

## Pairing in a three-component Fermi gas

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We consider pairing in a three-component gas of degenerate fermions. In particular, we solve the finite-temperature mean-field theory of an interacting gas for a system where both interaction strengths and fermion masses can be unequal. At zero temperature, we find the possibility of a quantum phase transition between states associated with pairing between different pairs of fermions. On the other hand, finite-temperature behavior of the three-component system reveals some qualitative differences from the two-component gas: for a range of parameters it is possible to have two different critical temperatures. The lower one corresponds to a transition between different pairing channels, while the higher one corresponds to the usual superfluid-normal transition. We discuss how these phase transitions could be observed in ultracold gases of fermionic atoms.

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### I. INTRODUCTION

Recently, the possibility of fermion pairing in a two-component system with unequal Fermi surfaces has attracted a considerable amount of attention [1]. In an electronic system, nonmatched Fermi surfaces could be due to the magnetic field interacting with electron spins and in color superconductivity, due to unequal quark masses. The newly realized strongly interacting superfluid Fermi gases [2–10] offer a promising playground for the study of pairing and superfluidity, also with imbalanced Fermi energies.

In ultracold degenerate gases, different components are typically atoms in different internal states of an atom, but different isotopes or elements can also be considered. In ultracold gases, the mismatch of the Fermi surfaces can be due to having an unequal number of atoms in different states. After the first experimental studies using a mixture of two internal states of <sup>6</sup>Li atoms [11,12], the properties of such systems, in a harmonic trapping potential, have been extensively discussed in the recent literature [13–23].

In principle, many different types of fermions can be trapped in the same trap. In order to reach long lifetimes, the atoms should have favorable collisional properties, but current knowledge of these collisional properties is limited. However, mixtures of either Bose condensed or fermionic atoms in a variety of different internal states have been experimentally demonstrated [24–28], and experimental effort toward realizing three-component Fermi gases is in progress. For this reason we explore the novel possibilities in a three-component Fermi gas by generalizing the BCS (Bardeen-Cooper-Schrieffer) theory into three components.

A related three-component Fermi system has been previously studied by Honerkamp and Hofstetter [29,30] and more recently by Bedaque and D’Incao [31]. The first reference employs a Hubbard lattice Hamiltonian and is focused on the rather special case in which all fermions have the same mass and interact with different fermions (as well as with fermions of the same type) with a single interaction

strength. The setting used in the latter reference includes the possibility of unequal interaction strengths between various components. Bedaque and D’Incao draw general qualitative conclusions on the symmetries of the possible zero-temperature phases, but all fermion masses are assumed equal.

In this paper, we discuss pairing in a three-component system both at zero as well as nonzero temperatures. Furthermore, we allow for the possibility that the third fermion type has a different mass from the other two, and since *a priori* there is little reason to expect identical scattering properties between different fermion components, we formulate our theory assuming different interaction strengths between the components. In ultracold gases, such a system could be realized by trapping, for instance, <sup>6</sup>Li and <sup>40</sup>K using atoms in two internal states for one of these and one internal state for the other. In order to restrict the parameter space somewhat, we make one simplifying assumption in our Hamiltonian. Generally, one expects three different interactions in a three-component system: one between the first and the second component, one between the second and the third component, and one between the third and the first component. In this paper, we assume that the interaction between the third and the first component is weaker than the other two interactions and can be ignored next to the dominant contributions. This restriction is simply a matter of convenience as it restricts parameter space to manageable proportions, but does not affect the qualitative picture we find.

We find that, within the BCS theory, the possible pairing always gives rise to just one order parameter of broken U(1) symmetry. Whether the pairing takes place between the first and the second component (1–2 channel) or between the second and the third component (2–3 channel) depends on the strengths of the interactions, atomic masses, as well as on the differences between the chemical potentials of different components. The unpaired component constitutes a normal Fermi sea. At zero temperature there is a possibility of a quantum phase transition from a phase with pairing in the 1–2 channel into a phase with pairing in the 2–3 channel as chemical potential differences are varied appropriately. This transition is of the first order. Furthermore, as the tempera-

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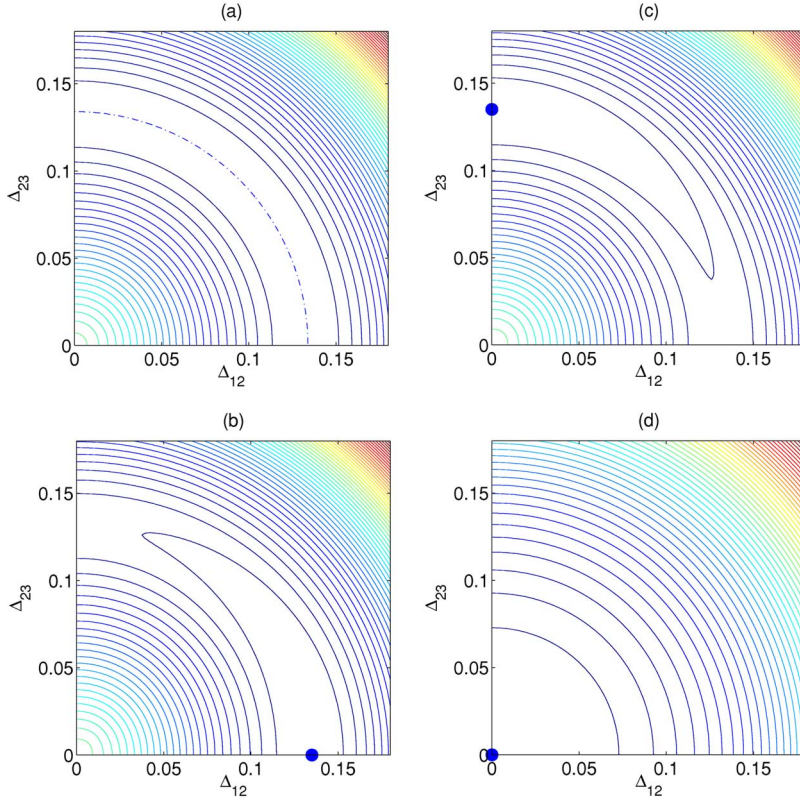


FIG. 1. (Color online) The free-energy landscape as a function of  $\Delta_{12}$  and  $\Delta_{23}$  when all three components have the same mass. The dash-dotted line in (a) and the filled circles in (b)–(d) show the location of the global minimum. We used equal coupling strengths  $g_{12}=g_{23}=-0.50$ , and (a)–(c) were calculated at zero temperature while (d) was calculated at  $k_B T / \epsilon_F = 0.08$ , which is above the critical temperature. The chemical potentials were such that in (a)  $\mu_1=\mu_2=\mu_3=1$ ; in (b)  $\mu_1=1.01$ ,  $\mu_2=1$ ,  $\mu_3=0.99$ ; in (c)  $\mu_1=0.99$ ,  $\mu_2=1$ ,  $\mu_3=1.01$ ; and finally in (d)  $\mu_1=\mu_2=\mu_3=1$ .

ture increases it is possible to have a second-order transition from a paired phase in the 2–3 channel into a paired phase in the 1–2 channel. At even higher temperature, there is another transition from the paired state into the normal state.

This paper is organized as follows. In Sec. II, we discuss the normal three-component Fermi gas and the possibility of phase separation in such a system. In Sec. III, we present the BCS-style mean-field theory and discuss the qualitative behavior of the associated grand potential at zero temperature. Also, we present the energy landscape of the grand potential for several different scenarios. In Sec. IV, we find the solutions to the gap equations that correspond to the global minimum of the grand potential for fermions where the third component has a different mass from the other two components. We end with some concluding remarks in Sec. V.

## II. NORMAL THREE-COMPONENT FERMION GAS

We study a homogeneous three-component Fermi gas whose components are either atoms in different internal states or different elements. For now we assume that an interaction between the first and the third component is sufficiently small, so that it is justified to focus on only the interactions between the first and the second component and the second and the third component. The second quantized Hamiltonian for this system is therefore

$$\begin{aligned}
 H = & \int d\mathbf{r} \left[ \sum_{\sigma=1,2,3} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \left( -\frac{\hbar^2 \nabla^2}{2m_{\sigma}} - \mu_{\sigma} \right) \hat{\psi}_{\sigma}(\mathbf{r}) \right] \\
 & + \tilde{g}_{12} \int d\mathbf{r} \hat{\psi}_{1}^{\dagger}(\mathbf{r}) \hat{\psi}_{2}^{\dagger}(\mathbf{r}) \hat{\psi}_2(\mathbf{r}) \hat{\psi}_1(\mathbf{r}) \\
 & + \tilde{g}_{23} \int d\mathbf{r} \hat{\psi}_{3}^{\dagger}(\mathbf{r}) \hat{\psi}_2^{\dagger}(\mathbf{r}) \hat{\psi}_2(\mathbf{r}) \hat{\psi}_3(\mathbf{r}), \quad (1)
 \end{aligned}$$

where  $\hat{\psi}_{\sigma}(\mathbf{r})$  and  $\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r})$  are the usual field operators which annihilate and create particles in state  $\sigma$ . In addition,  $m_{\sigma}$  is the atomic mass,  $\tilde{g}_{12}$  is the interaction strength between the first and the second component, and  $\tilde{g}_{23}$  is the interaction strength between the second and the third component. In terms of the scattering lengths  $a_{ij}$ , these interaction strengths are given by  $\tilde{g}_{ij} = 2\pi\hbar^2 a_{ij} \mu$ , where  $\mu = m_i m_j / (m_i + m_j)$  is the reduced mass of the scattering atoms.

Let us first discuss a mixture of three normal fermion components. If the mixture of normal three-component gas phase-separates spatially, it is clear that there is no possibility of a superfluid where all three components are mixed together and the problem is that of a two-component Fermi gas surrounded by the normal third component. Since the temperatures of interest are very low compared to the Fermi energies of the various components, we can consider the zero-temperature limit, in which the free-energy density  $f$  of the mixture of normal Fermi gases is given by

$$f = \frac{3\hbar^2}{10} (6\pi^2)^{2/3} \left( \frac{n_1^{5/3}}{m_1} + \frac{n_2^{5/3}}{m_2} + \frac{n_3^{5/3}}{m_3} \right) + \tilde{g}_{12} n_1 n_2 + \tilde{g}_{23} n_2 n_3, \quad (2)$$

where  $n_i$  are the component densities.

If both interaction strengths  $\tilde{g}_{12}$ ,  $\tilde{g}_{23}$ , are positive, then all three components separate. The reason for this is that then the positive definite free energy Eq. (2) is minimized when the interaction terms give vanishing contributions. If one of the interactions is positive and the other is negative, the components with attractive interaction mix and the third component separates. Therefore, the case in which all three components can coexist spatially occurs only when both

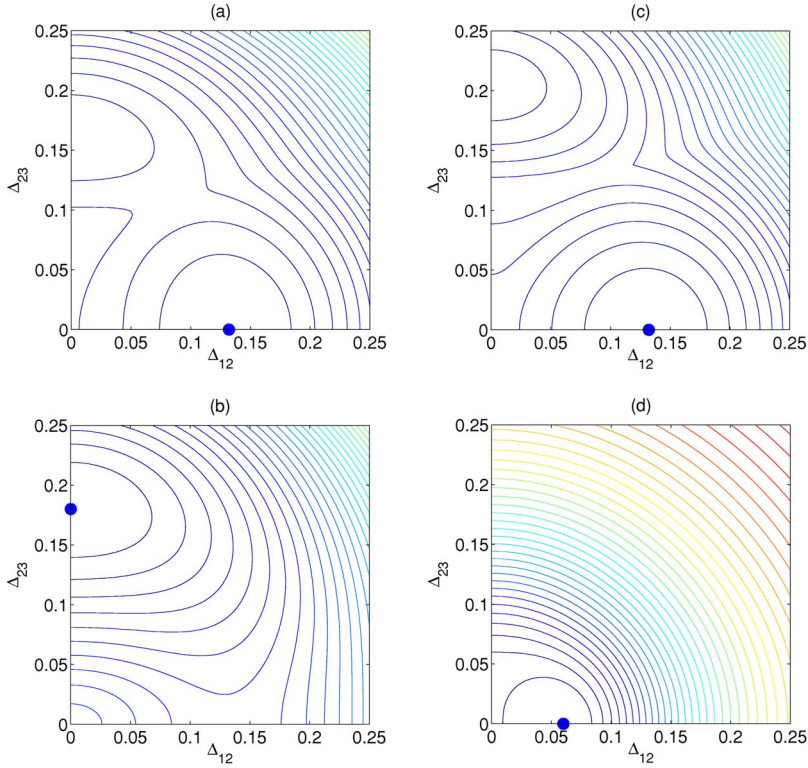


FIG. 2. (Color online) The free-energy landscape as a function of  $\Delta_{12}$  and  $\Delta_{23}$  with the mass ratio  $m_1/m_3=0.15$  and  $\mu_1=\mu_2=1.0$ . The filled circle shows the location of the global minimum. The coupling strengths were  $g_{12}=g_{23}=-0.5$ , and (a)–(c) were calculated at zero temperature while (d) was calculated at  $k_B T/\epsilon_F=0.07$ . In (a)  $\mu_3=0.07$ , in (b)  $\mu_3=0.15$ , in (c)  $\mu_3=0.25$ , and in (d)  $\mu_3=0.15$ . [In (d) we used a logarithmic scale to calculate the contour plot in order to enhance the relevant features.] The results show two types of transitions: a zero-temperature quantum phase transition between the two pairing channels [from (a) to (b) and from (b) to (c)] and a finite-temperature second-order transition between the pairing channels [from (b) to (d)].

interactions are attractive. If one of the interactions is attractive, then formally Eq. (2) has a global minimum at infinite density of the interacting components. This global minimum is not physically relevant since there is an energetic barrier separating this solution from the physically relevant regime of densities. In fact, the height of this barrier increases as the interactions become weaker. From now on we will focus on the most interesting region where both interactions are fairly large and negative.

### III. GRAND POTENTIAL OF THE THREE-COMPONENT FERMI GAS

The BCS theory involves approximating the Hamiltonian by the mean-field Hamiltonian density (in  $\mathbf{k}$  space)

$$\begin{aligned}
 H_{\text{BCS}} = & \frac{1}{V} \sum_{\mathbf{k}} \sum_{\sigma=1,2,3} \left( \frac{\hbar^2 k^2}{2m_{\sigma}} - \mu_{\sigma} \right) \hat{\psi}_{\sigma\mathbf{k}}^{\dagger} \hat{\psi}_{\sigma\mathbf{k}} + \Delta_{12} \hat{\psi}_{1,\mathbf{k}}^{\dagger} \hat{\psi}_{2,-\mathbf{k}} \\
 & + \Delta_{12}^* \hat{\psi}_{2,-\mathbf{k}} \hat{\psi}_{1,\mathbf{k}} + \Delta_{23} \hat{\psi}_{3,\mathbf{k}}^{\dagger} \hat{\psi}_{2,-\mathbf{k}} \\
 & + \Delta_{23}^* \hat{\psi}_{2,-\mathbf{k}} \hat{\psi}_{3,\mathbf{k}} - \frac{|\Delta_{12}|^2}{g_{12}} - \frac{|\Delta_{23}|^2}{g_{32}}, \quad (3)
 \end{aligned}$$

where

$$\Delta_{\sigma\sigma'} = \frac{g_{\sigma\sigma'}}{V} \sum_{\mathbf{k}} \langle \hat{\psi}_{\sigma\mathbf{k}} \hat{\psi}_{\sigma'-\mathbf{k}} \rangle$$

are the order parameters to be determined self-consistently. As a short-hand notation, we define the vector  $\mathbf{\Delta} = (\Delta_{12}, \Delta_{23})$  characterizing the state of the system.

Since the mean-field Hamiltonian is of second order in the operators, it can be easily diagonalized with a canonical

transformation. In this way, we can calculate the grand potential (or free energy)

$$\Omega(\Delta_{12}, \Delta_{23}) = -k_B T \log\{\text{Tr}[\exp(-\beta H_{\text{BCS}})]\}, \quad (4)$$

where  $k_B$  is the Boltzmann constant and  $\beta=1/k_B T$ . In the continuum limit, the grand potential is ultraviolet-divergent. This divergence is caused by the unphysical short distance behavior of the contact interaction and is removed, in the usual way, by subtracting the divergent contribution from the grand potential. We have done the diagonalization of the mean-field Hamiltonian which can be done analytically, but in the general case formulas are inconveniently long and not very informative. In order to get an overview of the expected system behavior, it is rather more instructive to focus on the behavior of the free energy.

We choose our units by assuming that the first and the second components are  ${}^6\text{Li}$  atoms and by using the ideal gas of the second component as a benchmark. The unit of energy is then  $\epsilon_F = \hbar^2 k_{F,2}^2 / 2m_2$ , where  $k_{F,2} = (6\pi^2 n_2)^{1/3}$  is the Fermi wave vector. Furthermore, we use the unit of length  $1/k_{F,2}$ . Using these units, we define the dimensionless coupling strengths as  $g_{12} = 2k_{F,2} a_{12} / \pi$  and  $g_{23} = (m_2 + m_3) k_{F,2} a_{23} / m_2 \pi$ .

#### A. Grand potential when all fermions have the same mass

Figure 1 demonstrates the behavior of the free-energy landscape as a function of the gaps  $\Delta_{12}$  and  $\Delta_{23}$  when all fermion components have the same mass. It is clear that when all chemical potentials are equal, the free-energy landscape is only a function of  $\Delta_{12}^2 + \Delta_{23}^2$  and at zero temperature displays a clear minimum corresponding to the solution of the BCS gap equation. With the parameters used in the fig-



ure, the minimum is located at  $\sqrt{\Delta_{12}^2 + \Delta_{23}^2} \approx 0.135$ ; see the quarter sphere in Fig. 1(a).

Any difference in the chemical potentials (or coupling strengths) breaks the above symmetry and makes it energetically favorable to have one of the phases  $\Delta = (\Delta_{12}, 0)$  or  $\Delta = (0, \Delta_{23})$ . When interactions are the same, which of these alternatives is chosen depends on the average chemical potential between the paired components. The channel corresponding to the higher average chemical potential has a lower free energy and is therefore physically realized. At zero temperature, the densities of the paired components are equal, as is to be expected from the BCS state. At higher temperatures, the normal state  $\Delta = (0, 0)$  eventually becomes the free-energy minimum. Figure 1 also demonstrates that generally the grand potential has several possible stationary points.

### B. Grand potential when the fermion masses differ

The different components could in principle have also different masses. For concreteness we assume that the first and the second component are different internal states of  ${}^6\text{Li}$  atoms while the third component is a  ${}^{40}\text{K}$ . This corresponds, therefore, to the mass ratio  $m_r = m_1/m_3 = 0.15$ . In Fig. 2, we show some typical free-energy landscapes in this case, when the chemical potential of the third component is varied. It is clear that the grand potential again has many different stationary points.

For small values of  $\mu_3$ , the pairing is only possible in the 1–2 channel. However, the Fermi surfaces are matched when  $\mu_3 = m_r$  and this is reflected as a possibility of pairing in the 2–3 channel around this value. The reason why pairing in this channel is favored for matched Fermi surfaces even when coupling strengths are equal is due to the higher density of states for atoms of higher mass. This higher density of states translates into reduction in energy. Naturally, if  $g_{23}$  is reduced sufficiently we enter a parameter region where pairing in the 2–3 channel will never take place. For the parameters used in the figure, this happens when  $|g_{23}| < 0.33$ .

Again we find that at zero temperature the densities of the paired components are always equal. It is also interesting to observe that by increasing the temperature, one can induce a transition from the  $\Delta = (0, \Delta_{23})$  phase into the  $\Delta = (\Delta_{12}, 0)$  phase before entering a normal state.

In summary, two transitions are visible: a zero-temperature quantum phase transition between the two pairing channels [transition from Fig. 2(a) to Fig. 2(b), and from Fig. 2(b) to Fig. 2(c)], and a finite temperature second-order transition between the pairing channels [transition from Fig. 2(b) to Fig. 2(d)].

## IV. SOLUTIONS OF THE GAP EQUATIONS OF THE THREE-COMPONENT FERMION GAS

For a given set of chemical potentials, the self-consistent BCS solution is found at the minimum of the grand potential. At the extremum value of the grand potential, the gap equations

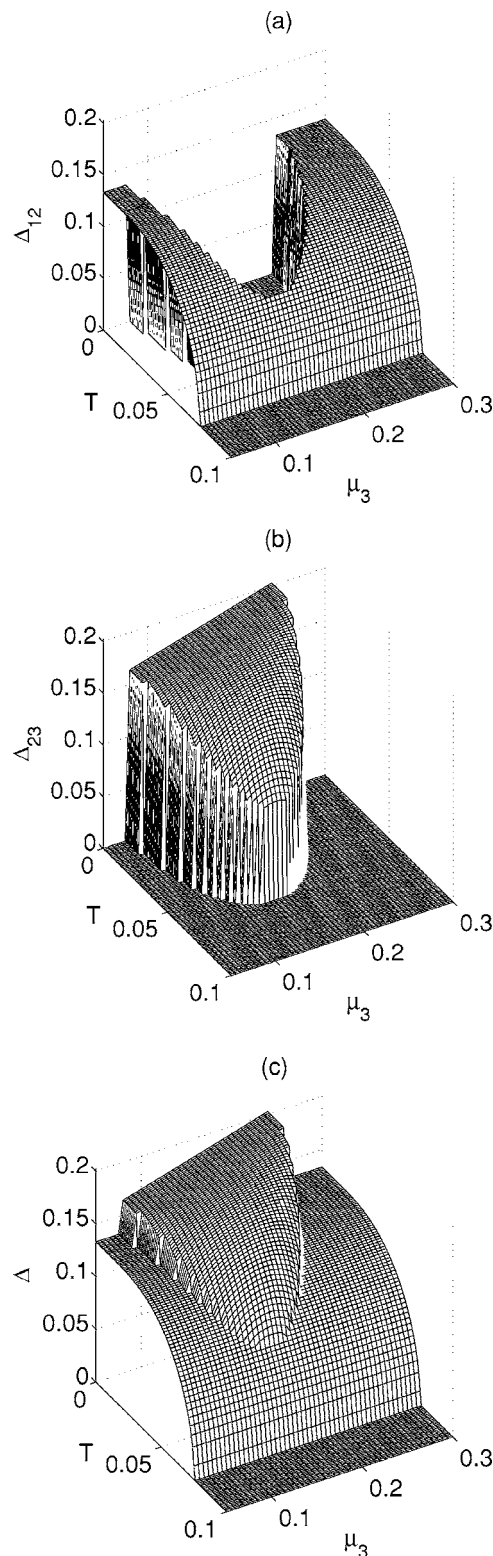


FIG. 3. The gap parameters as a function of temperature  $T$  and of the third-component chemical potential  $\mu_3$ . We used the mass ratio  $m_1/m_3 = 0.15$ ,  $\mu_1 = \mu_2 = 1$ , and the coupling strengths were  $g_{12} = g_{23} = -0.5$ . Panel (c) shows  $\Delta = \sqrt{\Delta_{12}^2 + \Delta_{23}^2}$  and demonstrates clearly the sharp change in the order parameter at zero temperature (the quantum phase transition) as well as the smoother transition from the  $\Delta_{23}$  superfluid to  $\Delta_{12}$  superfluid at a finite temperature.

$$\frac{\partial \Omega(\Delta_{12}, \Delta_{23})}{\partial \Delta_{12}} = 0 \quad (5)$$

and

$$\frac{\partial \Omega(\Delta_{12}, \Delta_{23})}{\partial \Delta_{23}} = 0 \quad (6)$$

are satisfied. These equations are satisfied at all extremal points of the grand potential, including local minima, local maxima, and saddle points. As we found out in the earlier section, the grand potential can have several extremal points so care must be taken in ensuring that numerics converges to the physically relevant global minimum of the grand potential rather than to a local stationary point.

We have found the global minima of the free energy by solving the gap equations under many different circumstances. Figure 3 shows typical results for the gaps as a function of temperature and  $\mu_3$ . At zero temperature there exists a first-order quantum phase transition, as the chemical potential is varied, from the  $\Delta=(\Delta_{12}, 0)$  phase into the  $\Delta=(0, \Delta_{23})$  phase. We also find that with increasing temperature there can be a second-order transition from the  $\Delta=(0, \Delta_{23})$  phase into the  $\Delta=(\Delta_{12}, 0)$  phase, which then makes a transition into the normal state at a higher temperature. However, whether this sequence of transitions takes place or not does depend on the strength of the interactions. For weaker interactions it is possible that the  $\Delta=(0, \Delta_{23})$  phase is not completely surrounded by the  $\Delta=(\Delta_{12}, 0)$  phase as it is in Fig. 3.

This overall behavior can be understood in the following way: The pairing between atoms of different masses happens around the point where their Fermi momenta are nearly equal (following from the condition  $\mu_3/\mu_1 \sim m_1/m_3$ ). This pairing is favored over the pairing with the same mass components due to the higher density of states for the more massive component. At finite temperature, the Fermi surfaces of both pairing components will be smeared out due to temperature; however, for components with different masses, this smoothening of the Fermi edge will happen differently (the higher mass component Fermi edge spreads more). Therefore, with increasing temperature, it becomes increasingly difficult to find a pairing partner with the same magnitude (but opposite sign) momentum, and also the advantage given by the higher density of states of the more massive component becomes less significant. This makes the pairing between the same mass components potentially more favorable at high temperatures.

## V. SUMMARY AND CONCLUSIONS

In this paper we have considered the mean-field theory of an interacting three-component Fermi gas. We found that in the highly symmetric case when all fermion masses as well as interactions strengths are equal, the free energy is only a function of  $\Delta_{12}^2 + \Delta_{23}^2$ . However, any deviation from the most symmetric situation, whether it is due to different atomic

masses, different interaction strengths, or different chemical potentials, breaks the above symmetry of the free energy and makes one of the paired states ( $\Delta_{12} \neq 0, \Delta_{23} = 0$ ), ( $\Delta_{12} = 0, \Delta_{23} \neq 0$ ), or the normal state ( $\Delta_{12} = 0, \Delta_{23} = 0$ ) energetically favored. Magnitudes of nonzero gaps as well as the point where the transition to the normal state occurs depend on parameters, but we have solved the global minima of the free energy for a fairly representative range of parameters.

When using a grand canonical ensemble, the average densities are quantities derived from the grand potential through  $n_i = -\partial \Omega / \partial \mu_i$ . In this work, we have explored the system behavior as a function of the chemical potentials by minimizing the grand potential. It is therefore useful to elaborate on what kind of density ratios different sets of chemical potentials actually correspond to. For the case investigated in the earlier section with a mass ratio  $m_1/m_3 = 0.15$  at zero temperature, we find at  $\mu_3 = 0.05$  pairing in the 1–2 channel and density ratios of  $n_3/n_1 = n_3/n_2 \approx 0.26$ . As the third-component chemical potential is increased to  $\mu_3 = 0.15$ , we find pairing in the 2–3 channel with density ratios  $n_2/n_1 = n_3/n_1 \approx 0.72$ . Finally, when  $\mu_3 = 0.25$ , the pairing is reverted back to the 1–2 channel and the mass ratios are  $n_3/n_1 = n_3/n_2 \approx 2.9$ . Therefore, this transition could be realized simply by varying the density of one component and keeping the other two fixed. Note that transitions could also be induced by changing the interaction strengths, i.e., the scattering lengths, between the three components as discussed in [31]. However, at present the method used for tuning the scattering lengths, i.e., the use of Feshbach resonances, does not allow us to tune the different scattering lengths independently, whereas the densities can be varied completely independent of each other. The change in the order gap related to the transitions could be observed using rf spectroscopy of the pairing gap [8,32,33] and corresponding condensate fraction by the pair projection method [4,5], and superfluidity could be directly demonstrated by the creation of vortices [10]—all these can be studied selectively for any choice for the pairing between the three components.

In this paper, we have limited ourselves for convenience to the special case in which interaction between the first and the third component is small enough to be neglected. This requirement can be relaxed easily and one could solve the most general case with unequal masses as well as with unequal interactions. We have checked that the presence of the omitted interaction between the first and the third component does not change the qualitative picture presented in this paper. For some parameter values, the new gap function  $\Delta_{13}$  can become nonzero, but otherwise the qualitative physics remains similar to the cases discussed in this paper.

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