Quantum demixing in binary mixtures of dipolar bosons

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Quantum Monte Carlo simulations of a two-component Bose mixture of trapped dipolar atoms of identical masses and dipole moments, provide numerical evidence of demixing at low finite temperatures. Demixing occurs as a consequence of quantum statistics, which results in an effective attraction between like bosons. Spatial separation of two components takes place at low temperature with the onset of long exchanges of identical particles, underlying Bose-Einstein condensation of both components. Conversely, at higher temperature the system is miscible due to the entropy of mixing. Exchanges are also found to enhance demixing in the case of mixtures of nonidentical and distinguishable species.

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I. INTRODUCTION

Phase separation or *demixing* in multicomponent mixtures has been a long-standing topic of interest in chemistry and physics. Closely following the achievement of Bose-Einstein condensation in dilute gases [1,2], there has been considerable interest in the study of binary mixtures of Bose-Einstein condensates (BECs). Of particular note, a two-component BEC was first reported in 1997 comprised of two hyperfine states of Rb [3], and then in 2001 using different atomic species (K and Rb) [4]. The advantage of these ultracold systems is that the entropy of mixing is small and demixing may be easily observed.

The conditions under which demixing occurs in binary BEC mixtures with hard-core repulsion, have been the focus of a number of theoretical works, including mean-field treatments at zero [5–10] and finite temperature [11] as well as quantum Monte Carlo (QMC) simulations [12,13]. Separation of species 1 and 2 is usually characterized in terms of a parameter $\Delta = U_{11}U_{22} - U_{12}^2$, defined in terms of the relative intraspecies (U_{11},U_{22}) and interspecies (U_{12}) interaction strengths. When $\Delta < 0$, so that particles of species 1 and 2 have a relatively strong repulsion, the system is predicted to phase separate, whereas for $\Delta \geqslant 0$ the system should remain mixed [5–13]. Recently, this criterion has been verified in experiments with binary BECs [14]. Earlier work on bosonic mixtures in the context of superfluid Helium have also predicted phase separation in the zero temperature limit for isotopes of different masses or concentrations [15,16]. Indeed, all predictions of phase separation in binary mixtures of bosons to date rely on a mismatch of interaction strengths or of some other physical parameters on which the Hamiltonian depends (such as different particle masses, concentrations, or external trapping potentials for each species). We refer to this scenario as *demixing through interactions*.

In this article, we report the prediction of demixing in a binary mixture of bosons with identical masses and interactions, due a very different mechanism—namely the effective attraction between indistinguishable bosons originating purely from quantum statistics. This prediction is made for $\Delta = 0$ in contrast to earlier work for which this value would lead to a miscible system. We refer to this scenario as *demixing through exchanges* or *quantum demixing*, which occurs when the system kinetic energy is reduced by the formation of long exchanges of identical particles, leading to the spatial separation of the two components. This is, of course, the same mechanism underlying Bose-Einstein condensation, as first established by Feynman [17] and subsequently elaborated on [18,19]. At low temperature, as the thermal wavelength becomes comparable to the interparticle distance, quantum exchanges involving two or more *indistinguishable* particles become frequent, and condensation sets in—this effect is also responsible for phase separation.

For this study, we have elected to use the dipole-dipole interaction potential to describe the inter- and intraspecies interactions, for which the condition $\Delta = 0$ is always satisfied. The physics of ultracold dipolar bosons has fast become the subject of intense research activity. Bose-Einstein condensation of dipolar chromium atoms has already been achieved [20]. The long-range and anisotropic nature of the interaction leads to many fascinating phenomena (see the review [21] and references contained therein).

So far, there have been few calculations explicitly dealing with binary mixtures of dipolar bosons [22,23]. In Ref. [22], the stability of a binary mixture with the components having oppositely oriented dipoles was investigated. In Ref. [23], spontaneous pattern formation associated with ferrofluidity was predicted and attributed to the anisotropic nature of the interaction. The role of finite range interactions in binary mixtures has also been addressed in previous studies [10,24]. In particular, it was found that increasing the range of the interactions leads to increased mixing [10].

II. FORMULATION

We consider here a system comprising N_a atoms of species a and N_b atoms of species b confined in a harmonic trapping potential. Let M_a, M_b be the masses of each species, and V_{aa}, V_{bb}, and V_{ab} be the inter- and intraspecies interaction potentials. We consider here a two-dimensional confined geometry, with a transverse polarization field in the z direction, for which the dipole-dipole interaction potential becomes isotropic and

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purely repulsive,[1] i.e., $V_{mm'}(r) = d_m d'_m / r^3$, between particles of species m and m', at a distance r from each other and with respective (electric or magnetic) dipole moments d_m and d'_m. Introducing a reference dipole moment $d_\circ$, we choose characteristic length and energy scales as $r_\circ = d_\circ^2 M_a/\hbar^2$ and $\epsilon_\circ = \hbar^2/(M_a r_\circ^2)$, respectively. The Hamiltonian for the two-component system is given, in dimensionless form, by

$$\hat{H} = \sum_{i=1}^{N_a}\left(-\frac{1}{2}\nabla_{ai}^2 + \Gamma \mathbf{r}_{ai}^2\right) + \sum_{i<j}\frac{\alpha^2}{|\mathbf{r}_{ai}-\mathbf{r}_{aj}|^3} + \sum_{i=1}^{N_2}\left[-\frac{1}{2}\left(\frac{M_a}{M_b}\right)\tilde{\nabla}_{bi}^2 + \Gamma\left(\frac{M_b}{M_a}\right)\mathbf{r}_{bi}^2\right] + \sum_{i<j}\frac{\beta^2}{|\mathbf{r}_{bi}-\mathbf{r}_{bj}|^3} + \sum_{i=1}^{N_a}\sum_{j=1}^{N_b}\frac{\alpha\beta}{|\mathbf{r}_{ai}-\mathbf{r}_{bj}|^3}, \quad (1)$$

where $\mathbf{r}_{mk}$ is the position of the kth particle of species m and $\Gamma = 1/2(L_\rho/r_\circ)^{-4}$ gives the trap strength, $L_\rho = \sqrt{\hbar/M_a\omega}$ being the harmonic oscillator length. For brevity, we write the relative dipole amplitudes as $\alpha = d_a/d_0$ and $\beta = d_b/d_0$.

If by analogy with the case of hardcore boson mixtures, we define a mixing parameter $\Delta \sim V_{aa}V_{aa} - V_{ab}^2$, then $\Delta = 0$ always.

III. NUMERICAL RESULTS

Henceforth, we choose $M_a = M_b$ and $N_a = N_b = N/2$. We have investigated the finite temperature equilibrium properties of the system by QMC simulations based on the Continuous-space Worm algorithm [25,26]. This technique is numerically exact, to within a controllable statistical error. We have carried out simulations with two values of N, namely 40 and 100, and with different values of the harmonic trap strength Γ, always chosen sufficiently small to keep the density in the middle of the trap below the crystallization threshold [27]. Our results are qualitatively the same for all cases considered. Other details of this calculation (e.g., the short-time approximation for the propagator [28]) are identical with other published works.

A. Identical and distinguishable species

We initially set the dipole moments of each species equal ($\alpha = \beta = 1$) so that the Hamiltonian (1) is symmetric to an interchange of labels a and b. Typical QMC configuration snapshots are shown in Fig. 1 for $N = 40$ with $\Gamma = 8$ (top) and $N = 100$ with $\Gamma = 0.5$ (bottom). In each case, the left plot shows the case where exchanges between indistinguishable (like) particles are included, whereas the right plot shows the same system but without exchanges (i.e., distinguishable particle statistics). For indistinguishable particle statistics like particles tend to aggregate, which is suggestive of demixing, whereas for distinguishable particle statistics the system remains mixed. Individual snapshots are not conclusive however,

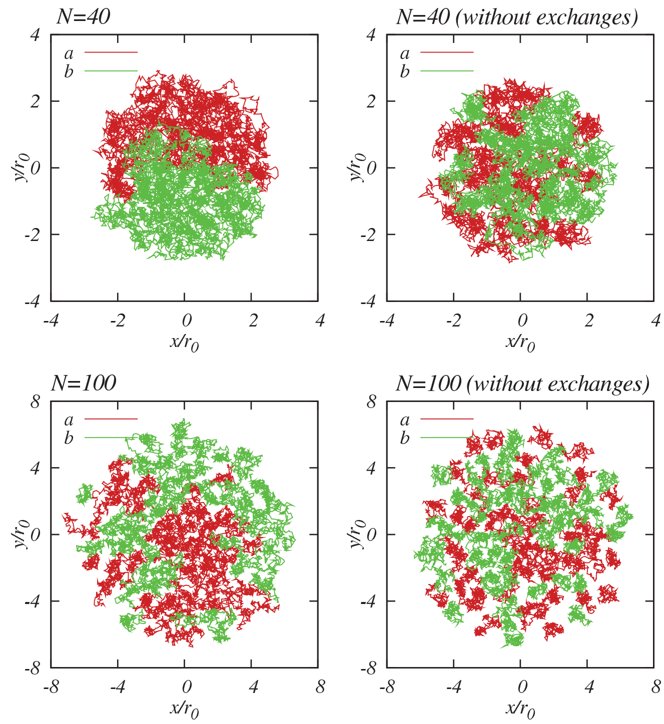

FIG. 1. (Color online) QMC configuration snapshots at temperature $T = 0.5$ for species a [red (dark gray) lines] and b [green (light gray) lines] in harmonic trap with $\alpha = \beta = 1$. Snapshots show particle world lines. In the upper plots $N = 40$ and $\Gamma = 8$ whereas in the lower plots $N = 100$ and $\Gamma = 0.5$.

so this prediction is verified first in Fig. 2 for the case $N = 40$ and $\Gamma = 8$ and then in Fig. 3 for a larger system size with $N = 100$ and $\Gamma = 0.5$. Both figures show the *integrated* [2] pair correlation function $g_{ab}(r)$, which for the lowest temperature shown, $T = 0.5$, becomes suppressed at short distances with respect to $g_{aa}(r)$. That is, the probability of finding *unlike* particles separated by r is less than that of finding *like* particles at the same distance. Differently phrased, a particle of a given species is preferentially surrounded by like particles. For both system sizes, at the highest temperature shown, there is no evidence of demixing, and the probability density of position for particles of either species only depends on the distance from the center of the trap. In this regime, entropy dominates.

As the temperature is lowered, the two components separate. To verify that exchanges are responsible for the observed demixing Figs. 2 (bottom) and 3 (bottom) also show the result for $T = 0.5$, but with exchanges turned off in the simulation (i.e., we regard particles as distinguishable). The resulting plots shows the system is fully mixed. The energetic mechanism leading to phase segregation, is that particles can lower their kinetic energy by exchanging with like particles, thereby enhancing their spatial delocalization. We also expect

[1] This is in fact a valid approximation for so-called *pancake* traps—highly anisotropic harmonic traps with transverse and planar trapping frequencies satisfying $\omega_z \gg \omega_\rho$.

[2] Clearly, since the system is not translationally invariant one ought more properly look at the two-point correlation function $g_{mm'}(\mathbf{r},\mathbf{r}')$, with $\mathbf{r},\mathbf{r}'$ measured with respect to the center of the trap. The function considered here is averaged over the whole trap; however, it still provides the quantitative information sought here.

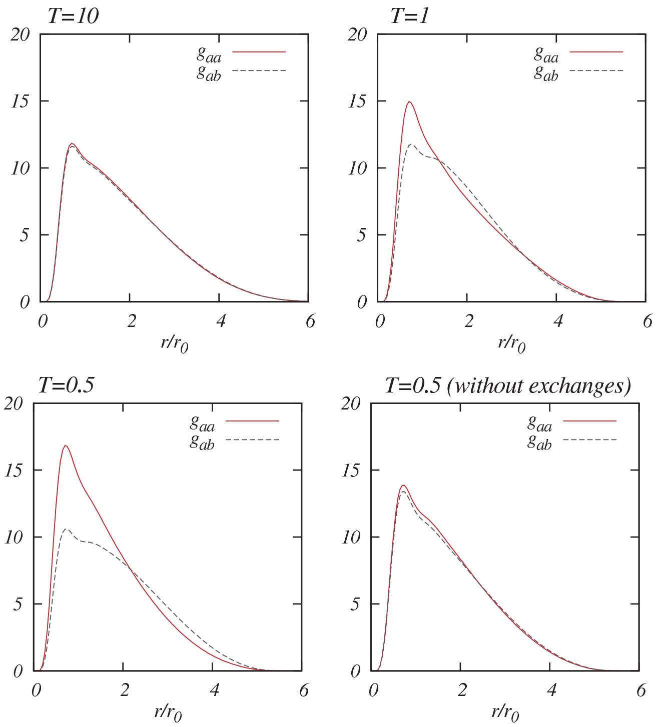

FIG. 2. (Color online) Integrated pair correlation function at temperatures $T = 10, 1, 0.5$ between like [g_{aa} (red solid curve)] and unlike [g_{ab} (black dashed curve)] particles for system in harmonic trap with $\Gamma = 8, \alpha^2 = \beta^2 = 1$, and $N = 40$. Errors are $\lesssim 7 \times 10^{-2}$ in all cases.

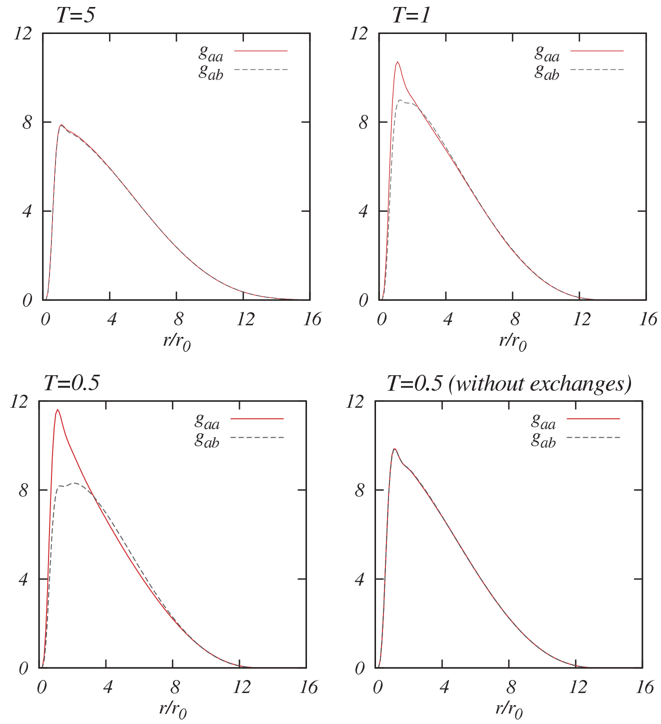

FIG. 3. (Color online) Integrated pair correlation function at temperatures $T = 5,1,0.5$ between like [g_{aa} (red solid curve)] and unlike [g_{ab} (black dashed curve)] particles for system in harmonic trap with $\Gamma = 0.5, \alpha^2 = \beta^2 = 1$, and $N = 100$. Errors are $\lesssim 2 \times 10^{-2}$ in all cases.

demixing to occur for larger N (relevant to experiments) as the relative interfacial energy decreases.

It should be emphasized that the demixing predicted here is a finite temperature effect. Finally, on lowering the temperature even further, the system remixes. This effect, also observed in hardcore boson mixtures [29], occurs when the temperature T is less than the level spacing $\hbar\omega = \sqrt{2\Gamma}$ of the confining harmonic potential. We have verified in our simulations that the remixing temperature decreases for smaller Γ.

We further elaborate on the connection between the appearance of long permutation cycles and demixing referring to Fig. 4, which shows the relative frequency of permutation cycles including different numbers L of particles, for a single species. Note that, as $T \to 0$, the frequency of occurrence of cycles of permutation (i.e., exchanges) involving almost all particles of each species (i.e., $L = 50$, in this case) increases dramatically. These exchanges are central to Bose-Einstein condensation, which in turn is responsible for the effective attraction between like atoms and therefore the observed phase separation. Such quantum demixing is not particular to our choice of interaction. Indeed, we have verified that it also occurs for potentials of the form $V(r) \sim 1/r^{12}$ (and with $\Delta = 0$), which emulate the usual hard-core repulsion appropriate for ultracold alkali atoms. In the more general case where $\Delta > 0$ the repulsive interaction energy would be offset by the decrease of kinetic energy due to exchanges, although this effect may not be large enough to lead to phase demixing.

It is instructive to note that only a technique which *explicitly* treats exchanges of indistinguishable particles at finite temperature, can yield predictions of demixing such as those shown here, for components of identical masses and interactions.

B. Nonidentical and distinguishable species

Next, we consider the situation where the dipole moments of each species are not equal (i.e., $\alpha \neq \beta$). In this case, the symmetry of the Hamiltonian with respect of exchange of

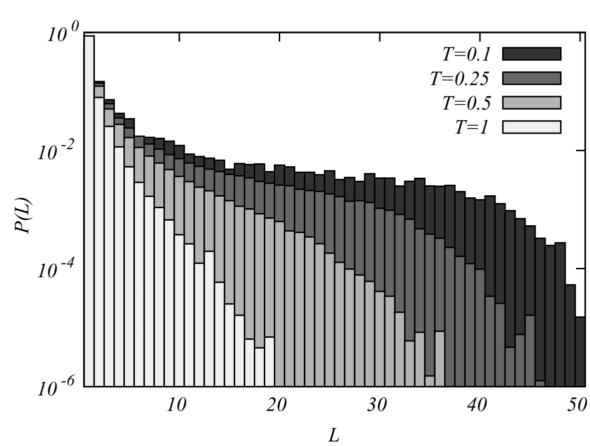

FIG. 4. Relative frequency of permutation cycles of length L for species a with $N = 100$, at four different temperatures for the case where $\alpha^2 = \beta^2 = 1$.

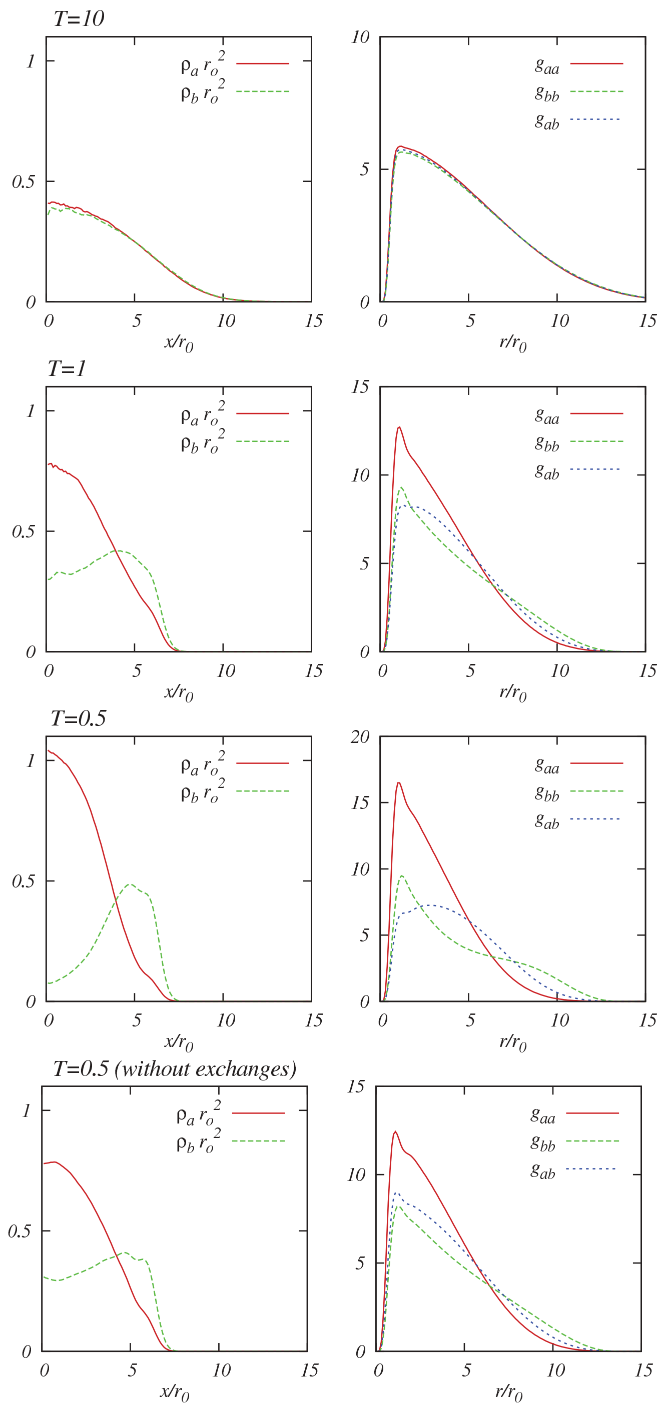

FIG. 5. (Color online) Left: Density profiles [ρ_a (red solid curve) and ρ_b (green dashed curve)] at temperatures $T = 10, 1, 0.5$, for species a and b in harmonic trap with $\Gamma = 0.5$, $\alpha^2 = 1$, $\beta^2 = 1.21$, and $N = 100$. Right: corresponding pair correlation functions [g_{aa} (red solid curve), g_{bb} (green dashed curve), and g_{ab} (blue dotted curve)]. Also repeated for comparison is the case $T = 0.5$ without exchanges (i.e., distinguishable quantum particles). Statistical errors are $\lesssim 2 \times 10^{-2}$ for all densities and $\lesssim 5 \times 10^{-2}$ for all pair correlation functions shown.

species a and b is explicitly broken, and we can expect phase separation to be evident in the radial density profiles $\rho_m(r)$, $m = a,b$, computed with respect to the center of the trap.

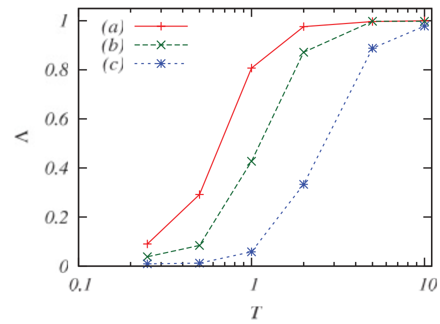

FIG. 6. (Color online) Radial mixing Λ as a function of temperature T for (a) $\alpha^2 = 1, \beta^2 = 1.21$ (red solid curve); (b) $\alpha^2 = 0.8, \beta^2 = 1.25$ (green dashed curve); and (c) $\alpha^2 = 0.5, \beta^2 = 2$ (blue dotted curve).

We consider for definiteness $\alpha < \beta$. In this case, species b forms a shell around species a due to the higher interaction energy of species b in the presence of the harmonic trap. That is, the larger interparticle repulsion of species b particles pushes that component to the outside of the trap. This can be seen in Fig. 5 for the case where $\alpha^2 = 1, \beta^2 = 1.21$. Specifically, as the temperature is lowered the partial overlap in density profiles between species a and b decreases, indicating the onset of demixing. It is worth noting that for binary mixtures of nondentical species the presence of demixing is due to the combined effects of interactions and quantum exchanges. To verify that exchanges do indeed enhance demixing, we show in Fig. 5 density profiles and pair correlation functions at $T = 0.5$, for the simulations both with and without exchanges.

The functions $\rho_m(r)$ can be used to quantify the degree of phase separation through the normalized overlap integral:

$$\Lambda = \frac{\left[\int \rho_a(r)\rho_b(r)\mathrm{d}r\right]^2}{\left[\int \rho_a(r)^2\mathrm{d}r\right]\left[\int \rho_b(r)^2\mathrm{d}r\right]}. \tag{2}$$

When there is complete overlap ($\rho_a \propto \rho_b$) then $\Lambda = 1$ indicating total mixing, whereas for complete phase separation we have $\Lambda = 0$. Note that Λ is not a good indicator of demixing when $\alpha = \beta$ since in this case the symmetry of the Hamiltonian means that the density profiles are identical when sufficient statistics are accumulated in the simulations. Figure 6 shows the radial mixing Λ as a function of temperature for three different combinations of dipole strengths (α and β). As the temperature decreases and/or the ratio between α and β decreases phase separation becomes more pronounced.

IV. CONCLUSIONS

In conclusion, low-temperature demixing purely due to Bose statistics is predicted to occur in a binary mixture of dipolar atoms, even when masses and the dipole moments of each species are equal, i.e., inter- and intraspecies interactions are identical. In the case where the dipole moments are unequal, interactions also contribute to demixing. As the temperature is raised, on the other hand, the system becomes miscible due to the entropy of mixing. The observation of the effect predicted here appears well within reach of current experimental efforts with cold dipolar systems. For our simulations the total peak density was $\rho\, r_o^2 \sim 1$, which for

^{52}Cr atoms gives $\rho \sim 10^{17}$ m^{-2}. This, while higher than those typical of magnetic traps, should be approachable using optical traps [27]. Moreover, optical traps allow for the simultaneous trapping of different hyperfine states [30], which in principle allows for two distinct but equal mass species. The integrated pair correlation function should be measurable by averaging over several "single shot" absorption images [31].

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