) \approx \frac{\Delta}{r}$ at short distances. The molecular wavefunction is $\phi(m) \approx a^{3/2}$ for $r < a_*$. Hence $|\langle \phi_c | | \phi_m \rangle|^2 \approx |\Delta|^2 a_*$. Figure 7 shows comparison of this simple model with the experimental results.

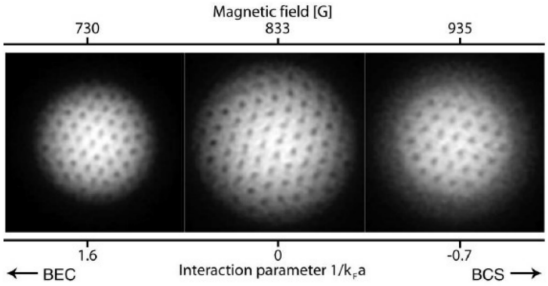

FIG. 9: Observation of vortices in a strongly interacting Fermi gas. Superfluidity, coherence, and vortex lattice were established at different value of the magnetic field. magnetic field was ramped to the BEC side for imaging. [2]