Ising Deconfinement Transition between Feshbach-Resonant Superfluids

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We investigate the phase diagram of bosons interacting via Feshbach-resonant pairing interactions in a one-dimensional lattice. Using large scale density matrix renormalization group and field theory techniques we explore the atomic and molecular correlations in this low-dimensional setting. We provide compelling evidence for an Ising deconfinement transition occurring between distinct superfluids and extract the Ising order parameter and correlation length of this unusual superfluid transition. This is supported by results for the entanglement entropy which reveal both the location of the transition and critical Ising degrees of freedom on the phase boundary.

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The ability to cool atoms to low temperatures, and control their interactions, has revolutionized the study of quantum many body systems. Important achievements include realizations of Bose-Einstein condensation (BEC), Bardeen-Cooper-Schrieffer (BCS) pairing in Fermi gases, and strongly correlated Mott insulators (MIs). In this development, the BEC-BCS crossover between a gas of tightly bound molecules and weakly bound Cooper pairs has played an instrumental role, and it has been widely explored using Feshbach resonances to induce pairing. This has led to diverse studies of the condensate fraction, single-particle gap, collective excitations, and vortices, and to pioneering approaches to molecular quantum chemistry. For a review see Ref. [1].

In recent work [2–6] it has been argued that the BEC-BCS "crossover" for bosons is strikingly different from the fermionic case since the atoms as well as molecules may undergo Bose-Einstein condensation. These studies have raised the exciting possibility of an Ising quantum phase transition between distinct molecular (MC) and atomic plus molecular (AC + MC) condensates. In addition to discrete $\mathbb{Z}_2$ symmetry breaking, this transition has a topological character and may be viewed as a confinement-deconfinement transition for vortices.

The principal aim of this Letter is to establish the presence of such novel $\mathbb{Z}_2$ transitions in 1D bosonic Feshbach systems, where strong quantum fluctuations destabilize long-range superfluid order. We combine large scale density matrix renormalization group (DMRG) [7] and field theory techniques to provide compelling evidence for Ising behavior. We elucidate a full characterization of the scaling regime and the proximate phases. Our results demonstrate that an Ising transition survives at strong coupling and large densities where field theory arguments are no longer justified. For related transitions in the attractive Bose-Hubbard model with three-body losses, see Refs. [8,9], and for analogues involving multicomponent fermions, see [10,11].

We consider the Hamiltonian [4,6,12]

$$H = \sum_{i\alpha} \epsilon_\alpha n_{i\alpha} - \sum_{\langle ij\rangle} \sum_{\alpha} t_\alpha (b^\dagger_{i\alpha} b_{j\alpha} + \text{H.c.}) + \sum_{i\alpha\alpha'} \frac{U_{\alpha\alpha'}}{2} :n_{i\alpha} n_{i\alpha'}: + H_F, \quad (1)$$

describing bosons $b_{i\alpha}$ hopping on a lattice with sites i, where $\alpha = a, m$ labels atoms and molecules. Here, ϵ_α are on-site potentials, t_α are hopping parameters, $\langle ij\rangle$ denotes summation over nearest neighbor bonds, and $U_{\alpha\alpha'}$ are interactions. Normal ordering yields $:n_{i\alpha}n_{i\alpha}: = n_{i\alpha}(n_{i\alpha} - 1)$ for like species and $:n_{i\alpha}n_{i\alpha'}: = n_{i\alpha}n_{i\alpha'}$ for distinct species. Molecules are formed by the Feshbach term, $H_F = g\sum_i (m_i^\dagger a_i a_i + \text{H.c.})$, where $m_i \equiv b_{im}$ and $a_i \equiv b_{ia}$. Atoms and molecules are not conserved, but the total, $N_T \equiv \sum_i (n_{ia} + 2n_{im})$, is preserved.

To orient the discussion, we present a section of the phase diagram in Fig. 1, with parameters chosen for comparison with previous studies [6]. In this Letter we use DMRG on a 1D system with up to $L = 512$ sites and adopt units where $t_a = 1$. We allow up to five atoms and five molecules per site and retain up to $m_\rho = 2400$ states in the density matrix so that the discarded weight is less than 1×10^{-10}. The phase boundaries correspond to the vanishing of the one-particle and two-particle excitation gaps, $E_{1g} \equiv \mu_{1p}(L) - \mu_{1h}(L)$ and $E_{2g} \equiv \mu_{2p}(L) - \mu_{2h}(L)$, respectively, where $\mu_{np}(L) = E_0(L, N_T + n) - E_0(L, N_T)$, $\mu_{nh}(L) = E_0(L, N_T) - E_0(L, N_T - n)$, and E_0 is the ground state energy. The diagram shows a MI with gaps for both excitations $E_{1g} \neq 0$ and $E_{2g} \neq 0$, a MC phase with a one-particle gap $E_{1g} \neq 0$ and $E_{2g} = 0$, and a coupled atomic plus molecular condensate (AC + MC) with $E_{1g} = 0$ and $E_{2g} = 0$. In contrast to the qualitative

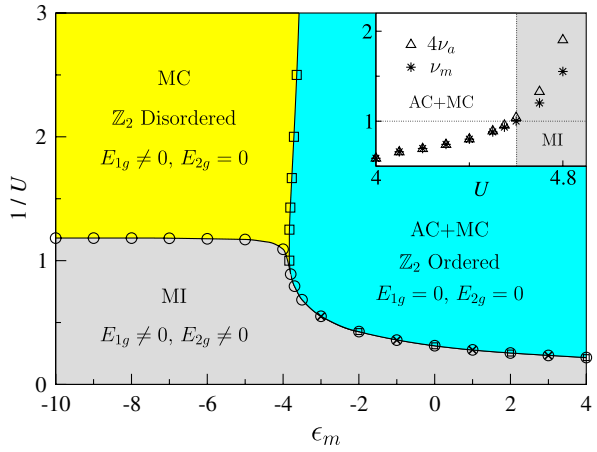

FIG. 1 (color online). Phase diagram of the 1D Hamiltonian (1) with total density $\rho_T = N_T/L = 2$, showing a Mott insulator (MI), a molecular condensate (MC), and a coupled atomic plus molecular condensate (AC + MC). We use DMRG with up to $L = 128$ and open boundaries, with $\epsilon_a = 0$, $U_{aa}/2 = U_{mm}/2 = U_{am} = g = U$, $t_a = 1$, $t_m = 1/2$. The squares and circles indicate the vanishing of the one-particle and two-particle gaps, E_{1g} and E_{2g}, as $L \to \infty$. The crosses show where the molecular correlation exponent ν_m reaches unity. Inset: AC + MC to MI transition at $\epsilon_m = 4$. The atomic and molecular exponents, ν_a and ν_m, are locked up to the MI boundary where $\nu_m = 1$, indicating the absence of an AC phase.

diagram in Ref. [6], inferred from quantum Monte Carlo simulations on smaller systems, we find no evidence for a single-component AC phase. This is in accord with expectations in higher dimensions [2]. As we will discuss, this is supported by direct evaluation of correlation functions using both DMRG and field theory. Throughout the AC + MC phase we find power laws for atoms *and* molecules with related exponents; see inset of Fig. 1. The conclusions of Ref. [6] are hampered by the slow divergence of the associated zero-momentum molecular occupation number with increasing L, close to the MI boundary. This also afflicts the molecular visibility. Here, our focus is on the transition between the MC and AC + MC superfluids. We begin with symmetry arguments and field theory predictions before comparison with DMRG.

An intuitive way to understand the origin of the proposed Ising transition between the MC and AC + MC phases is via the symmetry of the Hamiltonian (1) under $U(1) \times \mathbb{Z}_2$ transformations. This corresponds to invariance under $m \to e^{i\theta} m$ and $a \to e^{i(\theta/2 \pm \pi)} a$, where $\theta \in \mathbb{R}$. In general these symmetries may be broken independently. Before discussing the problem in 1D, where continuous $U(1)$ symmetry breaking is absent, let us first recall the situation in higher dimensions [2]. In this case, the MC phase has $\langle m \rangle \neq 0$ and $\langle a \rangle = 0$. This only breaks the $U(1)$ contribution and leaves the $\mathbb{Z}_2$ symmetry, $a \to -a$, intact; this corresponds to the disordered phase of an Ising model, coexisting with molecular superfluidity. On the other hand, the coupled atomic plus molecular condensate (AC + MC) phase has $\langle m \rangle \neq 0$ *and* $\langle a \rangle \neq 0$. This breaks the $U(1) \times \mathbb{Z}_2$ symmetry completely and corresponds to the ordered phase of an Ising model, coexisting with atomic and molecular superfluidity. Returning to the present 1D problem, where continuous $U(1)$ symmetry breaking is absent, the spontaneous formation of expectation values $\langle a \rangle$ and $\langle m \rangle$ is prohibited. Instead, superfluid order is characterized by long-range power law correlations, and the nature of the phases and transitions in Fig. 1 requires closer inspection.

Owing to the $U(1) \times \mathbb{Z}_2$ symmetry of the Hamiltonian, the low energy Lagrangian of the MC to AC + MC transition is given by $\mathcal{L} = \mathcal{L}_\vartheta + \mathcal{L}_\phi + \mathcal{L}_{\vartheta\phi}$ [2,3], where

$$\mathcal{L}_\vartheta = \frac{K_\vartheta}{2}[c_\vartheta^{-2}(\partial_\tau \vartheta)^2 + (\partial_x \vartheta)^2] \tag{2}$$

is a $U(1)$ invariant free scalar field, and

$$\mathcal{L}_\phi = \frac{K_\phi}{2}[c_\phi^{-2}(\partial_\tau \phi)^2 + (\partial_x \phi)^2] - \eta\phi^2 + \lambda\phi^4 \tag{3}$$

is an Ising model in the soft-spin ϕ^4 representation. The coupling, $\mathcal{L}_{\vartheta\phi} = i\phi^2 \partial_\tau \vartheta/2$, has a similar form to a Berry phase [2,3]. A similar action also emerges for quantum wires [13]. In the following we neglect $\mathcal{L}_{\vartheta\phi}$ and examine the reduced theory. Within mean field theory, $\mathcal{L}_{\vartheta\phi} \sim i\langle\phi\rangle^2 \partial_\tau \vartheta/2$ acts like a boundary term, and this is expected to provide a good description of the proximate phases. Near the transition, this cannot be neglected *a priori*, and $\mathcal{L}_{\vartheta\phi}$ may change the behavior on very large length scales and in other regions of the phase diagram [13]. Nonetheless, we find excellent agreement with bulk properties. The parameters K_ϑ, c_ϑ, K_ϕ, c_ϕ, η, λ are related to the coefficients of H. Atoms and molecules are described by the semiclassical number-phase relations, $m \sim \sqrt{\rho_m} e^{i\vartheta}$ and $a \sim \phi e^{i\vartheta/2}$, where ρ_m is the molecular density. We will explore the consequences of this correspondence in 1D, for local observables and correlations.

Let us first gather consequences of this correspondence for local observables. Deep within the $\mathbb{Z}_2$ disordered MC phase, $\eta \gg 0$ and $\langle\phi(x)\rangle = 0$. However, $\phi^2(x)$ may have a nonzero average. It follows that the densities of atoms and molecules, $\langle a^\dagger(x)a(x)\rangle \sim \langle\phi^2(x)\rangle$ and $\langle m^\dagger(x)m(x)\rangle \sim \rho_m$, are generically nonzero in *both* the AC + MC and MC phases. In addition, $\langle m^\dagger(x)a(x)a(x)\rangle \sim \sqrt{\rho_m}\langle\phi^2(x)\rangle$ acquires true long-range order, even in this 1D setting; H_F locks the atomic and molecular condensates as encoded in the number-phase relations. However, this local average is naively insensitive to the $\mathbb{Z}_2$ transition due to invariance under $a \to -a$. Insight is better gleaned from correlations.

It follows from the relation $m \sim \sqrt{\rho_m} e^{i\vartheta}$ that the molecular correlation function $\langle m^\dagger(x)m(0)\rangle \sim \rho_m\langle e^{-i\vartheta(x)} e^{i\vartheta(0)}\rangle \sim x^{-\nu_m}$ decays like a power law, where $\nu_m = 1/2\pi K_\vartheta$ varies throughout the phase diagram. In contrast, the behavior of the atomic correlations, $\langle a^\dagger(x)a(0)\rangle \sim \langle\phi(x)\phi(0)\rangle\langle e^{-i\vartheta(x)/2} e^{i\vartheta(0)/2}\rangle \sim \langle\phi(x)\phi(0)\rangle x^{-\nu_m/4}$, depends on the Ising prefactor. We consider the disordered and ordered phases in turn.

In the $\mathbb{Z}_2$ disordered MC phase, the atomic correlation function decays exponentially with a power law prefactor, $\langle a^\dagger(x)a(x)\rangle \sim x^{-\nu_m/4}K_0(x/\xi) \sim x^{-1/2-\nu_m/4}e^{-x/\xi}$. Here we use the result for the hard-spin Ising model, $\langle\phi(x)\phi(0)\rangle \sim K_0(x/\xi)$, where K_0 is a modified Bessel function and ξ is the Ising correlation length [14]. On the other hand, *pairs* of atoms condense and exhibit power law correlations, $\langle a^\dagger(x)a^\dagger(x)a(0)a(0)\rangle \sim \langle\phi^2\rangle^2 x^{-\nu_m}$, with the *same* exponent as the molecular two-point function ν_m. That is to say, the MC phase is a pairing phase of bosons without single-particle condensation [15]. In order to test these weak coupling predictions we perform DMRG on the 1D Hamiltonian (1). As predicted, this behavior is well supported by our simulations in Fig. 2(a), which reveal identical power laws for molecules and atomic bilinears, with exponential decay for atoms. This behavior extends throughout the MC phase, including the Mott boundary in the strongly coupled regime.

In contrast, in the $\mathbb{Z}_2$ ordered AC + MC phase, both molecules and atoms have power law correlations, $\langle m^\dagger(x)m(0)\rangle \sim x^{-\nu_m}$, $\langle a^\dagger(x)a(0)\rangle \sim \langle\phi\rangle^2 x^{-\nu_a}$, with locked exponents, $\nu_m = 4\nu_a$, that differ by a factor of 4 [2,3]. Again, these features are readily seen from our large scale DMRG simulations in Fig. 2(b) and the inset of Fig. 1. Likewise, this behavior persists into the strong coupling limit, where the field theory approach no longer strictly applies. In particular, we have checked that the molecular correlation function, $\langle m^\dagger(x)m(0)\rangle \sim x^{-\nu_m}$, remains a power law throughout the AC + MC phase and close to the Mott boundary in Fig. 1. This is consistent with the absence of an AC phase [2] in contrast to Ref. [6]. The latter employ the zero-momentum occupation $n(0)$. However, the Fourier transform of $x^{-\nu}$ gives $n(0) \sim$ const + const $L^{1-\nu}$; close to the MI where $\nu_m = 1$, one may miss the slow divergence of $n_m(0)$.

Having established a close connection between field theory and DMRG for the MC and AC + MC phases, let us now examine the transition. A key diagnostic is the central charge c, which counts critical degrees of freedom. This may be obtained from the entanglement entropy. For a block of length l in a periodic system of length L, the von Neumann entropy is given by $S_L(l) = -\mathrm{Tr}_l(\rho_l \ln\rho_l)$, where $\rho_l = \mathrm{Tr}_{L-l}(\rho)$ is the reduced density matrix. One obtains [16]

$$S_L(l) = \frac{c}{3}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi l}{L}\right)\right] + s_1, \tag{4}$$

where s_1 is a constant. As may be seen in Fig. 3, the numerically extracted central charge of the MC phase yields $c = 1$, as one would expect for a free boson, with coexisting gapped degrees of freedom. In addition, the AC + MC phase also has $c = 1$. Note that it is *not* $c = 2$ as would be the case

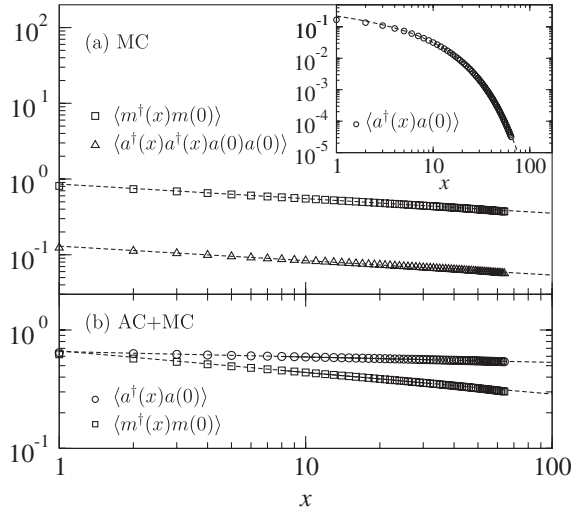

FIG. 2. Correlation functions using DMRG with $L = 128$ and open boundaries. We use the parameters in Fig. 1 with $U = 0.7$. (a) $\mathbb{Z}_2$ disordered MC phase with $\epsilon_m = -4$, revealing power laws for molecules and atomic bilinears with the same exponent; the fits are $y = 0.858x^{-0.1922}$ and $y = 0.130x^{-0.1909}$. Inset: Atomic correlations decay exponentially. We fit to the prediction $\langle a^\dagger(x)a(0)\rangle \sim x^{-\nu_m/4}K_0(x/\xi)$, where we input ν_m from (a) and extract $\xi \approx 9.28$. This establishes MC as a pairing phase without atomic condensation. (b) $\mathbb{Z}_2$ ordered AC + MC phase with $\epsilon_m = -3$. Atoms and molecules exhibit power law exponents locked by a factor of 4; the fits are $y = 0.667x^{-0.1827}$ and $y = 0.657x^{-0.0456}$.

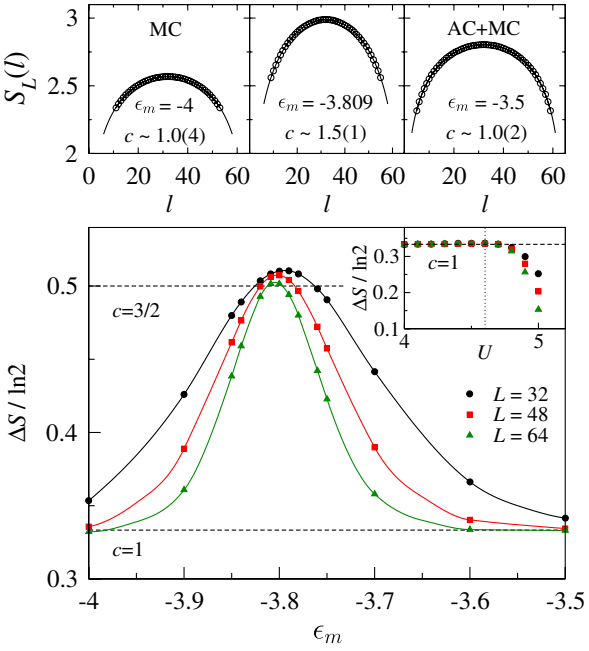

FIG. 3 (color online). Top: Entanglement entropy $S_L(l)$ obtained by DMRG in a periodic system with $L = 64$. We transit through the AC to AC + MC transition in Fig. 1 with $U = 0.7$. The fits to Eq. (4) yield $c \approx 1$ in the MC and AC + MC phases, and $c \approx 3/2$ close to the transition. This reflects additional critical $\mathbb{Z}_2$ degrees of freedom. Because of the asymptotic nature of Eq. (4), high quality fits are obtained from the central region away from the boundaries. Bottom: Entanglement entropy difference $\Delta S(L)$ showing an Ising transition at $\epsilon_m \approx -3.8$ for $U = 0.7$, in agreement with Fig. 1. The solid lines are spline fits. Inset: ΔS on passing through the AC + MC to MI transition at $\epsilon_m = 4$, suggesting an XY transition with $c = 1$.

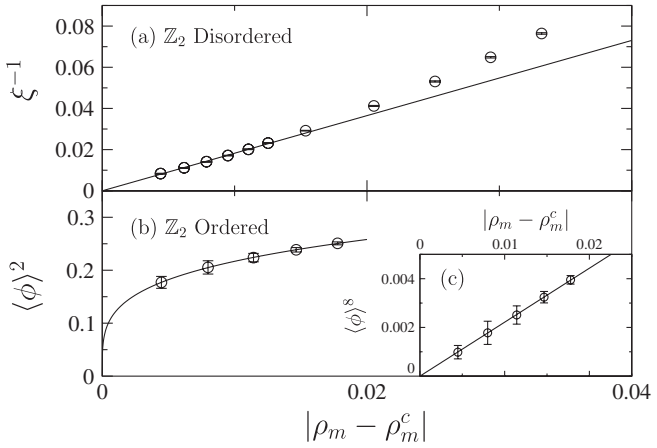

FIG. 4. DMRG with open boundaries. We use the parameters in Fig. 1 with $U = 0.7$ and transit from MC to AC + MC. $\mathbb{Z}_2$ disordered MC phase (a) ξ extracted from the atomic correlations with $L = 256$. $\xi^{-1} \sim |\rho_m - \rho_m^c|^\nu$, where ρ_m ($\rho_m^c \approx 0.85$) is the (critical) density of molecules and $\nu = 1$. $\mathbb{Z}_2$ ordered AC + MC phase (b) $\langle\phi\rangle^2$ up to a constant prefactor, obtained by finite size scaling of the atomic correlations with up to $L = 512$. (c) Replotting yields $\beta = 1/8$.

for two independent Luttinger liquids. This reflects the coupled nature of the atomic and molecular condensates in the AC + MC phase, with additional gapped Ising degrees of freedom; the Feshbach term is relevant and drives the $\mathbb{Z}_2$ sector massive. Close to the MC to AC + MC transition, where the anticipated Ising gap closes, one expects the central charge to increase to $c = 3/2$, due to *additional* critical Ising degrees of freedom with $c = 1/2$. This is confirmed by DMRG in Fig. 3. Further evidence is obtained from the difference [17], $\Delta S(L) \equiv S_L(L/2) - S_{L/2}(L/4) = \frac{c}{3} \times \ln(2) + \cdots$, as a function of ϵ_m; see Fig. 3. For a given L this displays a peak, whose location coincides with the MC to AC + MC transition obtained via the single-particle gap in Fig. 1. The evolution with increasing L is consistent with the passage towards $c = 1$ in the superfluid phases and $c = 3/2$ in the vicinity of the transition. Application of this method to the MI to superfluid transitions [4] yields $c = 1$ close to the MI boundary, suggesting XY behavior; see inset of Fig. 3. The absence of criticality within the MI phase is evidence against a super-Mott state [6] and correlations decay exponentially [12,18].

Having provided evidence for a $\mathbb{Z}_2$ superfluid transition, we now extract the Ising correlation length ξ and order parameter $\langle\phi\rangle$ via finite size scaling of the atomic and molecular correlations. Because of the absence of particle conservation, and the presence of additional superfluid degrees of freedom, these cannot be readily obtained from the energy spectra alone. Ising scaling close to the transition implies that $\xi^{-1} \sim |\mathcal{M} - \mathcal{M}_c|$ and $\langle\phi\rangle \sim |\mathcal{M} - \mathcal{M}_c|^{1/8}$, where $\mathcal{M}$ is a mass scale parametrizing the departure from criticality. We identify the molecular density, $\mathcal{M} \sim \rho_m$, as the appropriate scaling variable. As shown in Fig. 4, the DMRG results are in excellent agreement with Ising critical exponents. This is nontrivial since the Ising degrees of freedom are nonlocal with respect to the atoms and molecules themselves.

In summary, we have studied bosons interacting via Feshbach interactions in a 1D lattice. We provide evidence for an Ising quantum phase transition between distinct superfluids. We extract both the $\mathbb{Z}_2$ order parameter $\langle\phi\rangle$ and the Ising correlation length ξ. It would be interesting to see if this $\mathbb{Z}_2$ transition may be driven first order and the effect of higher bands [19]. One may also consider $\mathbb{Z}_N$ transitions involving N-particle pairing.

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