Observability of Quantum Criticality and a Continuous Supersolid in Atomic Gases

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We analyze the Bose-Hubbard model with a three-body hard-core constraint by mapping the system to a theory of two coupled bosonic degrees of freedom. We find striking features that could be observable in experiments, including a quantum Ising critical point on the transition from atomic to dimer superfluidity at unit filling, and a continuous supersolid phase for strongly bound dimers.

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Experiments with atomic quantum degenerate gases representing strongly interacting systems have reached a level of precision where quantitative tests of elaborate many-body theories have become possible [1–5]. In the interplay between experiment and theory, the challenge is now to identify realistic models where quantum fluctuations lead to qualitatively new features beyond mean field in quantum phases and phase transitions. We study below the Bose-Hubbard model with a three-body constraint, which arises naturally due to a dynamic suppression of three-body loss of atoms occupying a single lattice site [6,7], and can also be engineered via other methods [8]. This constraint stabilizes the system when two-body interactions are attractive, allowing for the formation of dimers—bound states of two atoms. The phase diagram then contains a dimer superfluid (DSF) phase connected to a conventional atomic superfluid (ASF). Remarkably, this simple but realistic model shows several nongeneric features, which are uniquely tied to the three-body constraint and could be observed with cold gases: (i) Emergence of an *Ising quantum critical point* (QCP) on the ASF-DSF phase transition line as a function of density—which generically is preempted by the Coleman-Weinberg mechanism [9], where quantum fluctuations drive the phase transition first order [10–12], with a finite correlation length; and (ii) a *bicritical point* [13] in the strongly correlated regime, which is characterized by energetically degenerate orders, in our case coexistence of superfluidity and a charge-density wave, representing a "continuous supersolid" with clear experimental signatures.

Below we describe the constrained model, and then present a new analytical formalism for a unified treatment of on site constraints in bosonic lattice models, based on an exact requantization of the Gutzwiller mean field theory. This allows for an analytical treatment of the phenomena arising here. At the end we discuss the experimental signatures of the latter.

Constrained model.—We consider the Bose-Hubbard model on a d-dimensional cubic lattice with a three-body on site hard-core constraint, $a_i^{\dagger 3} \equiv 0$,

$$H = -J\sum_{\langle i,j\rangle} a_i^\dagger a_j - \mu\sum_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1), \qquad (1)$$

where $\langle i, j\rangle$ denotes summation over nearest neighbors, J is the hopping matrix element, μ the chemical potential, and U the on site two-body interaction. The three-body constraint stabilizes the attractive bosonic many-body system with $U < 0$, which we focus on here.

The phase diagram of this model is shown in Fig. 1. The dominant phases are an ASF with order parameters $\langle a_i\rangle \neq 0$ and $\langle a_i^2\rangle \neq 0$, and a DSF with $\langle a_i^2\rangle \neq 0$ but $\langle a_i\rangle = 0$, formed at sufficiently strong interatomic attraction U. In the Gutzwiller mean field approximation [6] these two phases are separated by a second order phase transition of a special type, the Ising or ASF-DSF transition [12], at which the discrete Z_2 symmetry of DSF is spontaneously broken. One reason to question the mean field approach is the presence of two interacting soft modes close to the phase transition: the noncritical Goldstone mode, related to the $\langle a_i^2\rangle$ order parameter, and the critical Ising mode signaling the onset of atomic superfluidity with $\langle a_i\rangle \neq 0$. This

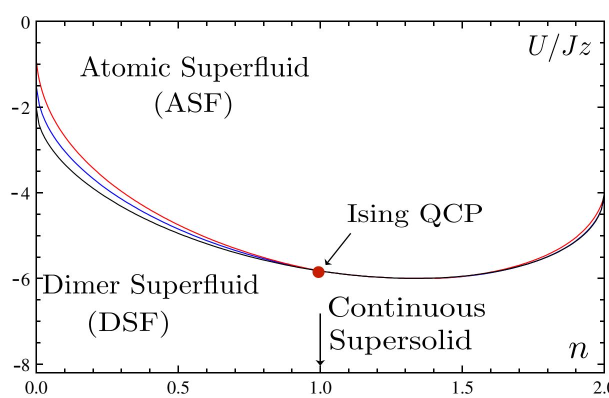

FIG. 1 (color online). Phase diagram for the Bose-Hubbard model with a three-body hard-core constraint, and $U < 0$. The black curve represents the mean field phase border, while red (light gray) and blue (dark gray) curves include shifts due to quantum fluctuations in $d = 2, 3$.

motivates the development of a fully quantum mechanical approach to the constrained Hamiltonian (1), with a *unified* description of interaction effects at various scales.

Formalism: Mapping the constrained model to a coupled boson theory.—Because of the constraint, the operators a_i, $a_i^\dagger$ are no longer standard bosonic ones and the on site Hilbert space is reduced to only three states $|\alpha\rangle$, corresponding to zero ($\alpha = 0$), single ($\alpha = 1$), and double ($\alpha = 2$) occupancy. Following Altman and Auerbach [14], for each lattice site i we introduce three operators $t_{\alpha,i}^\dagger$ creating these states out of an auxiliary vacuum state, $|\alpha\rangle_i = t_{\alpha,i}^\dagger|\mathrm{vac}\rangle = (\alpha!)^{-1/2}(a_i^\dagger)^\alpha|\mathrm{vac}\rangle$. By construction, these operators obey a holonomic constraint, $\sum_\alpha t_{\alpha,i}^\dagger t_{\alpha,i} = \mathbf{1}$. The Hamiltonian then reads

$$H = -J\sum_{\langle i,j\rangle}[t_{1,i}^\dagger t_{0,i} t_{0,j}^\dagger t_{1,j} + 2t_{2,i}^\dagger t_{1,i} t_{1,j}^\dagger t_{2,j} + \sqrt{2}(t_{2,i}^\dagger t_{1,i} t_{0,j}^\dagger t_{1,j} + t_{1,i}^\dagger t_{0,i} t_{1,j}^\dagger t_{2,j})] + U\sum_i \hat{n}_{2,i} - \mu\sum_i(\hat{n}_{1,i} + 2\hat{n}_{2,i}), \tag{2}$$

where $\hat{n}_{\alpha,i} = t_{\alpha,i}^\dagger t_{\alpha,i}$. This form is closely related to resonant Feshbach models describing, e.g., the BCS-BEC crossover [15]: The "Feshbach term" (second line, first term) allows interconversion of a "dimer" ($t_{2,i}$) into two "atoms" ($t_{1,i}$), and the detuning (second term), gives the corresponding energy difference. This detuning is given by the interaction U, in contrast to $\sim 1/U$ in resonant models.

Using the constraint, we can eliminate one of the operators $t_{\alpha,i}$ in Eq. (2), say $t_{0,i}$, as $t_{0,i} \to \sqrt{X_i}$ (and $t_{0,i}^\dagger \to \sqrt{X_i}$), where $X_i = 1 - \hat{n}_{1,i} - \hat{n}_{2,i}$. Noting that $X_i^2 = X_i$ on the constrained space, we replace $\sqrt{X_i}$ with X_i, yielding a *polynomial* Hamiltonian. The remaining operators t_1, t_2 can now be interpreted as standard bosonic ones. To demonstrate this, one divides the standard bosonic Hilbert space into a physical ($\mathcal{P}_i$) and an unphysical ($\mathcal{U}_i$) subspace, $\mathcal{H}_i = \mathcal{P}_i \oplus \mathcal{U}_i$, where the physical one consists of states obeying the three-body constraint. We see that H *does not couple* the physical $\mathcal{P} = \prod \mathcal{P}_i$ and unphysical $\mathcal{U} = \prod \mathcal{U}_i$ subspaces.

The distinction between the contributions from physical and unphysical spaces can most conveniently be achieved by using the quantum effective action $\Gamma[t_1, t_2]$ [16], which is a functional on classical fields and provides all one-particle irreducible correlation functions as coefficients of an expansion in powers of t_1 and t_2. Because Γ is formulated in terms of physical quantities, we can restrict its general form to a polynomial obeying the three-body constraint. The form of the effective action thus is restricted by the constraint, in addition to the symmetries of the microscopic theory.

To apply the above construction to a many-body system, one has to choose the proper ground state and the corresponding operators. Following Ref. [17], we introduce new operators $b_{\alpha,i} = (R_i)_{\alpha\beta} t_{\beta,i}$ ($\alpha, \beta = 0, 1, 2$), with a unitary transformation R. The parameters of R are such that $b_{0,i}$ creates the mean field vacuum, and $b_{1,i}$ and $b_{2,i}$ correspond to fluctuations on top of this state, with vanishing expectation values (see [18]). The DSF ground state, for example, corresponds to: $b_{0,i} = \cos(\theta/2)t_{0,i} + \sin(\theta/2)\exp(-i\phi)t_{2,i}$, $\quad b_{2,i} = \cos(\theta/2)t_{2,i} - \sin(\theta/2) \times \exp(i\phi)t_{0,i}$, and $b_{1,i} = t_{1,i}$, where ϕ is an arbitrary phase and the angle $\theta \in [0, \pi]$ is such that $2\sin^2(\theta/2) = n$, the density of atoms (on the mean field level for simplicity). The operators $b_{\alpha,i}$ are subject to the same constraint, $\sum_\alpha b_{\alpha,i}^\dagger b_{\alpha,i} = \mathbf{1}$, and we can eliminate $b_{0,i}^{(\dagger)}$ as described above. This results in a *polynomial* Hamiltonian for the remaining operators $b_{1,i}$ and $b_{2,i}$, where the operator independent part reproduces the Gutzwiller energy.

Application of the formalism.—The limit $n \to 0$ gives a stringent check of our formalism, where we recover the nonperturbative Schrödinger equation for the dimer bound state formation (see [18] for details). We now apply our method in the many-body context:

(i) Ising quantum critical point.—The polynomial Hamiltonian describes atomic ($b_{1,i}$) and dimer ($b_{2,i}$) fluctuations around the spatially uniform DSF state. After taking the long wavelength continuum limit, one can easily see that there are two soft modes in the vicinity of the ASF-DSF transition: the noncritical Goldstone mode $\pi \sim \mathrm{Im}(b_2)$ corresponding to the $\mathrm{U}(1)/Z_2$ gauge symmetry broken by the presence of the dimer condensate, and the critical atomic Ising mode $\varphi \sim \mathrm{Re}(b_1)$ signaling the appearance of an atomic condensate. The other two modes remain massive and do not affect the physics of the phase transition. Integrating out the latter we obtain an effective low energy action for the soft modes [18]:

$$S_{\mathrm{eff}}[\varphi, \pi] = \int_x \Big\{\frac{1}{2}\varphi(-Z_\varphi\partial_\tau^2 - \xi_+^2\Delta + m_+^2)\varphi + \lambda\varphi^4 + \frac{1}{2}\pi(-Z\partial_\tau^2 - \xi^2\Delta)\pi + i\kappa\varphi^2\partial_\tau\pi\Big\}. \tag{3}$$

It describes phonons π in the dimer superfluid coupled to a real scalar Ising field φ, in turn represented by an action of the Ginzburg-Landau type with the "mass" parameter m_+^2 crossing zero at the ASF-DSF transition. The coupling κ comes from the cubic coupling $-\sqrt{2}J\cos(\theta)b_{2,i}^\dagger b_{1,i} b_{1,j} + \mathrm{H.c.}$ which originated from the "Feshbach term" in the original Hamiltonian Eq. (2), such that $\kappa \sim \cos(\theta) \approx 1 - n$. This cubic coupling of Goldstone to Ising mode with linear time derivative has the same degree of relevance as the Ising coupling λ, leading to the Coleman-Weinberg (CW) phenomenon [10]: The renormalized value of the Ising coupling λ reaches zero at some *finite* scale ξ at which m_+^2 is still positive. As a result, terms with higher powers of φ, which are generated by fluctuations, become important. These self-interaction terms provide a new minimum with $\langle\varphi\rangle \neq 0$, which is reached via a first order phase transition with finite correlation length ξ. Therefore, the ASF-DSF phase transition is first order, contrary to the predictions of the mean field approach.

The coupling via a temporal derivative and, therefore, the CW phenomenon, is rather generic in nonrelativistic systems, in which an Ising field emerges as an effective low energy degree of freedom [10–12]. In our case, however, the coupling κ vanishes for $n \to 1$. The existence of such a decoupling point can be proven assuming a continuous, monotonic behavior of a particular compressibility, the μ derivative of the dimer mass term $K = -dm_d^2/d\mu|_n$ within the DSF phase: it then must have a unique zero crossing, because it is >0 (<0) for $n = 0$ (2) [18]. This argument is tied to the existence of a maximum filling, and thus to the three-body constraint. Using the Ward identities resulting from a temporally local gauge invariance $b_\alpha \to \exp[i\alpha\lambda(t)]b_\alpha$, $\alpha = 1, 2$, and $\mu \to \mu + i\lambda(t)$ [19], we see that $\kappa \propto K$. As a result, the first order Z_2 transition terminates into a true $(d+1)$-dimensional Ising quantum critical point in the vicinity of unit filling.

Fluctuations also shift the mean field phase boundary, cf. Fig. 1. This is only pronounced for $n \ll 1$, as dimer formation and atom criticality approach each other for $n \to 0$ [18].

(ii) Continuous supersolid.—Another peculiar consequence of the three-body constraint occurs for dimers in the strong coupling limit, where single particle excitations are strongly gapped ($\sim|U|/2$) and can be integrated out perturbatively. Taking the dominant nearest neighbor hopping t and interaction v into account, the effective lattice theory for hard-core bosons (dimers or diholes) can be conveniently rewritten as an antiferromagnetic Heisenberg spin Hamiltonian (see, e.g., [20]),

$$H_{\mathrm{AFM}} = 2t\sum_{\langle i,j\rangle}[s_{x,i}s_{x,j} + s_{y,i}s_{y,j} + \lambda s_{z,i}s_{z,j}] \qquad (4)$$

restricted to a subspace with a fixed projection of the total spin on the z-axis, $S_z = \sum_i s_{z,i} = L(n_d - 1/2)$, where L is the total number of the lattice sites, and $n_d = n/2$ the dimer filling. The anisotropy parameter λ is the ratio of the interaction and hopping, $\lambda = v/2t$. In the leading second order perturbation theory, we find $t = v/2 = 2J^2/|U|$, such that $\lambda = 1$ and the Hamiltonian (4) is SO(3) invariant, corresponding to a symmetry enhancement compared to the conventional SO(2) $\simeq$ U(1) phase symmetry for bosons. It parallels a similar effect for attractive lattice fermions [21], and is a peculiar feature of the three-body hard-core constraint—if virtual triple and higher occupancies are allowed, one finds $\lambda = 4$ [22]. The symmetry enhancement is operative for exactly half filling of dimers, $n_d = 1/2$, where $S_z = 0$, while for other dimer fillings $S_z \neq 0$ and the symmetry is reduced to U(1). In the first case, however, the ground state of the Hamiltonian (4) is the antiferromagnetic state parametrized by the direction of the Néel order parameter on the three-dimensional Bloch sphere. Generically, the Néel order parameter has components both in the xy plane and along the z axis. This means that the ground state of bosons has both DSF and charge-density wave (checkerboardlike, CDW) orders, i.e., is a supersolid. The specific feature, however, is that the SO(3) symmetry admits a continuous change in the ratio between the two order parameters without changing the energy, and this state may thus be called a continuous supersolid. A particular choice of the order parameters depends on the system preparation and boundary conditions, in contrast to supersolidity in other bosonic systems [23].

The spontaneously broken SO(3) symmetry in the continuous supersolid provides *two* massless Goldstone modes. A spin wave analysis yields their dispersion

$$\omega(\mathbf{q}) = tz[\tilde{\epsilon}_{\mathbf{q}}(1 + \lambda - \lambda\tilde{\epsilon}_{\mathbf{q}})]^{1/2}$$

with $\tilde{\epsilon}_{\mathbf{q}} = (1/d)\sum_\lambda(1 - \cos\mathbf{q}\cdot\mathbf{e}_\lambda)$, $\lambda \leq 1$. For $\lambda = 1$ the second Goldstone mode emerges at the edge of the Brillouin zone, adding to the one at zero momentum. In the next (fourth) order of perturbation theory, we find [18] $\lambda = 1 - 8(z-1)(J/|U|)^2 < 1$, and the DSF ground state is slightly favored over CDW order due to weak explicit breaking of SO(3). Still, the proximity to the continuous supersolid manifests itself in a weakly gapped ($\Delta \sim tz(1-\lambda)$) collective mode at the edge of the Brillouin zone, which may be probed experimentally, see below.

Experimental signatures.—We now discuss in detail the experimental signatures of the critical behavior and continuous supersolid. Above we showed that the ASF-DSF phase transition (see Fig. 1) terminates in an Ising quantum critical point at $n = 1$. The phase transition is thus second order at $n = 1$, with a diverging correlation length at the transition point. Away from $n = 1$ the transition is first order, with a finite correlation length estimated as $\xi/a \sim \kappa^{-6} \sim |1-n|^{-6}$ (a the lattice spacing) using the renormalization group flow of [10]. As typical of the radiatively induced first order transitions, the near-critical domain is large, with a correlation length exceeding the typical extent of optical lattices of 50 to 100 sites in a region $1/2 \lesssim n \lesssim 3/2$. This behavior can be measured directly in experiments probing the correlation length, as done in Ref. [1]. Alternatively, critical opalescence via damping of collective oscillations [24] could be probed.

The continuous supersolid appearing at strong attraction and unit filling can be detected by measurement of the coexisting spatial order and dimer superfluid correlations. The spatial structure could be detected via noise correlation measurements [25], and the dimer superfluid correlation functions in the momentum distribution of dimers, which could be imaged, e.g., by associating atoms to molecules, and measuring their momentum distribution. The CDW can also be stabilized with a weak ($\sim\Delta \ll tz$) superlattice, which acts as a staggered external field that rotates the Néel order parameter to the z axis.

We further elaborate on experimental signatures using exact numerical time-dependent density matrix renormalization group (t-DMRG) techniques [26] in 1D: Fig. 2(a) shows the density-density correlation function $\langle n_i n_{i+x}\rangle - \langle n_i\rangle\langle n_{i+x}\rangle$ characterizing CDW order, and the DSF correlator $\langle b_i^\dagger b_i^\dagger b_{i+x} b_{i+x}\rangle$ as a function of distance x in the ground state for realistic experimental size scales and

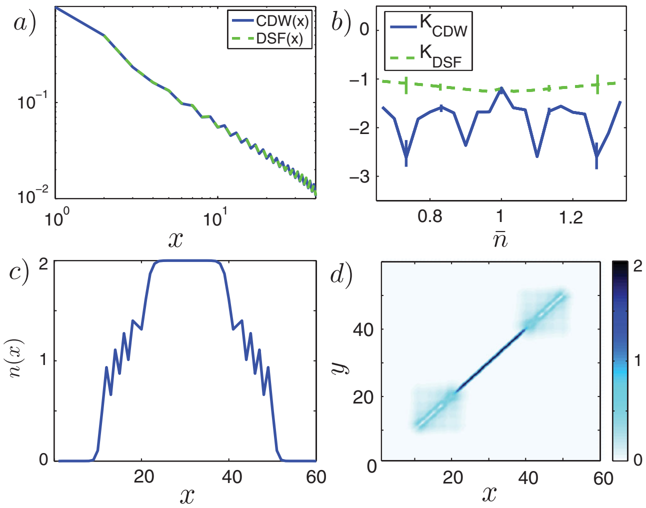

FIG. 2 (color online). Ground state computations on 60 lattice sites with $U/J = -20$ using t-DMRG. (a) Correlation functions characterizing the CDW and DSF orders for open boundary conditions at unit filling on a log-log scale as a function of distance x. (b) Fitted algebraic decay exponents K_{DSF} and K_{CDW} for varying n (error bars show estimates of the fitting error). (c) Density $n(x)$ for a system with a harmonic trapping potential $V(x)/J = (x - 30.5)^2/900$, $N = 60$ particles. (d) Shaded plot of the DSF correlation function $\langle b_x^\dagger b_x^\dagger b_y b_y \rangle$ with interpolated shading, indicating substantial DSF order where $n \sim 1$.

parameters. At unit filling, both decay algebraically and are essentially equal, indicating coexistence both orders. In Fig. 2(b) we show the result of fitting an algebraic decay $x^{K_{\mathrm{CDW,DSF}}}$ to the correlation functions. For $n = 1$ these are equal, but away from unit filling, the DSF correlations decay more slowly, so that DSF order dominates CDW. (The large fluctuations in K_{CDW} with varying n are due to the interplay between filling fraction and CDW order.) In experiments in a harmonic trap, where the filling factor varies across the system, this gives rise to further signatures. In Fig. 2(c), we plot the density in a trap, showing that a region exists near unit filling where oscillations in the density are present, characteristic of the appearance of CDW order. Figure 2(d) shows that in the same region the DSF correlations are significant, whereas in the center of the trap, a constraint-induced insulating phase with $n = 2$ appears. For more details see [18].

Conclusion.—We have demonstrated that an atomic Bose gas in an optical lattice with three-body on site constraint provides a realization of such fundamental physical concepts as the Coleman-Weinberg phenomenon of radiative mass generation and Ising quantum criticality. In addition, the ground state at unit filling in the strongly correlated limit is an example of a continuous supersolid—a supersolid with a tunable ratio between the superfluid and the charge-density wave order parameters.

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