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

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Starting with the two-band description of an orbital Feshbach resonance, we study superfluid properties of a trapped $^{173}$Yb Fermi gas under the assumptions of a local-density approximation for the trapping potential and a mean-field approximation for the intra-band Cooper pairings. In particular, we investigate the competition and interplay between the pair-breaking effect that is caused by the inter-band detuning energy, and the pair-breaking and thermal-broadening effects that are simultaneously caused by the temperature. We predict several experimental signatures that are directly caused by this interplay including a spatial separation of superfluid and normal phases within the trap, and could play decisive roles in probing two-band superfluidity in these systems.

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I. INTRODUCTION

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 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 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 inter-band 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 intra-band superfluid order parameters, but also the corresponding relative phase fluctuations and the resultant Gaussian collective modes around the equilibrium values, i.e., the phonon-like in-phase Goldstone mode and the exciton-like out-of-phase Leggett mode [7, 3, 10].

Encouraged by the recent realizations of an orbital Feshbach resonance in a $^{173}$Yb Fermi gas [1, 2], and unlike the followed up theoretical preprints appeared 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 intra-band Cooper pairings. We find that the interplay between the pair-breaking effect that is caused by the inter-band detuning energy, and the pair-breaking and thermal-broadening effects that are simultaneously caused by the temperature gives rise to non-monotonous 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 intra-band Cooper pairings, we derive the mean-field Hamiltonian density in Sec. [III] and obtain a set of self-consistency equations for the intra-band 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]. The experimental context is briefly discussed in the Appendix.

II. LOCAL-DENSITY APPROXIMATION FOR TRAP

The semi-classical method based on a local-density approximation for the trapping potential is probably one of the most convenient approaches for studying many-body effects in finite-sized systems. By shifting the confinement potential $V_{tr}(r)$ from the chemical potential $\mu$, one simply introduces a local chemical potential $\mu(r) = \mu - V_{tr}(r)$ that depends explicitly on the radial distance $r$. This assumption works best for large systems with slowly-varying potentials since the relevant Fermi energy scale becomes much larger than the confinement-induced energy separation between the quantum levels as the number of particles increases. For instance, within this approximation, the Hamiltonian density describing isotropically-trapped Fermi gases across an orbital Feshbach...
where the band index $i \equiv \{1,2\}$ refers to the particles in the open (lower band) and closed (upper band) channels with pseudo-spin projections $\sigma \equiv \{\uparrow, \downarrow\}$, and $k$ is momentum. The operator $c_{i\sigma k}^{\dagger}(r)$ creates a single particle at $r$ with quantum numbers $i$, $\sigma$ and $k$, and dispersion $\xi_{ik}(r) = \varepsilon_{k} - \mu_{i}(r)$. Here, $\varepsilon_{k} = k^{2}/(2m)$ is in units of $\hbar = 1$, and $\mu_{1}(r) = \mu - V_{tr}(r)$ for the lower and $\mu_{2}(r) = \mu - \delta/2 - V_{tr}(r)$ for the upper band, where $V_{tr}(r) = m\omega^{2}r^{2}/2$ 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 $b_{i\sigma q}^{\dagger}(r) = \sum_{k}c_{i\uparrow,k+q/2}^{\dagger}(r)c_{i\downarrow,-k+q/2}^{\dagger}(r)$ 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 intra-band $V_{11} = V_{22} = (g_{+} + g_{-})/2$ and local inter-band $V_{12} = V_{21} = (g_{+} - g_{-})/2$ interactions are related to the two-body scattering lengths in vacuum $a_{\pm}$ via the usual renormalization relations $1/g_{\pm} = -m\nu/4\pi a_{\pm} + \sum_{k}m/k^{2}$, where $\nu$ is the volume, in such a way that the orbital resonance occurs precisely when $\delta$ is tuned to a critical threshold $\delta_{rs} = 4/[m(a_{+} + a_{-})^{2}]$ [3]. These parameters have recently been determined for a $^{173}$Yb Fermi gas, and are given by $a_{+} \approx 1900\text{a}_{0}$ and $a_{-} \approx 200\text{a}_{0}$ with $a_{0}$ the Bohr radius [1] [2], for which both intra- and inter-band 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 intra-band order parameter $\Delta_{iq}(r) = -\sum_{j}V_{ij}(b_{jq}^{\dagger}(r))$ for each band [7], where $\langle \cdots \rangle$ is a thermal average. In addition, restricting ourselves solely to local BCS-like solutions, we set $\{0\}$ and determine the local complex parameter $\Delta_{i}(r) = \Delta_{i0}(r)$ self-consistently with the corresponding local number equation $n_{i}(r) = \sum_{k}c_{i\sigma k}^{\dagger}(r)c_{i\sigma k}(r)$ for each band at a given $r$. Once the total number of particles in a given band is obtained by $N_{i} = \langle /\rangle$ if $d^{2}n_{i}(r)$ 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 the literature, over the past decade or so, in the context of magnetic Feshbach resonances [8].

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

$$H_{mf}(r) = \sum_{ijq}V_{ij}b_{ijq}^{\dagger}(r)b_{ijq}(r),$$

where the matrix $U$ is the inverse of the amplitude matrix $V$, i.e., its elements can be written explicitly as $U_{11} = V_{22}/\det V$, $U_{22} = V_{11}/\det V$, $U_{12} = -V_{12}/\det V$ and $U_{21} = -V_{21}/\det V$ with $\det V = V_{11}V_{22} - V_{12}V_{21}$. Note that the inter-band coupling gives rise to a Josephson-type contribution to the Hamiltonian, $U_{12}(\Delta_{iq}^{\dagger}\Delta_{q} + \Delta_{iq}\Delta_{q}^{\dagger})$, depending explicitly on the relative phase between the intra-band 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]:

$$\begin{align*}
\Delta_{i}(r) &= \sum_{jk}V_{ij}\Delta_{j}(r)\tanh(\frac{E_{ik}(r)}{2T}), \\
n_{i}(r) &= \sum_{k}\left\{1 - \frac{\xi_{ik}(r)}{E_{ik}(r)}\tanh(\frac{E_{ik}(r)}{2T})\right\},
\end{align*}$$

where $E_{ik}(r) = \sqrt{\xi_{ik}^{2}(r) + \Delta_{i}^{2}(r)}$ is the energy of the local quasi-particle 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. (5) 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 alkali atoms across a magnetic Feshbach resonance [8], here we apply it to alkaline-earth 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., $\text{sign}(\Delta_{1}(r)) = -\text{sign}(\Delta_{2}(r))$ 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 $r_{F}$ in representing our numerical solutions. Assuming a total of $N$ non-interacting particles in a single-band Fermi gas at $T = 0$, and setting $\mu = \varepsilon_{F}$, we may write $\varepsilon_{F} = k_{F}^{2}(r)/(2m) + m\omega^{2}r^{2}/2$ for the lower band within the local-density approximation. This defines a local Fermi momentum $k_{F}(r)$ in such a way that the total number of particles is given by $n(r) = Vk_{F}^{2}(r)/(3\pi^{2})$ at a given $r$. Noting that $k_{F}(r_{F}) = 0$ at the edge of the system by definition, we may express $k_{F} = k_{F}(0) = m\omega_{F}$, leading to $N = k_{F}^{3}r_{F}^{3}/24$ or equivalently $\varepsilon_{F} = \omega(3N)^{1/3}$. Choosing a typical atomic density $n(r)/\nu \approx 10^{14}\text{cm}^{-3}$ at the center of the trap and using the scattering parameters of a $^{173}$Yb Fermi gas given in
Sec. II we find $1/(k_F a_{\pm}) \approx 0.693$, $1/(k_F a_{\mp}) \approx 6.582$ and $\delta_{res} \approx 3.144 \varepsilon_F$. 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 $k_0$.

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. (a) and (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 pair-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 (c), where we present the trap-averaged momentum distributions $n_i(k) = (1/V) \int d^2r n_i(r, k)$ as functions of $k$, where $n_i(r, k)$ is the summand of Eq. (4).

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 non-zero 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 inter-band 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 $\delta \gtrsim 4\varepsilon_F$, we find that the inter-band coupling is not locally strong enough to overcome the detuning barrier towards the edge of the gas, as a consequence of which the intra-band pairings vanish $|\Delta_{1,2}(r \to r_S)| \to 0^+$ simultaneously at some critical radius $r_S$. This naturally gives rise to $n_2(r) = 0$ and $n_1(r) \neq 0$ 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 non-interacting 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 $\mu$ in Fig. (a) 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 effect, leading eventually to $P \to 1$ or $N_1 \gg N_2 \to 0$ and $\mu \to \varepsilon_F$ in the $\delta \gg \varepsilon_F$ limit. The evolutions of $P$ and $\mu$ are smooth and monotonous across the resonance, at which point we find $P \approx 0.400$ and $\mu \approx 0.578 \varepsilon_F$. Similarly, in Fig. (b), we present $P$ and $\mu$ as functions of $T$ at $\delta = \delta_{res}$. While $\mu$ is a monotonically decreasing function of $T$, $P$ first increases to a peak value of $0.934$ at $T \approx 0.43 \varepsilon_F$ and then decreases. This temperature almost coincides with the critical one where $\mu \approx 0.342 \varepsilon_F$ and $P \approx 0.930$ at $T_c \approx 0.45 \varepsilon_F$.

The non-monotonous 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

![Graph](image-url)
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 non-interacting 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 $T$.

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 $n_1(0) = n_2(0)$ and $|\Delta_1(0)| = |\Delta_2(0)|$ at $\delta = 0$, the particles gradually transfer from the upper to the lower band with increased $\delta$ due to the simultaneous reduction of $|\Delta_2(0)| > |\Delta_1(0)|$. This eventually leads to $n_1(0) \gg n_2(0) \rightarrow 0$ and $|\Delta_{1,2}(0)| \rightarrow 0$ in the $\delta \gg \epsilon_F$ limit, and the problem reduces effectively to a single-band of non-interacting 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
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 intra-band pairings. One of our primary findings is that the interplay between the pair-breaking effect that is caused by the inter-band detuning energy $\delta$, and the pair-breaking and thermal-broadening effects that are simultaneously caused by the temperature $T$ gives rise to non-monotonous evolutions in some physical observables, including the band-population imbalance and trap-averaged momentum distributions. In addition, we found at $T = 0$ that while the entire trapped gas is a superfluid for $\delta \lesssim \delta_{\text{res}}$ with the resonance detuning $\delta_{\text{res}} \sim 3\epsilon_F$, 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 $\delta \gtrsim 4\epsilon_F$. 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.

VI. ACKNOWLEDGMENTS

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Appendix A: Experimental Context

First of all, we consider two different nuclear-spin states of a $^{173}$Yb atom and denote them with $|\uparrow\rangle$ and $|\downarrow\rangle$. In addition, assuming that a $\pi$-polarized clock laser light can be used to excite the atoms from their ground ($^1S_0$) state to a long-lived metastable ($^3P_0$) one, we also take into account two different internal-orbital states and denote them with $|e\rangle$ and $|s\rangle$ [1,2]. Then, in Eq. (1), the pseudo-spin projections $\sigma$ correspond precisely to $|1\uparrow\rangle \equiv |e\uparrow\rangle$ and $|1\downarrow\rangle \equiv |g\downarrow\rangle$ in the lower ($i = 1$) band, and to $|2\uparrow\rangle \equiv |g\uparrow\rangle$ and $|2\downarrow\rangle \equiv |e\downarrow\rangle$ in the upper ($i = 2$) band. This reorganization is in such a way that the nuclear-spin projections and orbital states are directly linked with each other in the two-particle scattering channels, where the anti-symmetric state $|e\uparrow; g\downarrow\rangle = (|e\uparrow\rangle|g\downarrow\rangle - |g\downarrow\rangle|e\uparrow\rangle)/\sqrt{2}$ corresponds to the open channel, and $|g\uparrow; e\downarrow\rangle = (|g\uparrow\rangle|e\downarrow\rangle - |e\downarrow\rangle|g\uparrow\rangle)/\sqrt{2}$ to the closed one [1,2].

Since the two-particle interaction between one $|g\rangle$ atom and one $|e\rangle$ atom in two different nuclear-spin states is characterized by the interplay between the orbital-singlet scattering length ($a_{s+}$) and the orbital-triplet ($a_{s-}$) one given in the main

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

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low-temperature ($T \ll T_c$) 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 non-monotonous 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.
text, it is possible to have both intra-channel spin-conserving (direct) interactions as well as an inter-channel spin-flipping (exchange) one. That is, the interaction between one $|g\rangle$ and one $|e\rangle$ atom may also involve a spin-flip. While the strengths of the former are equally proportional to an effective direct scattering length $(a_{s+} + a_{s-})/2$ in both open and closed channels, that of the latter one is proportional to an effective exchange scattering length $(a_{s+} - a_{s-})/2$ giving rise to a coupling between the open and closed channels when $a_{s+} \neq a_{s-}$.

Furthermore, the presence of an external magnetic field splits the nuclear-spin states depending on their Zeeman level, shifting relatively the energies of the scattering channels by varying the strength of the field. For instance, a strong magnetic field weakens the coupling between open and closed channels as the Zeeman energy dominates the spin-exchange interactions leading to well-defined nuclear-spin states. Therefore, the two-particle scattering channels may be strongly correlated with each other at small and intermediate magnetic fields, allowing for the creation of a new type of magnetically-tunable orbital Feshbach resonance, once the Zeeman energy matches the two-body binding energy of the least bound state in the closed channel $[1-4]$.

As the effective nuclear magnetic moments involved in orbital resonances are much smaller than the electronic ones in alkali-atom resonances, the widths of these resonances can be broad in magnetic field, despite their large and negative effective ranges which are characteristic features of narrow, i.e., closed-channel dominated, alkali-atom resonances. Therefore, in contrast to the broad alkali-atom resonances where it is sufficient to retain only the open channel with a single order parameter as the minimal description of the BCS-BEC crossover physics, here it is necessary to treat open and closed channels on an equal footing by introducing a coupled set of two mutually-coherent order parameters requiring a self-consistent solution, as discussed in the main text.

Lastly, we restrict ourselves to the balanced number of $\uparrow$ and $\downarrow$ atoms in each band for its simplicity, and set $\mu_{\uparrow} = \mu_{\downarrow} = \mu$ in Eq. (1). This is such that the total number $N$ of atoms is equally distributed over the two states $|e \uparrow\rangle$ and $|g \downarrow\rangle$ of the open channel in the non-interacting 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 $[1,2]$.

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