Symmetry protected topological Luttinger liquids and the phase transition between them

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Abstract

We show that a doped spin-1/2 ladder with antiferromagnetic intra-chain and ferromagnetic inter-chain coupling is a symmetry protected topologically non-trivial Luttinger liquid. Turning on a large easy-plane spin anisotropy drives the system to a topologically-trivial Luttinger liquid. Both phases have full spin gaps and exhibit power-law superconducting pair correlation. The Cooper pair symmetry is singlet $d_{xy}$ in the non-trivial phase and triplet $S_z = 0$ in the trivial phase. The topologically non-trivial Luttinger liquid exhibits gapless spin excitations in the presence of a boundary, and it has no non-interacting or mean-field theory analog even when the fluctuating phase in the charge sector is pinned. As a function of the strength of spin anisotropy there is a topological phase transition upon which the spin gap closes. We speculate these Luttinger liquids are relevant to the superconductivity in metalized integer spin ladders or chains.

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1. Introduction

Symmetry protected topological states (SPTs) [1–3] have attracted lots of interest in condensed matter physics recently. These states do not break any symmetry and are fully gapped, except at the boundary. The gapless boundary excitations of SPTs are protected by symmetry, hence are very different from “accidental boundary states” found at, say, semiconductor surfaces (due to “dangling bonds”). Searching for real materials realizing SPTs is a very active area of research.

The best known examples of SPT are topological insulators and superconductors [1,2]. In addition to these, there are “bosonic” SPTs [3]. A classic example is the antiferromagnetic (AF) spin-1 Heisenberg chain [4,5], which is gapped in the bulk but possesses gapless spin-1/2 excitations on the boundary [6]. These spin-1/2 boundary excitations are protected so long as the SO(3) spin rotation symmetry is respected (in fact even its $Z_2 \times Z_2$ subgroup is sufficient for the protection) [7,8]. Unlike topological insulators and superconductors, which can be realized in non-interacting (or mean-field) theories, the novel collective mode dynamics of spin-1 chains is caused by strong interaction. So long as the protective symmetry is unbroken, inequivalent SPTs are connected by topological phase transitions where the bulk gap closes.

In this paper we demonstrate that in one space dimension there exists topologically inequivalent (gapless) Luttinger liquids whose distinction is also protected by symmetry. The key signature of this gapless topological phase is the presence of gapless charge excitations and gapped spin excitations in the bulk, along with symmetry protected gapless spin-1/2 excitations at the boundary. These features render the phase studied here different from all gapless one-dimensional (1D) phases previously discussed within the Luttinger liquid paradigm (which lack protected gapless spin-1/2 excitations confined to the edge), as well as all other known 1D topological phases, as we argue in the following. Furthermore, these topologically non-trivial Luttinger liquids exhibit power-law Cooper pair correlation, hence are phase fluctuating superconductors. Interestingly the pairing symmetries are different in topologically inequivalent phases. Because the spin gap in the topologically non-trivial Luttinger liquid is due to collective mode dynamics, even after pinning the fluctuating phase in the charge sector it has no non-interacting or mean-field theory analog, hence is different from that discussed in Refs. [9–11]. They are also very different from the Weyl [12] or Dirac [13] semi-metals whose existence is not protected by a on-site (non-crystal) symmetry. We also study the phase transition between these Luttinger liquids and show that the quantum critical point exhibits central charge $c = 2$.

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2. The model

We begin by briefly reviewing a known topological phase transition between different phases of a spin-1 chain. The Hamiltonian under consideration is [14]

\[ H = J \sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + D \sum_{i=1}^{L} \mathbf{S}_i^2. \]  

(1)

In Eq. (1), \( i \) labels the sites of a one-dimensional lattice under periodic boundary condition (PBC) (i.e., \( L + 1 \equiv 1 \)) and \( \mathbf{S} \) is the spin-1 operator. The last term breaks the \( SO(3) \) spin rotation symmetry. The ground state is a product state with \( D = 0 \) on every site. Both phases have a full spin gap and do not break the \( U(1) \times Z_2 \) symmetry, but the Haldane phase possesses gapless boundary excitations while the “large D” phase does not [14]. As a function of \( D \) there is a topological phase transition occurring around \( D/J \approx 1 \). The central charge of the critical theory is estimated to be 1 [14].

Now we consider doping the above spin chain. To model doping we construct the following “t-J” type ladder Hamiltonian (see Fig. 1a):

\[ H = \sum_{i=1}^{L} \left( \frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + h.c. \right) + J_\perp \sum_{i=1}^{L} \left( \mathbf{S}_{i,\perp} \cdot \mathbf{S}_{i+1,\perp} + D \sum_{i=1}^{L} \left( \mathbf{S}_{i,\perp}^2 + \mathbf{S}_{i+1,\perp}^2 \right) \right) + t \sum_{i=1}^{L} \left( \mathbf{S}_{i,\perp} \cdot \mathbf{S}_{i+1,\perp} + D \sum_{i=1}^{L} \left( \mathbf{S}_{i,\perp}^2 + \mathbf{S}_{i+1,\perp}^2 \right) \right) \right). \]

(2)

Here \( z = 1, 2 \) labels the two chains and unlike the spin-1 operators in Eqs. (1) and (3), \( \mathbf{S}_{i,\perp} \) are spin-1/2 operators. We also note that only intra-chain hopping is allowed. This allows us to interpret \( z \) as labeling two different orbitals of an atom later, as atomic orbitals do not hybridize. In general as long as the strength of the inter-chain hopping is weak compared with \( J_t \), we do not expect any qualitative change in the results. Eq. (2) is supplemented with the Hilbert space constraint that there is at most one electron per site (i.e. \( n_{z,j} \leq 1 \)). Eq. (1) can be shown to be the effective Hamiltonian at half filling (one electron per site) under the conditions \( t = 0, J_t < 0 \) (FM) and \( J_t \gg J, D \).

Now consider doping holes into the system. We first consider large \( J_t \) so that minimizing the rung exchange energy requires doped holes to form “vertical pairs”. Under such condition the two electrons on each rung are effectively a spin-triplet boson which can hop into the empty rung created by doping via a second order virtual process \( t_s = \epsilon (\epsilon^2/J_t) \) (see Fig. 1b). The resulting effective Hamiltonian is given by

\[ H_0 = -t_s \sum_{j=1}^{L-1} \sum_{m=1}^{\beta_j} b_{j,m}^\dagger b_{j+1,m} + h.c. + J_b \sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + D_b \sum_{i=1}^{L} \mathbf{S}_i^2. \]

(3)

where \( m = 1 \) and \( \beta_j \) labels the three states of spin 1, \( \mathbf{S}_i \) is the total spin operator of the \( i \)th rung, \( J_b = \epsilon (\epsilon^2/D) \) and both are positive.

3. Factorization of the wave function and exact diagonalization

To illustrate the basic physics it is instructive to consider the limit \( t_s \gg J_b \) and \( t_s \gg D_b \). Under such condition, one can generalize the results of Refs. [15–18] and show that the ground state wave function exhibits spin-charge separation, namely,

\[ \langle 0|b_{x_1} \cdots b_{x_N} | \psi_0 \rangle = f(x_1 \cdots x_N) g(m_1 \cdots m_N) \] for \( x_1 < \cdots < x_N < x_1 + L. \]

(4)

In Eq. (4), \( f(x_1 \cdots x_N) \) is the charge and \( g(m_1 \cdots m_N) \) is the spin wavefunction, both are subjected to PBC. \( f(x_1 \cdots x_N) \) is the ground state of spinless hard-core bosons with nearest neighbor hopping. \( g(m_1 \cdots m_N) \) is the ground state of an effective spin Hamiltonian defined on the “squeezed” lattice, i.e. the lattice formed by deleting the holes. The effective spin Hamiltonian has the same form as the last two terms of Eq. (3) except the parameters are renormalized:

\[ J_{\perp} = J_\perp (n_{i,\perp}/L) \times L/N > 0 \] and \( D_{\perp} = D_{\perp} (n_{i,\perp}/L) \times L/N = D_{\perp} > 0 \), where \( n_{i,\perp} \) is the boson number operator and \( \langle ... \rangle \) denotes the expectation value computed using the hard-core boson wave function \( f \). In the case of \( D_{\perp} = 0, g \) is the ground state of the spin-1 AF Heisenberg chain [4,5]. For \( D_{\perp} \gg J_b, g \) is the ground state wavefunction of the large-\( D \) phase of Eq. (1) [14].

As a preliminary check of the validity of the factorized wavefunction we show in Fig. 1c the overlap of the exact ground state and the factorized wavefunction for a 12-site spin-1 chain doped with one bosonic hole. Although the factorized wavefunction only becomes exact in the \( J_b/t_s \approx 0 \) and \( D_b/t_s \approx 0 \) limit, the computed overlap is close to unity for a substantial range of \( J_b/t_s \) and \( D_b/t_s \). Due to spin-charge separation while both the \( D_b = 0 \) and the large-\( D_b \) phases are described by the same gapless Luttinger liquid in the charge sector, they differ topologically in the spin sector. Thus we have two topologically inequivalent Luttinger liquids!

Fig. 1. (Color online) Caricatures of Eqs. (2) and (3), and exact diagonalization results of ground state wave function. (a) A caricature of Eq. (2). The red vertical bonds are ferromagnetic while the black horizontal bonds are AF. (b) A caricature of Eq. (3). The triplet bosons are denoted by the light green ellipses. When doped these bosons can hop to nearest neighbor empty rungs. Each triplet boson experiences a spin anisotropy term and interacts with neighboring bosons via AF exchange interaction. (c) The overlap between the exact ground state of 11 triplet bosons on a 12 rung lattice and the factorized wavefunction, as a function of \( j_b/t_b \), for several value of \( D_b/j_b \).
Although the spin-charge separation limit provides an intuitive picture for the two Luttinger liquid phases, the parameters we used in the numerical study do not fall within the limit. In fact, the ground states of the two Luttinger liquid phases are spin-singlet and spin-triplet superconductors, with power-law pair-pair correlation, where the spin and charge do couple together. It is the \( Z_2 \times Z_2 \) spin symmetry group (\( \pi \) rotation of spin around the \( z \) and \( x \) axes) which protects these two Luttinger liquid phases as topologically distinct, hence requires a phase transition between them.

4. DMRG studies

In order to check whether the above Luttinger liquids survive when the parameters of Eq. (2) move away from the limit considered above, and to study the phase transition between these Luttinger liquids, we performed large scale density-matrix renormalization group [19] (DMRG) calculations. In the following, we specifically we study the ground state and spin excitations of Eq. (2) for \( D = 0 \); see inset of Fig. 2a we show the spin-1 gap when the rung coupling is \( J_3 = +3 \). As expected, the spin-1 excitation is gapped for OBC (and PBC).

Fig. 3a and b show the absolute value of the Cooper pair correlation function

\[
\Phi_{s(1),a}(r) = \langle \delta_{s(1),a}(i) \delta_{s(1),b}(i + r) \rangle, \quad \text{where} \\
\delta_{(s,t),a}(i) = \left( c_{i,1}^\dagger c_{i,2} - (+)^x c_{i,1}^\dagger c_{i-1,2} \right) / \sqrt{2}.
\]

In Eq. (5), \( i \) sits on the lower chain and \( a = x, y \). \((x \pm y)\) denotes the nearest neighbor (next nearest neighbor) along the chain, rung (diagonal) directions respectively. The symbols “s” and “t” stand for singlet and triplet. The triplet pair correlation, panel (a), exhibits exponential decay. On the surface this is counter-intuitive because the rung coupling is strongly FM. Upon further reflection this is expected because the spin sector is in the Haldane phase, hence all triplet spin correlation should decay exponentially. Fig. 3b shows the much slower decaying singlet pair correlation. The pairing channel which exhibits the strongest correlation (consistent with power-law decay, see inset in Fig. 3b) is associated with \( a = x \pm y \) and \( b = x \pm y \). The overlapping cyan and pink symbols in Fig. 3b denote \((a,b) = (x + y, x + y)\) and \((a,b) = (x + y, x - y)\), respectively. The degeneracy is caused by taking the absolute value. The actual correlations have opposite sign. Such sign structure can be interpreted as \( d_{xy} \)-pairing on the ladder.

If we view the \( x = 1 \) as labeling two orbitals of an atom and use \( c_{i,1,1}^\dagger \) and \( c_{i,2,1}^\dagger \) to denote the corresponding electron creation operator, then the Cooper pair which exhibits power-law correlation is created by

\[
(c_{i,1}^\dagger c_{i+1,1}^\dagger - c_{i,1}^\dagger c_{i+1,1}^\dagger) - (c_{i,2}^\dagger c_{i+1,1}^\dagger - c_{i,2}^\dagger c_{i+1,1}^\dagger).
\]

This is spin singlet, orbital antisymmetric and odd parity pairing. Our result suggests the doped spin-1 ladder studied above is a spin-gapped charge-gapless liquid with power-law superconducting correlations.

4.2. Transition into topologically trivial phase

Now let’s increase the value of \( D \). In Fig. 2c we show the spin gap under PBC as a function of \( D \). The gap reaches a minimum at \( D_c \approx 0.12 \) and the value decreases with increasing ladder length.

![Fig. 2. (Color online) DMRG results of spin gap. (a) The spin gap \( \Delta_s \) at \( D = 0 \) with 5\% hole doping for different ladder length \( L \). The black (red) symbols mark the spin-1(2) excitation gap. The main panel is for FM rung coupling and the inset shows the spin 1 gap for AF rung coupling. (b) A caricature for the spin-gapped and charge gapless bulk with spin-1/2 boundary excitations (red arrows). (c) The spin 1 gap as a function of \( D \) under PBC. (d) The spin-1 gap as a function of \( D \) under OBC.](image-url)
consistent with a zero spin gap at $D_c$. A closer inspection of Fig. 2c shows an even-odd effect in terms of the number of hole pairs. To understand this effect, we point out that the same even-odd effect should exist at half-filling as a function of the number of rungs (Eq. (2)) or the number of sites (Eq. (3)). This is because $Q = \prod_i S^x_i$, where $S^x_i$ is the total x-component spin operator on the ith rung (site) commutes with the Hamiltonian, hence is a good quantum number. It is straightforward to show that for the Haldane phase $Q = 1$ while for the large-$D$ phase $Q = (\pi D_0/\theta)^{1/6}$. Therefore for odd $L$ a $Q = -1$ excited state crosses the $Q = 1$ Haldane state at $D_c$. On the other hand for even $L$ such level crossing is avoided. This presence/absence of avoided crossing is responsible for the even-odd effect in $\Delta S = 1$. For the doped case the number of rungs (sites) in the "squeezed" spin ladder (chain) depends on the number of hole pairs (holes) which explains the even-odd effect in Fig. 2c.

In Fig. 2d we plot the spin-1 gap under OBC as a function of $D$ for several values of $L$ at 5% doping. The result is consistent with the absence of a spin gap for $D < D_c$, while a finite spin gap remains for $D > D_c$ as $L \rightarrow \infty$. The results of Fig. 2a, c, d support the statement that for $D < D_c$ the spin sector realizes a non-trivial SPT (the Haldane phase) with gapless edge excitation, while for $D > D_c$ the spin state is a trivial SPT (the large-$D$ phase) with no gapless edge excitations. A topological phase transition occurs at $D_c$ where the spin gap closes.

In Fig. 4a we plot the entanglement entropy as a function of number of rungs in an untraced subsystem for OBC. The oscillatory behavior is a consequence of the Friedel-like oscillation induced by the boundary effect due to the finite density wave susceptibility associated with hole pairs. This is common in 1D Luttinger liquids. Using the data of the longest ladder ($L = 200$) we fit the data with the formula for the entanglement entropy for a critical one-dimensional system with open boundary conditions [20],

$$S(x) = \frac{c}{6} \ln \left[ \frac{4(L+1)}{\pi} \sin \left( \frac{\pi(2x+1)}{2L+1} \right) \right] - \frac{\sin(k_F(2x+1))}{|\sin(k_F)|^{4L+1}} \left[ \sin \left( \frac{2\pi(2x+1)}{2L+1} \right) \right] + \text{const.}$$

(7)

where $L$ is the length of system and $x$ is the number of rungs in the untraced subsystem. $c$ is the central charge and $k_F$ is a fitting parameter. Performing the fit of $S(x)$ using Eq. (7) to the data in Fig. 4a
with different system sizes, we get $c \approx 1.08$ (consistent with $c = 1$) for $D = 0$ and $c \approx 1.96$ (consistent with $c = 2$) for $D = D_0$. The central charge at $D_0$ is consistent with the sum of the central charge associated with the gapless charge sector (namely $c_{\text{charge}} = 1$) and that of the spin sector (namely $c_{\text{spin}} = 1$) at the topological phase transition point.

Next we study the superconducting pair correlation in the large-$D$ phase. In Fig. 4b, c we show the absolute value of the spin triplet and spin singlet Cooper pair correlation function. In this case all singlet pair correlations decay exponentially. In contrast the triplet correlation decays much slower (consistent with power-law decay). In part (b) the cyan and pink symbols overlap signifying the same absolute value. The actual values have opposite sign. The spin state of the triplet Cooper pair that show the strongest correlation is $S = 1.5$. Again if we interpret the two chains as corresponding to the two atomic orbitals 1, 2 the triplet Cooper pair in question is created by

$$
(c_{1,i}^+ c_{2,i}^- + c_{2,i}^+ c_{1,i}^- + A(c_{1,i}^+ c_{2,i}^+ c_{1,i+1}^- + c_{1,i}^+ c_{2,i}^+ c_{1,i+1}^-) - A(c_{1,i}^+ c_{2,i}^+ c_{1,i+1}^- + c_{2,i}^+ c_{1,i}^- c_{1,i+1}^-),
$$

where $A$ is a constant. This is spin triplet, orbital anti-symmetric and even parity Cooper pairing.

5. Discussion and conclusion

The topologically non-trivial and trivial Luttinger liquids described so far can also be obtained from bosonization. However, for space consideration we refer to the Supplementary data.

In this work, we have used a combination of numerical and analytic techniques to demonstrate that the phase diagram of interacting 1D quantum systems exhibits a topologically non-trivial spin-gapped, charge-gapless phase with symmetry protected gapless spin-$1/2$ edge excitations. We have in particular discussed the emergence of this phase in the phase diagram of doped spin-ladder systems. Doped spin-ladders with AF rung coupling have been extensively studied (see Refs. [21–25]). At half-filling the spin state is a good example of the resonant-valence-bond state [26]. Upon doping the system becomes a spin-gapped Luttinger liquid with $d_{x^2-y^2}$ Cooper pairing. In this paper we studied doped spin ladders with FM rung coupling. At half-filling the spin state can be either a non-trivial SPT (Haldane phase) or a trivial one (the large-$D$ phase). Upon doping they also become phase fluctuating superconductors (spin-gapped Luttinger liquids) with different Cooper pair symmetries. This suggests the possibility of superconductivity in metalized integer spin ladders or chains. A particular interesting question is the relevance of our work to the superconductivity in FeSe. FeSe becomes nematic below 90K while maintains paramagnetic state due to the spontaneous formation of spin-1 chains. If so the superconducting pairing considered here could be relevant.

Conflict of interest

The authors declare that they have no conflict of interest.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.scib.2018.05.010.

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