Trapped $^{173}$Yb Fermi gas across an orbital Feshbach resonance

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Towards the end of last year, two experimental groups have independently identified a new type of two-body scattering resonance in an ultracold Fermi gas that is composed of neutral $^{173}$Yb atoms [1,2]. The possible creation of the so-called orbital interaction-induced Feshbach resonances was proposed a few months earlier as a result of the scattering between two (two-electron) alkaline-earth-metal atoms in different electronic-orbital and nuclear-spin states [3,4]. This is in contrast to the more familiar magnetic Feshbach resonances, which occur as a result of the coupling between two (one-electron) alkali-metal atoms in two different hyperfine states [5].

It turns out that these distinct resonance mechanisms give rise to important implications for the related many-body problems, e.g., in the contexts of Cooper pairing and associated BCS-BEC evolution [3,6,7]. While a single-band description taking only the open-channel scattering is typically sufficient for the entire evolution across a magnetic resonance [8], a two-band description taking both the open- and closed-channel scatterings on an equal footing is minimally required for an orbital resonance [3,4]. Thus, these new systems naturally break the ground for studies on two-band superfluidity and intrinsic Josephson effect in atomic settings with a high degree of precision and control [7]. In particular, depending on the details of the interband interactions, one can explore not only the competition between the 0-(in)-phase and $\pi$-(out-of)-phase solutions for the relative phase difference between the intraband superfluid order parameters, but also the corresponding relative phase fluctuations and the resultant Gaussian collective modes around the equilibrium values, i.e., the phononlike in-phase Goldstone mode and the excitonlike out-of-phase Leggett mode [7,9,10].

Encouraged by the recent realizations of an orbital Feshbach resonance in a $^{173}$Yb Fermi gas [1,2], and unlike the follow-up theoretical preprints appearing on uniform systems [3,6,7,9,10], here we focus on the confinement-induced signatures that can be decisively traced back to the existence of two-band superfluidity in trapped systems. For this purpose, we consider a two-band model under the assumptions of a local-density approximation for the trapping potential and a mean-field approximation for the intraband Cooper pairings. We find that the interplay between the pair-breaking effect that is caused by the interband detuning energy, and the pair-breaking and thermal-broadening effects that are simultaneously caused by the temperature gives rise to nonmonotonous evolutions in some physical observables. In particular to the zero temperature, we also find that while the entire trapped gas is a superfluid for low detunings, a spatial separation between the central superfluid core and the outer normal edge consisting only of particles in the lower band eventually appears beyond a detuning threshold that is of the order of the resonance value.

The rest of the paper is organized as follows. First, assuming a local-density approximation for the trapping potential, we introduce a two-band model for the Hamiltonian density in real space in Sec. II, and relate its bare theoretical parameters to the two-body scattering parameters of $^{173}$Yb atoms. Then, assuming a mean-field approximation for the intraband Cooper pairings, we derive the mean-field Hamiltonian density in Sec. III, and obtain a set of self-consistency equations for the intraband order parameters and number equations for the two bands. Having solved these equations numerically in Sec. IV and provided a thorough analysis for our findings, we end the paper with a brief summary of our conclusions in Sec. V.
pseudospin projections $\sigma \equiv \{\uparrow, \downarrow\}$, and $k$ is a momentum. The operator $c_{i\sigma k}^\dagger(r)$ creates a single particle at $r$ with quantum numbers $i, \sigma$, and $k$, and dispersion $\varepsilon_{i k}(r) = \varepsilon_k - \mu_i(r)$. Here, $\varepsilon_k = k^2/(2m)$ is in units of $\hbar = 1$, and $\mu_1(r) = \mu - V_i(r)$ is for the lower and $\mu_2(r) = \mu - \delta/2 - V_i(r)$ is for the upper band, where $V_i(r) = m\omega_r^2 r^2/2$ is assumed to be harmonic in space, and the energy shift $\delta/2 \geq 0$ between the two bands is a controllable detuning parameter that is used to access an orbital Feshbach resonance. Similarly, the operator $b_{i\sigma k}^\dagger(r) = \sum_k c_{i\sigma k+q/2}(r)c_{i\sigma k-q/2}^\dagger(r)$ creates pairs of $\uparrow$ and $\downarrow$ particles at $r$ with quantum numbers $i$ and center-of-mass momentum $q$. The bare amplitudes for the local intraband $V_{11} = V_{22} = (g_+ + g_-)/2$ and local interband $V_{12} = V_{21} = (g_- - g_+)$ are related to the two-body scattering lengths in vacuum $a_{i k}$ via the usual renormalization relations $1/g_k = -m V/(4\pi a_{i k}) + \sum_m m^2 k^2$, where $V$ is the volume, in such a way that the orbital resonance occurs precisely when $\delta$ is tuned to a critical threshold $\delta_{res} = 4/[m(a_{i+} + a_{i-}r^2)]^2$. These parameters have recently been determined for a $^{173}$Yb Fermi gas, and are given by $a_{i+} \approx 1900a_0$ and $a_{i-} \approx 200a_0$ with $a_0$ the Bohr radius $[1,2]$, for which both intra- and interband interactions turned out to be attractive with $V_{ij} > 0$.

### III. MEAN-FIELD APPROXIMATION FOR PAIRING

Assuming that the fluctuations of the pair-creation operators are small in comparison to their equilibrium values, we adopt a mean-field approximation for pairing, and introduce an intraband order parameter $\Delta_{i}(r) = -\sum_j V_{ij}(b_{j\sigma k}(r))$ for each band $[7]$, where $\langle \cdots \rangle$ is a thermal average. In addition, restricting ourselves solely to local BCS-like solutions, we set $q = 0$ and determine the local complex parameter $\Delta_i(r) = \Delta_0(r)$ self-consistently with the corresponding local number equation $n_i(r) = \sum_{\sigma k} (c^\dagger_{i\sigma k}(r)c_{i\sigma k}(r))$ for each band at a given $r$. Once the total number of particles in a given band is obtained by $N_i = \langle 1/V \rangle \int d^3r n_i(r)$, then $\mu$ is iterated until $N = N_1 + N_2$ is fixed to a specified value given in Sec. IV. This self-consistent construction is a straightforward extension of the usual mean-field approach that has extensively been employed for single-band Fermi gases, and it forms the fundamental basis for most of the BCS-BEC crossover studies in literatures, over the past decade or so, in the context of magnetic Feshbach resonances $[8]$.

Thus, within such a mean-field approximation for the intraband pairings, the local mean-field Hamiltonian can be reexpressed as

$$H_{mf} = \sum_{i\sigma k} \varepsilon_{i k}(r)c_{i\sigma k}^\dagger(r)c_{i\sigma k}(r)$$

$$+ \sum_{ijq} [\Delta_{i q}(r)b_{i q}^\dagger(r) + \Delta_{i q}^*(r)b_{i q}(r)]$$

$$+ \sum_{ijq} U_{i j} \Delta_{j q}^*(r)\Delta_{j q}(r),$$

(1)

where the matrix $U$ is the inverse of the amplitude matrix $V$. i.e., its elements can be written explicitly as $U_{11} = V_{22}/\det V$, $U_{22} = V_{11}/\det V$, $U_{12} = -V_{21}/\det V$, and $U_{21} = -V_{12}/\det V$ with $\det V = V_{11}V_{22} - V_{12}V_{21}$. Note that the interband coupling gives rise to a Josephson-type contribution to the Hamiltonian, $U_{ij}(\Delta_{i q}^\dagger \Delta_{j q} + \Delta_{i q}^* \Delta_{j q}^\dagger)$, depending explicitly on the relative phase between the intraband order parameters. Then, restricting to local BCS-like solutions, the resultant self-consistency equations can be compactly put in a more familiar form as follows $[7]$:

$$\Delta_i(r) = \sum_k V_{ij} \frac{\Delta_j(r)}{2E_{j k}(r)} \tanh \left[ \frac{E_{j k}(r)}{2T} \right],$$

(2)

$$n_i(r) = \sum_k \left[ 1 - \frac{\xi_k(r)}{E_{j k}(r)} \right] \tanh \left[ \frac{E_{j k}(r)}{2T} \right],$$

(3)

where $E_{j k}(r) = \sqrt{\xi_k(r)^2 + \Delta_i(r)^2}$ is the energy of the local quasiparticle excitations in the $i$th band with momentum $k$. $T$ is the temperature, and the Boltzmann constant $k_B$ is set to unity. The summand in Eq. (3) is the local momentum distribution $n_i(r,k)$ of particles in the $i$th band.

Motivated by the success of the analogous mean-field theories in describing the fundamental properties of alkalimetal atoms across a magnetic Feshbach resonance $[8]$, here we apply it to alkaline-earth-metal atoms across an orbital Feshbach resonance. Therefore, we are interested in the so-called $\pi$-phase solution for the local relative phases between the local order parameters, i.e., $\text{sgn}[\Delta_i(r)] = -\text{sgn}[\Delta_i(r)]$ at any given $r$, which is directly linked to the orbital Feshbach resonance found in a $^{173}$Yb Fermi gas $[3,7]$.

### IV. $\pi$-PHASE SOLUTIONS FOR A $^{173}$Yb FERMI GAS

We use the following definitions of an effective Fermi energy and the associated Fermi momentum $\varepsilon_F = k_F^2/(2m)$, and the corresponding Thomas-Fermi radius $r_T$ in presenting our numerical solutions. Assuming a total of $N$ noninteracting particles in a single-band Fermi gas at $T = 0$, and setting $\mu = \varepsilon_F$, we may write $\varepsilon_F = k_F^2/(2m) + m\omega_r^2 r^2/2$ for the lower band within the local-density approximation. This defines a local Fermi momentum $k_F(r)$ in such a way that the local number of particles is given by $n(r) = V(k_F^2(r))/(3\pi^2)$ at a given $r$. Noting that $\varepsilon_F = 0$ at the edge of the system by definition, we may express $k_F = k_F(0) = m\omega_r r_F/\varepsilon_F$ for $N = N_F r_F^3/24$ or equivalently $\varepsilon_F = \omega(3N)^{1/3}$. Choosing a typical atomic density of $n(0) = 10^{14}$ cm$^{-3}$ at the center of the trap and using the scattering parameters of a $^{173}$Yb Fermi gas given in Sec. II, we find $1/k_F a_{res} \approx 0.693, 1/(k_F a_{res}) \approx 6.582$, and $\delta_{res} \approx 3.14\varepsilon_F$. In addition, by choosing a large momentum cut-off $k_0 = 100k_F$ in $k$-space sums, we obtain $k_0$-independent solutions for the physical observables, even though all of the bare interaction amplitudes $V_{ij}$ themselves depend explicitly on $k_0$.

First we consider a resonant Fermi gas with $\delta = \delta_{res}$, and present typical $n_i(r)$ and $\Delta_i(r)$ profiles as functions of $r$. It is worth mentioning here that since were are presenting the $\pi$-(out-of)-phase excited-state solutions but not the $0$-(in)-phase ground-state ones, the higher $i = 2$ band has higher order parameters in spite of its lower density. As shown in Figs. 1(a) and 1(b), while $|\Delta_2(r)| > |\Delta_1(r)| > 0$ as long as $n_1(r) > n_2(r) > 0$ at $T = 0$, and therefore, the entire gas is found to be a superfluid, the pairing-breaking effect caused by finite $T$ weakens $|\Delta_i(r)|$ and turns the edge of the gas to normal beyond a
Critical radius $r > r_S$. Here, the critical radius $r_S$ for the spatial separation of superfluid and normal phases within the trap is determined by the simultaneous vanishing of $|\Delta_{1,2}(r_S)| \to 0^+$. Increasing $T$ gradually decreases $r_S$ towards the center of the trap, and eventually the entire gas turns to normal, i.e., $r_S \to 0$, beyond the critical superfluid-normal transition temperature $T_c \approx 0.45 \varepsilon_F$. The simultaneous disappearance of the order parameters leads not only to observable cusps in $n_i(r)$ precisely at $r = r_S$ but also to the thermal broadening of the outer normal regions. This is best seen in Fig. 1(c), where we present the trap-averaged momentum distributions $n_i(k)$ as functions of $k$, where $n_i(r,k)$ is the summand of Eq. (3).

We note the following in passing for the radial profiles at $T = 0$. Up until $\delta \sim \delta_{res}$, the local occupation of the upper band in the trap turns out to be nonzero as long as the lower band is also locally occupied there, i.e., if $n_1(r) \neq 0$, then $n_2(r) \neq 0$ for any given $r$. This is a direct result of the interband coupling, and the entire gas is a superfluid with $\Delta_2(r) \neq 0$ wherever $\Delta_1(r) \neq 0$, as illustrated above for a resonant Fermi gas. On the other hand, when $\delta \geq 4 \varepsilon_F$, we find that the interband coupling is not locally strong enough to overcome the detuning barrier towards the edge of the gas, as a consequence of which the intraband pairings vanish $|\Delta_{1,2}(r \to r_S)| \to 0^+$ simultaneously at some critical radius $r_S$. This naturally gives rise to $n_2(r_S) = 0$ and $n_1(r_S) \neq 0$ for $r > r_S$, and hence, a spatial separation appears between the central superfluid core and the outer normal edge consisting only of particles in the lower band. When $r_S$ eventually reduces to 0 as $\delta \gg \varepsilon_F$, then the entire trap is effectively occupied by a single band of noninteracting Fermi gas in the lower band.

To understand the general trends, next we present the band-population imbalance $P = (N_1 - N_2)/N$ and chemical potential $\mu$ as functions of $\delta$ at $T = 0$. It is clearly seen that while $P = 0$ or $N_1 = N_2$ and $\mu < 0$ at $\delta = 0$, the particles gradually transfer from the upper to the lower band as a result of the increased energy difference $\delta/2$ between the bands and its pair-breaking
FIG. 3. Central parameters at resonance detuning. (a) The numbers of particles $n_i(r = 0)$ [in units of $NV/(4\pi r_j^3)$], (b) the order parameters $\Delta_i(r = 0)$, and (c) the trap-averaged momentum distributions $n_i(k = 0)$ (in units of $4\pi r_j^3 F / V$) are shown as functions of temperature $T$.

The nonmonotonous evolution of $P$ with $T$ at fixed $\delta$ is a direct consequence of the competition between the pair-breaking and thermal-broadening effects of $T$. To illustrate this competition, we present the central parameters $n_i(r = 0)$ and $\Delta_i(r = 0)$ in Figs. 3(a) and 3(b), respectively, as functions of $T$ for a resonant Fermi gas. In accordance with our definition of $\epsilon_F$ given above for a noninteracting single-band Fermi gas at $T = 0$, the upper band is completely empty for $\epsilon_F < \delta / 2$. Since $\delta_{\text{res}} \approx 3.144 \epsilon_F$ in this paper, $\Delta_i(r) \neq 0$ promotes some of the particles to the upper band causing $N_2 \neq 0$ at $T = 0$ in the first place, and thus, the reduction of $|\Delta_i(r)|$ at finite but low $T \lesssim T_c$ naturally demotes particles back to the lower band. However, in the mean time, the particles are thermally excited back to the upper band as well, leading to the aforementioned competition as a function of $T$. The isolated effects of pair-breaking and thermal-broadening mechanisms on the occupations of the bands are evidently seen in Fig. 3(c), where we present $n_i(k = 0)$ as functions of $T$. 

FIG. 4. Central parameters at zero temperature. (a) The numbers of particles $n_i(r = 0)$ [in units of $NV/(4\pi r_j^3)$], (b) the order parameters $\Delta_i(r = 0)$, and (c) the trap-averaged momentum distributions $n_i(k = 0)$ (in units of $4\pi r_j^3 F / V$) are shown as functions of detuning $\delta$. 

The effect, leading eventually to $P \to 1$ or $N_1 \gg N_2 \to 0$ and $\mu \to \epsilon_F$ in the $\delta \gg \epsilon_F$ limit. The evolutions of $P$ and $\mu$ are smooth and monotonous across the resonance, at which point we find $P \approx 0.400$ and $\mu \approx 0.578 \epsilon_F$. Similarly, in Fig. 2(b), we present $P$ and $\mu$ as functions of $T$ at $\delta = \delta_{\text{res}}$. While $\mu$ is a monotonically decreasing function of $T$, $P$ first increases to a peak value of 0.934 at $T \approx 0.43 \epsilon_F$ and then decreases. This temperature almost coincides with the critical one where $\mu \approx 0.342 \epsilon_F$ and $P \approx 0.930$ at $T_c \approx 0.45 \epsilon_F$. 

The nonmonotonous evolution of $P$ with $T$ at fixed $\delta$ is a direct consequence of the competition between the pair-breaking and thermal-broadening effects of $T$. To illustrate this competition, we present the central parameters $n_i(r = 0)$ and $\Delta_i(r = 0)$ in Figs. 3(a) and 3(b), respectively, as functions of $T$ for a resonant Fermi gas. In accordance with our definition of $\epsilon_F$ given above for a noninteracting single-band Fermi gas at $T = 0$, the upper band is completely empty for $\epsilon_F < \delta / 2$. Since $\delta_{\text{res}} \approx 3.144 \epsilon_F$ in this paper, $\Delta_i(r) \neq 0$ promotes some of the particles to the upper band causing $N_2 \neq 0$ at $T = 0$ in the first place, and thus, the reduction of $|\Delta_i(r)|$ at finite but low $T \lesssim T_c$ naturally demotes particles back to the lower band. However, in the mean time, the particles are thermally excited back to the upper band as well, leading to the aforementioned competition as a function of $T$. The isolated effects of pair-breaking and thermal-broadening mechanisms on the occupations of the bands are evidently seen in Fig. 3(c), where we present $n_i(k = 0)$ as functions of $T$. 

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For completeness, next we discuss the central parameters $n_i(r = 0), \Delta_i(r = 0)$, and $n_i(k = 0)$ as functions of $\delta$ at $T = 0$, showing purely the crucial role played by the pair-breaking effect of $\delta$ in the absence of thermal effects. As shown in Fig. 4, while $n_i(0) = n_\Delta(0)$ and $|\Delta_i(0)| = |\Delta_\Delta(0)|$ at $\delta = 0$, the particles gradually transfer from the upper to the lower band with increased $\delta$ due to the simultaneous reduction of $|\Delta_\Delta(0)| > |\Delta_i(0)|$. This eventually leads to $n_1(0) > n_2(0) \rightarrow 0$ and $|\Delta_\Delta(0)| \rightarrow 0$ in the $\delta \approx \varepsilon_F$ limit, and the problem reduces effectively to a single band of noninteracting Fermi gas in the lower band.

We would like to remark here that the physical picture outlined just above in understanding the general trends presented in this paper goes beyond the simple mean-field approximation that is assumed in our numerical calculations. It is widely believed that while this approximation reliably describes the low-temperature ($T < T_c$) properties of a weakly interacting Fermi gas in general, the inclusion of (at least) the Gaussian pair fluctuations is necessary in order to produce a qualitatively correct $T_c$ in the strongly interacting regime, especially near the resonance [6]. However, the nonmonotonic evolutions caused by the competition between the pair-breaking and thermal-broadening mechanisms should be manifested in beyond mean-field calculations as well, apart from expected minor quantitative differences.

V. CONCLUSIONS

In summary, we analyzed how a trapped $^{173}$Yb Fermi gas and its superfluid properties evolve across an orbital Feshbach resonance. We used a two-band description for this purpose, under the assumptions of a local-density approximation for the trapping potential and a mean-field approximation for the intraband pairings. One of our primary findings is that the interplay between the pair-breaking effect that is caused by the interband detuning energy $\delta$, and the pair-breaking and thermal-broadening effects that are simultaneously caused by the temperature $T$ gives rise to nonmonotonic evolutions in some physical observables, including the band-population imbalance and trap-averaged momentum distributions. In addition, we found that at $T = 0$ while the entire trapped gas is a superfluid for $\delta \lesssim \delta_{\text{res}}$ with the resonance detuning $\delta_{\text{res}} \sim 3\varepsilon_F$, a spatial separation between the central superfluid core and the outer normal edge which consists only of particles in the lower band eventually appears beyond a critical detuning that is of the order of $\delta \gtrsim 4\varepsilon_F$. We also argued that, since these predictions are physically intuitive and not caused by any of the approximations used, they may play decisive roles in probing two-band superfluidity in the cold-atom context. As an immediate outlook, we look forward to further research along these lines by especially taking the beyond local-density and/or mean-field corrections into account for quantitatively more accurate predictions.

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in Eq. (1). This is such that the total number $N$ of atoms are equally distributed over the two states $|\epsilon \uparrow\rangle$ and $|\epsilon \downarrow\rangle$ of the open channel in the noninteracting limit when $\delta > 2\epsilon_F$. For instance, if all of the atoms are initially prepared in the ground state $|g\rangle$, then one can achieve a balanced system by exciting all of the $\uparrow$ atoms from $|g\rangle$ to the excited state $|e\rangle$. The formalism developed in this paper can easily be extended to the analysis of the imbalanced problem, and this is one of the immediate experimental interests to be addressed in the near future. Furthermore, we assume a common trapping potential for all atoms, independent of their orbital and nuclear-spin degrees of freedom [1,2].