Dynamical probing of a topological phase of bosons in one dimension

Emanuele G Dalla Torre

Department of Physics, Harvard University, Cambridge, MA 02138, USA
E-mail: emanuele@physics.harvard.edu

Received 18 December 2012, in final form 14 March 2013
Published 11 April 2013
Online at stacks.iop.org/JPhysB/46/085303

Abstract

We study the linear response to time-dependent probes of a symmetry-protected topological phase of bosons in one dimension, the Haldane insulator (HI). This phase is separated from the ordinary Mott insulator (MI) and density-wave (DW) phases by continuous transitions, whose field theoretical description is reviewed here. Using this technique, we compute the absorption spectrum to two types of periodic perturbations and relate the findings to the nature of the critical excitations at the transition between the different phases. The HI–MI phase transition is topological and the critical excitations possess trivial quantum numbers: they correspond to particles and holes at zero momentum. Our findings are corroborated by a non-local mean-field approach, which allows us to directly relate the predicted spectrum to the known microscopic theory.

1. Introduction

According to the Landau paradigm, any two phases with the same symmetries can be adiabatically connected through some path in parameter space (the best known example being the liquid and gas phases of water). For many years, the only counter-examples were the quantum Hall states, which do not break any local symmetry, but nevertheless cannot be connected without crossing a phase transition. In recent years, this phenomenon has been extended to a broader class of phases known as ‘topological band insulators’ [1–4]. Lacking a local order parameter, topological insulators may possibly be used to realize quantum circuits unaffected by the local sources of dissipation, such as disorder and time-dependent noise [5]. However, for the same reason, their experimental characterization is generally very hard: local probes are unable to distinguish the bulk of a topological insulator from the bulk of a conventional insulator.

This problem is usually overcome by studying interfaces between topological phases and trivial phases (such as vacuum), where protected edge states must appear. In the case of the integer quantum Hall states, the number of edge modes coincides with the number of filled Landau levels and leads to a quantized transverse conductance. Similarly, the appearance of topologically protected zero-energy modes at the boundaries between different phases constituted the first experimental evidence of topological insulators [6–8]. The second strategy consists in measuring non-local ‘string’ order parameters, characteristic of topological phases in one dimension. A proof-of-principle experiment has already been successfully demonstrated using ultracold atoms in optical lattices [9], following our predictions [10, 11].

In the context of ultracold atoms, a third alternative method consists in probing the dynamic response of the system in the vicinity of transitions between different phases [12, 13]. Here, we specifically refer to continuous phase transitions, which can be detected by the closing of a gap in the response to a local probe\(^1\). In the vicinity of these transitions, the low-frequency excitations hold information about the nature of the transition. In particular, because transitions between the topologically trivial and non-trivial phases do not break any local symmetry, their low-frequency excitations possess trivial quantum numbers. In contrast, if a transition breaks a particular symmetry, its low-frequency excitations possess the same quantum number as the order parameter of the symmetry-broken phase. Dynamical probes couple to these low-frequency excitations and may provide useful information about the nature of the transition.

\(^1\) Local probes do not couple distinct ground states across a first-order transition. As a consequence, the closing of a spectral gap in the response to a local probe is generically associated with continuous phase transitions.
In the case of translational invariance, for example, at the transition from a homogeneous phase to a density-wave (DW) phase, the critical excitations possess the same momentum as the DW order parameter. In contrast, at a topological phase transition the critical excitations possess zero momentum. Similarly, systems that conserve the total number of particles possess an additional $U(1)$ ‘gauge’ symmetry, which is spontaneously broken at the transition to a superfluid phase. At this transition the critical excitations are Bogoliubov quasi-particles, which do not conserve the total number of particles (or to be more precise, shift the number of particles by a non-integer amount). In contrast, at a transition between a normal and topological phase, the symmetry is preserved and, accordingly, the critical excitations carry an integer charge.

In this paper, we consider a particular example of one-dimensional symmetry-protected topological insulator, the ‘Haldane insulator’ (HI) [10, 11, 14, 15]. This phase arises in models of interacting bosons on a one-dimensional lattice, which are relevant to ultracold dipolar atoms [16] or molecules [17] and Rydberg atoms [18], in optical lattices [19]. These systems support additional phases that are topologically trivial, such as the Mott insulator (MI) and the DW phase. In the simplest DW phase, the density oscillates between even and odd sites, spontaneously breaking the discrete translational invariance modulo two lattice sites. As we will see, the dynamic response demonstrates that the critical excitations of the HI–DW transition are phonons at momentum $k = \pi$. In contrast, at the topological MI–HI transition the dynamic response demonstrates that the critical excitations are simply particles and holes at zero momentum.

This paper is organized as follows. In section 2, we describe the ground-state properties of the HI and present new numerical results aimed to characterize its low-lying excitations. In sections 3 and 4, we introduce the field theoretical description of the HI and use this method to predict the dynamic response of the system. Our findings are in contrast with the predictions of [10], obtained through a non-local mean field approach. In section 5, we show how to correctly apply the mean-field approach to obtain results consistent with the field-theoretical description. Section 6 concludes the paper with a summary of the results and an outlook to future research directions.

2. The Haldane insulator

Lattice bosons with non-local interactions can form a zoo of different phases with local order parameters, including superfluids (SF), DW, supersolids and dimerized phases (see for example [20–22]). Traditionally, the only phases without a local parameter were MIs at integer filling. These phases are topologically trivial because their ground states can be adiabatically deformed to site-factorizable states with an exact (integer) number of atoms per site ((11 11 11 . . . ), (22 22 22 . . . ), . . . states). In this sense, the MIs of bosons are analogous to the trivial band insulators of fermions. In [10], we found that non-local (short-ranged) interactions can stabilize a non-trivial topological phase, the HI.

In our theoretical study, we considered the one-dimensional Bose–Hubbard model with extended interactions:

$$
H = \sum_i \left[ -t(b_i^\dagger b_{i+1} + H.c.) + \frac{U}{2} n_i(n_i - 1) \right] + \sum_i \sum_{j=0}^{\bar{L}} V_j n_i n_{i+j}.
$$

Figure 1. Phase diagram of the extended Bose–Hubbard model (1) at filling of $\bar{n} = 1$ particles per site, as obtained by density matrix renormalization group (DMRG) calculations with $L_{\text{max}} = 256$ sites and $M_{\text{max}} = 250$ states per block. Inset: excitation gaps $\Delta_c$ and $\Delta_e$ (defined in the text) along the path $V/t = 6$. The phase transitions are located at the points in which the gap vanishes ($V/t \approx 4$ and $V/t \approx 4.75$).

At $V = 0$ and integer filling, the Bose–Hubbard model describes a quantum phase transition between neighbouring sites, the second term $U$ describes the effective interactions between atoms on the same site and $V_j$ describes non-local interactions. This model applies to atoms and molecules with fixed electric or magnetic dipoles [16, 17, 23], and to Rydberg atoms with induced dipoles [22]. For simplicity, we will assume that only the nearest-neighbour term $V_1 = V$ is non-zero. This assumption is not essential for the present analysis, provided that $V_j$ decays fast enough.

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lattice-inversion symmetry. In the presence of this symmetry, the HI cannot be adiabatically connected to a site-factorizable state. Remarkably, the lattice-inversion symmetry is trivially broken at the edges of the lattice, and therefore the HI does not have protected edge states.

Because both the MI and the HI do not break any local symmetry, they cannot be distinguished by any local order parameter. Exploiting an analogy to spin chains, we demonstrated that these two phases can nevertheless be characterized by two ‘string’ order parameters [11]. These order parameters are non-local in the sense that they consist of an infinite product of operators acting on different sites [28, 29]. Their experimental detection therefore requires the simultaneous measurement of all the sites in the lattice. Using new microscopic techniques for ultracold atoms [30, 31], the string order of the MI has been recently measured [9].

The existence of a string order is however specific to one dimension and, at the moment, does not seem to extend to other topological phases. In this paper, we present an alternative approach in probing the low-energy excitations of the different phases. It is therefore not specific to one dimension and can be easily generalized to higher dimensions. In one dimension, both methods apply and can be used to complement and verify one another.

**Elementary excitations**

As explained in the introduction, we propose here to study the topological properties of the Mott and Haldane phases by probing the low-energy excitations at the transition between the two phases. To characterize their nature, let us consider again the inset of figure 1. This graph shows two independent curves. One curve (diamonds) represents the ‘neutral gap’ \( \Delta_0 = E_{N=0}^{(1)} - E_{N=0}^{(0)} \), which is the gap to the first excited state with the same number of particles as in the ground state (\( \delta N = 0 \)). It was calculated by targeting the first excited state in the density matrix renormalization group (DMRG) calculation. The second curve (squares) represents the ‘particle–hole gap’ \( 2\Delta_p = E_{N=1}^{(0)} - E_{N=0}^{(0)} - 2E_{N=0}^{(0)} \), which was calculated by adding or subtracting one particle (\( \delta N = \pm 1 \)) and computing the new ground state.

At the MI–HI phase transition the particle–hole gap closes, indicating that at this point the energy needed to create a particle or a hole (‘the mass term’, in the field-theoretical terminology) becomes zero. At the HI–DW phase transition, on the other hand, the particle–hole gap remains open, indicating that the phase transition is due to a different type of excitation. We can easily guess the nature of these excitations by recalling that the HI–DW phase transition involves the spontaneous breaking of a local \( Z_2 \) symmetry, related to translational invariance modulo two lattice sites. In order to break this symmetry, the ground state has to mix with a phonon at the edge of the Brillouin zone (i.e. at momentum \( k = \pi \)), whose excitation gap must be closed at the phase transition.

To verify this hypothesis, we compute the overlap between the lowest excited state in the vicinity of the HI–DW phase transition and a trial wavefunction for a phonon at momentum \( k \):

\[
|\Psi_k^{\text{Phonon}}\rangle = \sum_j e^{ikx_j} \delta n_j |\Psi_{gs}\rangle.
\]

Here, \( |\Psi_{gs}\rangle \) is the ground state wavefunction as given by the DMRG algorithm and \( \delta n_j = n_j - \bar{n} \) is the difference between the local occupation and the average occupation \( \bar{n} \). As shown in figure 2, the numeric result confirms the existence of a large overlap with a phonon at momentum \( k = \pi \), supporting our assumption.

**3. Critical theory of the phase transitions**

The properties of any system near a continuous phase transitions do not depend on the details of the microscopic model and are determined by a universal critical theory. The critical theories of the MI–HI and HI–DW phase transitions were derived in [11] using a field-theoretical approach, the ‘bosonization of bosons’ [26, 27]. In what follows, we outline the properties of these theories, which will be used to compute the dynamic response of the system in section 4.

**MI–HI phase transition**

The critical theory of the MI–HI phase transition is described by the sine-Gordon model

\[
H = \int dx \left[ \frac{K}{2} (\partial_x \theta)^2 + \frac{1}{2K} (\partial_x \phi)^2 - g \cos(2\phi) \right].
\]

Here, the field \( \phi(x) \) measures the displacement of the particles with respect to a fixed lattice and is related to the particles’ density by \( n(x) \approx n_0 - (1/\pi) \partial_x \phi \), where \( n_0 = \bar{n}/a \), \( \bar{n} \) is...
the average number of particles per site and $a$ is the lattice constant. The field $\theta(x)$ is canonically conjugate to $n(x)$ and corresponds to the coherent phase of the bosons.

The quadratic part of the Hamiltonian (3) simply describes linear phonons, i.e. the Goldstone mode associated with translational invariance in one dimension. The unitless prefactor $K$ is non-universal and it varies along the MI–HI phase boundary. A renormalization group (RG) analysis [32] shows that, in order for a direct MI–HI phase transition to occur, $K$ must be bounded between 1/2 and 2. For $K > 2$, the MI and HI phases would be separated by a superfluid phase, and for $K < 1/2$, by a third gaped phase.

The cosine term in equation (3) describes the effects of the periodic potential (lattice). This term pins the field $\phi(x)$ to a fixed value, modulo $\pi$. The MI–HI phase transition corresponds to a change in the sign of the prefactor. In the MI, $g > 0$ and the field $\phi$ is pinned to zero, indicating that the particles are centred at the lattice sites. In the HI, $g < 0$ and $\phi$ is pinned to $\pi/2$. The particles are centred at the lattice bonds, and live in a coherent superposition of two (or more) neighbouring sites. A weak-coupling analysis leads to $g \approx n_0(U - V)$, indicating that the MI–HI phase transition is located approximately at $U = V$.

The low-energy excitations of the MI–HI phase transition correspond to jumps of $\pm \pi$ in the field $\phi(x)$, termed ‘kinks’ or ‘solitons’. Because the density of particles is proportional to the derivative of $\phi$, each kink involves the addition, or subtraction, of one particle. Using a perturbative RG approach it is possible to show that each kink increases the energy of the state by a charge gap $\Delta_c \sim g^{1/(2-K)}$. In addition, depending on the value of $K$, the kinks may either repel (for $K > 1$) or attract (for $K < 1$). In the former case, the neutral excitation gap is given by twice the energy cost of a kink, $\Delta_n = 2\Delta_c$. In the latter case, particles and holes form bound states (‘breathers’). Their total mass is lowered by the binding energy of the pair. In what follows, we consider only $1 < K < 2$, corresponding to intermediate values of the lattice depth.

The sine-Gordon model (3) is a useful representation of the critical theory of the MI–HI phase transition because it is exactly solvable. In particular, the matrix elements between the ground state and any excited state can be obtained following the ‘form factor’ approach introduced by Smirnov [33]. This approach relies on the exact expression for the scattering-matrix between kinks and breathers.

**HI–DW phase transition**

The transition from the HI to the DW phase breaks a local $Z_2$ symmetry. In [111] we showed that, indeed, this transition belongs to the universality class of the Ising transition in 1+1 dimensions. The critical theory of this transition is captured, for instance, by the spin-1/2 transverse-field Ising chain

$$H = \sum_i \left[ -\sigma_i^y\sigma_{i+1}^y + \lambda \sigma_i^z \right].$$

Here $\sigma_i^y$ and $\sigma_i^z$ are Pauli matrices. The model (4) shows a quantum phase transition at $\lambda = 1$ between a paramagnet, with zero magnetization $\langle \sigma_i^z \rangle = 0$, and a ferromagnet, with $\langle \sigma_i^z \rangle \neq 0$. The ferromagnet breaks the $Z_2$ symmetry, related to the rotation of $\pi$ around the $z$-axis. The transverse-field Ising model (4) has an exact solution in terms of free fermions, based on the Jordan–Wigner transformation [34, 35]. This mapping shows that the excitation gap vanishes linearly and symmetrically around the phase transition

$$\Delta = |1 - \lambda|.$$ 

The exact solution also shows that the nature of the low-energy excitations changes dramatically across the phase transition. In the paramagnetic phase, the low-energy excitations are local spin-flips, created by the operator $\sigma_i^z$. In the ferromagnetic phase, on the other hand, the elementary excitations are domain walls between spin-up and spin-down regions.

In the original Bose–Hubbard model, the paramagnetic and ferromagnetic phases correspond respectively to the HI and DW phases. The spin-up and spin-down states correspond to the two possible configurations of the DW ($\langle 02020 \ldots \rangle$ and $\langle 02020 \ldots \rangle$) leading to the mapping

$$\sigma_i^z \leftrightarrow (-1)^{m_i - \bar{n}_i}.$$ 

Equation (6) indicates that the low-energy excitations of the HI are density fluctuations (phonons) with momentum $\pi$. In contrast, the low-energy excitations of the DW phase are non-local domain walls.

**4. Dynamic probes: absorption spectra**

We now apply the above field-theoretical description to compute the dynamic response of the system in the vicinity of the MI–HI and HI–DW phase transitions. In particular, we focus on two specific perturbations: lattice modulations and Bragg spectroscopy at momentum $k = \pi$. As we will see, these perturbations are easily realizable with ultra-cold atoms and best capture the differences between the two transitions. The results obtained by this method are summarized in figures 3 and 4.

In an idealized version of the proposed experiment, the system is initially prepared in the ground state, a periodic
perturbation is applied with a frequency \( \omega \) for a given time \( t_{\text{pert}} \gg 1/\omega \), and finally the amount of absorbed energy \( \Delta t \) is computed by measuring the increase in temperature of the system. The absorption spectrum is defined as the ratio between the absorbed energy and the perturbation time \( t_{\text{pert}} \). According to the Fermi golden rule, this ratio is independent of \( \omega \) and \( \Delta \), and is equal to

\[
S(\omega) = \sum_a |\langle \psi_a | T | \Psi_{gs} \rangle|^2 (\epsilon_a - \epsilon_{gs}) \delta(\omega + \epsilon_{gs} - \epsilon_a).
\]  

Here \( |\Psi_{gs}\rangle \) and \( |\psi_a\rangle \) are, respectively, the ground- and excited-states of the unperturbed Hamiltonian, with energies \( \epsilon_{gs} \) and \( \epsilon_a \) (we work in units where \( \hbar = 1 \)). The operator \( T \) models the perturbation and will be derived below for two specific cases, denoted by \( T_{\text{hop}} \) and \( T_{k=\pi} \).

The first perturbation consists of small modulations of the lattice strength. It mainly influences the tunnelling matrix element between two neighbouring sites and corresponds to the operator

\[
T_{\text{hop}} \equiv \delta t \sum_i \left[ b_i^\dagger b_{i+1} + \text{H.c.} \right].
\]  

The second perturbation corresponds to the addition of a superlattice with a given momentum \( k \), which locally modifies both the tunnelling and the chemical potential. In the case of \( k = \pi \), the tunnelling is modulated uniformly along the lattice, while the chemical potentials of odd and even sites are shifted in opposite directions. The correspondent operator is the sum of (8) and

\[
T_{k=\pi} \equiv \delta \mu \sum_i (-1)^i \delta n_i,
\]

where \( \delta n_i = b_i^\dagger b_i - \bar{n} \). In the following, we will assume that Bragg spectroscopy is performed by modulating both the lattice and the superlattice in such a way that only \( T_{k=\pi} \) is applied.

**MI–HI phase transition**

The critical theory of the MI–HI phase transition can be expressed in terms of the sine-Gordon model (3). In this language, the modulation of the lattice corresponds to

\[
T_{\text{hop}} \approx \delta t \int dx \cos(2\phi).
\]  

This term creates kink–anti-kink pairs, corresponding to particle–hole excitations. The total energy of the pair is given by the sum of two positive terms: the chemical potential, \( \Delta_\sigma = 2\Delta_c \), and the kinetic energy of the pair. As a consequence, the resulting absorption spectrum \( S_{\text{hop}}(\omega) \) is non-zero only for frequencies \( \omega > 2\Delta_c \). The relevant matrix elements can be computed using the form-factor approach [33, 36, 37], leading to the formulas summarized in appendix A. Close to the lowest edge of the continuum \( 0 < \omega < 2\Delta_c \), the spectrum follows the power law

\[
S_{\text{hop}}(\omega) \sim (\omega - 2\Delta_c)^2.
\]  

Bragg spectroscopy, on the other hand, does not couple to the low-energy excitations of the MI–HI phase transitions. The critical excitations of this phase transition are particles and holes with zero momentum, while \( T_{k=\pi} \) couples only to excitations with total momentum \( k = \pi \). Thus, Bragg spectroscopy at momentum \( k = \pi \) does not show any particular low-frequency feature at the MI–HI phase transition, despite the closing of the gap. This observation will allow us to clearly distinguish between this transition and the HI–DW transition to be considered below.

**HI–DW phase transition**

The critical theory of the HI–DW phase transition is captured by the transverse-field Ising model (4). The operator \( T_{\text{hop}} \) corresponds to the term of the Hamiltonian (1) which stabilizes the HI, and therefore maps to the \( \sum_i \sigma_i^z \) term of equation (4) which stabilizes the paramagnetic phase. In appendix B, we show how to compute the response of this term by mapping equation (4) to a theory of free fermions, through the subsequent application of the Jordan–Wigner and Bogoliubov transformations. The resulting absorption spectrum is

\[
S_{\text{hop}}(\omega) \equiv \delta t \frac{\sqrt{\omega^2 - (2\Delta_n)^2}}{\omega} \Theta(\omega - 2\Delta_n).
\]  

Here, \( \Theta \) is the Heaviside theta function and \( \Delta_n = |1 - \lambda| \) is the neutral excitation gap. As explained in section 2, the gap \( \Delta_n \) separates the ground state from a phonon at momentum \( k = \pi \). Lattice modulations correspond to a translational invariant operator and can couple only to excitations with zero total momentum, such as, in this case, a pair of counter-propagating phonons. The absorption spectrum (12) shows a broad feature, corresponding to the continuum of two-particle excitations. This result is in contrast with the analysis of [10], which predicted the appearance of a sharp peak in the response to lattice modulations. As we will see in section 5, the mean-field approach can be fixed by a more accurate characterization of the elementary excitations.

The operator corresponding to Bragg spectroscopy (9) is a modulation of the local operator \( (-1)^i \delta n_i \), which corresponds to the order parameter of the symmetry-breaking phase and, in the effective Ising model, maps to the local magnetization \( \sigma_i^z \) (see equation (6)). In the paramagnetic phase (HI), this
operator couples directly to the low-energy excitations of the phase: spin-flips at zero-momentum. The corresponding matrix element can be computed through conformal field theory methods [38], leading to

$$S_{k=\pi}(\omega) \approx |\Delta|^{2\eta-1} \delta(\omega - \Delta_n).$$

(13)

Here, $\eta = 1/8$ is the anomalous dimension of the operator $\sigma^z$. The operator $T_{k=\pi}$ can additionally couple to any state with an odd number of spin-flips. Therefore, we expect a continuum of three-particle excitations in $S_{k=\pi}$ for $\omega > 3\Delta_n$.

In the DW phase (ferromagnet), the elementary excitations are domain walls in the ferromagnetic order parameter ($\sigma^z$). The operator $\sigma^z$ is local and can excite only an even number of domain walls. Thus, in this phase we expect a broad continuum, whose lowest edge is located at $\omega = 2\Delta_n$.

Figures 3 and 4 summarize graphically our findings for the MI, HI and DW phases. This model supports three gapped phases, the 'large-U', the Haldane and the Neel phases, corresponding respectively to the phase: spin-flips at zero-momentum. The corresponding operator couples directly to the low-energy excitations of the system. The narrow absorption peak in Bragg spectroscopy at the MI–HI and HI–DW phase transitions.

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5. Non-local mean field

We now present an alternative method to compute the dynamic response of the HI, based on a non-local mean field introduced by Kennedy and Tasaki [39]. This approach is valid deep in the gapped phase, and it complements the field-theoretical approach presented above, which is valid only in the vicinity of a phase transition.

The first step of this method is an approximate mapping between the HI and the Haldane gapped phase of spin-1 chains [10]. The mapping can be made explicit by truncating the Hilbert space of the Bose system to three occupation states per site (for example, for a system with $n = 1$ particles per site, we keep only the occupation states $n = 0, 1, 2$ for every site). This defines an effective spin-1 model with $S_i^z = n_i - \bar{n}$. If we neglect particle–hole symmetry breaking terms, the analogous spin-1 model is the well-known antiferromagnetic XXZ model

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

(14)

This model supports three gapped phases, the ‘large-U’, the Haldane and the Neel phases, corresponding respectively to the MI, HI and DW phases.

Kennedy and Tasaki [39] introduced a non-local mean-field theory which captures the whole phase diagram of the XXZ chain. Their approach relies on a unitary transformation [40] that transforms the string operators into local spin operators:

$$O_{\text{string}}^\text{string} = S_i^j \exp \left( i \pi \sum_{j<i} S_j^z \right) U^{-1} S_j U = \tilde{S}_i^j,$$

$$O_{\text{string}}^\text{string} = \exp \left( i \pi \sum_{j<i} S_j^z \right) S_i^z U^{-1} S_j U = \tilde{S}_i^z.$$  

(15)

Table 1. Four-field mean-ground-states of the transformed Hamiltonian (17) and the respective signs of $(\tilde{S}^z)$

| State\(\langle \text{Order parameter} \rangle\) | Sign($\tilde{S}^z$) | Sign($\tilde{\Psi}_1^\alpha$) |
|---------------------------------------------|-----------------|------------------|
| $|\psi_1\rangle = \cos \theta \langle 0 \rangle + \sin \theta \langle 1 \rangle$ | $+$ | $+$ |
| $|\psi_2\rangle = \cos \theta \langle 0 \rangle - \sin \theta \langle 1 \rangle$ | $-$ | $+$ |
| $|\psi_3\rangle = \cos \theta \langle 0 \rangle + \sin \theta \langle -1 \rangle$ | $+$ | $-$ |
| $|\psi_4\rangle = \cos \theta \langle 0 \rangle - \sin \theta \langle -1 \rangle$ | $-$ | $-$ |

The operator $U$ flips every second site with $S_i^z = \pm 1$, skipping those with $S_i^z = 0$. It is given explicitly by [40]

$$U = \prod_{\forall j,k \neq j} e^{\pi \tilde{S}_j^z} \equiv \prod_{\forall j,k \neq j} E_{j,k}.$$  

(16)

The unitary operator $U$ transforms the Hamiltonian (14) into an unusual, but nevertheless local form

$$\tilde{H} = U H U = -2t \sum_j \left( \tilde{S}_j^x \tilde{S}_{j+1}^x - \tilde{S}_j^y \exp (\pm i \pi \tilde{S}_i^z) \tilde{S}_{j+1}^y \right)$$

$$- V \sum_j \left( \tilde{S}_j^z \tilde{S}_{j+1}^z \right) + \frac{U}{2} \sum_j \tilde{S}_j^z.$$  

(17)

The transformed Hamiltonian $\tilde{H}$ has an explicit $Z_2 \times Z_2$ symmetry, generated by $\pi$ rotations of the spins around the main axes. In the Haldane phase, this symmetry is spontaneously broken and the two order parameters $\tilde{S}^z$ acquire a non-zero mean value. These properties enable a variational mean-field approximation [39] for the ground state. It consists in considering only site-factorizable wavefunctions of the form

$$|\Psi_{\text{GS}}^\alpha\rangle = \prod_{1 \leq i \leq L} |\psi_\alpha\rangle_i \equiv |\alpha \ldots \alpha\rangle,$$

(18)

where $|\psi_\alpha\rangle = \cos \theta \langle 0 \rangle \pm \sin \theta \langle 1 \rangle$.

In the HI, the minimal variational energy is obtained for $\cos^2 \theta = (U - 2V + 4t)/(8t - 2V)$ and the ground state is fourfold degenerate. As shown in table 1, the four different states can be characterized by the signs of the two order parameters and reflect the broken $Z_2 \times Z_2$ symmetry. In the DW phase, $\cos \theta = 0$ and the ground state is doubly degenerate. In the MI phase, $\cos \theta = 1$ and the ground state is non-degenerate. The resulting phase boundaries, first obtained in [39], are given in figure 5.

Variational wavefunctions of the excitations

The non-local mean field allows us to describe the elementary excitations of the different phases in terms of domain walls (‘kinks’) of the two order parameters [41]. A domain wall localized at site $i$ may be represented by the site-factorizable wavefunction

$$|\Psi_{i\beta}^{\alpha}\rangle = \prod_{1 \leq j \leq i} |\psi_\alpha\rangle_j \prod_{i+1 \leq j \leq L} |\psi_\beta\rangle_j \equiv |\alpha \ldots \alpha \beta \ldots \beta\rangle.$$  

(19)

This wavefunction can be symmetrized with respect to lattice translations to obtain a variational ansatz for the elementary excitations:

$$|\Psi_{k\beta}^{\alpha}\rangle = \sum_j e^{ikx_j} |\Psi_{i\beta}^{\alpha}\rangle \equiv |\alpha \ldots \alpha \beta \ldots \beta\rangle_k.$$  

(20)
In the HI, the domain walls can flip either one of the hidden $Z_2$ symmetries or both, giving rise to three different excitations. Note that these excitations do not coincide with those predicted in [10]. As we will see, the present approach correctly reproduces the findings of the field-theoretical approach.

A kink that flips only $\tilde{S}^y$ is described by the wavefunction $|\Psi^i_k\rangle = |\Psi^{1,2}_k\rangle \triangleq |11\ldots 1122\ldots 22\rangle_k$ (see table 1) and is created by the untransformed operator $S^y_k$. In terms of the original Bose–Hubbard model, this ‘neutral’ excitation corresponds to a phonon (2) with momentum $k = \pi$. In contrast, the operators $S^x_k$ and $S^z_k$ change the total number of particles by one. The resulting excitations $|\Psi^x_k\rangle = |\Psi^{1,3}_k\rangle \pm |\Psi^{2,5}_k\rangle \equiv |11\ldots 1133\ldots 33\rangle_k + |22\ldots 2233\ldots 33\rangle_k$, correspond to a superposition of two types of kinks: $|11\ldots 1133\ldots 33\rangle_k$, which is a kink only in $\tilde{S}^x$, and $|22\ldots 2233\ldots 33\rangle_k$, which is a kink in both $\tilde{S}^x$ and $\tilde{S}^z$. In the original Bose–Hubbard model, these ‘charged’ excitations correspond to the creation or annihilation of one boson with momentum $k$.

The energy of the three collective excitations can be calculated variationally: $E^u = \langle \Psi^u_k | H | \Psi^u_k \rangle - \langle \Psi^u | H | \Psi^u \rangle$, leading to

\[
\Delta_u = E^u_k = 2\theta \left( 1 + \cos^2 \theta \right)
\]

\[
\Delta_x = E^x_k = E^z_k = 2V \frac{1 - \cos^2 \theta}{1 + \cos^2 \theta} \left( 1 + \cos^3 \theta + \cos^2 \theta \right) \cos k.
\]

We find that: (i) at the transition to the MI ($\theta \to 0$), the energies of both excitations vanish at momentum $k = 0$; (ii) at the transition to the DW phase ($\theta \to \pi/2$), only the energy of the neutral mode (22) vanishes at wavevector $k = \pi$. Both observations are in agreement with the numerical and field-theoretical approaches presented above.

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**Absorption spectrum: selection rules**

Having described the elementary excitations of the HI, we can now calculate the absorption spectra $S(\omega)$. For this task, we should compute the matrix elements between the different excitations and the perturbation operators defined in equations (8) and (9). Unfortunately, these calculations are extremely complicated, due to the unknown interactions between the kinks. Nevertheless, we can formulate simple selection rules that determine when these matrix elements can be finite and when they must vanish.

To establish the selection rules, we classify all excited states in four topological sectors, defined by the parity of the number of kinks in the $x$ and $z$ string order parameters, denoted by $N^x$ and $N^z$. Because the string order parameters of the original model correspond to the local spin operators of the transformed model (equation (15)), we can define the Boolean numbers $N^x$ and $N^z$ according to

\[
N^a = \lim_{j \to \infty} \text{sign}(\tilde{S}^x_{j+1} \tilde{S}^y_{j+1}).
\]

The perturbations (8) and (9) can connect the ground state only to excitations belonging to a well-defined topological sector. In particular, the operator corresponding to lattice modulations, $T_{\text{hop}}$, remains local after the unitary transformation (16)

\[
UT_{\text{hop}}U^{-1} = \sum_i S^x_i S^x_{i+1} - S^z_i \exp(i\pi S^y_i + i\pi S^y_{i+1}) S^y_{i+1}.
\]

As a consequence, $T_{\text{hop}}$ can excite only states with an even number of domain walls, and

\[
\langle \psi_a | T_{\text{hop}} | \psi_b \rangle \neq 0 \text{ only if } (N^x, N^z)_a = (+, +).
\]

Bragg spectroscopy transforms as

\[
UT_{\text{hop}}U^{-1} = \sum_i e^{ikx_i} \tilde{S}^x_i \prod_{j<i} \exp(i\pi S^z_j).
\]

Noting that $\exp(i\pi S^z_j)$ flips $\tilde{S}^y_j \to -\tilde{S}^y_j$, we deduce that $T_{\text{hop}}$ flips $N^x \to -N^x$. Consequently, $T_{\text{hop}} | \psi_{\text{gs}} \rangle$ overlaps only with states containing an odd number of kinks of the $x$ string order parameter and

\[
\langle \psi_a | T_{\text{hop}} | \psi_{\text{gs}} \rangle \neq 0 \text{ only if } (N^x, N^z)_a = (-, +).
\]

Using these selection rules, we conclude that lattice modulations can excite only pairs of charged or neutral excitations and therefore its absorption spectrum is dominated by two particle continua. Bragg spectroscopy $T_{\text{hop}}$ can couple to a neutral excitation at momentum $k = \pi$: we therefore expect a sharp resonance in the absorption spectrum, whose energy goes to zero at the HI–DW phase transition.

The resulting absorption spectra are shown in figures 6 and 7. We find excellent agreement with the results obtained from the critical theories shown in figures 3 and 4. As expected, the mean-field approach does not capture the precise shape of the excitation gap in the vicinity of the transition. It does however provide a reliable method to quantitatively predict the position of the peaks and continua, deep in the HI, starting from the microscopic Hamiltonian (1).
particle conservation. Symmetries of the problem, i.e. translational invariance and topological phase transition trivially commute with all the symmetries of the systems.

At the MI–HI phase transition, the low-energy excitations are particles and holes at zero momentum. They appear as a broad peak in the response to lattice modulations, and do not couple to Bragg spectroscopy at \( k = \pi \). This observation indicates that the phase transition between the MI and the HI is of topological origin: the critical excitations at a topological phase transition trivially commute with all the symmetries of the problem, i.e. translational invariance and particle conservation.

At the HI–DW phase transition, the low-energy excitations are phonons at the edge of the Brillouin zone. These excitations appear as a narrow peak in the response to Bragg spectroscopy at \( k = \pi \). They possess a non-trivial quantum number (momentum), showing that the HI–DW phase transition is not topological, and spontaneously breaks a local symmetry (translational invariance).

These qualitative features are confirmed by the field-theoretical analysis of the phase transitions. More quantitative predictions are obtained using a non-local mean-field approach. In contrast to the analysis of \([10]\), the present approach correctly reproduces the shape of the spectra predicted by the field-theoretical calculations, at both the MI–HI and HI–DW phase transitions. The non-local mean-field can be therefore used to interpolate between the two phase transitions, and is expected to provide reliable results deep in the topological phase (HI), where the field theories cease to apply. This method does not rely on effective parameters of the continuum theory, which are in general not known, but rather applies directly to the microscopic Bose–Hubbard model.

The techniques developed here can be extended to other types of dynamic probes, such as Bragg spectroscopy at a general momentum \( k \), local perturbations, small quenches \([42]\), as well as to quantum phase transitions of other systems. Among those, we would like to briefly discuss quantum systems of interacting fermions in one dimension. The extended Bose–Hubbard model considered here can be approximately mapped into a fermionic problem, by splitting the single chain at integer filling into two chains at half-integer filling, and then applying the Jordan–Wigner transformation. This transformation maps the local occupation \( n_i \) and the nearest-neighbour tunnelling \( b_i^\dagger b_{i+1} \) of the bosons into the corresponding operators of the fermions. As a consequence, we expect the absorption spectrum of fermions to be identical to the one of bosons. The topological phase transition between the MI and the HI maps into a phase transition between two topological phases of interacting fermions in one dimension, belonging to the more general \( Z_8 \) group of \([43]\). (The fermionic model possesses additional symmetries which map into local symmetries of the bosonic model.) It would be interesting to extend this result to the transitions to the other six phases.

Field-theoretical techniques should allow us to extend the present approach to topological phases of fermions and bosons in higher dimensions. Recently, field theories describing gapped phases of fermions \([44]\) and bosons \([45]\) have been found. However, less is known about the critical theory of the quantum phase transitions between the different topological phases. In the case of topological band insulators, it is natural to expect these critical theories to be non-interacting (Gaussian), in analogy to the present case. In general, it should be possible to compute the response to physical probes by expressing the corresponding perturbations in terms of the critical theories. One should then be able to experimentally probe whether the critical excitations of the topological phase transition respect all the symmetries of the systems.

Acknowledgments

We wish to thank E Berg, T Giamarchi, S Huber and S Kivelson for many useful discussions. Part of the results presented in this work has been submitted to the Feinberg Graduate School, as a chapter of the Ph.D. thesis of the author, under the supervision of E Altman.
Appendix A. Form-factor approach

According to the form-factor approach [33, 36, 37], the spectrum of lattice modulations is given by

$$S_{\text{hop}}(\omega) = \frac{1}{\omega \sqrt{\omega^2 - 4\Delta_c^2}} |F_{\text{cos}}[\theta(\omega, g)]|^2,$$

(A.1)

where $\Delta_c$ is the charge gap (‘soliton mass’) and

$$\theta(\omega, g) = 2 \log \left( \frac{\omega}{2\Delta} + \sqrt{\frac{\omega^2}{4\Delta_c^2} - 1} \right).$$

(A.2)

$$F_{\text{cos}}(\theta) = \frac{\cosh(\theta/2)}{\sinh\left[\frac{\pi}{2\lambda}(\theta - i\pi)\right]} F(\theta),$$

(A.3)

$$F(\theta) = \sinh(\theta/2) \exp \left( \int_0^{\infty} \frac{dx K(\theta, x)}{x} \right),$$

(A.4)

$$K(\theta, x) = \frac{(\sin(\theta + i\pi/2)x/2)^2 \sin(\pi x/2)}{x \sin(\pi x) \cos(\pi x/2) \sin(\gamma x/2)},$$

(A.5)

$$\gamma = \frac{\pi K}{2 - K}.$$

(A.6)

Appendix B. Jordan–Wigner and Bogoliubov transformations

In this appendix, we compute the absorption spectrum of

$$T_{\text{hop}} = \sum_i S_i^z$$

through the subsequent application of the Jordan–Wigner and Bogoliubov transformations. Applying the Jordan–Wigner transformation to (4), we obtain

$$H_{\text{ising}} = \sum_i n_i - \lambda(\nu_i^\dagger + \nu_i)(\nu_{i+1}^\dagger + \nu_{i+1})$$

$$= \sum_k (1 - \lambda \cos(k)) \nu_k^\dagger \nu_k + \lambda \sin(k) \nu_k \nu_k + \text{H.c.}.$$

(B.1)

Here $u = 2\lambda a$ and $\Delta = 2(\lambda - 1)$. We now diagonalize (B.1) by the Bogoliubov transform: $
u_k = \cos(\theta_k/2) \psi_k + i \sin(\theta_k/2) \psi_{k+1}^\dagger$, where $\tan(\theta_k) = k/\Delta$.

We now express $\sigma_i^\tau$ in terms of Bogoliubov quasi-particles creation and annihilation:

$$\sum_i \sigma_i^\tau = \sin(\theta_k) \gamma_k^\dagger \gamma_{-k} + \cos(\theta_k) \gamma_k \gamma_k + \text{H.c.}. $$

(B.2)

The required matrix element is

$$M_{k,0} \equiv \left( \nu_k \left( \sum_i \sigma_i^\tau \Psi_{gs} \right) \right) = \sin(\theta_k) \approx \frac{k}{\epsilon_k}.$$

(B.3)

Here, $|\psi_k\rangle$ is a state with two Bogoliubov quasi-particles (at momenta $k$ and $-k$) and energy $2\epsilon_k = 2\sqrt{K^2 + \Delta^2}$. The computation of the absorption spectrum is straightforward:

$$S_{\text{hop}}(\omega) \approx \sum_k |M_{k,0}|^2 \delta(\omega - 2\epsilon_k) \approx \left( \frac{k}{\epsilon_k} \right)^2 \frac{\partial k}{\partial \epsilon_k} \delta(\omega - 2\epsilon_k)$$

$$= \left( \frac{k}{\epsilon_k} \right) \frac{\omega^2 - (2\Delta)^2}{\omega^2} \Theta(\omega - 2\Delta).$$

(B.4)

Here $\Theta(\omega)$ is the Heaviside step function.

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