Crossovers and quantum phase transitions in two-band superfluids: The evolution from BCS to Bose pairing by tuning interactions and band offset

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(Dated: April 20, 2022)

We show that in two-band $s$-wave superfluids it is possible to induce quantum phase transitions (QPTs) by tuning intraband and interband $s$-wave interactions, in sharp contrast to single-band $s$-wave superfluids, where only a crossover between Bardeen-Cooper-Schrieffer (BCS) and Bose-Einstein condensation (BEC) superfluidity occurs. For non-zero interband and attractive intraband interactions, we demonstrate that the ground state has always two interpenetrating superfluids possessing three spectroscopically distinct regions where pairing is qualitatively different: (I) BCS pairing in both bands (BCS-BCS), (II) BCS pairing in one band and BEC pairing in the other (BCS-BEC), and (III) Bose pairing in both bands (BEC-BEC). Furthermore, we show that by fine tuning the interband interactions to zero one can induce QPTs in the ground state between three distinct superfluid phases. There are two phases where only one band is superfluid ($S_1$ or $S_2$), and one phase where both bands are superfluid ($S_1 + S_2$), a situation which is absent in one-band $s$-wave systems. Lastly, we suggest that these crossovers and QPTs may be observed in $^{173}$Yb and $^{87}$Sr.

Introduction: The evolution from Bardeen-Cooper-Schrieffer (BCS) to Bose pairing in one-band superfluids is a topic of intensive recent experimental [1–4], and theoretical [5–8] research, because it is the simplest system addressing the deep theoretical connection between BCS and Bose superfluidity [9–11] that arises in many areas of physics: condensed matter (superconductivity), atomic physics (ultracold Fermi superfluids), astrophysics (ultracold neutron stars) and quantum chromodynamics (color superconductivity) [12]. Unfortunately, in quantum chromodynamics, astrophysics and condensed matter the tunability of interactions is extremely limited or nonexistent. However, for low density one-band Fermi atoms ($^6$Li or $^{40}$K) it is possible to tune $s$-wave interactions and study the crossover from BCS to Bose-Einstein condensation (BEC) superfluidity [12–14], where large Cooper pairs evolve into tightly bound pairs, when interactions change from weak to strong.

Although the BCS-BEC crossover is interesting, its physics is not as striking as that occurring in quantum phase transitions (QPTs), where singular behavior emerges. In one-band superfluids, topological QPTs were theoretically predicted as a function of interaction strength for higher angular momentum pairing, such as $p$- or $d$-wave [15–20], leading to superfluid phases in the BCS and BEC regimes which are qualitatively different. However, the experimental observation of this phenomenon in cold gases has failed, because $p$-wave fermion pairs dissociate by tunneling out of the centrifugal barrier, that is, their lifetime is just not long enough to observe superfluidity [21,22]. This experimental fact, makes it impossible to study predicted QPTs in the superfluid state of $p$-wave or higher angular momentum pairing [23] as a function of interactions.

In this paper, we propose an alternative idea to study elusive QPTs between qualitatively different superfluid states during the BCS to BEC evolution: tune only $s$-wave interactions, but enlarge the Hilbert space of states to two bands. The tuning of $s$-wave interactions creates stable fermion pairs, while the existence of two bands allows for the emergence of QPTs. Experimental candidates include systems with four internal states such as $^6$Li and $^{40}$K, where interactions may be tuned via magnetic Feshbach resonances [13–16], and $^{173}$Yb [25,26] and $^{87}$Sr [27,28], where interactions may be tuned via optical Feshbach resonances [29,30]. We investigate a Fermi gas with two parabolic bands per spin label (four internal states) separated by a band offset $\varepsilon_0$, whose physical origin can be a quadratic Zeeman shift. We allow for $s$-wave intraband and interband interactions, where the latter is described by pair tunneling $J$.

We find two types of crossovers and two types of QPTs. For non-zero $J$, the ground state phase diagram always exhibits superfluidity in both bands for any chosen values of the intraband interactions, this means that there are no QPTs, but there are two crossovers. Typical crossover lines separate regions which are spectroscopically distinct with respect to their quasiparticle excitation spectrum: I) both bands have indirect gaps (BCS-BCS); II) one band has an indirect gap and the other has a direct gap (BCS-BEC); III) both bands have direct gaps (BEC-BEC). The first type of QPT is a $0-\pi$ phase transition, where the relative phases of the $s$-wave order parameters in the two bands changes from $0$ ($J > 0$) to $\pi$ ($J < 0$). However, the second type of QPT occurs for $J = 0$, and leads to three different ground states as intraband interactions are changed: a) two phases where only one band is superfluid ($S_1$ or $S_2$); and b) one phase where both bands are superfluid ($S_1 + S_2$). Thus, QPTs in two-band $s$-wave superfluids are found, rather than standard crossover physics in the evolution from BCS to BEC superfluidity.
Hamiltonian: To explore QPTs in two-band s-wave superfluids, we start from the Hamiltonian
\[
H = \sum_{jks} \xi_j(k)c_{jk}\dagger c_{jk} + \sum_{ij\ell\ell'q} V_{ij}(k,k')b_{ij}\dagger b_{ij}, \tag{1}
\]
where pair operators \(b_{ij\ell\ell'q} = c_{j-k+q/2,\ell}c_{j-k-q/2,\ell'}\) are defined in terms of fermion operators \(c_{jk}\) with band index \(j = \{1, 2\}\), momentum \(k\) and spin labels \(s = \{\uparrow, \downarrow\}\). We work in three dimensions (3D) and choose units where \(\hbar = k_B = 1\). The term \(\xi_j(k) = \varepsilon_j(k) - \mu\) is the kinetic energy for band \(j\) with respect to the chemical potential \(\mu\), with \(\varepsilon_0 = \varepsilon_{10} = 0\) and \(\varepsilon_{20} = \varepsilon_0 > 0\), where \(\varepsilon_0\) is the energy offset between the two bands, as shown in Fig. 1. The solid blue line (red line) represents band 1 (band 2), and \(E_{F_1} = k_B^2/2m_1\) (\(E_{F_2} = k_B^2/2m_2\)) is the Fermi energy with Fermi momentum \(k_{F_1}\) (\(k_{F_2}\)). In Eq. (1), \(V_{ij}(k,k')\) are intraband and interband interactions. The intraband interactions are written in the separable form \(V_{ij}(k,k') = V_{ij}\Gamma_j(k)\Gamma_j(k')\) with \(\Gamma_j(k) = [1 + k^2/k_B^2]^{-1/2}\), with \(k_B \sim R^{-1}\). Here, \(R\) is the interaction range in real space. The symmetry factor \(\Gamma_j(k)\) in \(V_{11}(k,k')\) and \(V_{22}(k,k')\) represents s-wave pairing interactions. The interband terms \(V_{12}(k,k') = V_{12}\) and \(V_{21}(k,k') = V_{21}\) are Josephson couplings, where s-wave pairs tunnel between bands, that is, there is a momentum space proximity effect, where superfluidity in one band can induce superfluidity in the other.

Physical picture: The parameters of the Hamiltonian in Eq. (1) are: masses \(m_1\) and \(m_2\), interactions \(V_{11} = -|V_{11}|, V_{22} = -|V_{22}|,\) and \(V_{12} = V_{21} = -J\), band offset \(\varepsilon_0\), and chemical potential \(\mu\) fixing the total number of particles \(N = N_1 + N_2\). Next, we set \(m_1 = m_2 = m\), but the arguments presented are based on energetics and are also valid for \(m_1 \neq m_2\) [11]. To compare interactions to Fermi energies \(E_{F_1}, E_{F_2}\) we write the interaction energy scales \(\lambda_j = |V_{11}/N_1, \lambda_2 = |V_{22}/N_2,\) and \(\lambda_J = J\sqrt{N_1N_2}\).

In Fig. 1, Fermi energies \(E_{F_1}\) and \(E_{F_2}\) are compared to interaction energies \(\lambda_1\) and \(\lambda_2\). The Josephson energy scale \(\lambda_J\), not shown in the figure, is considered to the smallest of all. A simple analysis of these energy scales leads to four general outcomes. The first case is illustrated in panel (a), where the pairing energy scales \(\lambda_1 < E_{F_1}\) and \(\lambda_2 < E_{F_2}\) leading to BCS pairing in both bands (BCS-BCS), and pair sizes \(\xi_1 \gg k_{F_1}^{-1}\) and \(\xi_2 \gg k_{F_2}^{-1}\), where \(k_{F_1}\) is the Fermi momentum associated with band 1. The second case is illustrated in panel (b), where \(\lambda_1 < E_{F_1}\) and \(\lambda_2 > E_{F_2}\) leading to BCS pairing in band 1 and BEC pairing in band 2 (BCS-BEC), and pair sizes \(\xi_1 \gg k_{F_1}^{-1}\) and \(\xi_2 < k_{F_2}^{-1}\). The third case is illustrated in panel (c), where \(\lambda_1 > E_{F_1}\) and \(\lambda_2 < E_{F_2}\) leading to BEC pairing in both bands (BEC-BCS), and pair sizes \(\xi_1 < k_{F_1}^{-1}\) and \(\xi_2 \gg k_{F_2}^{-1}\). The fourth case is illustrated in panel (d), where \(\lambda_1 > E_{F_1}\) and \(\lambda_2 > E_{F_2}\) leading to BEC pairing in both bands (BEC-BEC), and pair sizes \(\xi_1 < k_{F_1}^{-1}\) and \(\xi_2 < k_{F_2}^{-1}\). The effect of \(\lambda_J\) is to transfer fermion pairs from one band to the other, thus guaranteeing that the ground state is always superfluid with both bands participating. Thus, when \(\lambda_J \neq 0\), we can have only crossovers between BCS-BCS, BCS-BEC, BEC-BCS and BEC-BEC regions. The case of \(\lambda_J = 0\) is very special, because it blocks pair transfer from one band to the other, and allows for ground states where superfluidity exists not only in both bands, but also in just one band, as either interactions or band offset are changed. Thus, fine tuning \(\lambda_J\) to zero allows for QPT’s between different superfluid phases rather than crossovers, even with only s-wave interactions. As discussed below, this physical picture is further constrained by \(\mu\), because only the total number operator \(\hat{N} = \sum_{jks} c_{jk}\dagger c_{jk}\) is conserved.

Thermodynamic Potential: To obtain the thermodynamic potential \(\Omega = -T \ln Z\), where \(Z\) is the grand canonical partition function, we choose pairing to be independent of time and to occur at zero center-of-mass momentum \(\langle \mathbf{q} = 0 \rangle\), that is, the pairing field is \(\Delta_j(k) = \Delta_0\delta_{kq}\), where \(\Delta_0\) is the order parameter for the \(j\)th band. This approximation leads to \(\Omega = \Omega_p + \Omega_c\). The first term is \(\Omega_p = -\sum_{ij\ell\ell'} \Delta_0 \delta_{ij\ell\ell'}\). The second term, arising from the fermionic degrees of freedom, is \(\Omega_c = T \sum_{j} \beta \{ \Delta_j(k) - E_j(k) - 2 \ln [1 + e^{-\beta E_j(k)}] \}\), where the quasiparticle excitation energy is
\[
E_j(k) = \sqrt{\varepsilon_j^2(k) + \Delta_j(k)^2}, \tag{2}
\]
Since $\mu < \varepsilon_0$ and both $E_1(k)$ and $E_2(k)$ have indirect BCS-like gaps (BCS-BCS); (II) where $\varepsilon_0 > \mu > 0$ and $E_1(k)$ has an indirect BCS-like gap and $E_2(k)$ has a direct BCS-like gap (BCS-BEC); and (III) where $\mu < 0$ and both $E_1(k)$ and $E_2(k)$ have direct BEC-like gaps (BEC-BEC).

Notice that, while $\Omega_\ast$ depends only on the moduli $|\Delta_{10}|$, we can write $\Omega_\ast = -g_{11}|\Delta_{10}|^2 - g_{22}|\Delta_{20}|^2 - 2g_{12}|\Delta_{10}|^2|\cos \delta \varphi$, where $\delta \varphi = \varphi_2 - \varphi_1$ is the relative phase between the two order parameters. Here, $g_{11} = -V_{22}/\text{det } V$, $g_{22} = -V_{11}/\text{det } V$, and $g_{12} = -V_{12}/\text{det } V$ with $\text{det } V = (V_{11}V_{22} - V_{12}V_{21}) > 0$. Since $V_{12} = V_{21} = -J$, then $g_{12} = J/\text{det } V$ defines the sign of the prefactor of $\cos \delta \varphi$. When $|\Delta_{10}|$ and $|\Delta_{20}|$ are non-zero and $J > 0$, the thermodynamic potential $\Omega$ is minimized when the phases of the order parameters are the same (differ by $\pi$), that is, $\varphi_2 = \varphi_1 \pm \pi$. When $J = 0$, $\varphi_1$ and $\varphi_2$ are completely independent. Thus, the limit $J \to 0$ is singular, that is, there is a phase transition between the $0$-phase with $\delta \varphi = 0$ and the $\pi$-phase with $\delta \varphi = \pm \pi$. This means that keeping $V_{11}, V_{22}, \varepsilon_0$, and $\mu$ fixed, and switching $J \to -J$ leads to a $0$-$\pi$ QPT for any values of the order parameters.

**Order Parameters:** From the condition $\delta \Omega/\delta \Delta_{10} = 0$, we obtain the order parameter equations

$$\Delta_{10} = -\sum_{j,k} V_{1j} \frac{\Delta_{10} \Gamma_j(k)}{E_j(k)^2} \tanh \left( \frac{\beta E_j(k)}{2} \right).$$

The number equation is $N = -\partial \Omega/\partial \mu|_{T,V}$, leading to $N = N_1 + N_2$, where $N_j = \sum_k n_j(k)$ is the number of particles in band $j = \{1,2\}$, and $n_j(k) = \frac{1}{2} \left[ 1 - \frac{\delta_j(k)}{E_j(k)} \tanh \left( \frac{\beta E_j(k)}{2} \right) \right]$ is the momentum distribution. For each internal (spin) state of the $j$th band. For $J > 0$ with $\varphi_1 = \varphi_2$ or $J = 0$ with $\varphi_1$ and $\varphi_2$ being independent, we obtain $|\Delta_{10}|$ and $\mu$ from the order parameter and number equations by writing $V_{11} = -|V_{11}|$ and $V_{22} = -|V_{22}|$ in terms of the $s$-wave scattering lengths $a_{s_j}$ via $\frac{1}{|V_{11}|} = -\frac{mL^2}{4\pi a_{s_j}} + \sum_k \frac{|\Gamma_j(k)|^2}{2E_j(k)}$. We use the total particle density $N/V$ to define an effective Fermi momentum $k_F$ via $n = k_F^3/3\pi^2$ and an effective Fermi energy $\varepsilon_F = k_F^2/2m$ as momentum and energy scales, since we choose $m_1 = m_2 = m$ from now on. Note that $k_F^3 = k_F^3 + k_F^3$. In Fig. 2 we show $|\Delta_{10}|/\varepsilon_F$ and $|\Delta_{20}|/\varepsilon_F$ versus $1/k_F a_{s_2}$ for fixed $1/k_F a_{s_1} = -1.5$, but different values of $(\varepsilon_0/\varepsilon_F, J/\varepsilon_F)$: (a) $(0,10^{-3})$, (b) $(0.9,10^{-3})$, (c) $(0,0)$, (d) $(0.9,0)$. In (a) and (b): the BCS-BCS region (I, purple), BCS-BEC region (II, gray), and BEC-BEC region (III, green) are shown. In (c) and (d): three phases of $S_1 + S_2$ (yellow) with $|\Delta_{10}|/\varepsilon_F \neq 0$, $S_1$ (blue) with $|\Delta_{10}| \neq 0$ and $|\Delta_{20}| = 0$, and $S_2$ (orange) with $|\Delta_{10}| = 0$ and $|\Delta_{20}| \neq 0$ are depicted. The solid red line is for $\mu = \varepsilon_0$ and the dotted blue line is for $\mu = 0$.

**Phase Diagrams:** The ground state phase diagrams in the $1/k_F a_{s_1}$ versus $1/k_F a_{s_2}$ plane, shown in Fig. 4, are determined by analyzing $|\Delta_{10}|$, $|\Delta_{20}|$, and $\mu$. The solid red (dotted blue) line corresponds to $\mu = \varepsilon_0$ ($\mu = 0$). In panels (a) and (b), where $J/\varepsilon_F \neq 0$, su-
perfluidity arises in both bands for all values of $1/k_Fa_{s_1}$ and $1/k_Fa_{s_2}$, that is, $|\Delta_{10}|$ and $|\Delta_{20}|$ are always non-zero. Thus, there are only crossovers between spectroscopically different superfluids phases: (I) BCS-BCS (purple) with $\mu > \epsilon_0$, (II) BCS-BEC (gray) with $\epsilon_0 > \mu > 0$, and (III) BEC-BEC (green) with $\mu < 0$. However, in panels (c) and (d), where $J/\varepsilon_F = 0$, there are three different phases and QPTs between them. The phases are $S_1$ (blue) with $|\Delta_{10}| \neq 0$ and $|\Delta_{20}| = 0$, $S_2$ (orange) with $|\Delta_{10}| = 0$ and $|\Delta_{20}| \neq 0$, and $S_1 + S_2$ (yellow) with $|\Delta_{10}| \neq 0$ and $|\Delta_{20}| \neq 0$. For $J/\varepsilon_F = 0$, there is no superfluid proximity effect, thus, the strongest-coupled band depletes the weakest-coupled band forcing the order parameter of the latter to zero. At the boundaries between $S_1 + S_2$ and $S_1$ ($S_2$), $|\Delta_{20}|$ ($|\Delta_{10}|$) vanish and the transitions are continuous. Furthermore, when $\mu < \epsilon_0$ ($\mu < 0$), $N_2$ ($N_1$) also vanish where $|\Delta_{20}| = 0$ ($|\Delta_{10}| = 0$). These calculations confirm previous conjectures [31] and shine light on earlier works that missed the full phase diagrams containing double crossovers and QPTs [33–38].

**Pair size:** To characterize further the spectroscopic regions (I, II, III) and the QPTs for $J/\varepsilon_F = 0$, we discuss the pair sizes $\xi_j$ within the $j^{th}$ band [17, 39]:

$$
\xi_j^2 = \left( \sum_k \phi_j^*(k) \left[ -\nabla_k^2 \right] \phi_j(k) \right) / \sum_k |\phi_j(k)|^2 ,
$$

where $\phi_j(k) = \Delta_j(k)/(2E_j(k))$ is the non-normalized pair wave function. In Fig. 4, we show $k_F\xi_1$ (dotted blue line) and $k_F\xi_2$ (solid red line) versus scattering parameter $1/k_Fa_{s_1}$ for fixed $1/k_Fa_{s_1} = -1.5$ and different values of $(\epsilon_0/\varepsilon_F, J/\varepsilon_F)$: (a) $(0, 10^{-3})$, (b) $(0.9, 10^{-3})$, (c) $(0, 10^{-4})$, (d) $(0.9, 10^{-4})$, (e) $(0, 0)$, and (f) $(0.9, 0)$. Background color codes are the same as in Fig. 3. The value $k_F\xi_1 = 1$ approximately separates the BCS-like ($k_F\xi_j \gg 1$) and BEC-like ($k_F\xi_j \ll 1$) regimes. The coherence lengths $k_F\xi_{1c}$ (dashed magenta line) and $k_F\xi_{2c}$ (dotted green line) are shown in panels (e) and (f).

**Ginzburg-Landau Theory:** As shown in Fig. 2, QPTs occur only for $J/\varepsilon_F = 0$. In the vicinity of the phase boundaries between the $S_1 + S_2$ (yellow) and $S_1$ (blue) or $S_2$ (orange) phases, a Ginzburg-Landau (GL) theory is possible. Writing the order parameter as $\Delta_j(q) = |\Delta_{j0}| \delta_{q,0} + \Lambda_j(q)$, and setting $|\Delta_{j0}| = 0$ at the appropriate boundary, the GL thermodynamic potential becomes

$$
\Omega_{GL} = \Omega_i + \Omega_{JN} + \int d^d \mathbf{r} \left[ \frac{1}{L^d} \left( \Lambda_j^*(\mathbf{r}) M_j(\mathbf{q}) \Lambda_j(\mathbf{r}) + b_j |\Lambda_j(\mathbf{r})|^4 \right) \right] ,
$$

where $\Omega_i$ ($\Omega_{JN}$), with $i \neq j$, is the thermodynamic potential of band $i$ ($j$) which remains superconducting (becomes normal) at the phase boundary. The fluctuation terms under the integral are $M_j(\mathbf{q}) = a_j + c_j \bar{q}^2/2m_j$, and $b_j > 0$. The GL coherence length $\xi_{jc}$ for pairing in the $j^{th}$ band is $\xi_{jc}^2 = c_j/2m_j a_j$, where $a_j = M_j(0)$ and $c_j = 2m_j [\partial^2 M_j(q)/\partial q^2]_{q=0}$, with

$$
M_j(q) = -g_{jj} - \sum_{k, \lambda} \left[ \Gamma(k) \right] \alpha_j^\lambda(k_+, k_-) \beta_j^\lambda(k_+, k_-) ,
$$

where $k_\pm = k \pm q/2$. The index $\lambda = \{p, h\}$ represents quasiparticle ($p$) or quasihole ($h$) contributions. The functions within the sum are

$$
\alpha_j^\lambda(k_+, k_-) = \frac{\tan \left[ E_j(k_+)/2T \right] \pm \tan \left[ E_j(k_-)/2T \right]}{E_j(k_+) \pm E_j(k_-)} ,
$$

with the $+$ ($-$) sign being for $\lambda = p$ ($\lambda = h$), and

$$
\beta_j^\lambda(k_+, k_-) = \frac{1}{4} \left[ 1 \pm \frac{\xi_j(k_+)\xi_j(k_-)}{E_j(k_+)E_j(k_-)} \right] .
$$
are the coherence factors. Near the phase boundary at $T = 0$, $\xi_{jc} = \xi_{j0} |\eta_j - \eta_j^*|^{-1/2}$, where $\eta_j = 1/k_F a_{s_j}$ and $\eta_j^* = 1/k_F a_{s_j}^*$ is the critical interaction parameter. When corresponding phase boundaries are crossed, $\xi_{jc}$ diverges similarly to the pair size $\eta_j$, signaling continuous phase transitions over all phase boundaries in the $1/k_F a_{s_j}$ versus $1/k_F a_{s_{j'}}$ plane. This is illustrated in panels (e) and (f) of Fig. 1 where we can also see that in the BEC regime ($1/k_F a_{s_2} \to \infty$), the pair size $k_F \xi_2 \to 0$, while the coherence length $k_F \xi_{2c} \to C$, where $C \neq 0$.

**Conclusions:** We showed that, during the evolution from BCS to BEC superfluidity, elusive quantum phase transitions (QPTs) occur by tuning $s$-wave interactions and band offset in two-band superfluids. This in sharp contrast with single-band $s$-wave systems where only a crossover is possible. Our results may bypass long standing experimental difficulties in the search of QPTs for ultracold fermions with one-band, where at least $p$-wave pairing is required, but unfortunately $p$-wave Cooper pairs are short-lived. In addition to QPTs, we have also established three spectroscopically distinct superfluid regions - (I) BCS-BCS, (II) BCS-BEC, and (III) BEC-BEC - possessing crossovers between them, where pair sizes from each band can be dramatically different. We analyzed pair sizes and coherence lengths, within the Ginzburg-Landau theory, and showed that they diverge at the appropriate phase boundaries. Lastly, our results may motivate the experimental search for multiband superfluidity and QPTs in ultracold $^{173}$Yb and $^{87}$Sr.

We thank the National Natural Science Foundation of China (Grants 11522436 & 11774425), the Beijing Natural Science Foundation (Grant Z180013), and the National Key R&D Program of China (Grant 2018YFA0306501) for financial support.

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