Edge Theories in Projected Entangled Pair State Models

S. Yang,[1] L. Lehman,[2] D. Poilblanc,[3] K. Van Acoleyen,[4] F. Verstraete,[4,5] J. I. Cirac,[1] and N. Schuch[2]
[1]*Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany*
[2]*Institut für Quanteninformation, RWTH Aachen University, D-52056 Aachen, Germany*
[3]*Laboratoire de Physique Théorique, C.N.R.S. and Université de Toulouse, F-31062 Toulouse, France*
[4]*Department of Physics and Astronomy, Ghent University, Krijgslaan 281, S9, 9000 Gent, Belgium*
[5]*Vienna Center for Quantum Science and Technology, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria*
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We analyze the low energy excitations of spin lattice systems in two dimensions at zero temperature within the framework of projected entangled pair state models. Perturbations in the bulk give rise to physical excitations located at the edge. We identify the corresponding degrees of freedom, give a procedure to derive the edge Hamiltonian, and illustrate that it can exhibit a rich phase diagram. For topological models, the edge Hamiltonian is constrained by the topological order in the bulk, which gives rise to one-dimensional edge models with unconventional properties; for instance, a topologically ordered bulk can protect a ferromagnetic Ising chain at the edge against spontaneous symmetry breaking.

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The edge of strongly correlated quantum systems can display very intriguing phenomena. For instance, in two-dimensional (2D) quantum Hall systems the low energy behavior can be described in terms of chiral modes which live at the edge of the material [1–4], a behavior also discovered later in topological insulators [5,6]. In contrast to the gapped bulk, these edge modes are gapless and cannot be gapped out by any perturbation of the system, giving rise to protected edge currents. Interestingly, this property cannot be described by a conventional one-dimensional (1D) theory, and is dictated by the presence of the topologically ordered bulk, exposing an intimate connection between the seemingly different physics in the bulk and at the edge.

In this Letter, we study the low-energy physics for a class of spin systems on 2D lattices. We show that the Hilbert space of the effective low-energy theory can be identified with the entanglement degrees of freedom which live at the edge of the system. This allows us to construct 1D edge Hamiltonians which describe the low-energy physics of the system, and investigate how they change under perturbations in the bulk. We find that bulk perturbations can induce phase transitions at the boundary, and explicitly investigate one particular example where we find a rich phase diagram with gapped, gapless, and symmetry-broken phases at the boundary. We also study the effect of topological order in the bulk and find that it induces constraints on the edge Hamiltonian which cannot occur in conventional 1D spin systems, a direct consequence of the topological protection [7,8]; for instance, we give a model based on the Toric code (TC) [9] whose edge Hamiltonian is an Ising chain, but which is protected against spontaneous symmetry breaking by the topological properties of the bulk.

We restrict our attention to projected entangled pair state (PEPS) models, and perturbations thereof. PEPS models consist of a Hamiltonian H together with its ground space which are both derived from a single tensor which describes the entanglement structure of the system locally [10–13]. We focus on models where $H = \sum h$ is translationally invariant, i.e., a sum of identical local terms, and gapped for periodic boundaries. Many paradigmatic models such as the AKLT model [10], topologically ordered systems [14–16], or resonating valence bond (RVB) states [14,17] are PEPS models, and we will illustrate our results with particular perturbations of these models.

We start by introducing PEPS models. For simplicity, we restrict to square lattices and translationally invariant systems. The central object is a five-index tensor $A^i_{\mu_1,\mu_2,\mu_3,\mu_4}$, with physical index $i = 1, \ldots, d$ and virtual indices $\mu_k = 1, \ldots, D$. For a given region R, these tensors are arranged on a 2D grid as shown in Fig. 1(a). Adjacent virtual indices μ_k in the bulk are contracted (i.e., identified and summed over), while the "open" virtual indices at the boundary are set to $\alpha \equiv (\alpha_1, \ldots, \alpha_{|\partial R|})$. One remains with a tensor $c_{i_1,\ldots,i_N}(\boldsymbol{\alpha})$, which describes a physical state (a PEPS) $|\Phi_{\boldsymbol{\alpha}}\rangle = \sum c_{i_1,\ldots,i_N}(\boldsymbol{\alpha})|i_1, \ldots, i_N\rangle$. This defines a linear map $\mathcal{X}\colon |\boldsymbol{\alpha})\mapsto\mathcal{X}|\boldsymbol{\alpha}) \equiv |\Phi_{\boldsymbol{\alpha}}\rangle$ between states $|\boldsymbol{\alpha}) \in (\mathbb{C}^D)^{\otimes|\partial R|}$ on the boundary and the subspace $\mathcal{S} \equiv \mathrm{span}\{|\Phi_{\boldsymbol{\alpha}}\rangle\} \subset (\mathbb{C}^d)^{\otimes|R|}$ of physical states. [We use $|\cdots)$ to denote states on the virtual boundary.] Note that equivalently, one can construct $|\Phi_{\boldsymbol{\alpha}}\rangle$ by placing virtual *bonds* $\sum_{\mu=1}^D |\mu,\mu)$ with bond dimension D along the edges, the state $|\boldsymbol{\alpha})$ at the boundary, and applying the linear map described by A at every site [11].

Having defined the PEPS states $|\Phi_{\boldsymbol{\alpha}}\rangle$ and the PEPS subspace $\mathcal{S} = \mathrm{span}\{|\Phi_{\boldsymbol{\alpha}}\rangle\}$, let us now turn towards

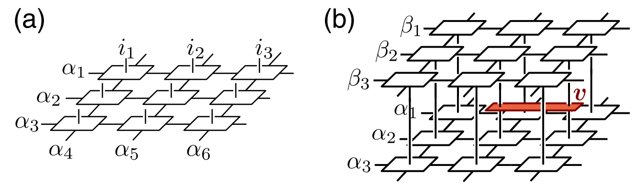

FIG. 1 (color online). (a) Construction of a PEPS by contracting local tensors. PEPS give a map from the boundary indices $(\alpha_1, \alpha_2, \ldots)$ to the bulk indices $(i_1, i_2, \ldots)$. (b) Using this map, any bulk Hamiltonian v naturally induces a Hamiltonian on the boundary by sandwiching v in between the PEPS. Note that the boundary degrees of freedom still need to be orthogonalized.

Hamiltonians for PEPS models. A parent Hamiltonian is a local Hamiltonian $H = \sum h$ such that for any (sufficiently large) region R (i) $h \geq 0$, and $H|\Phi_{\boldsymbol{\alpha}}\rangle = 0\,\forall|\boldsymbol{\alpha})$, i.e., H is frustration free and all states in $\mathcal{S}$ are ground states of H, and (ii) all ground states of H are of the form $|\Phi_{\boldsymbol{\alpha}}\rangle$, ker $H = \mathcal{S}$; this is known as the intersection property [10,12,13]. Given a PEPS, a parent Hamiltonian can be constructed by choosing ker $h = \mathcal{S}$ for some small region (e.g., as a projector), where appropriate conditions on A (which hold for generic tensors) ensure the intersection property [12,13]; since rank $\mathcal{S} \leq D^{|\partial R|}$ for large enough R, such h always exist. The paradigmatic example of a PEPS model is the AKLT model [10], which is constructed by placing spin-$\frac{1}{2}$ singlet bonds along the edges and subsequently projecting onto the maximal spin subspace ($S = 2$ on the square lattice); the parent Hamiltonian is obtained by observing that for any two adjacent sites, the total spin cannot be $S = 4$, and choosing $h = \Pi_{S=4}$ (the projector onto the $S = 4$ subspace).

We now start from a PEPS model, specified by $H = \sum h$ and a tensor A characterizing its ground space $\mathcal{S}$, with a gap Δ above the ground space, and consider an arbitrary perturbation to this model, $H' = H + V = \sum(h + v)$, where $\|V\| \ll \|H\|$. What is the low-energy physics of the perturbed model $H + V$? In leading order, it is given by the effective Hamiltonian $H_{\text{eff}} = \Pi_{\mathcal{S}} V \Pi_{\mathcal{S}}$, where $\Pi_{\mathcal{S}}$ is the projector onto the ground space $\mathcal{S}$ of H; i.e., the low-energy physics takes place in the subspace $\mathcal{S}$. Since $\mathcal{S} = \text{span}\{|\Phi_{\boldsymbol{\alpha}}\rangle\}$, this implies that the states which describe the low-energy physics are in one-to-one correspondence with states $|\boldsymbol{\alpha})$ on the virtual edge (via the inverse of the map $\mathcal{X}$), and thus, the low-energy states exhibit a 1D structure which is associated to the edge. Even more, if the system does not break local symmetries (more technically, if it satisfies the weak LTQO condition [18,19]), these states are exponentially localized at the edge; i.e., different $|\Phi_{\boldsymbol{\alpha}}\rangle$ do not differ in the bulk. Together, this shows that the low-energy Hamiltonian H_{eff} can indeed be understood as a 1D Hamiltonian acting on degrees of freedom localized at the edge.

Let us now show how to determine the 1D model which describes the effective low-energy physics. To this end, we work in the 1D basis $|\boldsymbol{\alpha})$ which lives on the virtual edge indices. There, the perturbation induces a term $(\boldsymbol{\alpha}'|\mathcal{M}|\boldsymbol{\alpha}) = \langle\Phi_{\boldsymbol{\alpha}'}|V|\Phi_{\boldsymbol{\alpha}}\rangle$; that is, $\mathcal{M}$ is obtained by sandwiching the Hamiltonian between a ket PEPS and a bra PEPS, as shown in Fig. 1(b). However, the map $\mathcal{X}\colon |\boldsymbol{\alpha})\mapsto|\Phi_{\boldsymbol{\alpha}}\rangle$ does not preserve orthogonality, and thus, in order to obtain an edge Hamiltonian $\mathcal{H}$ which is isomorphic to H_{eff}, we need to orthogonalize $\mathcal{M}$, $\mathcal{H} = \mathcal{P}^{-1}\mathcal{M}\mathcal{P}^{-1}$, where $\mathcal{P} = \sqrt{\mathcal{Q}}$, $(\boldsymbol{\alpha}'|\mathcal{Q}|\boldsymbol{\alpha}) = \langle\Phi_{\boldsymbol{\alpha}'}|\Phi_{\boldsymbol{\alpha}}\rangle$. Put more formally, we can write $\mathcal{X} = \mathcal{W}\mathcal{P}$, with $\mathcal{P}$ a positive map acting on the virtual indices and $\mathcal{W}$ an isometry from the virtual to the physical system; then, the edge Hamiltonian is $\mathcal{H} = \mathcal{W}^\dagger V \mathcal{W} = \mathcal{P}^{-1}\mathcal{X}^\dagger V \mathcal{X}\mathcal{P}^{-1}$ [where $\mathcal{X}^\dagger V \mathcal{X}$ is the tensor network in Fig. 1(b)], and thus indeed isomorphic to H_{eff}.

An essential point to note about the structure of the edge Hamiltonian is that it inherits all (on-site) symmetries shared by the PEPS and the bulk perturbation: Any symmetry action on a PEPS can be moved from the physical index to an action of the same symmetry on the virtual indices [20], and thus ultimately any symmetry shared by V shows up as a symmetry at the edge degrees of freedom and thus in $\mathcal{H}$; the argument generalizes to other symmetries such as reflection or time reversal.

As an example, we have numerically studied the edge Hamiltonian $\mathcal{H}$ of the square lattice AKLT model on an infinitely long cylinder of circumference N_v; since the transfer operator of the AKLT model has a unique fixed point, the two boundaries decouple and we can restrict our study to a single boundary (see Supplemental Material for a description of the numerical method [21]). We have considered the class of U(1) invariant perturbations

$$V = \sum_{\langle ij\rangle}[J\boldsymbol{S}_i \cdot \boldsymbol{S}_j + gS_i^z S_j^z] + h\sum_i S_i^z, \tag{1}$$

i.e., an anisotropic Heisenberg Hamiltonian with a magnetic field. Since $\mathcal{H}$ is linear in V, we can write $\mathcal{H} = J\mathcal{H}_J + g\mathcal{H}_g + h\mathcal{H}_h$; as $D = 2$, the $\mathcal{H}_\bullet$ ($\bullet = J, g, h$) are spin-$\frac{1}{2}$ Hamiltonians with translational and U(1) symmetry [SU(2) for $\mathcal{H}_J$]. Note that due to symmetry, $\mathcal{H}_J$ is completely determined by $\mathcal{H}_g$.

First, let us see whether the $\mathcal{H}_\bullet$ are sums of local terms. To this end, we decompose $\mathcal{H}_\bullet$ in a Pauli basis, and denote by d_r the total weight of all terms which span r contiguous sites (see [22,23]). Figure 2 shows the result for $\mathcal{H}_J$ and $\mathcal{H}_g$: In both cases d_r decays exponentially with r, indicating that the edge Hamiltonian is approximately local. Let us now have a closer look at the individual terms. For $\mathcal{H}_J$, symmetries restrict the possible two- and three-body terms to Heisenberg couplings, which following Fig. 2 are the dominating terms. More generally, we find

$$\mathcal{H}_J \approx \sum_{\ell\geq 1}\eta_\ell \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\ell} \tag{2}$$

where $\eta_1 \approx 2.298$ and $\eta_2 \approx -2.394$, longer range η_ℓ decay exponentially, and many-body terms are strongly

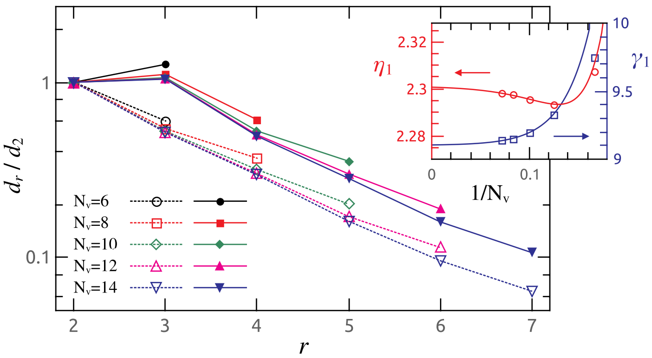

FIG. 2 (color online). Edge Hamiltonian for the perturbed AKLT model: Exponential decay of the interaction strength of range-r terms, d_r, with distance, for different N_v, for $\mathcal{H}_J$ (solid lines) and $\mathcal{H}_g$ (dotted lines). Inset: Finite size scaling of η_1 (red circles) and γ_1 (blue squares) vs $1/N_v$.

suppressed. Remarkably, the nearest neighbor (NN) and next-nearest neighbor (NNN) Heisenberg terms in $\mathcal{H}_J$ have essentially the same strength, but opposite sign (this staggering repeats in the longer-range η_ℓ and arises from the alternating parity of singlets connecting the bulk perturbation to the boundary). Adding an $S_i^z S_j^z$ anisotropy in the bulk leads to an anisotropy at the edge with a similarly staggered structure and a renormalized Heisenberg term,

$$\mathcal{H}_g \approx \sum_{\ell \geq 1} \left[\gamma_\ell \sum_i S_i^z S_{i+\ell}^z + \frac{\eta_\ell - \gamma_\ell}{3} \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+\ell} \right] \qquad (3)$$

but with suppressed NNN amplitudes $\gamma_1 \approx 9.137$, $\gamma_2 \approx -4.493$. (The dependence between the coefficients is due to symmetries.) Finally, a local magnetic field induces exactly a field of identical strength at the boundary, $\mathcal{H}_h = \sum S_i^z$, as can be shown analytically based on symmetries of the state [24].

We have studied the phase diagram of the edge for $J > 0$ using exact diagonalization supplemented by DMRG and analytical arguments, see Fig. 3. We find that the model exhibits three phases—a fully polarized ferromagnetic phase, an antiferromagnetic phase, and an XY Luttinger liquid phase. By choosing the appropriate bulk perturbation V, we can thus achieve either gapped, gapless, or symmetry broken phases at the edge, and induce phase transitions between them. Note that the phase diagram at the edge only depends on the relative strength of the terms in V, and thus all phases can be realized within the perturbative regime; generally, the perturbative treatment will be valid as long as V is sufficiently smaller than the bulk gap.

A natural question is whether we can achieve any edge Hamiltonian $\mathcal{H}$ we want. Since for a trivial bulk phase the mapping $\mathcal{X}$ from the edge to the bulk is injective, the answer there is indeed yes. Even more, any local $\mathcal{H}$ can be obtained from an approximately local bulk perturbation: At the RG fixed point where A is the identity, this is clear. Now for any model connected to it via a gapped path, we

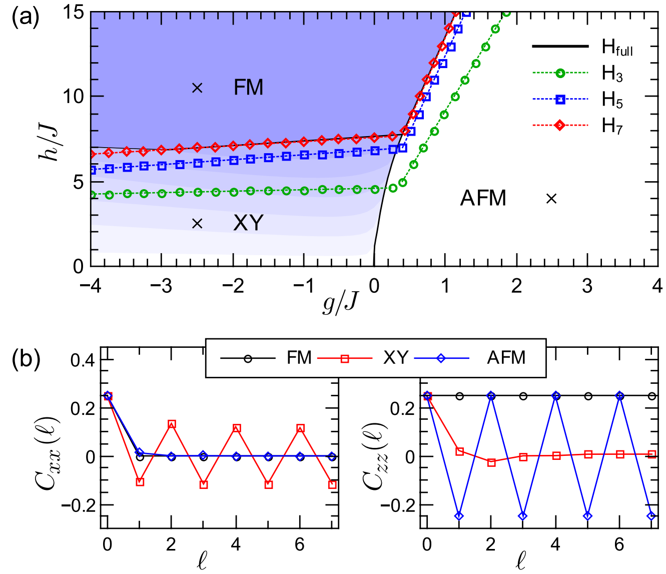

FIG. 3 (color online). Edge Hamiltonian for the perturbed AKLT model, Eq. (1). (a) Phase diagram as a function of anisotropy g/J and field h/J, for $J > 0$. Three phases are observed: a fully polarized ferromagnetic (FM) phase (with magnetization $m_z = \frac{1}{2}$), an antiferromagnetic (AFM) phase ($m_z = 0$), and an XY Luttinger liquid phase. The shading shows m_z for the ground state of the full edge Hamiltonian $\mathcal{H}$ for $N_v = 14$; the solid lines give phase boundaries determined analytically using fully polarized and mean-field AFM Ansätze, both for $\mathcal{H}$ and Hamiltonians $\mathcal{H}_k$ where the sum in (2) and (3) is restricted to $\ell < k$. (b) Correlation functions $C_{xx}(\ell) = \langle S_i^x S_{i+\ell}^x \rangle$ and $C_{zz}(\ell) = \langle S_i^z S_{i+\ell}^z \rangle$ for the three phases, computed at the points marked × in (a). DMRG calculations for $\mathcal{H}_k$ show that in the XY phase, C_{xx} decays algebraically.

can obtain its ground space via a quasiadiabatic evolution [25] of the original ground space; the correspondingly evolved bulk perturbation is then quasilocal and yields the desired $\mathcal{H}$. Thus, we find that for a trivial bulk phase, the edge is never protected [26].

We now turn towards topologically ordered systems, and investigate whether the bulk order can protect the physics at the edge. In these systems, the PEPS tensor is invariant under a symmetry action on the virtual indices which can be identified with particle types (charges) p of the topological model. Therefore, on the cylinder the transfer operator $\mathbb{E}$ of a column (cf. Supplemental Material [21]) is degenerate, with its maximal eigenvectors ρ_{fp}^p being supported on the sector with total topological charge p [23]. In particular, the fixed point $\mathbb{E}^\infty$ is of the form $\mathbb{E}^\infty = \sum_p |\rho_{\text{fp},L}^p\rangle\langle\rho_{\text{fp},R}^{p^*}|$, with p^* the antiparticle of p.

Let us now for a moment fix p in the sum: Then, we are essentially back in the scenario which we had for nondegenerate $\mathbb{E}$, in that any perturbation induces an effective edge Hamiltonian on the two edges independently. However, there is an important difference: $\rho_{\text{fp},L}^p$ does not have full rank, but is supported on the sector with topological charge p. Thus, only boundary conditions $|\boldsymbol{\alpha})$ in this sector will correspond to a nonzero physical state $|\Phi_{\boldsymbol{\alpha}}\rangle$ and thus to admissible gapless excitations. At the same time, the label p is also preserved by $\mathbb{E}_V$ (since it emerges from a symmetry acting solely on the virtual indices of the PEPS tensor [13]), and thus, $\mathcal{M}_L^p$ is also supported only in that sector. Thus, we can still orthogonalize it using the pseudoinverse of $(\rho_{\mathrm{fp},L}^p)^{1/2}$, and obtain an effective edge Hamiltonian $\mathcal{H}_L^p$ for the sector with charge p (and analogously $\mathcal{H}_R^{p^*}$ for the right edge).

The full edge Hamiltonian is now obtained by putting both edges together and summing over p; it is of the form

$$\mathcal{H} = \Pi_0(\mathcal{H}_L \otimes \mathbb{1}_R + \mathbb{1}_L \otimes \mathcal{H}_R)\Pi_0,$$

where $\mathcal{H}_{L,R} = \sum_p \mathcal{H}_{L,R}^p$, and Π_0 is the projector onto the sector with total charge $p = 0$ for both boundaries together. This implies that the edge Hamiltonian for a single edge must conserve the topological charge; this edge symmetry is protected by the topological order in the bulk and can stabilize nontrivial properties of the edge Hamiltonian [7]. Let us illustrate this for the Toric code [9], where the spin-$\frac{1}{2}$ edge Hamiltonian is constrained by a quasifermionic $\mathbb{Z}_2$ parity superselection rule. Since the TC is an RG fixed point, there is a one-to-one local unitary correspondence between virtual and physical degrees of freedom at the edge up to the parity constraint [13], allowing us to engineer any parity-preserving edge Hamiltonian. In particular, $V = -\sum_{\langle ij\rangle} S_i^x S_j^x$ yields Ising models $\mathcal{H}_L = \mathcal{H}_R = -\sum S_i^x S_{i+1}^x$ at the edges, whose even and odd parity ground states are the GHZ states $|+\ldots+\rangle \pm |-\ldots-\rangle$. Thus, each of the edges is an Ising model in a GHZ state—a macroscopic superposition—which is protected against spontaneous symmetry breaking by *arbitrary* local perturbations, something that is impossible in a conventional 1D spin system; this is in close analogy to the protection of a fermionic Majorana chain [27].

We have computed the edge Hamiltonian for the topological RVB state on the kagome lattice, which is a $D = 3$ PEPS [14,17], for a bulk perturbation $V = \sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$. We find that $\mathcal{H}_L$ and $\mathcal{H}_R$ are again approximately local, while the per-sector Hamiltonians $\mathcal{H}_{L/R}^p$ are not; the latter is due to the fact that $\mathcal{H}_{L/R}^p$ contain a projector onto a superselection sector, in direct analogy to what has been found for the Hamiltonians reproducing the entanglement spectrum in the case of topological models [23]. The symmetry of the RVB PEPS strongly restricts the possible local terms, implying that the structure of the edge is that of a spinful particle or a hole, similar to a *t-J* model [28]; explicitly, we find that the leading terms of the edge Hamiltonian for $N_v = 8$ are (using the notation of [28])

$$\mathcal{H} \approx \sum_i \bigg[t_1 \sum_s (a_{s,i}^\dagger a_{s,i+1} + \mathrm{H.c.}) + J_1 \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \frac{3c_2}{\sqrt{2}}\left(n_i - \frac{2}{3}\right) + \Delta_1 (a_{\downarrow,i} a_{\uparrow,i+1} - a_{\uparrow,i} a_{\downarrow,i+1} + \mathrm{H.c.}) \bigg]$$

where the $a_{s,i}$ denote hardcore bosons, and with $t_1 \approx -0.158$, $J_1 \approx 0.233$, $c_2 \approx 0.177$, and $\Delta_1 \approx -0.086$. We have also considered a chiral perturbation $V = \sum \boldsymbol{S}_i \cdot (\boldsymbol{S}_j \times \boldsymbol{S}_k)$, where the sum runs over all triangles, and found that the dominant term at the edge is given by a chiral current of particles, $\mathcal{H}_L \approx \sum i a_{s,k}^\dagger a_{s,k+1} + \mathrm{H.c.}$, carrying 64.5% of the total weight in $\mathcal{H}_L$. Note, however, that such a term by itself does not give rise to a protected chiral edge mode. [A similar chiral perturbation to the AKLT model gives, in leading order, rise to a chiral spin current $\mathcal{H} \approx \sum \boldsymbol{S}_k \cdot (\boldsymbol{S}_{k+1} \times \boldsymbol{S}_{k+2})$; note that this is the simplest SU(2) invariant chiral spin-$\frac{1}{2}$ Hamiltonian.]

In this Letter, we have studied edge theories in the framework of PEPS models. We have demonstrated that the effective low-energy theory lives on the virtual degrees of freedom at the boundary, which allows us to explicitly obtain the edge Hamiltonian in the vicinity of these models. In the trivial phase, this allows us to engineer arbitrary edge Hamiltonians, while topological bulk phases carry symmetries at their boundary which can protect the physics at the edge. Thus, protected physics at the edge is a signature of topological order in the bulk, and we expect that one can characterize the type of bulk topological order from the protected properties of the edge [29]. All results equally apply to fermionic systems [30]. While we focused on a perturbative regime around PEPS models, we expect our findings to apply more generally: First, PEPS approximate ground states of local Hamiltonians well [31] and any (generic) PEPS has a parent Hamiltonian associated with it [12,13], suggesting that many systems have a PEPS model closeby; and second, the identification of the low-energy physics with the virtual degrees of freedom at the edge extends to any system connected to a PEPS model by a gapped path, by quasiadiabatic evolution of the ground space [25].

One question left open is the possible correspondence between entanglement spectrum and edge physics [32–35] beyond that emerging from their joint symmetries. For example, for the RVB model the Heisenberg term in $\mathcal{H}$ is much enhanced as compared to the Hamiltonian derived from the entanglement spectrum [22,28], which can be seen as a trace of the Heisenberg bulk perturbation. To study this further, one can apply our framework to frustrated PEPS models (e.g., variationally minimized iPEPS) which exhibit edge dynamics without perturbations.

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