Resonance theory of the crossover from Bardeen-Cooper-Schrieffer superfluidity to Bose-Einstein condensation in a dilute Fermi gas

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We present a description of the behavior of a superfluid gas of fermions in the presence of a Feshbach resonance over the complete range of magnetic field detunings. Starting from a resonance Hamiltonian, we exploit a functional method to describe the continuous behavior from Bardeen-Cooper-Schrieffer to Bose-Einstein condensation type superfluidity. Our results show an ability for a resonance system to exhibit a high critical temperature comparable to the Fermi temperature. The results are derived in a manner that is shown to be consistent with the underlying microscopic scattering physics.

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I. INTRODUCTION

The ability to cool a gas of fermionic atoms well into the regime of quantum degeneracy hints at the exciting possibility of allowing one to study the mechanisms of superfluidity in an entirely new context [1]. Since these systems remain extremely dilute and are not complicated by long-range Coulomb interactions or lattice effects, cold degenerate gases seem ideal for the study of the fundamental physics behind the exotic behavior of superfluidity. Unfortunately, temperatures of around 0.2T_F are the current state of the art in cooling [1–6]. To obtain such high critical temperatures a strong coupling mechanism is required forcing the theoretical description to extend beyond the standard Bardeen-Cooper-Schrieffer (BCS) approach.

Several theoretical papers have studied the effects of increasing the two-particle interactions [7–9], characterizing the coupling processes by large negative scattering lengths. We have focused in detail upon a related yet distinct approach [10], which is to significantly increase the interatomic couplings by making use of a Feshbach resonance. The difference is that, in the neighborhood of the resonance, the interactions can no longer be adequately described by a scattering length, since the scattering length diverges as one approaches the resonance. This is an artifact of the approximations made in formulating the theory since the full energy-dependent scattering T-matrix, which is the true descriptor of the two-particle interactions, does not diverge at finite scattering energy. This leads us to explicitly incorporate the physics of the resonance into our microscopic description of the interatomic couplings. A much more detailed discussion of this can be found in Ref. [10].

So far, we have not discussed in detail the role of fluctuations, which can have a significant effect on the critical behavior [11]. How we incorporate these fluctuations proves crucial in describing the physics correctly within the crossover regime where we find a significant population of tightly bound composite particles. The aim, therefore, of this paper will be to account for fluctuations in such a way as to properly describe the behavior of a superfluid Fermi gas at all detunings from the resonance. Recently, a complimentary treatment was independently developed by Ohashi and Griffin [13]. The slight quantitative differences between their results for the critical superfluid transition temperature and the values we will present here appear to arise primarily from the use of quite different two-body scattering parameters and a distinct renormalization procedure.

The problem of describing a superfluid Fermi gas at all coupling strengths has been extensively studied in recent years, motivated by a desire to explain the properties of “exotic” high-T_c superconductors, whose behavior seems to lie in a region somewhere between BCS superconductivity and Bose-Einstein condensation (BEC). An early description of the crossover from BCS to BEC superconductivity was put forth by Nozières and Schmitt-Rink (NSR) [14], after the pioneering work of Eagles [15] and Leggett [16], and later expanded upon by various authors [17–19]. A functional analysis of the crossover behavior, which is the method that we will employ, was equated to the NSR method by Rand-era et al. [19]. We will adapt this method to a resonant system as necessary to describe the relevant physics of superfluidity in dilute atomic gases. It should be stressed that our method contains the multichannel interatomic couplings intrinsic to the Feshbach resonance. This was not considered in previous calculations in the context of condensed matter systems.

II. RESONANT ACTION

We consider the Feshbach resonance [20] for s-wave scattering of atoms in the lowest two hyperfine states of a fermionic alkali atom, denoted symbolically by \( \sigma \in \{ \uparrow, \downarrow \} \). For a homogeneous system we have the following generalized Hamiltonian:

\[
\hat{H}(t) = \sum_\sigma \int \psi_\sigma^\dagger(x)(\hat{H}_\sigma - \mu)\psi_\sigma(x)d^3x
\]

\[+\sum_j \int \psi_m^\dagger(x)(\hat{H}_{mj} - 2\mu + \nu_j)\psi_m(x)d^3x\]

\[+\int U(x-x')\psi_\uparrow^\dagger(x)\psi_\downarrow^\dagger(x')\psi_\downarrow(x)\psi_\uparrow(x)d^3xd^3x'\]

\[+\sum_j \int \left[ g_j(x-x')\psi_m^\dagger(x)\left(\frac{x+x'}{2}\right)\psi_\downarrow(x)\psi_\downarrow(x')\right]
\]

\[+\text{H.c.}]d^3xd^3x', \quad (1)
\]
where the operators \( \psi^\dagger_\sigma(\psi_\sigma) \) create (annihilate) fermions at \( x=(x,t) \), and \( \psi^\dagger_{m}\, (\psi_{m}) \) create (annihilate) composite bosons. The free dispersion Hamiltonian for fermions (bosons) is \( \hat{H}_f \, (\hat{H}_m) \) and \( \nu_j \) is the detuning of the \( j \)th molecular state from the collision continuum. The collisional interactions are described by both background fermion scattering \( (U) \) and an interconversion between composite bosons and fermion pairs \( (g_j) \).

Functional methods prove to be especially convenient in describing the thermodynamics of the resonant system. For a finite temperature action:

\[
S_M = \sum_{q,j} \left( iv - \frac{q^2}{4m} - \nu_j + 2\mu \right) b^*_j(q)b_j(q) - \frac{1}{\sqrt{BV}} \sum_{q,p_1+p_2,j} g_j[b^*_j(q)a_j(p_1)a_j(p_2) + a^*_j(p_2)a^*_j(p_1)b^*_j(q)].
\] (5)

In deriving Eqs. (4) and (5) we have inserted contact potentials for the couplings \( U(x-x') \rightarrow Ud(x-x') \) and \( g_j(x-x') \rightarrow g_jd(x-x') \). The full partition function for our resonant system, under the model Hamiltonian of Eq. (2), can now be written as

\[
Z = \int \left( \prod_{\sigma} Da^*_\sigma Da_\sigma \right) \left( \prod_{j} Db^*_j Db_j \right) e^{S_{\text{BCS}} + S_M},
\] (6)

with the functional integral, \( Dc = \Pi_i dc^i \), ranging over all Fermi and Bose fields.

### III. Saddle-Point Approximation

From the form of the action in Eq. (6), it should be apparent that all of the resonant contributions are contained within the molecular action. In practice this gives rise to the integral of a displaced Gaussian that can be easily evaluated. After integrating out the molecular degrees of freedom, we are left with the partition function:

\[
Z = \int \left( \prod_{\sigma} Z_B(q^2/4m + \nu_j - 2\mu) \right) Da^*_\sigma Da_\sigma e^{S_{\text{BCS}}}'.
\] (7)

Here \( Z_B(q^2/4m + \nu_j - 2\mu) \) is a Bose partition function describing the formation of bound molecules and \( S_{\text{BCS}}' \) is the BCS action with a potential that is now dependent on both thermal frequencies and momentum. The interaction potential in the BCS action is, therefore, modified in the presence of a Feshbach resonance in the following way:

\[
U \rightarrow U - \sum_j \frac{g_j^2}{q^2_j/4m + \nu_j - 2\mu - iv}.
\] (8)

With the above partition function, Eq. (7), we may go on to calculate all thermodynamic properties of interest. Here, we are primarily interested in calculating the critical temperature of the superfluid phase transition. This can be done by solving for the gap and number equation, and then self-consistently solving these two equations for both the chemical potential and the critical temperature. The procedure is straightforward since the full resonant calculation has been reduced to the usual BCS calculation, only with a more complicated potential. Following Popov’s derivation [22], introducing the complex auxiliary Bose field \( c(q) \) and expanding about the neighborhood of its zero value (which is equivalent to saying that we expand about the zero of the gap near \( T_c \)), we derive the gap equation at the critical point.
The second self-consistent equation, the number equation, is found in the saddle-point approximation by expanding the action to lowest order, i.e., \( c(q) = c^*(q) = 0 \), and using the thermodynamic identity \( N = -\partial \ln Z / \partial \mu \) giving

\[
N = 2 \sum_{j,k} \frac{1}{e^{\beta (k^2/2m + v_j - 2\mu)} - 1} + 2 \sum_k \frac{1}{e^{\beta (k^2/2m - \mu)} + 1}.
\]

(10)

Thus our number equation counts all free fermions, \( N_f \), plus an additional boson population \( N_b \). Equations (9) and (10) provide for us a set of equations for determining \( T_c \) and \( \mu \) at the critical point. In the usual BCS theory, this level of approximation proves reasonable for calculating \( T_c \) in the BCS limit (small negative scattering length), but diverges as the scattering length grows, and is wholly inapplicable for positive scattering lengths. The reason for this is that the primary mechanism for the phase transition within the weak coupling BCS limit is the formation and disassociation of Cooper pairs. As the coupling increases the particles tend to pair up at higher and higher temperatures which means that the critical transition is no longer signaled by the formation of Cooper pairs, but rather by a coherence across the sample caused by condensation of preformed Cooper pairs. Since we are interested in describing the resonant system at all detunings, by condensation of preformed Cooper pairs, the method of Nozieres and Schmitt-Rink incorporates the true microscopic physics into the problem, removing the unphysical divergence.

For the resonant case, a more sophisticated approach is required, which we have extensively studied previously [10]. In the case of a single resonance (i.e., the \( j \) sum has only a single term) the renormalization is performed by the following relations: \( U = \Gamma \bar{U} \), \( g = \Gamma \bar{g} \), and \( \nu = \bar{\nu} + \alpha g \bar{g} \). The chemical potential of each atomic state is modified to \( \mu = \bar{\mu} - \langle T(k) n_k \rangle \) to include the proper mean-field shifts induced by all two-body scattering processes, where \( n_k \) is the Fermi distribution, \( T(k) \) is the two-body scattering matrix for the resonant system [10], and \( \langle \cdot \rangle \) denotes an averaging. This shift, however, is sufficiently small to neglect; inclusion has demonstrated corrections of the order of 1% or less. By replacing the bare values in Eqs. (9) and (13) with the renormalized values, all of the results to be discussed have been shown to be independent of the introduced momentum cutoff \( K_{cut} \).

The renormalization of the resonance theory forces us to take a closer look at the bound state physics of the system. In Fig. 1 we show the bound state energies for a single resonance system with a positive background scattering length. The figure results from a coupled square well calculation of the bound state energies [10] and shows the avoided crossing of two molecular states. The upper state behaves to a fairly good approximation as \( E_b = (m a_g^2)^{-1} \), which is the molecular binding energy regularly associated with a contact interaction [23]. The lower state, however, is offset from the detuning by an energy \( \sim \kappa \) and goes linear with the detuning. We find a similar behavior as in the lower state in the first term of Eq. (13). Taking the cutoff to infinity, which is justified since this term does not diverge, the renormalized detuning approaches \( \nu \rightarrow \nu - g^2/\bar{U} \). This produces a constant
shift of $\gamma^2/\bar{U} = \kappa$ between the detuning and the molecular binding energy. Keeping this term in the number equation would incorrectly cause a transfer of the entire population into the wrong molecular state. In order to avoid this unwanted behavior we set this term to zero, i.e., $N_{B} = 0$. In the case of a negative background scattering length, we would not have encountered this problem, and only one molecular state would have appeared (see Fig. 2). We will show in the next section that the pairing term fully accounts for the correct population of molecules in this system with $a_{bg} > 0$.

Before we present the full crossover solution for the case of $^{40}$K, let us look at the analytical solutions to Eqs. (9) and (13) in the strong (BEC) and weak (BCS) coupling regimes. We will first turn our attention to the weak coupling (BCS) regime. In this limit we would expect only free fermions to contribute to the population, so from Eq. (13) we find that the chemical potential is at the Fermi surface ($\mu = E_F$). With this information, we solve the gap equation for the critical temperature. The result is the usual exponential dependence on the effective scattering length

$$T_c/T_F \approx \frac{8}{\pi} e^{-\gamma} \exp\left(\frac{-\pi}{2k_F|a_{eff}|}\right),$$

where $\gamma \approx 0.5772$ is the Euler-Mascheroni constant, $k_F$ is the Fermi wave number, and $a_{eff} < 0$ is the effective scattering length produced by the Feshbach resonance $a_{bg} = a_{bg}(1 - \kappa/v)$.

The other limit we may consider is the strong coupling (BEC) limit. When the argument of the tanh function in the gap equation (9) becomes sufficiently negative, it is a good approximation to use its asymptotic value of unity. What this means physically is that the fermion statistics are unimportant in determining the value of the gap. This allows us to solve the gap equation for the chemical potential as a function of detuning. In the limit of large negative detuning we find that $\mu \rightarrow -E_F/2$, where $E_F \approx 1ma^2_{bg}$. Within this limit the entire population has been converted to molecules and we can solve the number equation to get the BEC condensation temperature of $T_c/T_F \approx 0.218$.

V. NUMERICAL RESULTS

To study the transition between the BEC and BCS regimes, we numerically solve Eqs. (9) and (13) for $^{40}$K. The single resonance curve is produced using a background scattering length of $176a_0$ and $\kappa = 7.68$ G at a density of $10^{14}$ cm$^{-3}$.

Figure 3 shows the critical temperature as a function of magnetic field detuning. The crossover calculation clearly merges with the BEC result for large-positive detunings and smoothly connects between positive and negative detunings, limiting to the Bose condensation temperature of $T_c/T_F \approx 0.218$ for large negative detuning. This approach gives a maximum near zero detuning ($T_c/T_F \approx 0.26$), but the maximum critical temperature we find is less than the predictions of the HFB approach in our earlier papers ($T_F/T_F \approx 0.5$) [24]. We believe this is due to the inclusion of fluctuations in the beyond saddle point approximation which act to reduce the gap at zero temperature and therefore the critical temperature for the formation of a superfluid.

Figure 4 shows the chemical potential as a function of detuning, beginning at the Fermi energy for positive detuning and approaching half the bound state energy at large negative detuning $\mu \rightarrow -E_F/2$. Figure 5 shows the change in population as a function of detuning. For large positive detuning, the system is composed solely of free fermions. As the detuning is decreased (i.e., from positive to negative) the contribution of the fermions begins to decrease until all the population is transferred into the atom pairs at $\nu \approx -0.5$ G.
The chemical potential is then equal to $-E_p/2$ and we may identify the atom pairs from that point as the molecules. The superfluid behavior then comes from the condensation of these molecules, which are no longer disassociating into free fermions.

**VI. CONCLUSION**

We have presented a crossover model to describe the behavior of a gas of fermionic atoms for all detunings from a Feshbach resonance. The model is able to smoothly connect between the BCS and BEC regimes and accounts for the microscopic two-body physics throughout. We find a smooth behavior of the transition temperature in the entire crossover regime, with a maximum near zero detuning of $T_c/T_F \approx 0.26$, and agreeing with the appropriate BEC and BCS behaviors in the respective large detuning limits. The maximum is below the value predicted by the Hartree-Fock-Bogoliubov theory for the uniform gas derived in earlier work. This result is a direct indication of the important role of preformed atom pairs which are neglected above $T_c$ in the Hartree-Fock-Bogoliubov theory. Such atomic pairing is represented as fluctuations in the fermion pairing field and modify the elementary excitation spectrum even in the normal phase. We emphasize, however, that in this paper we have only accounted for the pairing physics by including the second order fluctuations in order to be able to account for the correct molecular binding energy as derived from the two-body scattering physics. While the inclusion of this order of fluctuations is the main ingredient necessary to encapsulate essential aspects of the behavior of the system in the crossover regime, it would be interesting to extend the approach to consider the effect of higher order interactions which have not been accounted for. For example, we have only included interactions between free fermion atoms, neglecting all other contributions such as the interactions between pairs. This is most clearly seen in the BEC limit, where our solution adopts the thermodynamic behavior of the ideal Bose gas, rather than the dilute interacting Bose gas. A more sophisticated treatment could extend our approach to consider all these factors. Nevertheless, the results we have presented here illustrate the realistic potential in this realizable system for increasing the superfluid transition temperature, with the aid of the Feshbach resonance, to a significant fraction of the Fermi temperature. This is an important and timely aspect from a practical perspective because the maximum value we predict is in the region of the temperature range which is currently experimentally accessible.

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[11] Gorkov finds, by including fluctuations within a higher order diagrammatic calculation, a factor of approximately 2 reduction in $T_c$ within the BCS regime [12].