Proceedings of the International Conference "Quantum Optics V", Kościelisko, Poland, 2001

Resonance Superfluidity in a Quantum Degenerate Fermi Gas

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We consider the superfluid phase transition that arises when a Feshbach resonance pairing occurs in a dilute Fermi gas. This is related to the phenomenon of superconductivity described by the seminal Bardeen–Cooper–Schrieffer theory. In superconductivity, the phase transition is caused by a coupling between pairs of electrons within the medium. This coupling is perturbative and leads to a critical temperature $T_{\rm c}$ which is small compared to the Fermi temperature $T_{\rm F}$. Even high-$T_{\rm c}$ superconductors typically have a critical temperature which is two orders of magnitude below $T_{\rm F}$. Here we describe a resonance pairing mechanism in a quantum degenerate gas of potassium (^{40}K) atoms which leads to superfluidity in a novel regime — a regime that promises the unique opportunity to experimentally study the cross-over from the Bardeen–Cooper–Schrieffer phase of weakly-coupled fermions to the Bose–Einstein condensate of strongly-bound composite bosons. We find that the transition to a superfluid phase is possible at the high critical temperature of about $0.5T_{\rm F}$. It should be straightforward to verify this prediction, since these temperatures can already be achieved experimentally.

PACS numbers: 03.75.Fi, 67.60.–g, 74.20.–z

1. Introduction

The phenomenon of superfluidity is closely related to Bose–Einstein condensation (BEC), as was shown in the foundation of the microscopic theory of superfluid ^{4}He in the 1960's. In bosonic fluids the phase transition is marked by the appearance of a macroscopic number of bosons in the lowest quantum state. In fermionic systems the occurrence of superconductivity and superfluidity in su-

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perconductors and liquid ^{3}He, is due to the rise of a pairing field and thereby, in a generalized sense, to a condensation of Cooper pairs.

The study of superfluid phase transitions in fermion and boson systems has played an important role in the development of many areas of quantum physics. Their characteristics determine the observed properties of some of the most distinct systems imaginable, including the cosmology of neutron stars, the non-viscous flow of superfluid liquid helium, the non-resistive currents in superconductors, and the structure and dynamics of microscopic elemental nuclei. Recently, physicists have succeeded in demonstrating the creation of weakly interacting quantum fluids by cooling dilute gases to temperatures in the nanokelvin scale. For these near ideal gases, reaching such incredibly low temperatures is required in order to cross the threshold for superfluid properties to emerge. These systems offer great opportunities for study since they can be created in table-top experiments, manipulated by laser and magnetic fields which can be controlled with high precision, and directly observed using conventional optics. Furthermore their microscopic behavior can be understood theoretically from first principles. Observations of Bose–Einstein condensation [1], and demonstrations of the near ideal degenerate Fermi gas [2], are becoming fairly routine in atomic physics — something which would have been hard to foresee even ten years ago.

The phenomenology of superfluid dilute gases can be quite distinct from that of condensed matter systems. In this letter, we present a striking illustration of this

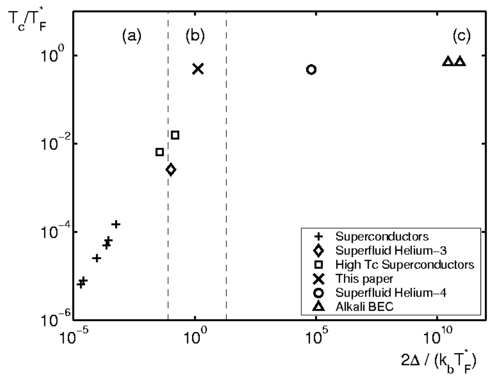

Fig. 1. A log–log plot showing six distinct regimes for quantum fluids. The transition temperature T_c is shown as a function of the relevant gap energy 2Δ. Both quantities are normalized by an effective Fermi temperature T_F^*. For the BCS systems in region (a), and the systems in the cross-over region (b), 2Δ is the energy needed to break up a fermion pair, and T_F^* is the Fermi energy. For the systems in region (c), which are all strongly bound composite bosons and exhibit BEC phenomenology, 2Δ is the smallest energy needed to break the composite boson up into two fermions, i.e. ionization to a charged atomic core and an electron, and T_F^* is the ionic Fermi temperature.

point by predicting the existence of a Feshbach resonance superfluidity in a gas of fermionic potassium atoms. This system has an ultrahigh critical phase transition temperature in close proximity to the Fermi temperature. This is a novel regime for quantum fluids, as illustrated in Fig. 1, where our system and others which exhibit superfluidity or BEC are compared. Simply by modifying a control parameter, in this case the strength of magnetic field, the system we consider can potentially explore the cross-over regime between the Bardeen–Cooper–Schrieffer (BCS) [3] transition of weakly-coupled fermion pairs and the Bose–Einstein condensation of strongly-bound composite particles [4]. This is an intriguing regime for quantum fluids as it bridges the physics of superconductors and superfluid ^{3}He, and the physics of superfluid ^{4}He and bosonic alkali gases. Non-resonant pairing applied to a dilute gas yields a T_c that depends exponentially on the inverse scattering length [5], as will be pointed out in the following section. Typically this results in a critical temperature of order $T_c \approx 10^{-4} T_F$ or $T_c \approx 10^{-10}$ K, which is way out of reach in current experiments. Many qualitative features of the nature of the superfluid phase transition are modified in the presence of a resonance coupling, including the participation of all fermions in the pairing field and the formation of a Bose–Einstein condensate of molecules at the critical point. This is illustrated

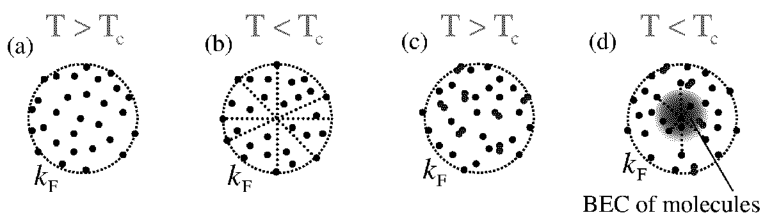

Fig. 2. Schematic illustration of the nature of the pairing fields in the cases of resonance and non-resonance coupling. The dashed circles illustrate the Fermi surface as a two-dimensional $\boldsymbol{k}$-space projection of the Fermi sphere ($\boldsymbol{k}$ is the wavevector). All plots are for temperatures in the quantum degenerate regime below T_F, so that a large number of the quantum states inside the Fermi surface are occupied. A sample of occupied quantum states are illustrated by the single dots. (a) Non-resonance-pairing for $T > T_c$. This situation is closely approximated by the non-interacting quantum degenerate Fermi gas. (b) Non-resonance-pairing for $T < T_c$. Superfluidity arises from Cooper-pairs which are composed of fermions in states near the Fermi sphere with opposite wavevectors. Only a small band of energies near the Fermi energy participates in the pairing. (c) Resonance-pairing for $T > T_c$. In addition to the quantum degenerate fermions, quasi-bound molecules are present and are shown by double dots. (d) Resonance-pairing for $T < T_c$. In this system T_c may be comparable to T_F, so that pairing is no longer restricted to fermions in close proximity to the Fermi sphere. The entire distribution contributes to the superfluidity and a Bose-Einstein condensate of molecules is present (shown as a shaded region).

in Fig. 2, where the nature of a resonance pairing mechanism is compared to the case of non-resonance pairing.

The system we study consists of an ensemble of fermionic ^{40}K atoms equally distributed between the two hyperfine states which have the lowest internal energy in the presence of a magnetic field. We calculate the full thermodynamics for this resonant superfluid system via a renormalized low energy field theory [6]. We treat explicitly a short range quasibound resonant state by extending the theory given in Refs. [7]. The parameters of the theory are uniquely specified by the known dependence of the scattering properties on magnetic field. In a dilute gas, all interactions are assumed to occur through binary collisions described by a two-body interaction. The properties of the scattering are determined by the positions of the bound states in the interaction potentials. In the low energy regime, only the highest bound states play an important role, and the scattering is completely described by the s-wave phase shift characterized by the scattering length a. In a two-body potential, a bound state may lie near threshold and give rise to a very large value of the scattering length. This occurs, for example, in the triplet potential of ^{6}Li which yields a scattering length of about $-2000a_0$ [8]. According to the conventional BCS theory, this would imply a much larger value for the critical temperature [9] than the typical value for nonresonant scattering mentioned previously. Moreover, in a multi-channel system, a bound state may cross the threshold energy as a function of magnetic field and enter the continuum, resulting in a field-dependent Feshbach scattering resonance [10]. As this occurs, a dramatic modification of the scattering length is observed (see Fig. 3).

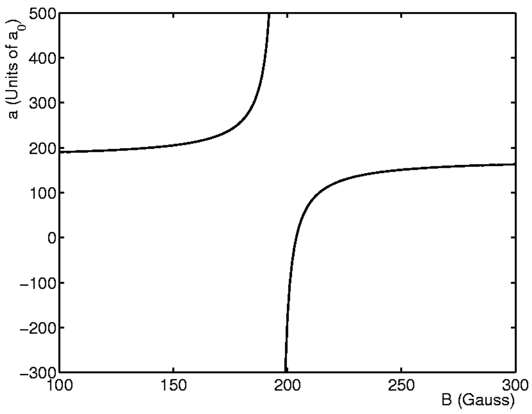

Fig. 3. Scattering length as a function of magnetic field, for a collision between ^{40}K atoms prepared in the two lowest hyperfine states. The resonance field value is $B =$ 196 gauss and the width is equal to 7.7 gauss [16]. The asymptotic behavior is caused by a Feshbach resonance.

2. Problems with BCS theory close to resonance

The BCS theory of superconductivity applied to a dilute gas considers binary interactions between particles in two distinguishable quantum states, say $|\uparrow\rangle$ and $|\downarrow\rangle$. For a uniform system, the fermionic field operators may be Fourier-expanded in a box with periodic boundary conditions giving wavevector-$\boldsymbol{k}$ dependent creation and annihilation operators $a^\dagger_{\boldsymbol{k}\sigma}$ and $a_{\boldsymbol{k}\sigma}$ for states $|\sigma\rangle$. At low energy, the binary scattering processes are assumed to be completely characterized by the s-wave scattering length a in terms of a contact quasipotential $U = 4\pi\hbar^2 an/m$, where n is the number density. The Hamiltonian describing such a system is given by

$$H = \sum_{\boldsymbol{k}} \epsilon_k \left(a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\uparrow} + a^\dagger_{\boldsymbol{k}\downarrow} a_{\boldsymbol{k}\downarrow} \right) + U \sum_{\boldsymbol{k}_1 \ldots \boldsymbol{k}_3} a^\dagger_{\boldsymbol{k}_1\uparrow} a^\dagger_{\boldsymbol{k}_2\downarrow} a_{\boldsymbol{k}_3\downarrow} a_{\boldsymbol{k}_4\uparrow}, \tag{1}$$

where $\epsilon_k = \hbar^2 k^2/2m$ is the kinetic energy, m is the mass, and the constraint $\boldsymbol{k}_4 = \boldsymbol{k}_1 + \boldsymbol{k}_2 - \boldsymbol{k}_3$ gives momentum conservation.

For a negative scattering length, the thermodynamic properties of the gas show a superfluid phase transition at a critical temperature T_c which arises due to an instability towards the formation of Cooper-pairs. When the gas is dilute, as characterized by the inequality $n|a|^3 \ll 1$ (or equivalently $k_F|a| \ll 1$, where k_F is the Fermi wavenumber), the application of mean-field theory gives a well-known solution for the ratio of T_c to the Fermi temperature T_F [5]

$$\frac{T_c}{T_F} \sim \exp\left(-\frac{\pi}{2|a|k_F} \right). \tag{2}$$

The exact prefactor to the exponential depends on the precise form of the analytic integral approximations made in the derivation. Several papers have pointed out that the presence of a scattering resonance in dilute alkali gases can be used to obtain a very large negative value for the scattering length [9]. This promises the opportunity for the system to enter the high-T_c superfluidity regime as the ratio in Eq. (2) approaches unity. However, direct application of the BCS theory close to resonance then becomes speculative due to the potential breakdown of a number of underlying assumptions:

1. Exactly on resonance the theory fails as the scattering length passes through $\pm\infty$ and the Hamiltonian in Eq. (1) cannot be defined.
2. For the mean field approach to be accurate it is required that there are many particles inside a volume associated with the spatial scale of a Cooper-pair. This condition begins to break down as T_c approaches T_F.
3. The theory of the dilute gas is formulated on a perturbation approach based on an expansion in the small parameter $n|a|^3$. When this parameter approaches unity the perturbation theory fails to converge.

These points show that care should be taken in applying Eq. (2) near the point of resonance where the basis for the conventional mean-field theory is not well founded.

Despite these limitations, on general grounds, one would expect to be able to derive a renormalizable low-energy effective field theory even in close proximity to a resonance. This statement is based on the identification that at relevant densities the range of the interparticle potential is always orders of magnitude smaller than the interparticle spacing. Here we present a theory of superfluidity in a gas of dilute fermionic atoms which handles correctly the scattering resonance and places the transition temperature to the superfluid state in the experimentally accessible range.

While the scattering length a usually characterizes the range of the interatomic potential for a collision, this is a poor approximation in the vicinity of a scattering resonance. The scattering properties are completely determined by the positions of the bound states in the interaction potentials. In a multichannel system, a bound state may cross the threshold as a function of magnetic field and enter the continuum, resulting in a field-dependent Feshbach scattering resonance [10]. As this occurs, the scattering length becomes strongly dependent on the field, and exactly at threshold it changes sign by passing through $\pm\infty$.

3. Resonance pairing theory

When such resonance processes occur, it is necessary to formulate the Hamiltonian by separating out the resonance state and treating it explicitly. This is motivated by the microscopic identification of two types of scattering contributions: one from the scattering resonance, and one from the background non-resonant processes that includes the contributions from all the other bound states. The non-resonant contributions give rise to a background scattering length $a_{\rm bg}$ which is a good characterization of the potential range. The corresponding quasipotential in that case is given by $U_{\rm bg} = 4\pi\hbar^2 a_{\rm bg} n/m$. The Feshbach resonance occurs due to a coupling with a molecular state, that is long-lived in comparison with characteristic non-resonant collision timescales. This state is a composite boson which is described by bosonic annihilation operators $b_{\boldsymbol{k}}$. It is parameterized by a detuning energy from threshold, denoted by 2ν, that is dependent on the value of the magnetic field. The coupling strength of $b_{\boldsymbol{k}}$ to the two-particle continuum is well characterized by a single coupling constant g, independent of $\boldsymbol{k}$. These considerations imply that the Hamiltonian given in Eq. (1) is not sufficient to account for the important resonance processes and must be extended to incorporate explicitly the coupling between the atomic and molecular gases

$$H = 2\nu \sum_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}} b_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} \epsilon_k (a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\uparrow} + a^\dagger_{\boldsymbol{k}\downarrow} a_{\boldsymbol{k}\downarrow}) + U_{\rm bg} \sum_{\boldsymbol{k}_1 \ldots \boldsymbol{k}_3} a^\dagger_{\boldsymbol{k}_1\uparrow} a^\dagger_{\boldsymbol{k}_2\downarrow} a_{\boldsymbol{k}_3\downarrow} a_{\boldsymbol{k}_4\uparrow}$$
$$+ g \sum_{\boldsymbol{k},\boldsymbol{q}} b^\dagger_{\boldsymbol{q}} a_{\frac{\boldsymbol{q}}{2}+\boldsymbol{k}\uparrow} a_{\frac{\boldsymbol{q}}{2}-\boldsymbol{k}\downarrow} + b_{\boldsymbol{q}} a^\dagger_{\frac{\boldsymbol{q}}{2}-\boldsymbol{k}\downarrow} a^\dagger_{\frac{\boldsymbol{q}}{2}+\boldsymbol{k}\uparrow}. \tag{3}$$

Evolution generated by this Hamiltonian conserves the particle number $N = \sum_{\boldsymbol{k}} (a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\uparrow} + a^\dagger_{\boldsymbol{k}\downarrow} a_{\boldsymbol{k}\downarrow}) + 2\sum_{\boldsymbol{k}} b^\dagger_{\boldsymbol{k}} b_{\boldsymbol{k}}$. Note that the Hamiltonian does not contain

a explicitly, and that the field dependence of the scattering is completely characterized by the parameters: g, ν, and $U_{\rm bg}$. The magnitude of g is derived in the following way. We define κ as the product of the magnetic field width of the resonance and the magnetic moment difference of the Feshbach state and the continuum state. For large values of ν, the boson field $b_{\boldsymbol{k}}$ can be adiabatically eliminated from the theory, and then $g = \sqrt{\kappa U_{\rm bg}}$ is required in order for the scattering properties to have the correct dependence on magnetic field†.

The essential point is that this Hamiltonian, founded on the microscopic basis of resonance scattering, is well-behaved at all detunings ν; even for the pathological case of exact resonance. The diluteness criterion is now given by constraints which require both the potential range and the spatial extent of the Feshbach resonance state, to be much smaller than the interparticle spacing (e.g. $n|a_{\rm bg}|^3 \ll 1$).

We apply this Hamiltonian to derive the self-consistent mean-fields for given thermodynamic constraints by formulating a Hartree–Fock–Bogoliubov theory‡. The mean-fields present include the fermion number $f = \sum_{\boldsymbol{k}} \langle a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\uparrow}\rangle$, the molecule field $\phi_m = \langle b_{\boldsymbol{k}=0}\rangle$ taken to be a classical field, and the pairing-field $p = \sum_{\boldsymbol{k}} \langle a_{\boldsymbol{k}\uparrow} a_{-\boldsymbol{k}\downarrow}\rangle^\S$. It is well known that such a theory must be renormalized in order to remove the ultraviolet divergence which arises from the incorporation of second-order vacuum contributions. This implies replacing the physical parameters in the Hamiltonian, U, g, and ν, by renormalized values so that observables are independent of a high momentum cut-off used in the formulation of the effective field-theory [13]. In order to diagonalize the Hamiltonian, we construct Bogoliubov quasiparticles according to the general canonical transformation [14]

$$\begin{pmatrix} \alpha_{\boldsymbol{k}\uparrow} \\ \alpha^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} = \begin{pmatrix} \cos\theta & -e^{i\gamma}\sin\theta \\ e^{i\gamma}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} a_{\boldsymbol{k}\uparrow} \\ a^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix}. \tag{4}$$

Given single particle energies, $U_k = \epsilon_k - \mu + Uf$, where μ is the chemical potential, and the gap parameter in the quasiparticle spectrum $\Delta = Up - g\phi_m$, the two transformation angles are specified as $\tan(2\theta) = |\Delta|/U_k$ and $\phi_m = |\phi_m|\exp(i\gamma)$. The corresponding quasiparticle spectrum is $E_k = \sqrt{U_k^2 + \Delta^2}$. Dropping terms of higher order than quadratic in the fermion operators, gives the resulting many-body Hamiltonian

$$H - \mu N = 2(\nu - \mu)|\phi_m|^2 + \sum_{\boldsymbol{k}} \left[U_k + E_k(\alpha^\dagger_{\boldsymbol{k}\uparrow}\alpha_{\boldsymbol{k}\uparrow} + \alpha^\dagger_{\boldsymbol{k}\downarrow}\alpha_{\boldsymbol{k}\downarrow} - 1)\right], \tag{5}$$

which is now in diagonal form.

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†This expression for g is chosen so that a obeys the correct field dependence. For further discussion see Ref. [11].

‡An analogous field-theory is derived for a bosonic model in Ref. [12].

§A magnetization field $\sum_{\boldsymbol{k}} \langle a^\dagger_{\boldsymbol{k}\uparrow} a_{\boldsymbol{k}\downarrow}\rangle$ is also included in our formulation. However, we drop this term in our discussion since it is identically zero in the spin-symmetric case considered here. Inclusion gives a slightly more general treatment, and requires the addition of a spin-rotation following the transformation to Bogoliubov quasiparticles.

4. Thermodynamic solutions

The next task is to calculate the thermodynamic solutions. Equilibrium populations for the quasiparticles are given by the Fermi–Dirac distribution. The fermion number and pairing field are not only inputs to the Hamiltonian, but also determine the quasiparticle spectrum. Therefore, they must be self-consistent with the values derived by summing the relevant equilibrium density matrix elements over all wave numbers. In practice, at a given temperature, chemical potential, and molecule number ϕ_m, this requires an iterative method to locate self-consistent values for f and p. The value of ϕ_m is calculated by minimizing the grand potential $\Phi_{\rm G} = -k_{\rm b}T \ln \Xi$ at fixed temperature and chemical potential, with $k_{\rm b}$ denoting Boltzmann's constant. The partition function $\Xi = {\rm Tr}[\exp(-(H - \mu N)/k_{\rm b}T)]$ is found from Eq. (5). This procedure is mathematically equivalent to minimizing the Helmholtz free-energy at fixed temperature and density and corresponds uniquely to the maximum entropy solution. This solution has an associated particle number, $\langle N \rangle = -\partial \Phi_{\rm G}/\partial \mu$, taken at constant temperature and volume, which must match the actual particle density of the gas, so that the final step is to adjust the chemical potential until this condition is satisfied. The whole procedure is repeated over a range of temperatures to determine the locus of thermodynamic equilibrium points. For large positive detunings, where the molecule field could be eliminated from the theory entirely, regular BCS theory emerges. For this case, when the scattering length a is negative the behaviour of the critical temperature on $1/a$ is given by the usual exponential law [5].

In this paper, we use fermionic ^{40}K atoms as an example of the application of this theory. The values of our interaction parameters $a_{\rm bg} = 176 a_0$ and $\kappa/k_{\rm b} = 657$ μK are obtained from [15]. We fix the total density to be $n = 10^{14}$ cm^{-3}, a typical experimental value expected for this quantum degenerate gas in an optical trap. We set the detuning to be $\nu = +E_{\rm F}$, so that the quasi-bound state is detuned slightly above the atomic resonance. For a temperature above $T_{\rm c}$, the grand potential surface is shaped like a bowl, and the value of ϕ_m which minimizes the grand potential is $\phi_m = 0$, associated with the self-consistent solution $p = 0$. For $T < T_{\rm c}$, the grand potential surface is shaped like a Mexican hat, and its minimum is given by ϕ_m with a non-zero amplitude and an undetermined phase. The superfluid phase transition therefore leads to a spontaneously broken symmetry. The value of $T_{\rm c}$ can be clearly found from Figs. 4 and 5, where we show the chemical potential, the molecular density, and the gap as a function of temperature. We find for our parameter set for ^{40}K and almost zero detuning a remarkably high value for the critical temperature $T_{\rm c} \approx 0.5 T_{\rm F}$, i.e. $T_{\rm c} \approx 0.6$ μK. Furthermore, we find a weak dependence of $T_{\rm c} \approx 0.5 T_{\rm F}$ on the density, so that the value of $T_{\rm c}$ has more-or-less the same density behavior as $T_{\rm F}$. When we increase the detuning to $\nu = +17.6 E_{\rm F}$ (this corresponds to a magnetic field detuning of 0.5 Gs away from the Feshbach resonance), the value of $T_{\rm c}$ drops to approximately $0.25 T_{\rm F}$.

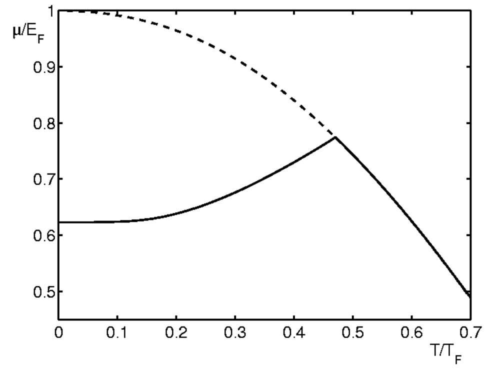

Fig. 4. Chemical potential as a function of temperature for the system of resonance pairing (solid line). The second order phase transition occurs at $T_c \approx 0.5 T_F$, where a clear cusp is visible. The dashed line shows the chemical potential of a non-interacting Fermi gas.

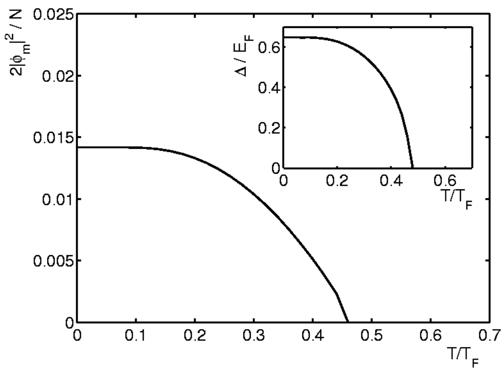

Fig. 5. The temperature at the phase transition is also visible from the amplitude of the molecular field. This amplitude is non-zero only when the broken symmetry exists in the region $T < T_c$. For $T = 0$, the molecules form a Bose condensed fraction of 1.5% of the total gas sample. The inset shows the behaviour of the gap $\Delta = Up - g\phi_m$. The critical temperature T_c can be related to the value of the gap at $T = 0$. For comparison, in superconductors the analogous gap is simply the binding energy of a fermion pair.

The system of ^{40}K atoms, equally distributed among the two lowest hyperfine states, is a good candidate for demonstrating the superfluid phase transition. It not only exhibits a Feshbach resonance, but also, the inelastic binary collision events are energetically forbidden. Three-body interactions are highly suppressed, since the asymptotic three-body wave function should consist of a product of three s-wave two-body scattering wave functions. In a three-body interaction, two-particles are always in the same initial hyperfine state, and therefore the corresponding s-wave state is forbidden. The only three-body relaxation could come from asymptotic p-waves, but these have very little contribution at the low temperatures considered. Although the detailed three-body collision problem is an intricate one, this asymptotic statistical effect should lead to a large suppression of the vibrational relaxation of quasi-bound molecules.

Current experimental techniques for ultracold gases do not produce samples which are spatially uniform. An optical dipole trap may be needed to confine the high field seeking atoms, and the conditions for the superfluid phase transition would be satisfied first in the trap center where the density is highest. The presence of the quasi-bound molecules may be a very useful aspect allowing direct observation of the phase transition through imaging the molecular field.

In conclusion, we have shown that resonance pairing in an alkali gas yields a quantum fluid that can undergo a superfluid phase transition at a temperature comparable to the Fermi temperature. This extraordinary property places this system in a regime which lies in between BCS-like superconductors, and bosonic systems which may undergo BEC. Since the transition temperature is larger than the lowest temperatures already achieved in a degenerate Fermi gas, it should be possible to study this new type of quantum matter and to quantitatively compare with our predictions.

Acknowledgments

We thank J. Cooper, E. Cornell, D. Jin, C. Wieman, and B. DeMarco for very stimulating discussions. Support is acknowledged for M.H. from the National Science Foundation, for S.K. from the U.S. Department of Energy, Office of Basic Energy Sciences via the Chemical Sciences, Geosciences and Biosciences Division, for M.C. from the INFM and SNS, Pisa (Italy), and for R.W. from the Austrian Academy of Sciences.

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