Quantum criticality in a trapped binary Bose gas

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We demonstrate that measurements of number fluctuations within finite cells provide a direct means to study critical scaling in a trapped two-component, or binary Bose gas. This system supports a second-order quantum phase transition between miscible (co-spatial) and immiscible states that is driven by a diverging susceptibility to magnetic fluctuations. As the transition is approached from the miscible side, the magnetic susceptibility is found to scale critically, but with an exponent that depends strongly on the geometry and orientation of the observation cell. We show that the critical behavior expected in the homogeneous gas, with scaling exponent $\gamma = 1$, can be recovered by using an observation cell that covers half of the trapped system. Interestingly, as the transition is approached from the immiscible (symmetry-broken) side, the magnetic susceptibility exhibits a critical scaling, but with a non-trivial exponent $\gamma \approx 1.30$.

Ultracold quantum gases play an important role in our understanding of phase transitions; they provide us with a number of experimental controls and observational tools that are not available in conventional condensed matter systems. For example, modern experiments with laser-cooled atoms have demonstrated thermal phase transitions such as Bose-Einstein condensation [1-6] and the Berezinskii-Kosterlitz-Thouless transition in two-dimensional (2D) superfluids [7,10], and quantum phase transitions such as the Mott insulator/superfluid transition [11-13] and Dicke super-radiant self-organization [15,17]. Recently, a great deal of interest has been generated by quantum gases of bosons with spin or pseudo-spin degrees of freedom, including spinor [18,19] and spin-orbit coupled BECs [20-22], which are ideal for studying a variety of magnetic and topological phase transitions in quantum-degenerate matter.

Perhaps the most simple, yet robust quantum Bose gas with a pseudo-spin (1/2) degree of freedom is the two-component, or binary Bose-Einstein condensate (BEC). At ultracold temperatures, this system supports a second-order quantum phase transition between miscible and immiscible states as the interaction strength between the components ($g_{12}$) is tuned across a critical threshold $g_c$, reminiscent of a para-to-ferromagnetic Ising transition. To date, a great deal of experimental [23,24] and theoretical [25,26] work has been dedicated to understanding these states and the dynamics of the transition between them. A number of groups have performed theoretical studies of quenches across the miscible-immiscible transition [27,41], demonstrating, for example, a Kibble-Zurek scaling of domain formation [42] and long-time coarsening behavior of the “ferromagnetic” domains [43]. These studies were motivated in part by the fact that ultracold atomic systems equilibrate on relatively long time scales, allowing for resolved measurements of their dynamics. Modern methods for in-situ imaging, however, allow for the direct measurement of number fluctuations, and thus for statistical studies of equilibrium states that were previously unobtainable [10,44-49].

In this Letter, we study the equilibrium properties of a binary Bose gas near the miscible-immiscible transition threshold at very low but finite temperature, and show how measurements of number fluctuations can reveal universal critical physics in this system. Focusing on the experimentally realistic case of an oblate harmonic trapping potential, we numerically calculate the quantum and low-lying thermal contributions to the magnetic (pseudo-spin) fluctuations within a finite observation cell. We extract critical scaling exponents for the gap energy $\Delta$ and the magnetic susceptibility $\chi$ as [50]

$$\Delta \sim |\delta|^{\nu z} , \quad \chi \sim |\delta|^{-\gamma} \quad (1)$$

where $\delta \equiv 1 - g_{12}/g_c$, and show how the latter exhibits a strong dependence on the cell orientation and geometry. Perhaps counterintuitively, the scaling of the homogeneous binary BEC ($\gamma = 1$) can be recovered in the harmonically trapped system by choosing a large cell that encapsulates half the atoms. We also study the miscible-immiscible transition as it is approached from the immiscible side, and find a non-trivial scaling exponent $\gamma \approx 1.30$. Finally, we compare our results with a local density approximation (LDA), and find qualitative agreement only for very specific orientations of the observation cell.

Formalism— We consider an ultracold Bose gas with two distinguishable components that have equal mass $m$ and are trapped by the same harmonic potential $V(r) = m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2$, where $\omega_i$ are the trapping frequencies along each direction. Additionally, we consider the case where the confinement along the $z$-direction is tight ($\omega_z \gg \omega_x,\omega_y$) so the axial degree of freedom is effectively frozen out. This oblate geometry is ideal for ex-
perimental measurements of number fluctuations, which can be made via in situ column density imaging [10]. Analytically integrating over the $z$-coordinate then allows us to work in the quasi-two-dimensional (quasi-2D) regime with the spatial coordinates $\mathbf{r} = \{x, y\}$. The two-body scattering is still three dimensional (3D), however, provided that $a_{ij} \ll a_z$, where $a_{ij}$ is the 3D $s$-wave scattering length between components $i$ and $j$, and $a_z = \sqrt{\hbar/m a_z}$ [21]. In the weakly interacting limit, the condensate order parameters $\psi_k(\mathbf{r}) = \langle \hat{\Psi}_k(\mathbf{r}) \rangle$, where $k = 1, 2$, are solutions of the coupled Gross-Pitaevskii equations (GPEs) [25 26 53],

$$\left[ -\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) + \sum_i g_{ij} n_i^0(\mathbf{r}) \right] \psi_k(\mathbf{r}) = \mu_k \psi_k(\mathbf{r}),$$

where $n_i^0(\mathbf{r}) = |\psi_i(\mathbf{r})|^2$ is the areal density of component $i$ and $g_{ij} = N \sqrt{8\pi \hbar^2 a_{ij}} / m a_z$. We obtain the condensate excitations by linearizing the coupled Eqs. (2) about the stationary solutions $\psi_k(\mathbf{r})$ and solving the resulting Bogoliubov de Gennes (BdG) equations [29 52 54 55].

In the thermodynamic limit, the fluctuation-dissipation theorem relates the magnetic susceptibility $\chi = 2\partial(N_1 - N_2)/\partial(\mu_1 - \mu_2)\Gamma$ to the magnetic number fluctuations $\delta M^2$ as [56 57]

$$k_B T \chi = \frac{\delta M^2}{N_\sigma} = \frac{(\langle \hat{M}_\sigma \rangle - \langle \hat{M}_\sigma \rangle^2)}{N_\sigma}, \tag{3}$$

where $\hat{M}_\sigma = \int_\sigma d\mathbf{r} [\hat{n}_1(\mathbf{r}) - \hat{n}_2(\mathbf{r})]$ is the net magnetization operator and $N_\sigma = \langle \hat{N}_\sigma \rangle = \int_\sigma d\mathbf{r} [\hat{n}_1(\mathbf{r}) + \hat{n}_2(\mathbf{r})]$ is the total particle number in the cell $\sigma$, $\mu_k$ is the chemical potential, and $\hat{n}_k(\mathbf{r}) = \hat{\Psi}_k^\dagger(\mathbf{r}) \hat{\Psi}_k(\mathbf{r})$ is the density operator for component $k$. At the level of Bogoliubov theory, which is expected to give good quantitative results in the ultracold, dilute regime we consider here, we evaluate $\delta M^2$ at quadratic order in the field fluctuations $\hat{\Psi}_k(\mathbf{r}) - \langle \hat{\Psi}_k(\mathbf{r}) \rangle$, and neglect higher order contributions, which are vanishingly small away from the miscible-immiscible phase transition threshold. For detailed discussions of density fluctuations in condensed systems, see Refs. [46 48].

In practice, we solve the coupled GPEs (Eq. 2) and the BdG equations with a basis of ideal harmonic oscillator modes beneath the single-particle energy cutoff $E_{\text{cut}} = 100\hbar \omega_x$. We use 8800 modes when evaluating Eq. (3) in the normally ordered form, which produces a converged result [60].

**Results**—Without loss of generality, we consider a system with interaction strengths $g_{12} = g_{22} \equiv g = 500\hbar^2/m$ in a slightly asymmetric trap with $\omega_y/\omega_x = 1.1$ to avoid the ambiguity of choosing a boundary axis. For this system, the critical interspecies interaction strength, which defines the threshold of the miscible-immiscible transition, is $g_c = 1.0072(8)g$ [61], where the deviation from unity is due to finite size effects.

![FIG. 1](image-url) (c) Component separation in the $x$-direction, where $\langle x_k \rangle = \int d\mathbf{r} n_k^1(\mathbf{r})$. Short red (gray) vertical lines mark the five smallest $g_{12}/g_c$ plotted in Fig. 3. (d) Bogoliubov energy spectrum. The red (gray) solid curves are scaling fits with $\nu z = 0.505$ for the miscible and $\nu z = 0.60(3)$ for the immiscible region (see text). The vertical dashed lines show the interaction parameters for (a) and (b).

The most fundamental properties of this system undergo qualitative changes across this transition. Figs. 1(a) and (b) show examples of the condensate densities for miscible and immiscible solutions, respectively. The component separation, shown in Fig. 1(c), is zero until $g_{12} = g_c$, above which it grows abruptly before plateauing for larger $g_{12}$. The low-lying excitation energies, which are eigenvalues of the BdG equations, are plotted in Fig. 1(d) as a function of the interspecies interaction strength. On the miscible side ($g_{12} < g_c$), the two lowest-lying modes are out-of-phase “slosh” modes, which soften at the transition threshold. We perform a scaling fit $\sim |\delta|^{\nu z}$ (see Eq. 1) to the lowest mode in the region near the transition, over $g_{12}/g_c = 0.6-1$, and find that $\nu z \simeq 0.505$, consistent with square root behavior. On the immiscible side ($g_{12} > g_c$), we ignore the modes corresponding to interface bending, as they do not contribute to the transition instability [58], and instead focus on the out-of-phase “mixing” modes [59 60]. For these modes, there is a clear deviation from a square root behavior over the fitting range $g_{12}/g_c = 1-1.3$, where we find $\nu z = 0.60(3)$. The uncertainty arises because of fitting ambiguity, possibly due to avoided crossings, and is
We study number fluctuations in the low temperature regime with $T = 7.8\hbar \omega_c/k_B = T_c^0/10$, where $T_c^0 = \sqrt{6\hbar \omega_c/\pi k_B}$ is the ideal 2D condensation temperature [60], with $N = 10^4$ atoms per component. In Fig. 2 we plot number fluctuations as a function of $g_{12}/g_c$ for three square cells of various width $L$. The cells are positioned symmetrically about the $y$-axis with their edges placed at $x = 0$ (see insets). This cell location makes them highly sensitive to fluctuations that separate (mix) the components in the miscible (immiscible) phase. Deep in the miscible regime ($g_{12}/g_c \ll 1$), the magnetic ($\delta M^2$) and normal ($\delta N^2$) number fluctuations are small and equal. The magnetic fluctuations diverge as the transition is approached from the miscible side, $g_{12}/g_c \rightarrow 1$, whereas the normal fluctuations steadily decrease.

For the uniform binary Bose gas in the thermodynamic limit, the magnetic fluctuations scale as (c.f. the susceptibility for the coherently coupled system [61])

$$\frac{\delta M^2}{N_1} = \frac{k_B T}{n_1 g_c \delta^2}, \tag{4}$$

where $n_1$ is the areal density of component 1, which is equal to that of component 2 in the balanced case we consider here. Together, Eqs. (4) and (1) imply that this system has a critical exponent $\gamma = 1$. Motivated by this result, we explore the scaling of magnetic fluctuations in the trapped system by fitting our numerical results to Eq. (4). We first perform fits over the broad range $g_{12}/g_c = 0.1-1$, which are shown by the dashed teal lines in Fig. 2. For cell A (the smallest cell) we find $\gamma = 0.84$, for cell B we find $\gamma = 0.94$, and for cell C (the largest cell, which encompasses half the system) the exponent is nearly unity with $\gamma = 0.98$. As the cell size is increased, the fit parameter $\gamma$ approaches unity and the fit quality improves, i.e. the divergence of $\delta M^2$ becomes more algebraic.

We also perform fits over the ranges $g_{12}/g_c = 0.1-0.9$ and $g_{12}/g_c = 0.9-1$, the results of which are shown in Table I. Interestingly, fitting over the range $g_{12}/g_c = 0.1-0.9$ (excluding the transition region) results in fitting parameters $\gamma$ that are close to unity for all cell sizes. In contrast, fitting only near the transition region ($g_{12}/g_c = 0.9-1$) results in $\gamma$ parameters that are further from unity, particularly for the smallest cell (cell A). The deviation from $\gamma = 1$ in smaller cells is a finite size effect, reflecting the fact that the critical magnetic fluctuations are long-wavelength in nature; when their characteristic length (the spin healing length $\xi$) exceeds the cell size, deviations from the thermodynamic limit scaling (Eq. (4)) are expected. For cell C, this cannot occur, as $\xi$ is limited by the size of the system itself. Thus, cell C represents the closest analog to the thermodynamic limit that is achievable in the trapped system, which is represented by our findings. Additionally, in contrast to the uniform system, the local condensate densities in the trapped system decrease with increasing $g_{12}$. Thus, it is not surprising that the fit parameters exhibit a dependence on the fit range.

We employ a local density approximation (LDA) by applying the uniform result (Eq. (4)) to our numerical solutions; we replace $n_1$ with the cell-weighted average.
for the trapped system, \( \gamma \) magnetic fluctuations is less evident. To its small size), and the free-particle character of the calculation, as seen in Fig. 2, where the LDA results are how well the LDA results agree with the full numerical calculation, as seen in Fig. 2, where the LDA results are shown by the short red (gray) curves. Inset shows cell size and location relative to the condensate for \( g_{12}/g_c = 0.897 \).

\[
\bar{n}_{1\sigma} = \int d\rho \frac{n_{1\sigma}^0(\rho)}{N_{\sigma1}} - n_{1\sigma}^0(\rho),
\]

where \( N_{\sigma1} = \int n_{1\sigma}^0(\rho) d\rho \), and we use the critical point for the trapped system, \( g_c = 1.0072(8)g \). It is remarkable how well the LDA results agree with the full numerical calculation, as seen in Fig. 2 where the LDA results are shown by the red solid lines. Away from the transition, the LDA is more accurate when applied to cell A. In this case, the density is more uniform across the cell (due to its small size), and the free-particle character of the magnetic fluctuations is less evident.

As the transition is approached from the immiscible side, the behavior is more complicated. Again, we fit our numerical results to Eq. (1) over various ranges of \( g_{12}/g_c \), and show the fitting parameters \( \gamma \) in Table I. In this case, \( \gamma \) increases significantly with increasing cell size for all fitting ranges. Furthermore, for cells A and B, \( \gamma \) is significantly larger for fits near the transition \( (g_{12}/g_c = 1.05) \) compared to the region further from the transition \( (g_{12}/g_c = 1.05-1.2) \). In contrast, the fits for cell C are more consistent over the various fitting ranges, giving \( \gamma = 1.29 \) near the transition, \( \gamma = 1.24 \) away from the transition, and \( \gamma = 1.30 \) over the broad range \( g_{12}/g_c = 1-1.2 \). As shown in Fig. 1(c), the spatial overlap between the components increases as \( g_c \) is approached from the immiscible side; this is also the case in the uniform system. Thus, deviations from purely algebraic scaling behavior are not surprising.

In Fig. 2, we show how magnetic fluctuations depend on cell position in the miscible regime, with \( L = 5a_x \) (same as cell B). We calculate fluctuations for cells centered at different points along the \( y = 0 \) axis (see inset in Fig. 3). For the case of essentially uncoupled condensates, \( g_{12}/g_c = 0.01 \), the behavior is similar to that of number fluctuations in a single component gas, which are superpoissonian at high density and superpoissonian at the low density condensate surface (see Fig. 5(a) of Ref. [17]). For cells positioned off-center, the magnetic fluctuations tend to diverge near the transition. In contrast, the fluctuations clearly converge for cells positioned at the trap center. Here, the cells become insensitive to the out-of-phase “slosh” modes, since magnetic fluctuations on opposite sides correlate and nullify. Instead, the cells are most sensitive to the out-of-phase breathing modes (third and fourth-to-lowest modes in Fig. 1(c)), which converge to a finite value at the transition. The LDA prediction is also plotted for \( g_{12}/g_c = 0.01 \) and 0.9997, shown by the solid red lines. While these results compare reasonably well with the full-numerical calculation at \( \sim 3L_z \), the LDA completely fails to capture the convergence of fluctuations at the trap center.

**Discussion**— The experimental realization of the system at hand could be achieved with two hyperfine states of the same atomic species \([22, 63]\) or with different species \([44, 65]\). Assuming \( 10^4 \) \(^{87}\)Rb atoms in each component and \( a_{11} = a_{22} = 100a_0 \), where \( a_0 \) is the Bohr radius, having \( g = 500\hbar^2/m \) implies a \( z \)-confinement strength of \( \omega_z = 2\pi \times 413 \) Hz. To observe magnetic fluctuations over two orders of magnitude, as we predict here, requires control of \( a_{12} \) in the range \( 5a_0 \) to \( 100a_0 \). In the quasi-2D geometry, the interaction strengths can be scaled by varying \( \omega_z \). Finally, we note that we calculated the magnetic fluctuations at various temperatures, and found that the low temperature used here, \( T = T_0/10 \), produces considerably enhanced fluctuations. This should be contrasted to the \( T = 0 \) case, where fluctuations do not diverge near the transition (see Eq. 3). We also investigated the case of slightly unequal populations and found the same critical scaling; the case of significantly unbalanced populations is a question for future work.

**Summary**— We proposed an experimentally accessible scheme to extract the critical exponent \( \gamma \), associated with a diverging magnetic susceptibility, for the second-order miscible-immiscible transition in a trapped binary Bose gas at very low but finite temperature. Importantly, this involves \textit{in situ} density measurements, which do not require high-resolution imaging. On the miscible side of the transition, we found qualitative differences between the fully trapped and the uniform system in the thermodynamic limit, but ultimately the same scaling, \( \gamma = 1 \), is predicted over two decades of fluctuation size for both systems. Additionally, we find the gap exponent to be \( \nu z = 0.505 \). Fluctuations of the trapped system strongly depend on cell geometry and orientation. A large cell that spans half the system, e.g. the region corresponding...
to $x > 0$, is the closest analogue to the thermodynamic limit. Interestingly, fluctuations do not diverge for cell placements at the trap center, due to symmetry. On the immiscible side, we found non-trivial critical scaling, $\gamma \simeq 1.30$, and an associated non-square root gap exponent, $\nu_z \simeq 0.60(3)$. We also developed and tested an LDA theory that does not require the numerically intensive calculation of Bogoliubov modes, and find that it provides reasonable agreement with the numerics in certain regimes.

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[66] We correct for the error introduced by such an approach, i.e. that \( \langle \psi_k^*(\mathbf{r})\psi_k^*(\mathbf{r})\psi_k(\mathbf{r})\psi_k(\mathbf{r}) \rangle = (n_0^k)^4 \) instead of \( n_0^k(n_0^k - 1) \). In practice this amounts to correcting the poissonian fluctuation contributions i.e. \( N_{sk}^{0} \rightarrow N_{sk}^{0} - (N_{sk}^{0})^2/N_{k}^{0} \) where \( N_{sk}^{0} = \int n_{sk}^{0}(\mathbf{r})d^3r \) and \( N_{k}^{0} = \int n_{k}^{0}(\mathbf{r})d^3r \).
[67] The uncertainty of the critical point occurs due to a small region or coexistence exhibiting both a stable miscible and an immiscible solution.