Hidden order in bosonic gases confined in one-dimensional optical lattices

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Abstract. We analyze the effective Hamiltonian arising from a suitable power series expansion of the overlap integrals of Wannier functions for confined bosonic atoms in a one-dimensional (1D) optical lattice. For certain constraints between the coupling constants, we construct an explicit relationship between such an effective bosonic Hamiltonian and the integrable spin-$S$ anisotropic Heisenberg model. The former results are therefore integrable by construction. The field theory is governed by an anisotropic nonlinear $\sigma$-model with singlet and triplet massive excitations; this result holds also in the generic non-integrable cases. The criticality of the bosonic system is investigated. The schematic phase diagram is drawn. Our study sheds light on the hidden symmetry of the Haldane type for 1D bosons.

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1. Introduction

Systems of cold atoms trapped in optical lattices provide a remarkable tool to simulate quantum many-body physics in engineered quantum systems [1, 2]. In this context, new perspectives are provided by the ability to handle atoms or molecules with large dipole moment [3]. For these systems, the Bose–Hubbard models can be employed [4], provided that processes arising from the long-range interaction are considered. The corresponding ‘extended’ Bose–Hubbard Hamiltonian can display a variety of quantum phase transitions between superfluid and Mott insulator (MI) states (for instance see [5]).

Recent investigations by Altman and co-workers indicate that a strongly interacting bosonic system can display a further gapped phase with ‘exotic’ order [6]. Based on numerical analysis of a Bose–Hubbard type model, such a phase was shown to be characterized by a non-local hidden order of the Haldane type. Originally discovered in spin systems [7, 8], Haldane phases are believed to play a crucial role in many different contexts, including quantum chromodynamics (QCD) [10] and high-\(T_C\) superconductivity [11]. Recently, the hidden order was noticed also in different types of electronic insulator [12, 13].

Evidence for the Haldane order in the bosonic systems was obtained by rephrasing the physical concepts provided for the study of the hidden order for spin systems. Although Altman and co-workers constructed a variational scenario in order to interpret their results, it is desirable to trace how the bosonic hidden order emerges from the Haldane order in spin systems. This is a major purpose of the present work.

Based on exact methods, we construct a precise relationship between the bosonic and spin hidden orders. Relying on this, the quantum criticality of the bosonic system is investigated. We construct the nonlinear-\(\sigma\) model (NL\(\sigma\)M) that describes the system at long wavelengths. The phase diagram is investigated within the saddle point approximation of the NL\(\sigma\)M. Our results shed light on the structure of the hidden order in bosonic systems, suggesting that the bosonic excitations in the Haldane insulator (HI) are of triplet nature.

The paper is organized as follows. In section 2, we derive the model Hamiltonian from the microscopic dynamics of a dilute system of interacting dipolar bosons. The emerging Hamiltonian defines a type of extended Bose–Hubbard model of interacting bosons in the lowest Bloch band. In section 3, we establish the mapping between the bosonic model and the integrable higher spin-\(S \ XXZ\) Hamiltonian [18] (see equations (4)–(10)). Because of the integrability of the spin model, the bosonic Hamiltonian is integrable by construction as long as
Figure 1. Saddle-point phase diagram for the NLσM. Based on the behavior of the gaps (inset), the different phases are identified through the indications we reported in the text; the small offsets in the decay of $\Delta_z$ and $\Delta_\perp$ are artefacts of the saddle-point approximation. The plot corresponds to $t = 15/4$. Along the orange continuous line $U_1 = 1 + kU_0$ the lattice model (2) is integrable. The green-dotted continuous line indicates the degeneration of the gaps, $\Delta_z = \Delta_\perp$ (a similar phenomenon was evidenced for $S = 1$ [28, 29, 31]). Inset: behavior of the gaps $\Delta_z$ (dashed lines) and $\Delta_\perp$ for $U_0 = 1$ and for different $t$ (the leftmost blue lines correspond to $t = 15/4$, and the red lines to $t = 23/4$). For increasing $t$ the HI is shrunk.

the microscopic parameters entered into it fulfill certain relations (see equation (11)). Relying on this result, the quantum criticality of the bosonic system is investigated in section 4, where we construct the NLσM that describes the system at long wavelengths. The phase diagram is constructed, beyond integrability, within the saddle-point approximation of the NLσM (see figure 1; we note that the results are not restricted by equation (11)). In section 4, we discuss and suggest experimental protocols to detect the Haldane insulating phase. Finally, we draw our conclusions.

2. The bosonic model Hamiltonian

We start by analyzing the order of magnitude of the amplitudes involved in the one-dimensional (1D) Lattice Hamiltonian for trapped bosonic atoms; we include dipole–dipole interaction. We will obtain an effective model with density–density interaction and higher-order hopping processes. The general Hamiltonian for the atomic (of mass $m$) gas reads $\hat{H} = H_0 + H_{\text{int}}$ with

$$H_0 = - \int d\vec{r} \hat{\Psi}^* (\vec{r}) \left[ \frac{\hbar^2}{2m} \nabla^2 - V (\vec{r}) \right] \hat{\Psi} (\vec{r}),$$

$$H_{\text{int}} = \int d\vec{r} \int d\vec{r}' \hat{\Psi}^* (\vec{r}) \hat{\Psi}^* (\vec{r}') V_{\text{int}} (\vec{r} - \vec{r}') \hat{\Psi} (\vec{r}') \hat{\Psi} (\vec{r}),$$

(1)
where \( V \) results from a combination of harmonic confinement with the optical lattice, \( V = V_{\text{harm}} + V_{\text{lat}} \). We consider a 'cigar-shaped' configuration \( V_{\text{harm}} = m\omega^2(x^2 + y^2 + 2y^2z^2)/2 \), where the harmonic potential has a frequency \( \omega \) along the \( x \)-direction and is much more confined to an anisotropy factor \( \gamma \gg 1 \) in the \( y, z \)-directions. The 1D lattice, \( V_{\text{lat}} = sE_r \sin^2(\pi x/a) \), is arranged along the \( x \)-direction. \( E_r = (\hbar^2 \pi^2/2a^2m) \) is the photon recoil energy, \( a \) is the lattice spacing and \( s \) measures the optical lattice depth in terms of \( E_r \).

The interaction potential \( V_{\text{int}} = V_{\text{sr}} + V_{\text{dd}} \) contains two terms: an 'on-site' short-range potential \( V_{\text{sr}}(\vec{r}) = 4\pi\hbar^2a_{\text{BB}}\delta(\vec{r})/m \) characterized by the s-wave scattering length \( a_{\text{BB}} \); and a 'long-range' anisotropic dipole–dipole potential \( V_{\text{dd}}(\vec{r} - \vec{r}') = \mu_0\mu^2(1-3 \cos^2 \theta)/(4\pi |\vec{r} - \vec{r}'|^3) \), \( \mu \) being the atomic magnetic dipole \( (\mu_0) \) is the vacuum magnetic permeability) and \( \theta \) being the angle of \( \vec{r} - \vec{r}' \) with the dipole's orientation.

The bosonic field operator can be realized through Wannier functions \( w(\vec{r} - \vec{r}_i) \) localized around \( \vec{r}_i \); \( \hat{\Psi}(\vec{r}) = \sum_i b_i w(\vec{r} - \vec{r}_i) \), where \( b_i \) annihilates a boson at the lattice site \( i \). In this formalism, the Hamiltonian reads

\[
H = \sum_{i,j} t_{ij} b_i^\dagger b_j + \sum_{ijkl} t_{ijkl} b_i^\dagger b_j^\dagger b_k b_l, \quad \text{where} \quad t_{ij} \text{ and } t_{ijkl} \text{ are the standard Wannier functions integrals} \ [1].
\]

They can be expanded as power series of the so-called 'lattice attenuation parameter' \( \varepsilon \equiv \exp(-a^2/4l_{\text{opt}}^2) = \exp[-(\pi/2)^2\sqrt{\varepsilon}] \), with \( l_{\text{opt}} = a/(\pi s^{1/4}) \ll a \ [2] \); \( w(\vec{r} - \vec{r}_i) \) are assumed to factorize, \( w(\vec{r} - \vec{r}_i) = w(x - x_i)w(y)w(z) \) and approximated as \( w(v) = (\pi^{-1/4}e^{-v^2/2})\exp(-v^2/2l_{\perp}^2) \), \( v = x, y, z \), with \( l_{\perp} \equiv l_{\text{opt}} \) and \( l_{x} = l_{z} = l = (\hbar/m\gamma\omega)^{1/2} \).

The effective lattice (grand canonical) Hamiltonian emerging from the analysis above is

\[
H_b = -\kappa \sum_i n_i - t \sum_i b_i^\dagger b_{i+1} + U_0 \sum_i n_i(n_i - 1)
+ U_1 \sum_i n_i n_{i+1} - t_c \sum_i (n_i + n_{i+1}) b_i^\dagger b_{i+1}
+ t_p \sum_i (b_i^\dagger)^2 b_{i+1}^2 + \cdots,
\]

(2)

where \( n_i = b_i^\dagger b_i \) is the number operator. Terms in the ellipses involve higher powers in \( \varepsilon \) (see also [14]). The first two terms, with \( \kappa \) being the chemical potential and \( t \) the nearest neighbor hopping (in units of \( E_r \)), are the only low-order terms from \( H_b \) since the matrix elements \( t_{ij} \) decrease as \( e^{|i-j|} \). \( U_0 = (2/\pi)^3 a_{\text{BB}}a^2s^{1/4}/l_{\perp}^2 \) is the on-site interaction neglecting the renormalization due to \( V_{\text{dd}} \) (that is of the order of \( \varepsilon^2 \)). Defining \( I_{\text{dd}} = m\mu_0\omega^2/(2a^3\hbar^2) \), the contributions of \( V_{\text{dd}} \) to the integral \( t_{ii+1;i;i+1} \), the coupling constants in (2) read

\[
t_c = U_0\varepsilon^{3/2} + I_{\text{dd}}\varepsilon,
U_1 = 2t_p = (U_0 + I_{\text{dd}})\varepsilon^2.
\]

(3)

We comment that the (form of the) second-quantized Hamiltonian (2) is not affected by the Gaussian approximation of the Wannier function, which can only modify the expression of the coupling constants in (3).

Besides the density–density interaction \( U_1 \), \( H_b \) provides for correlated \( t_c \) and bosonic pair \( t_p \) nearest-neighbors hopping processes. It is important to note that experimentally there are different ways of manipulating the relative strength of the coupling constants, e.g. it is possible to change the optical lattice parameters [15], or use appropriate Feshbach resonances [16] to

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separately tune $I_{dd}$ and $U_0$, independently from the expansion in terms of the parameter $\varepsilon$. This opens the possibility of exploring a large portion of phase space.

Below we demonstrate that the 1D bosonic Hamiltonian (equation (2)) is obtained as large $S$ limit of the integrable spin model generalizing the XXZ model to higher spin [17]. This will prove that the model (2) is integrable (see, however, the discussion below (10)).

3. The integrable Heisenberg model for higher spin

Integrable XXZ models for higher spin [18, 19] were intensively studied in the framework of the quantum inverse scattering method [20]. The Hamiltonian ($E_i$ is assumed as the energy’s unit) is obtained as logarithmic derivative of the transfer matrix [21]

$$H_{XXZ} = -\sum_i \psi_\alpha [J(\alpha)_{i,i+1} + 1] + \psi_\alpha (1),$$

where

$$\psi_\alpha [x] = \Gamma'_\alpha (x) / \Gamma_\alpha (x),$$

$$\Gamma_\alpha (x) = (1 - e^x)^{1-x} \prod_{n=0}^{\infty} [1 - e^{x(n+1)}]/[1 - e^{x(n+1)}],$$

reducing to the ordinary gamma function for $\alpha \to 0$. The quantity $J(\alpha)$ is related to the (co-product $\Delta$ of) Casimir operator $C_S = S^+S^- + \sinh \alpha S^z \sinh (S^z + 1)/\sinh^2 \alpha$ of the quantum algebra $su_\alpha (2)$ underlying the integrability of the theory

$$\Delta C_S = \frac{\sinh \alpha J(\alpha) \sinh \alpha (J(\alpha) + 1)}{2 \sinh^2 \alpha}.$$ (6)

We remark that the anisotropy $\alpha$ enters into (4), deforming both the gamma function and the ‘representation’ $J(\alpha)$ of $su_\alpha (2)$.

The limit of large $S$, with small $\alpha S$, is interesting for us. The first ‘effect’ of this limit is that the $\psi_\alpha (x)$ in (4) reduces to the ordinary digamma function $\psi (x) = \Gamma'(x)/\Gamma (x)$. In this limit the quantity $J(\alpha)$ can be obtained explicitly by resorting to the explicit expression of $\Delta C_S$

$$\Delta C_S^{(i,i+1)} = e^{\alpha S_i^z} \left[ \frac{1}{2} S^+_{i+1} S^-_{i+1} + \sinh \alpha S_i^z \sinh \alpha S^z_{i+1} \frac{\cosh \alpha S \cosh \alpha (S + 1)}{\sinh^2 \alpha} \right] e^{-\alpha S_i^z}.$$ (7)

By retaining the terms up to the second order in $\alpha S$, we obtain

$$\Delta C_S^{(i,i+1)} = S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \lambda S^z_i S^z_{i+1} + \frac{\alpha^2}{2} ((S^x_i)^2 + (S^y_{i+1})^2) + S(S + 1),$$ (8)

where $\lambda = 1 + \alpha^2 k$ with $k = S(S + 1) + 1/2$. By exploiting its relation with $\Delta C_S$, $J(\alpha)$ can be written as $1/S$ perturbative expansion, $J(\alpha)_{i,i+1} = A(\alpha)_{i,i+1} + B(\alpha)_{i,i+1} S$, to finally give

$$J(\alpha)_{i,i+1} = 2S + 1/2 \left[ -3\alpha^2/8 + (1 - 3\alpha^2/8) \left( \hat{b}_i^+ \hat{b}_{i+1} + \text{h.c.} \right) - (1 + 9\alpha^2/8) \left( \hat{n}_i + \hat{n}_{i+1} \right) \right].$$ (9)

The quantum lattice gas ($U_0 \to \infty$) can be obtained from the spin model following the procedure in [17].
where we used the Holstein–Primakoff realization of \( su(2) \) [22]. The bosonic model (2) is obtained, first by employing the Stirling formula for the asymptotics of the digamma function \( \psi(x) \approx \ln(x) \), then by expanding the equation resulting from (4) at second order in \( 1/S \)

\[
H_{\text{XXX}} = H_0 + \text{const.,}
\]

where \( \text{const.} = N \ln[S(2 + 3\alpha^2/4)] - N\psi(1). \) Translational invariance has been assumed. The spin \( S \) and the anisotropy \( \alpha \) are obtained by comparison of (10) with (2); \( S = t/(2U_0 + U_1), \) \( \alpha^2 = 2(U_0 - U_1)/(3U_1), \) with the constraints

\[
t_c = \frac{U_1}{2}, \quad t_p = \frac{2t_c - U_0}{2}, \quad \frac{(2U_0 + U_1)^2}{2} = \frac{8(2U_0 - 3U_1)^2}{8t^2}, \quad 8t^2U_1 = (2U_0 + U_1)^2.
\]

We note that only one parameter’s results are adjustable in (2) when achieved from (4); we remark that restrictions (11) can be achieved by tuning the relative strength of contact versus dipole interactions. The resulting one-parameter \( H_b \) is integrable by construction (see also [23]); the exact solution will be studied elsewhere. In the isotropic case, \( \alpha = 0, \) \( H_b \) is obtained from the Faddeev–Takhtajan–Tarasov–Babujian model [24]. In this case, \( U_1 = 2U_0 = 2t^2 = 2t_c = 4t_p [25]. \)

The ground state of (4) is a singlet, \( S_{\text{tot}}^z = 0. \) For imaginary \( \alpha, \) the spectrum is gapless. For real \( \alpha, \) it was proved that the excitations are gapped [19]. Given the relation (10), it is intriguing to study the low-energy spectrum of \( H_{\text{XXX}} \) in the limit of large \( S. \) This is what we will do by exploiting the NL\( \sigma \)M.

4. NL\( \sigma \)M

As is customary, the large \( S \) limit is combined with the continuous limit \( a \to 0. \) The action

\[
\mathcal{S} = iS\omega[\Omega] + \int dt dx \mathcal{H}[\Omega](\tau, x) \quad \text{is obtained within the spin-coherent state path integral formalism,} \quad \mathcal{H}[\Omega] = \langle \Omega | H | \Omega \rangle \quad \text{and} \quad \omega[\Omega] \quad \text{is the Berry phase [22]}. \]

The semiclassical continuous Hamiltonian arising from gradient expansion of (4) is

\[
\mathcal{H} = \langle \Omega(x, \tau) | \Delta C_S[\Omega(x, \tau)] + \cdots \rangle, \quad \text{where the ellipses indicate terms with higher powers of} \quad a \quad \text{and} \quad 1/S, \quad \text{or combinations thereof}. \quad \mathcal{H} \quad \text{has the} \quad \lambda - D \quad \text{form with} \quad D = a^2. \]

The gradient expansion procedure spoils the integrability of the lattice model (10), since the \( t_c \) and \( t_p \) terms turn out of higher order in \( a [26]; \) nevertheless integrability manifests in the field theory in the form of the restriction \( \lambda = 1 + kD, \) with \( k = S(S - 1)/2 \), arising from the lattice theory. Generic values of \( \lambda, D \) can be considered through the \( 1/S \) expansion of the \( \lambda - D \) lattice model (that is not integrable), providing a different parameterization of the spin parameters in bosonic terms

\[
S = \frac{4t + 1}{8}, \quad \lambda = U_1, \quad D = U_0.
\]

The large-scale behavior of the system is captured by the large \( S \) realization of the coherent state spin variables in terms of staggered magnetization \( \vec{n}_j(\tau) \) and quasi-homogeneous \( \vec{l}_j(\tau) \) fluctuating fields through the Haldane mapping [7]

\[
\langle \Omega | \vec{S}_j(\tau) | \Omega \rangle = (-1)^j \vec{n}_j(\tau) \sqrt{1 - \frac{|\vec{u}_j(\tau)|^2}{S^2}} + \frac{\vec{l}_j(\tau)}{S},
\]

where \( |\vec{n}_j(\tau)| = 1 \) and \( \vec{l}_j(\tau) \cdot \vec{n}_j(\tau) = 0. \) The NL\( \sigma \)M description of (4) is obtained following a variation of the procedure originally adopted in [7, 29, 31] to deal with the \( S = 1, \lambda - D \).
model. Due to the anisotropy of the $\lambda - D$ model, we separate the staggered magnetization and its fluctuation in their perpendicular and transversal components, $\vec{n} = (\vec{n}_\perp, n_z)$ and $\vec{l} = (\vec{l}_\perp, l_z)$. In order to obtain the Lagrangian of the NL$\sigma$M, one needs to integrate out the $\vec{l}$ field in the Hamiltonian, together with the terms coming from the Berry phase. After taking the continuum limit one finds

$$\mathcal{L} = \frac{a^2}{2} \left[ S^2 |\partial_\perp \vec{n}|^2 + \frac{c_\perp}{2} |\partial_\perp \vec{n}|^2 \right] + \frac{a^2}{2} \left[ S^2 \lambda (\partial_z n_z)^2 + \frac{c_z}{2} (\partial_z n_z)^2 \right] + MS^2 n_z^2,$$

with $M = 1 + S(S - 1/2)U_0 - U_1$, plus the topological phase associated with the Néel field $\vec{n} = (\vec{n}_\perp, n_z)$

$$T = \frac{1}{4\pi} \int \! d\tau \, d\vec{x} \vec{n} \cdot (\partial_\perp \vec{n} \times \partial_z \vec{n}).$$

$T$ can assume only integer values, for it is the winding number of the mapping $\vec{n} : \mathbb{R}_{comp} \rightarrow S^2$, which is classified by the second homotopy group $\pi_2(S^2) = \mathbb{Z}$. $T$ contributes in the partition function as $e^{2\pi i TS}$, with $T \in \mathbb{Z}$, so that it does not contribute for integer spins. In equation (14), the Néel field satisfies the constraint $|\vec{n}|^2 = 1$. The coefficients are

$$c_\perp = 2 \frac{1 - n_z^2 (1 - U_1)}{\mu - M n_z^2 (2 - M n_z^2)},$$

$$c_z = \frac{\mu - 2n_z^2 (1 - U_1)}{\mu - M n_z^2 (2 - M n_z^2)},$$

with $\mu = 1 + U_1 + kU_0$. The coefficients provide an additional interaction between the components of the Néel field. For $M = 0$, equation (14) is the sum of an $O(2)$ NL$\sigma$M in the field $\vec{n}_\perp$ and a scalar model in $n_z$. The former describes a free Gaussian model with a bosonic compactified field, which is known to be a conformal field theory with central charge $c = 1$; the latter is also integrable.

One of the most striking features of the Haldane phase is that the gap is provided by a triplet structure [7, 27]. The masses of the particles $\Delta_\perp$ and $\Delta_z$ belong to the sectors $S_z = 0$ and $S_z = \pm 1$, respectively. For the case $S_z = 1$, $\Delta_z$ and $\Delta_\perp$ play the role of the excitations of a conformal field theory with $c = 1/2$ and $c = 1$, respectively [29]. Even though the Haldane order in the bosonic systems was made evident through a non-local ‘order parameter’ defined in analogy with the spin string order parameter [9], the phase diagram can also be studied by analyzing the low-energy properties of the system, and specifically the particle-hole $\delta \mathcal{E}_n$ and the neutral $\delta \mathcal{E}_n$ energy gaps [6]. We shall see that $\Delta_z$ and $\Delta_\perp$ play the role of $\delta \mathcal{E}_z$ and $\delta \mathcal{E}_n$, respectively.

To obtain such quantities from the continuous field theory, we treat (14) by saddle-point approximation ($S = 1$). The method assumes that $\langle n_z^2 \rangle := \zeta$. This means that $\|\delta n_j\|^2 - \delta n_j \delta n_{j+1} \ll 1$ with $\delta n = n - n$, indicating that only sparse charge-fluctuations around ‘diluted density wave (DW) states’ (so-called ‘zero defects states’ [30]) are considered. The constraint on the field $\vec{n}$ is taken into account by introducing a uniform Lagrangian multiplier $\eta$

$$\mathcal{L} = \frac{a^2}{2} \left[ \frac{v_\perp}{g_\perp} |\partial_\perp \vec{n}|^2 + \frac{|\partial_\perp \vec{n}|^2}{v_\perp g_\perp} \right] + MS^2 n_z^2 + \frac{a^2}{2} \left[ \frac{v_z}{g_z} \lambda (\partial_z n_z)^2 + \frac{(\partial_z n_z)^2}{v_z g_z} \right] + \eta(x, \tau)(|\vec{n}|^2 - 1),$$

where $v_\perp / g_\perp = S^2$, $v_z / g_z = S^2 \lambda$, and $1/(v_i g_i) = c_i/2$ with $i = \{\perp, z\}$. There are two poles in the propagators of the effective action, providing the expressions in terms of $\zeta$ for the gaps.
in the $z$ and in the perpendicular direction, respectively, $\Delta_z$ and $\Delta_\perp$, to be determined self-consistently [31]. In order to derive the expression for the gaps, we need to calculate the propagator. We substitute in the action the Fourier transform of the field $\mathbf{n}$ and of the Lagrange multiplier $\eta$, respectively, $\tilde{n}$ and $\tilde{\eta}$. After performing a Gaussian integration on the field $\mathbf{n}$, the effective action becomes

$$S[\tilde{n}] = \sum_{q,n,j} \{ \ln(K^{-1})^{ij} \} (q, n; q', n') - \tilde{n}(0, 0),$$

where $(K^{-1})^{ij}$ are the diagonal entries of the inverse propagator

$$(K^{-1})^{ij} = \frac{1}{\beta L} \left\{ \begin{array}{c} \delta_{nn'} \delta_{qq'} (\Omega_n^2 + q^2 v_j) - i \tilde{n} \varepsilon q \frac{\eta}{\beta L} (\Delta q, \Delta n') + \mu \delta_{j3} \\ \end{array} \right\},$$

with $\Delta q := q - q'$, $\Delta n := n - n'$ and $j = \{1, 2, 3\}$. The notation $v_j$, $g_j$ stands for $v_\perp$ if $j = \{1, 2\}$ or $v_z$ and $g_z$ if $j = 3$. $\Omega_n$ are the Matsubara–Bose frequencies, $\Omega_n = 2\pi n/\beta$. $(K^{-1})^{33}$ provides an expression for $\xi$.

With the ansatz $\tilde{n}(q, n) = (\beta L)\delta_{n0}\delta_{q0} \eta$, we can derive the saddle-point equation $(\partial S/\partial \eta = 0)$. For low temperatures $(\beta \to \infty)$ and in the thermodynamic limit $(L \to \infty)$ one finds

$$\left\{ \begin{array}{c} 1 = \frac{g_\perp}{\pi} \ln \left[ \Lambda \xi + \sqrt{\Lambda^2 \xi^2 + 1} \right] + \zeta, \\
\xi = \frac{g_z}{2\pi} \ln \left[ \frac{\Lambda}{\sqrt{\xi^{-2} + \nu^{-2}}} + \sqrt{\frac{\Lambda^2}{\xi^{-2} + \nu^{-2}} + 1} \right], \\ \end{array} \right.$$ (20)

where the ultraviolet cut-off $\Lambda$ is a free parameter to be determined by fitting the gap to the known value for the isotropic point $\Delta_{\text{iso}} = 0.41048$, where $\xi_\perp = \xi_z$. The notation stands for $\xi_{\gamma}^{-2} := 2g_\gamma \eta/\nu_\gamma$ with $\gamma = \{\perp, z\}$, $\xi_{\perp}^{-2} := \xi_z^{-2}/\lambda$ and $\nu_z^{-2} := 2M g_z/\nu_z$. The expressions for the gaps are

$$\left\{ \begin{array}{c} \Delta_\perp = v_\perp \xi_\perp^{-1}, \\
\Delta_z = v_z \sqrt{\xi_z^{-2} + \nu_z^{-2}}. \\ \end{array} \right.$$ (21)

We can solve the numerically self-consistent equations (20) for different values of $U_1$ and $U_0$, and of the spin $S$ (or equivalently $t$). From the numerical study of the gaps one can draw a (qualitative) phase diagram (see figure 1).

We see that $\Delta_z$ and $\Delta_\perp$ display behavior very similar to that of $\delta \xi_c$ and $\delta \xi_n$, respectively (see figure 1). In such a view, the phenomenology of the bosonic excitations in the HI would arise from the triplet nature of $\Delta_z$ and $\Delta_\perp$. In particular, the line $\delta \xi_c = \delta \xi_n$ that was evidenced numerically in [6] can be interpreted as the degeneracy of the triplet excitations of the field theory (14) (that includes the $O(3)$ model [27]).

Further insights into the criticality of the bosonic system can be obtained by adapting the results for the spin $S$, $\lambda = D$ model [32]. Specifically, the onset of the HI-density wave phase is suggested to be of the Ising type (second order), $c = 1/2$, and it is characterized by $\Delta_z = 0$ with $\Delta_\perp \neq 0$; the MI–HI phase transition is with $c = 1$ and it is caused by $\Delta_z \neq 0$ with $\Delta_\perp = 0$. Similar behavior of $\delta \xi_c$ and $\delta \xi_n$ was noticed in [6] (except that additionally $\delta \xi_c = 0$ was shown to vanish at the MI–HI transition). The DW phase–MI transition is predicted to be of the first order; the $c = 1/2$ and $c = 1$ lines meet in a point that is governed by the continuous limit of the $\alpha = 0$ integrable theory, with $c = 3S/(1 + S), S = 1/(2t)$ [33]. The phase diagram of the system is summarized in figure 1.

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5. Experimental feasibility

Although a detailed analysis would go far beyond the scope of the present paper, we would like to sketch a possible method that could serve for detecting the HI experimentally (complementing the observations in [6]). The basic idea relies on the detection of the atomic current, tracing back to the early experimental evidence of MI phase [34]; the MI conductivity is probed by applying a washboard potential to the lattice. A resonance in the atomic conductivity appears when the tilt between adjacent sites reaches the energy gap $U_0$, i.e. when it is resonant with the particle-hole pair excitation energy. Because of the peculiar solitonic non-local order [30] of the HI, the resonance peak in the conductivity is narrowed, as already noticed with a different experimental situation (parametric resonance) by the authors of [6]. Placing the bosonic chain in a washboard potential, the distinctive feature of the HI phase would be a dependence of the atomic current on the length of the chain (this is the analogue of the diffusive spin transport evidenced in Haldane compounds [35]). We observe that, being an incompressible phase, the HI is expected to be robust to the parabolic confinement whenever the induced total energy offset (between center and the trap edges) is of the order of the energy gap. Following the numerical indications provided in [6], this gap is estimated to be of the same order of magnitude as the MI's, $\Delta \approx t$. We can therefore estimate the magnitude of the allowed harmonic confinement to be $m \omega^2 x_M^2 < t = 2sE_r$, $x_M$ being the size of the condensate along the optical lattice. It would be interesting to trace the analogue for the HI of the ‘wedding cake’ structure that appears in MI in the presence of a strong confinement.

Finally, ring-shaped (with circumference $L$) optical lattices with twisted boundary conditions [36] could be exploited to show the HI in an expansion experiment (we note that the energy offset due to harmonic confinement can be minimized in this case). In fact, adapting the results obtained for the spin diffusion in twisted Heisenberg integer spin rings [37], the atomic density current would display a characteristic parametric dependence on the boundary twist; a sawtooth-like behavior for correlation length $\xi \gg L$, which would be exponentially suppressed, with sinusoidal oscillations for $\xi \ll L$. This could be a fingerprint of the Haldane gap for (finite) ultracold atomic systems.

6. Conclusions

By exploiting a suitable expansion of the matrix elements in terms of the lattice attenuation parameter $\varepsilon \ll 1$, we derived an effective model for bosonic atoms in a 1D lattice (2). Additional terms enter the Hamiltonian with respect to the standard Bose–Hubbard model. For one choice of the coupling constants, the model results are integrable through mapping with the spin-$S$-XXZ integrable model (see equation (10)). We note that the possibility of independently tuning the onsite interaction relative to the density–density interaction is available in the bosonic model Hamiltonian only in the presence of dipole–dipole interactions. This is precisely what allows degenerate quantum gases to explore different portions of the phase diagram beyond the MI region.

The direct relationship between the spin and bosonic pictures is exploited to investigate the critical properties of the bosonic systems. From the present work, it is suggested that the correct context is provided by the spin $S$, $\lambda$-$D$ model. The HI is investigated by studying the continuous field theory arising from gradient expansion of the lattice model; the Lagrangian has the form of an NL$\sigma$M with further interactions between the components of the Neel field (see...
equations (14) and (16)). We comment that the terms \( t_p \) and \( t_c \) entering (2) do not contribute to the NL\( \sigma \)M formulation, indicating that such terms are irrelevant for the criticality studied. Such an effect is a physical manifestation of the Affleck analysis [26]. The difference between integrable and non-integrable lattice theories is reflected in a different parameterization of the coupling constants entering the NL\( \sigma \)M. Interestingly, the integrable parameterization of the continuous model (14) we found should be closely related to the so-called principal chiral fields [38], indicating an emergent \( SU(2) \times SU(2) \) symmetry of the bosonic Haldane phase, but we notice that the phase diagram of the system (14) is investigated, beyond the integrability, by means of the saddle-point approximation; the integrable case might need separate discussion. The Haldane phase is found for any finite range of the interaction. This should be relevant for experiments where the scattering length can be tuned around zero, thus evidencing the interaction between light-induced dipoles [16].

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