Hidden Order in 1D Bose Insulators

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We investigate the phase diagram of spinless bosons with long range ($\propto 1/r^3$) repulsive interactions, relevant to ultracold polarized atoms or molecules, using density matrix renormalization group. Between the two conventional insulating phases, the Mott and density wave phases, we find a new phase possessing hidden order revealed by nonlocal string correlations analogous to those characterizing the Haldane gapped phase of integer spin chains. We develop a mean field theory that describes the low-energy excitations in all three insulating phases. This is used to calculate the absorption spectrum due to oscillatory lattice modulation. We predict a sharp resonance in the spectrum due to a collective excitation of the new phase that would provide clear evidence for the existence of this phase.

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Introduction.—Systems of ultracold atoms in optical lattices hold significant promise in the study of correlated quantum matter. Experimental realization of the Bose-Hubbard model has been an important step in this direction, not least of all because it facilitated the first observation of a quantum insulating state of bosons [1]. Localization of bosons in the Mott insulator is driven by strong on site interactions leading to an extremely simple state, well described by a site-factorizable mean field wave function. An interesting question is what other phases, perhaps with a nontrivial structure, may be stabilized by longer range interactions [2–6]. This issue has been given added urgency by recent advances in trapping and cooling of atoms [7] and molecules [8] with large dipole moments.

Ultracold dipolar bosons, in one-dimensional optical lattices can be described by the Hamiltonian

$$H = -t\sum_i (b_i^\dagger b_{i+1} + \text{H.c.}) + \frac{U}{2}\sum_i n_i(n_i - 1) + \sum_{i,r>0} \frac{V}{r^3} n_i n_{i+r}, \quad (1)$$

where we assumed that the dipoles are polarized by an external field perpendicular to the lattice. The three parameters appearing in the Hamiltonian can be tuned independently in experiments [2]. The conventional phases of this system at *integer filling* are known from mean field studies [2,3]. They include the Mott insulator (MI) at large U, a density wave (DW) for large V, and a superfluid (SF) for large t.

In this Letter we use the density matrix renormalization group (DMRG) method [9] to show that a new gapped insulating phase with nontrivial structure obtains in a wide parameter regime between the two conventional insulators. The new phase is separated from the conventional insulators by lines of second order transitions and is found to possess particularly subtle order that is revealed only by highly nonlocal string correlation functions. Correlations of similar nature exist in the Haldane gapped [10] phase of quantum spin-1 chains [11,12]. We shall therefore term the new phase as the Haldane Bose insulator (HI). The analogy can be made more explicit by truncating the Hilbert space of the Bose system to three occupation states per site (for example, for a system with $\bar{n} = 1$ particles per site, we keep only the occupation states $n = 0, 1, 2$ for every site). This defines an effective spin-1 model with $S_i^z = n_i - \bar{n}$ and $\bar{n}$ the average filling. In this space the DW phase corresponds to antiferromagnetic ordering of the pseudospins in the z direction. The MI ground state, on the other hand, includes a large amplitude of the state with $S_i^z = 0$ on every site and small admixture of states containing tightly bound particle-hole fluctuations ($S^z = \pm 1$ on nearby sites). The Haldane phase may also contain mostly sites with $S^z = 0$ at large U, but the ordering of the fluctuations is unusual. The string correlations imply that particle and hole fluctuations appear in an alternating order along the chain separated by strings of zeros of arbitrary length [11,12]. The truncation to three states is justified only at large U when fluctuations in site occupancy are strongly suppressed. However, from the numerical results we conclude that the long-ranged string order of the actual bosons survives fluctuations in the occupancy beyond the effective spin-1 description.

After a description of the DMRG results, we will show how the new phase can be detected experimentally. The challenge lies in the fact that standard experimental probes couple to local observables and are blind to the highly nonlocal string correlations. We shall therefore look for signatures of the new phase in the excitation spectrum rather than the ground state properties by considering the response to lattice modulation [13]. We develop an approximation scheme that enables us to calculate the response functions in all three insulating phases. We predict a sharp resonance in the absorption due to a neutral collective mode ($S^z = 0$ in the pseudospin terminology), that is special to the Haldane insulator and can serve to identify this phase.

Numerical results.—We investigate ground state and lowest excitations of the Hamiltonian (1) in a space of the parameters U and V using the DMRG algorithm [9]. Throughout we consider a filling of $\bar{n} = 1$ particles per site in the ground state. The maximal length of the system is $N = 256$ sites, and up to $M = 200$ states are kept per block. In most of the parameter regime we found that the results do not change significantly when the cutoff in boson occupation number per site is increased beyond 4. The $1/r^3$ interactions was included up to the next nearest neighbor range. Open boundary conditions were used, and opposite external chemical potentials were applied on the first and last site in order to lift the ground state degeneracy in the HI and DW phases.

The phase diagram of (1) in the (U, V) plane is shown in Fig. 1. The nature of the phases in the DMRG simulation was elucidated by a direct calculation of the ground state correlation functions:

$$R_{\mathrm{SF}}(|i-j|) = \langle b_i^\dagger b_j \rangle, \tag{2}$$

$$R_{\mathrm{DW}}(|i-j|) = (-1)^{|i-j|}\langle \delta n_i \delta n_j \rangle, \tag{3}$$

$$R_{\mathrm{string}}(|i-j|) = \langle \delta n_i e^{i\pi \sum_{k=i}^{j} \delta n_k} \delta n_j \rangle. \tag{4}$$

Here $\delta n_i \equiv n_i - \bar{n}$. The superfluid phase is characterized by a power law decay of $R_{\mathrm{SF}} \propto |i-j|^{-1/2K}$ with Luttinger parameter $K \geq 2$. In the MI phase, all the correlation functions decay exponentially to zero. In the DW phase $R_{\mathrm{DW}}(|i-j|)$ approaches a constant at long distances [note that also $R_{\mathrm{string}}(|i-j|) \rightarrow \mathrm{const} \neq 0$], and the lattice translation symmetry is spontaneously broken. In analogy to the $S = 1$ XXZ chain [11,12,14,15], we expect the appearance of another phase (the Haldane phase) between the MI and DW phases. This phase is characterized by $R_{\mathrm{string}}(|i-j|) \rightarrow \mathrm{const} \neq 0$, while the DW correlations decay exponentially. Unlike the density wave phase, this phase does not break the lattice translation symmetry. It does, however, break a hidden Z_2 symmetry related to the string order parameter [12,16]. Figure 2(a) presents an example of how the phase boundaries were determined: we show the string and DW order parameters (defined as the square root of the asymptotic values of the corresponding correlation functions) as a function of V along the line $U = 6t$. The phase transitions from MI to HI and from HI to DW are clearly visible and seem to be of second order.

The phase diagram does not change qualitatively if we keep only the nearest-neighbor interactions in (1). However, further range interactions act to frustrate the DW order and thereby widen the domain of the HI phase. We note that previous DMRG studies of the Bose-Hubbard model with nearest neighbor interaction [17] did not look for the string correlations and therefore did not find the subtle HI phase.

In addition to the ground state, the energies of the first few excited states were calculated. The gap to the first excited state with the same number of particles as the ground state, $\Delta_0 = E^{(1)}_{\delta n=0} - E^{(0)}_{\delta n=0}$, was calculated by targeting also the first excited state in the DMRG calculation. Here δn is the number of particles relative to a state with exactly $\bar{n} = 1$ particles per site. The charge gap of the system $\Delta_1 = E^{(0)}_{\delta n=1} + E^{(0)}_{\delta n=-1} - 2E^{(0)}_{\delta n=0}$ was calculated by targeting the ground states of the $\delta n = \pm 1$ sectors.

The gaps Δ_0, Δ_1 along the line $U = 6t$ in the (U, V) plane are shown in Fig. 2(b). At the transition point between the MI and HI phases, both Δ_0 and Δ_1 vanish, while at the transition between the HI and DW phases only Δ_0 vanishes. This indicates that both transitions are second

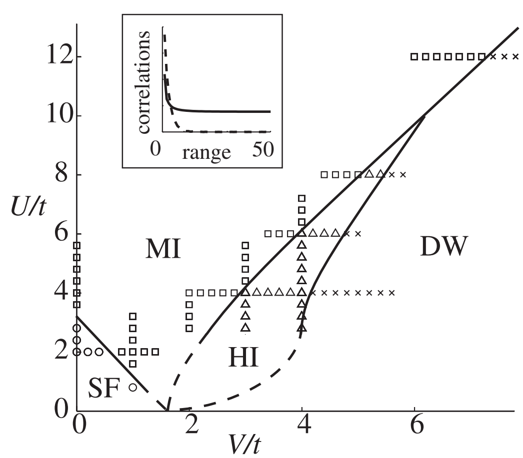

FIG. 1. Phase diagram of the Hamiltonian (1) in the (U, V) plane, obtained from DMRG. The phases that appear in the diagram are: superfluid (○), Mott insulator (□), density wave (x) and Haldane insulator (△). Inset: density wave (dashed line) and string (solid line) correlations at a particular (U, V) point [see (3) and (4),]. This point is in the HI phase, as can be seen from the fact that string correlations do not decay, whereas DW correlations decay rapidly.

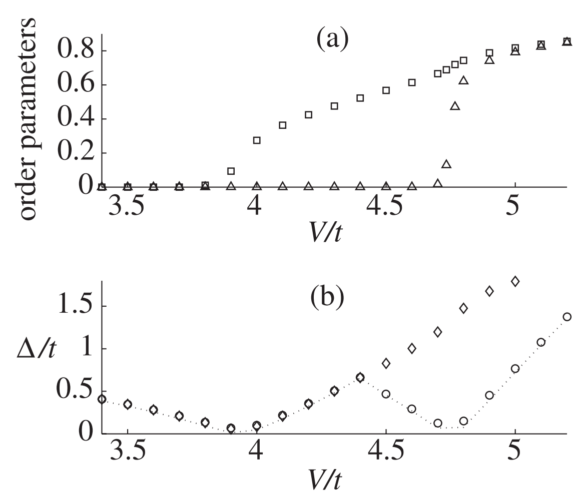

FIG. 2. (a) DW order parameter (△) and string order parameter (□) as a function of V along the line $U = 6t$. (b) Gaps to neutral and charged excitations, Δ_0 (○) and Δ_1 (◇), respectively, (see text) along the same line.

order, but the nature of the critical excitations at the transition is different.

In the MI phase, the lowest excitations are particle and hole excitations. This is clear from the fact that $\Delta_1 = \Delta_0$; i.e., the first excitation with $\delta n = 0$ is an unbound particle-hole pair. The gaps to these particle and hole excitations vanish at the transition to the HI. The Haldane phase displays another low-energy excitation. In a certain region of the phase diagram Δ_0 goes below the charge gap indicating the presence of a genuine *neutral* mode with $\delta n = 0$. In Fig. 2(b) the crossing point between the two states is clearly seen as a cusp in the Δ_0 curve near the middle of the HI phase region. At the transition to the DW phase, only the neutral gap vanishes. The presence of the neutral mode seems to be characteristic of the Haldane phase, and can be used to detect it, as will be discussed below.

Experimental detection.—In the numerical simulation we were able to establish the presence of the string ordered insulating phase HI by measuring the nonlocal ground state correlations (4) directly. By contrast, experimental probes naturally couple to local operators, such as the charge density. Our detection strategy will focus on probes of the excitation spectrum, which may exhibit distinct (albeit indirect) signatures of the HI phase.

Let us consider in some detail the response to parametric excitation of the optical lattice. This technique was used successfully to probe the excitations in both the MI and SF phases [13]. The idea is to apply a periodic modulation of the lattice intensity. Within the lowest Bloch band this perturbation simply corresponds to uniform modulation of the hopping matrix element in (1). The perturbed Hamiltonian can be written as $H + h\cos(\omega t)\hat{T}$, where $\hat{T}$ is the kinetic energy operator $\hat{T} = \sum_i b_i^\dagger b_{i+1} + \text{H.c.}$. Within linear response, the absorption rate is

$$I(\omega) \sim \sum_\alpha |\langle\psi_\alpha|\hat{T}|\psi_0\rangle|^2 \delta(\omega_{\alpha 0} - \omega). \tag{5}$$

We shall calculate $I(\omega)$ within the effective spin-1 Hamiltonian

$$H = J\sum_i (S_i^+ S_{i+1}^- + \text{H.c.}) + \sum_i V S_i^z S_{i+1}^z + \frac{U}{2}(S_i^z)^2, \tag{6}$$

using the corresponding perturbation operator $\hat{T} = \sum_i S_i^+ S_{i+1}^- + \text{H.c.}$ The mapping to a spin model amounts to projecting (1) on the subspace including only three occupation states per site ($\delta n_i = 0, \pm 1$). This is justified in the insulating phases at large U, where multiple particle or hole occupancy is suppressed. The U term in (6) corresponds to on site interaction, V to nearest neighbor interactions, and J to boson hopping. The projection of the hopping term in (1) gives another contribution to the spin model, that breaks the particle-hole symmetry. Omitting this term, as we have done in (6), does not lead to qualitative changes in the phase diagram. The advantage in using the model (6) is that it is amenable to a mean field theory, developed by Kennedy and Tasaki [12], that captures all three insulating phases.

Kennedy and Tasaki introduced a nonlocal unitary operator that transforms the string correlation (4) to conventional spin correlations $\langle S_i^z S_j^z\rangle$, which admit a local mean field treatment. At the same time the Hamiltonian (6) assumes a rather unusual, but nevertheless local form:

$$\tilde{H} = -J\sum_j S_j^x S_{j+1}^x - S_j^y \exp(i\pi S_j^z + i\pi S_{j+1}^x) S_{j+1}^y - V\sum_j S_j^z S_{j+1}^z + \frac{U}{2}\sum_j (S_j^z)^2. \tag{7}$$

The $U(1)$ symmetry of the original Hamiltonian seems to have been broken down to $Z_2 \times Z_2$. In fact the full $U(1)$ symmetry is preserved but is generated by a highly nonlocal operator in the new representation.

The mean field theory of (7) consists of finding the best site-factorizable wave function for this Hamiltonian. The solutions are of the general form [12] $|\Psi\rangle = \prod_i(\cos\theta|0\rangle_i \pm \sin\theta|\pm 1\rangle_i)$. The resulting phase diagram is shown in the inset of Fig. 3. In the Haldane phase $0 < \theta < \pi/2$ and the ground state is fourfold degenerate, which reflects broken $Z_2 \times Z_2$ symmetry. θ is given explicitly by the expression $\cos^2\theta = (U - 2V + 4J)/(8J - 2V)$. The DW phase is characterized by $\sin\theta = 1$, i.e., doubly degenerate ground state. Finally, in the MI there is a nondegenerate ground state with $\cos\theta = 1$. The fact that the superfluid phase is pushed to negative V is an artifact of the projection to three occupation states.

The collective excitations are found, following a standard scheme [18], by quantizing the small fluctuations around the mean field minima. We obtain an effective

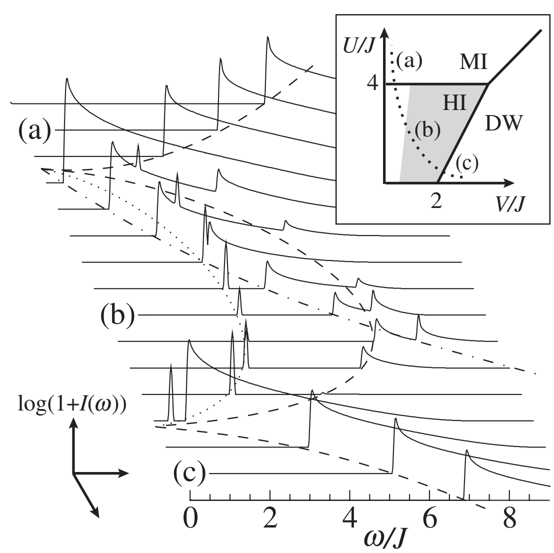

FIG. 3. Absorption spectrum (5) calculated from the mean field theory along the dotted line in the inset [mean field phase diagram of (7)]. The dotted line in the spectra marks the position of a quasiparticle peak seen only in the HI phase (b). The dashed and dash-dotted lines mark the edges of two particle continua.

Hamiltonian of the form $H_{\rm eff} = \sum_{\alpha k} \omega_{\alpha k} \beta^\dagger_{\alpha k} \beta_{\alpha k}$ for the two collective modes $\beta_{\alpha k}$ ($\alpha = 1, 2$). Likewise, we expand the perturbation $\hat{T}$ in terms of the collective mode operators. Finally, we compute $I(\omega)$ using (5).

Figure 3 displays the results at different points along a line in the (U, V) plane that cuts through the three phases. As expected, we see the gap in the spectrum closing at the two quantum phase transitions. The most distinct signature of the Haldane phase is a delta-function peak in the absorption spectrum corresponding to creation of a single quasiparticle. This resonance can serve as a "smoking gun" experimental evidence of the HI phase. The fact that this quasiparticle couples to $\hat{T}$, which does not change particle number, suggests that it must be a neutral excitation (quantum number $\delta n = 0$). Similarly, we infer that the other quasiparticle, which does not couple to $\hat{T}$, is a charged mode. The other two peaks seen in the spectra are the bottom edges of the two particle continua corresponding to a pair of "charged" and a pair of neutral excitations, respectively.

While the mean field treatment is approximate and cannot be expected to capture details such as the location of phase boundaries, it agrees with the DMRG results on the qualitative features. In both calculations the signature neutral mode is below the particle-hole continuum in a wide region inside the HI phase [see Fig. 2(b) and 3, gray region in the inset]. The mean field theory also captures the fact that only the neutral mode becomes critical at the transition from the HI to the DW state. Because of the lattice symmetry breaking in the DW phase, we expect a neutral excitation with momentum $k = \pi$ to drop to zero energy at the transition to this phase. This mode is adiabatically connected to the $S^z = 0$ magnon of the spin-1 Heisenberg chain. However, it cannot be identified with the delta-function peak in Fig. 3, because the operator $\hat{T}$ couples only to $k = 0$ excitations. The delta-function peak is therefore interpreted as a $k = 0$ bound state of two such $k = \pi$ excitations. A single $k = \pi$ excitation will show up as a sharp peak in Bragg spectroscopy [19], in which the lattice is modulated with another laser of wave vector $k = \pi$.

We now discuss the possibility of realizing the HI phase experimentally in a system of ultracold atoms in a one-dimensional optical lattice. From Fig. 1 we see that this requires $V \sim U$. This condition can be expressed in terms of the elastic scattering length, a_s, and the effective scattering length associated with a dipole d, $a_d = -md^2/4\pi\hbar^2$. For a typical optical lattice potential, with wavelength k_L and effective depth of the order of $10E_R$ [$E_R = (\hbar k_L)^2/2m$], we estimate [20] $U \approx 12(k_L a_s)E_R$. The nearest neighbor interaction energy is $V = d^2/r^3 \approx d^2 k_L^3/\pi^3$ and therefore the condition $V \sim U$ is equivalent to $|a_d| \sim 30 a_s$. Since the typical scattering length of atoms is of the order of tens of angstroms, we need an effective dipole scattering length of order 1000 Å. Dipoles of this magnitude can be obtained with ultracold dipolar molecules [21]. Alternatively, it might be possible to use Cr atoms with $a_d \approx 6$ Å if the other energy scales t and U are reduced proportionally. Of course, the temperature would have to be lowered to the same scale, below the gap $\Delta \sim t \sim V$ seen in Fig. 2(a). This is achieved automatically by adiabatic cooling as the optical lattice potential is increased slowly to the desired value. The fact that the HI phase is incompressible implies that in the presence of a harmonic confinement it will form a plateau structure, similar to the usual Mott insulator.

Discussion and conclusions.—We have shown that addition of further range interactions to the Bose-Hubbard model can give rise to a new insulating phase with nonlocal string order, analogous to the Haldane gapped phase of integer spin chains. The new phase can be realized in systems of ultracold dipolar atoms or molecules in optical lattices. We predicted unique signatures of the new phase in the parametric excitation spectra. These include low-energy critical excitations that appear near the phase transitions to the conventional phases, and a sharp resonance in the response seen only in the new phase.

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