

Quantum criticality of spin-1 bosons in a one-dimensional harmonic trap

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We investigate universal thermodynamics and quantum criticality of spin-1 bosons with strongly repulsive density-density and antiferromagnetic spin-exchange interactions in a one-dimensional harmonic trap. From the equation of state, we find that a partially polarized core is surrounded by two wings composed of either spin-singlet pairs or a fully spin-aligned Tonks-Girardeau gas depending on the polarization. We describe how the scaling behavior of density profiles can reveal the universal nature of quantum criticality and map out the quantum phase diagram. We further show that at quantum criticality the dynamical critical exponent $z = 2$ and correlation length exponent $\nu = 1/2$. This reveals a subtle resemblance to the physics of the spin-1/2 attractive Fermi gas.

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Alkali bosons with hyperfine spins in an optical trap provide exciting opportunities to simulate a variety of macroscopic quantum phenomena. In the spinor gas, the spin-dipolar collisions significantly change the spin states producing rich Zeeman effects. In particular, spinor Bose gases with density-density interaction and antiferromagnetic spin-exchange interaction [1,2] exhibit various phases of strongly correlated quantum liquids and are thus particularly valuable to study quantum magnetism and criticality. The experimental study of quantum criticality and universal scaling behavior has recently been initiated in low-dimensional cold atomic matter [3,4]. These advances build on theoretical schemes for mapping out quantum criticality in cold-atom systems [5–7]. In this framework, exactly solved models of cold atoms, exhibiting quantum phase transitions, provide a rigorous way to investigate quantum criticality [8].

One-dimensional (1D) spinor Bose gases with short-range δ -function interaction and antiferromagnetic spin-exchange interaction are particularly interesting due to the existence of various phases of quantum liquids associated with exact Bethe ansatz solutions [9–12]. The antiferromagnetic interaction leads to an effective attraction in the spin-singlet channel that gives rise to a quasicondensate of singlet bosonic pairs when the external field is less than a lower critical field at zero temperature. In this phase, the low-energy physics can be characterized by a spin-charge separation theory of the U(1) Tomonaga-Luttinger liquid (TLL) describing the charge sector and a O(3) nonlinear σ model describing the spin sector [10]. However, if the external field exceeds an upper critical field, we have a solely ferromagnetic quasicondensate of unpaired bosons with spins aligned along the external field. For an intermediate magnetic field, the spin-singlet pairs and spin-aligned bosons form a two-component TLL with a magnetization (see Fig. 1).

Quantum critical phenomena in the spin-1 Bose gas associated with phase transitions at zero temperature can be explored by varying the magnetic field and chemical potential. In this Rapid Communication we use the exact thermodynamic Bethe ansatz (TBA) solution for spin-1 bosons to illustrate the microscopic origin of the quantum criticality of different spin states in a 1D harmonic trap.

The model and equation of state. We consider N particles of mass m confined in one dimension to a length L with δ -interacting-type density-density and spin-exchange interactions between two atoms. The Hamiltonian is [1,9]

$$\mathcal{H} = - \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + \sum_{i<j} [c_0 + c_2 S_i S_j] \delta(x_i - x_j) + E_z, \quad (1)$$

where S_i is a spin-1 operator with z component ($s = 1, 0, -1$), $E_z = -H S^z$ is the Zeeman energy, with H the external field and S^z the total spin in the z component. The 1D interaction parameters $c_0 = (g_0 + 2g_2)/3$ and $c_2 = (g_2 - g_0)/3$ with $g_s = -2\hbar^2/m a_s$. Here m is the particle mass and a_s represents the 1D s -wave scattering length in the total spin $S = 0, 2$ channels. Following Refs. [13,14] the effective 1D coupling constant g_s can be expressed in terms of the known 3D scattering lengths.

Extending Yang's method [15], Cao *et al.* [9] solved the model (1) for the case $c = c_0 = c_2$. For convenience, we define the linear density $n = N/L$ and use dimensionless quantities $\tilde{\mu} = \mu/\varepsilon_b$, $h = H/\varepsilon_b$, $t = T/\varepsilon_b$, and $\tilde{p} = p/|c|\varepsilon_b$. Here energy and length are measured in units of the binding energy $\varepsilon_b = \hbar^2 c^2/16m$ and c^{-1} , respectively. We set $\hbar = 2m = 1$ in the following.

The model (1) has two conserved quantities, S^z and the total particle number N . The number of particles in a particular spin state ($s = 1, 0, -1$) is no longer conserved. For instance the scattering between two particles of spin $s = \pm 1$ can produce two particles of spin $s = 0$ and vice versa. Therefore, the model can have two types of pairing between two spin ± 1 atoms or between two spin-0 atoms (see Refs. [1,9,11]).

The ground-state properties of the system were studied in Refs. [10–12]. Analytic results can be extracted from the TBA equations for strong coupling $\gamma \gg 1$ and low temperature $t \ll 1$ (see Ref. [16] for details). The pressure of the system can be written as $\tilde{p} = \tilde{p}_1 + \tilde{p}_2$ in terms of the pressure \tilde{p}_1 for unpaired and \tilde{p}_2 for paired bosons (Boltzmann constant $k_B = 1$)

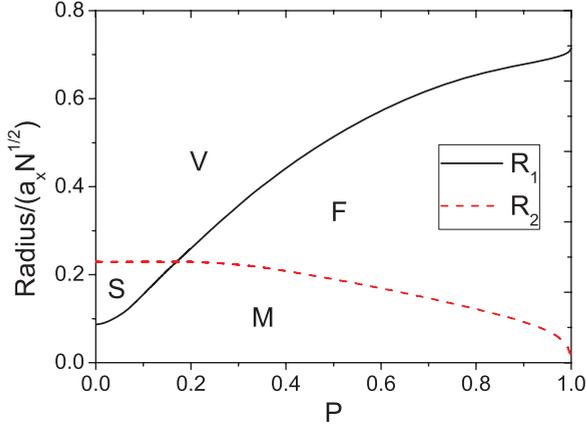


FIG. 1. (Color online) Phase diagram of the spin-1 Bose gas at $T = 0$ in terms of the rescaled axial radius $R/a_x N^{1/2}$ versus the polarization $P = N_1/N$ for $N/a_x^2 c^2 = 0.05$. The lines R_1 and R_2 denote the phase boundaries of vanishing density of singlet pairs and vanishing density of spin-aligned bosons. The model exhibits three quantum phases: spin-singlet-paired bosons S , ferromagnetic spin-aligned bosons F , and a mixed phase of the pairs and unpaired bosons. V stands for the vacuum.

where

$$\begin{aligned} \tilde{p}_1 &= -\frac{t^{3/2}}{4\sqrt{2\pi}} f_{\frac{3}{2}}^1 \left(1 + \frac{t^{3/2}}{32\sqrt{2\pi}} f_{\frac{3}{2}}^1 - \frac{124t^{3/2}}{125\sqrt{\pi}} f_{\frac{3}{2}}^2 \right), \\ \tilde{p}_2 &= -\frac{t^{3/2}}{4\sqrt{\pi}} f_{\frac{3}{2}}^2 \left(1 - \frac{124t^{3/2}}{125\sqrt{2\pi}} f_{\frac{3}{2}}^1 - \frac{181t^{3/2}}{3456\sqrt{\pi}} f_{\frac{3}{2}}^2 \right). \end{aligned} \quad (2)$$

Here $f_n^j = \text{Li}_n(-e^{A_j/t})$ with $j = 1, 2$ denotes the standard polylog function $\text{Li}_n(x)$, with

$$\begin{aligned} A_1 &= \tilde{\mu} + h + 2\tilde{p}_1 - \frac{16\tilde{p}_2}{5} \\ &\quad + \frac{t^{5/2}}{16\sqrt{2}} \left(\frac{1}{2\sqrt{\pi}} f_{\frac{5}{2}}^1 - \frac{1984}{125\sqrt{2\pi}} f_{\frac{5}{2}}^2 \right) + f_s, \\ A_2 &= 1 + 2\tilde{\mu} - \frac{32\tilde{p}_1}{5} - \frac{\tilde{p}_2}{3} \\ &\quad - \frac{t^{5/2}}{16\sqrt{2}} \left(\frac{3968}{125\sqrt{\pi}} f_{\frac{5}{2}}^1 + \frac{181}{108\sqrt{2\pi}} f_{\frac{5}{2}}^2 \right). \end{aligned} \quad (3)$$

The terms $f_s = te^{-h/t} e^{-2\tilde{p}_1/t} I_0(2\tilde{p}_1/t)$ with $I_0(z) = \sum_{k=0}^{\infty} \frac{(z/2)^{2k}}{k!^2}$ are extracted from the spin wave bound states [16].

The above result for the pressure serves as the equation of state, from which thermodynamic quantities such as the particle density n , the density of unpaired bosons n_1 , the density of spin-singlet pairs n_2 , the entropy, and the compressibility of the system can be determined through the standard thermodynamic relations. Moreover, the equation of state allows an exact description of TLLs and quantum criticality of the system.

Phase diagram and density profiles. In order to study quantum criticality in the spin-1 Bose gas in a 1D harmonic trap, the equation of state (2) can be reformulated within the local density approximation (LDA) by a replacement $\mu(x) = \mu(0) - \frac{1}{2}m\omega_x^2 x^2$ in which x is the position and ω_x is

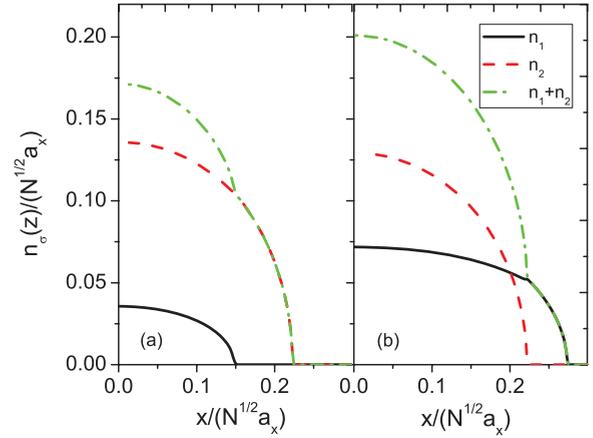


FIG. 2. (Color online) The density distribution profiles for trapped bosons at zero temperature with $N/a_x^2 c^2 \simeq 0.05$ for (a) $P \approx 12.22\%$ (or $h = 0.49$) and (b) $P \approx 22.33\%$ (or $h = 0.51$).

the trapping frequency (see Ref. [17]). Using the dimensionless chemical potential $\tilde{\mu}(\tilde{x}) = \tilde{\mu}(0) - 8\tilde{x}^2$, where $\tilde{x} = x/a_x^2|c|$ is a rescaled distance and $a_x = \sqrt{\hbar/m\omega_x}$ is the harmonic characteristic radius, the total particle number and the polarization are given by

$$\begin{aligned} \frac{N}{a_x^2 c^2} &= \int_{-\infty}^{\infty} \tilde{n}(\tilde{x}) d\tilde{x}, \\ P &= \int_{-\infty}^{\infty} \tilde{n}_1(\tilde{x}) d\tilde{x} / [N / (a_x^2 c^2)]. \end{aligned} \quad (4)$$

We extract the phase boundaries from the equation of state (2) within the LDA (4) in the limit $t \rightarrow 0$ (see Fig. 1). The line R_1 (R_2) indicates the vanishing density of unpaired bosons (spin-singlet pairs). The intersection of the phase boundaries occurs at $h = 0.5$ and $\mu = 0.5$ yielding the critical polarization $P_c \approx 16.97\%$. This phase diagram resembles that of the spin-1/2 attractive Fermi gas, recently confirmed by Liao *et al.* [18]. Here the critical properties of the spin-1 Bose gas are described by two Tonks-Girardeau gases with masses m and $2m$, which are likely to mimic the free fermions and bosonic bound pairs in the spin-1/2 attractive Fermi gas.

Figure 2 shows the density distribution profiles in the limit $t \rightarrow 0$ for $N/a_x^2 c^2 \simeq 0.05$ for (a) low polarization ($P < P_c$) $P \approx 12.22\%$ and (b) large polarization ($P > P_c$) $P \approx 22.33\%$. We find a partially polarized core surrounded by two wings composed of either spin-singlet pairs or a fully spin-aligned Tonks-Girardeau gas. The threshold values of the phase boundaries are consistent with the phase diagram Fig. 1. Our result convincingly indicates that spinor Bose gases in a 1D harmonic trap constitute an excellent quantum simulator of strongly correlated TLLs which could be probed by *in situ* imaging, analogously to the trapped Fermi gas [18].

Quantum criticality. The equation of state (2), capturing the entire thermal fluctuation in the quantum critical regimes, illustrates the microscopic origin of the quantum criticality. The thermodynamic functions can be cast in a universal scaling form [19,20]. For example, the density and compressibility are

given by

$$n(\mu, T, x) = n_0 + T^{\frac{d}{z}+1-\frac{1}{\nu z}} \mathcal{G}\left(\frac{\mu(x) - \mu_c}{T^{\frac{1}{\nu z}}}\right), \quad (5)$$

$$\kappa(\mu, T, x) = \kappa_0 + T^{\frac{d}{z}+1-\frac{2}{\nu z}} \mathcal{F}\left(\frac{\mu(x) - \mu_c}{T^{\frac{1}{\nu z}}}\right), \quad (6)$$

with dimensionality $d = 1$. Here we find the scaling functions $\mathcal{G}(x) = \lambda_\alpha \text{Li}_{1/2}(-e^x)$ and $\mathcal{F}(x) = \lambda_\beta \text{Li}_{-1/2}(-e^x)$, from which follow the dynamical critical exponent $z = 2$ and correlation length exponent $\nu = 1/2$ for different phases of the spin states. In the above, n_0 , κ_0 , λ_α , and λ_β are constants associated with the background near the critical points (see details in Ref. [16]). Moreover, quantum criticality driven by the external field H leads to similar scaling, where now $\mathcal{G}(x) = \lambda_g \text{Li}_{1/2}(-e^{\Lambda_0 x})$ and $\mathcal{F}(x) = \lambda_f \text{Li}_{-1/2}(-e^{\Lambda_0 x})$ with a dimensionless factor Λ_0 and the same critical exponents [16]. Here $\lambda_{g,f}$ are different constants associated with critical points.

The critical exponents appearing in the scaling functions are analytically determined from the exact Bethe ansatz solution. We observe that the 1D spin-1 Bose gas belongs to the same universality class as spin-1/2 attractive fermions [8] due to the hard-core nature of the two coupled Tonks-Girardeau gases. This demonstrates a significant feature of 1D many-body physics—quantum criticality involves a universal crossover from a TLL with linear dispersion to free fermions with a quadratic dispersion in the low-energy physics [21]. In addition, the critical exponents of 1D spin-1 bosons have the same values as the critical exponents of the Mott transition in 1D and 2D Bose-Hubbard models (see Refs. [22,23]).

The universal scaling behavior of the homogenous system can be mapped out through the density profiles of the trapped gas at finite temperatures. Although a finite-size scaling effect is evident in the scaling analysis [5,6,24], the finite-size error lies within the current experimental accuracy [23]. Here we show that all thermodynamic observables are given in terms of the rescaled temperature and chemical potential. Thus one can either lower the temperature or increase the interaction strength (by tuning the transverse frequency) such that all data curves for the physical properties in the trapped gas collapse at different temperatures into a single curve with a proper scaling. This collapse signature can be used to confirm the quantum critical law, see the experimental measurements given in Ref. [23].

In the regime of low polarization ($P < P_c$), the phase transitions from the vacuum into the spin-singlet paired phase and from the pure paired phase into the mixture of spin-singlet pairs and spin-aligned bosons occur as the chemical potential passes the lower critical point $\tilde{\mu}_{c2} = -0.5$ and the upper critical point $\tilde{\mu}_{c4} = -h + \frac{32\sqrt{2}}{15\pi}(\frac{1}{2} - h)^{\frac{3}{2}} + \frac{2912}{225\pi^2}(\frac{1}{2} - h)^2$, respectively.

The universal scaling behavior can be identified following the scheme proposed in Ref. [6] by plotting the “rescaled density” versus the chemical potential for different values of temperature. Figures 3(a) and 3(b) show the rescaled density normalized by $N^{1/2}/(a_x)$ versus the rescaled distance at different temperatures. All curves intersect at the critical points $\tilde{\mu}_{c2}$ and $\tilde{\mu}_{c4}$ after a subtraction of the background density n_0 . We also see in Fig. 3 that all data points collapse onto a

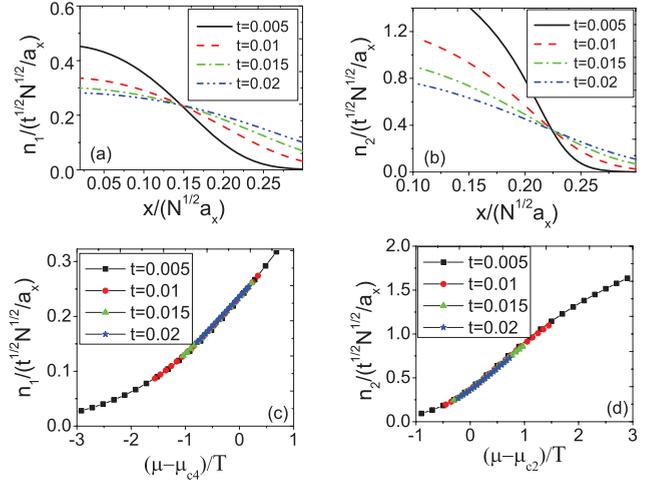


FIG. 3. (Color online) Quantum criticality for low polarization. The rescaled density profiles are plotted within LDA near the critical points (a) $\tilde{\mu}_{c4}$ and (b) $\tilde{\mu}_{c2}$ at different temperatures $t = 0.005, 0.01, 0.015,$ and 0.02 . All curves intersect at the critical points. The rescaled density vs (c) $[\mu(x) - \mu_{c4}]/T^{z\nu}$ and (d) $[\mu(x) - \mu_{c2}]/T^{z\nu}$ at different temperatures $t = 0.005, 0.01, 0.015,$ and 0.02 . All data points collapse onto a single curve.

single curve near (c) $\tilde{\mu}_{c4}$ and (d) $\tilde{\mu}_{c2}$, which is the scaling function for these quantum critical points.

For large polarization ($P > P_c$), the phase transitions from vacuum into the ferromagnetic spin-aligned boson phase and from the spin-aligned boson phase into the mixture of spin-singlet pairs and spin-aligned bosons occur as the chemical potential varies across the lower critical point $\tilde{\mu}_{c1} = -h$ and the upper critical point $\tilde{\mu}_{c3} = -\frac{1}{2} + \frac{8\sqrt{2}}{15\pi}(h - \frac{1}{2})^{\frac{3}{2}} + \frac{104}{75\pi^2}(h - \frac{1}{2})^2$, respectively. A similar analysis is presented in Fig. 4 near the critical points $\tilde{\mu}_{c1}$ and $\tilde{\mu}_{c3}$.

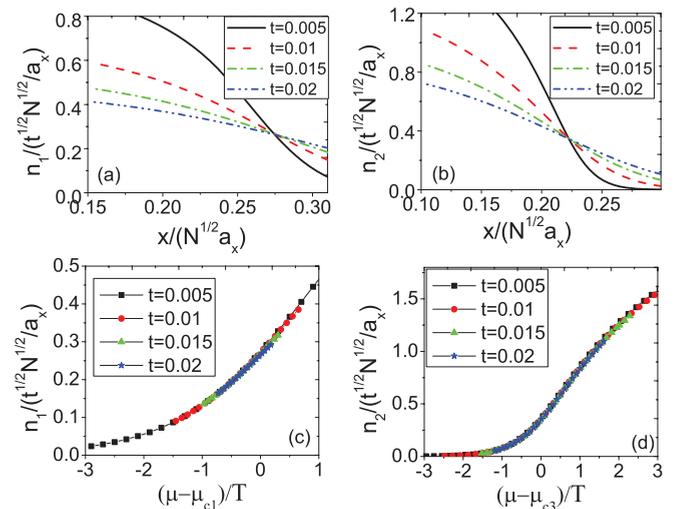


FIG. 4. (Color online) Quantum criticality for high polarization. The rescaled density profiles are plotted within LDA near the critical points (a) $\tilde{\mu}_{c1}$ and (b) $\tilde{\mu}_{c3}$. The rescaled density vs (c) $[\mu(x) - \mu_{c1}]/T^{z\nu}$ and (d) $[\mu(x) - \mu_{c3}]/T^{z\nu}$. As in Fig. 3 the curves and data points are indicative of scaling behavior at quantum criticality.

Similar plots can be made for the rescaled compressibility in agreement with the universal scaling result (6). The compressibility curves at different temperatures collapse into a single curve obeying the scaling law. The compressibility always develops a peak near the phase boundary on the side with higher density of state. However, the experimental measurement of the compressibility is more difficult than the density profiles. Nevertheless, progress in measuring the compressibility of an ultracold Fermi gas has recently been made [25].

In conclusion, we have discussed the equation of state, the density profiles, TLL thermodynamics, and universal scaling at quantum criticality for the spin-1 Bose gas with strongly repulsive density-density and antiferromagnetic spin-exchange interactions in a 1D harmonic trap. We have shown that the quantum criticality of different spin states belongs to the universality class with critical exponents $z = 2$ and

$\nu = 1/2$. This remains true in general for the 1D model even for the nonintegrable case $c_0 \neq c_2$. We have also demonstrated that the phase diagram, the TLLs, and critical properties of the bulk system can be mapped out from the density profiles of the trapped spinor gas at finite temperatures. Current experiments [3,4,18,26] are capable of measuring such universal features of 1D many-body physics.

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