

Generalized Haldane map from the matrix product state path integral to the critical theory of the J_1 - J_2 chain

F. Azad^{1,2,*}, Adam J. McRoberts^{3,4,*}, Chris Hooley⁴, and A. G. Green²

¹Electrical Engineering and Computer Science Department, *Technische Universität Berlin*, 10587 Berlin, Germany

²London Centre for Nanotechnology, University College London, Gordon Street, London WC1H 0AH, United Kingdom

³International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy

⁴Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany



(Received 29 April 2024; revised 2 December 2024; accepted 17 January 2025; published 19 February 2025)

We study the J_1 - J_2 spin-1/2 chain using a path integral constructed over matrix product states (MPS). By virtue of its nontrivial entanglement structure, the MPS ansatz captures the key phases of the model even at a semiclassical, saddle-point level, and, as a variational state, is in good agreement with the field theory obtained by Abelian bosonization. Going beyond the semiclassical level, we show that the MPS ansatz facilitates a physically motivated derivation of the field theory of the critical phase: By carefully taking the continuum limit—a generalization of the Haldane map—we recover from the MPS path integral a field theory with the correct topological term and emergent $SO(4)$ symmetry, constructively linking the microscopic states and topological field-theoretic structures. Moreover, the dimerization transition is particularly clear in the MPS formulation—an explicit dimerization potential becomes relevant, gapping out the magnetic fluctuations.

DOI: [10.1103/PhysRevResearch.7.L012037](https://doi.org/10.1103/PhysRevResearch.7.L012037)

The attempt to combine variational methods with quantum field theory has a long history [1], with a significant advance coming from the formulation of matrix product states directly in the continuum limit [2,3]. An alternative approach, that follows the traditional route of condensed matter physics more directly [4,5], is to develop a spatially discrete path integral over an appropriate variational manifold [6] and then to construct a field theory as a continuum limit. The question of how the topological terms of conventional field-theoretical approaches emerge in this prescription has up to now been unclear.

The J_1 - J_2 chain has provided an archetypal model in which to investigate the role of topology in quantum systems, and harbors a rich phase diagram. Semiclassically, an incommensurate helimagnetic phase interpolates between the ferromagnetic and antiferromagnetic (Néel) phases, and a plethora of numerical and analytical approaches have revealed further features [7–13]. We will be most concerned with the transition in the quantum $S = \frac{1}{2}$ chain between a critical antiferromagnetic phase and the dimer phase, where competing first- and second-neighbor antiferromagnetic terms drive adjacent spins into singlets.

Under Abelian bosonization [4,5,14,15], this transition appears to be of Kosterlitz-Thouless (KT) character. In obscuring the $SU(2)$ symmetry, however, this misses the spacetime topology of the quantum states, and the fact that

topological defects in one phase are bound to the charges of the other—the boundary between two singlet covers has a single (delocalized) spin. Field-theoretically, this is encoded in additional topological Wess-Zumino (WZ) terms [16–18] (generalizations of the Haldane Θ term [19]), which measure the winding of the joint Néel-singlet order parameter during the tunneling events (instantons) that drive the transition out of the dimer phase.

These ideas are central to the understanding of deconfined quantum criticality [20] and underpin a rich network of dualities between different two-dimensional quantum states. In the J_1 - J_2 model, these terms may be derived via a mapping of the spins to fermionic degrees of freedom [16–18]. In this Letter, we give an alternative derivation working with the original spin degrees of freedom, mirroring the derivation of the Θ term in the antiferromagnet [19], and drawing an explicit, constructive connection between tensor network states and field-theoretic topological terms.

A matrix product state (MPS) ansatz encompassing the key physics of the different phases is the basis of our approach—even as a variational wave function, it captures a continuous phase transition between the critical and dimer phases. Reparametrizing in terms of the order parameters of these phases, we construct the path integral over the MPS ansatz [6], and demonstrate how the resulting effective action recovers the nonlinear sigma model (NLSM) of the critical phase, with the $SO(4)$ WZ term (cf. Ref. [19]), explicitly linking these topological field-theoretic structures to the microscopic states. Further, the MPS field theory clarifies the nature of the dimerization transition, with an explicit potential term which breaks the $SO(4)$ symmetry and opens the gap.

Model and MPS ansatz. The Hamiltonian of the J_1 - J_2 chain consists of competing Heisenberg interactions between

*These authors contributed equally to this work.

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

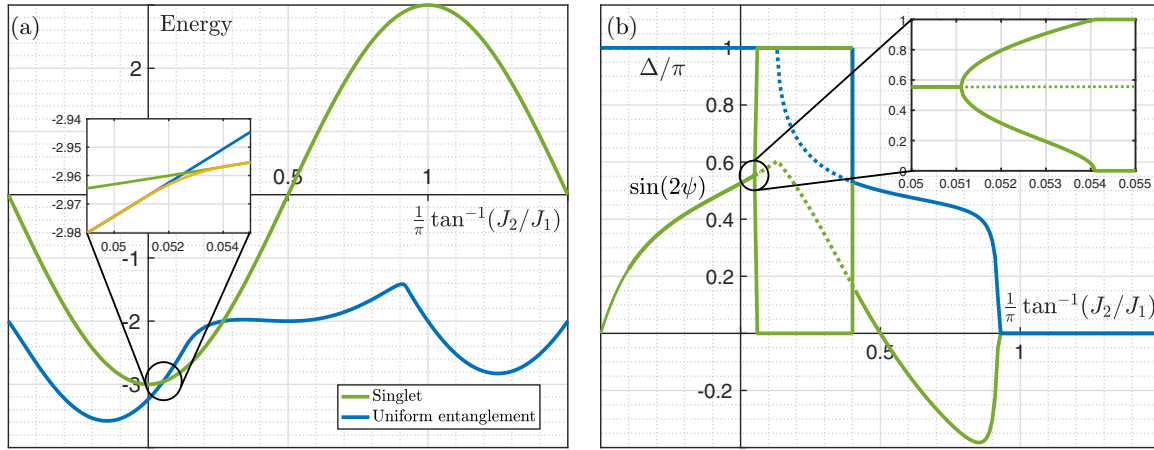


FIG. 1. Saddle-point phase diagram as a function of $\tan^{-1}(J_2/J_1)/\pi$. (a) Variational ground state energy: The blue curve shows the energy of the uniform entanglement saddle point ($\psi_A = \psi_B$), and the green curve the energy of a singlet cover. Near the crossover (inset), another saddle-point solution emerges (see Supplemental Material [21]), so that the transition is continuous even at this level. (b) The helimagnetic pitch Δ/π (blue) and the entanglement $\sin(2\psi)$ (green). The entanglement is uniform except in the singlet phase, and near the transition (inset). The singlet phase suppresses the development of an incommensurate spiral (dashed curves show the optimum uniform entanglement state).

nearest and next-nearest neighbors,

$$\hat{H} = \sum_i (J_1 \hat{\sigma}_i \cdot \hat{\sigma}_{i+1} + J_2 \hat{\sigma}_i \cdot \hat{\sigma}_{i+2}), \quad (1)$$

where $\hat{\sigma} = (\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z)$ is the vector of Pauli matrices. We introduce our variational state as an MPS ansatz with bond-dimension two,

$$|\Psi\rangle = \sum_{\{\sigma\}} \bigotimes_i (A_{[i]}^{\sigma_i} |\sigma_i \hat{n}_i\rangle), \quad A_{[i]}^+ = \begin{pmatrix} \cos \psi_i & 0 \\ 0 & ie^{i\xi_i} \sin \psi_i \end{pmatrix},$$

$$A_{[i]}^- = e^{i\pi/4} \begin{pmatrix} 0 & \cos \psi_i \\ ie^{i\xi_i} \sin \psi_i & 0 \end{pmatrix}, \quad (2)$$

where $|\hat{n}\rangle$ represents a spin-coherent state polarized in the direction of the unit vector $\hat{n}$. [We discuss the gauge fixing in the Supplemental Material (SM) [21]]. The angle ξ allows tuning between singlet and $S = 0$ triplet configurations and will generally not appear in the following.

This state captures the key phases of the J_1 - J_2 model. In particular, it can represent a product state antiferromagnet with $\psi = 0$ or $\pi/2$, and $|\hat{n}_i\rangle = |(-1)^i \hat{n}\rangle$, and the singlet covers are obtained by setting $\psi_{2i} = \pi/4$, $\psi_{2i-1} = 0$ (or vice versa), with $|\hat{n}_i\rangle = |(-1)^i \hat{n}\rangle$.

Saddle-point phase diagram. Before turning to the connections to the field theory, let us first discuss the phase diagram that results from the ansatz (2). The finite, two-site correlation length implies that $\langle \hat{H} \rangle$ can be calculated and manipulated analytically; Eq. (2) is in left canonical form with left-environment $\mathbb{1}$ and right-environment $R_i = (\mathbb{1} + \sigma^z \cos 2\psi_{i+1})/2$.

In order to simplify the optimization, we restrict $\hat{n}$ to lie in the xy plane with a constant pitch angle $\Delta \in [0, \pi]$, such that $\hat{n}_i \cdot \hat{n}_{i+1} = \cos \Delta$. Further, we assume that the entanglement parameters ψ_i will at most alternate between two values ψ_A on even sites and ψ_B on odd sites. Now, the expectation value of the Hamiltonian (1), over the MPS ansatz (2) with these

restrictions, is

$$E = J_1[(\cos^2 2\psi_A + \cos^2 2\psi_B) \cos \Delta - \sin[2(\psi_A + \psi_B)](1 - \cos \Delta)] + J_2[2 \cos^2 2\psi_A \cos^2 2\psi_B \cos 2\Delta + \sin 4\psi_A \sin 4\psi_B (1 + \cos 2\Delta)/4]. \quad (3)$$

The variational (saddle-point) phase diagram (Fig. 1) follows by minimizing Eq. (3) over ψ_A , ψ_B , and Δ . The pitch angle follows the classical result for most of the phase diagram—an (incommensurate) helimagnetic phase with $\Delta = \cos^{-1}[-J_1/(4J_2)]$ interpolates between ferromagnetic and Néel order at $J_1/J_2 < -4$ and $J_1/J_2 > 4$, respectively, dressed with some uniform entanglement. The helimagnetic order is suppressed, however, by the dimerized singlet phase for $0.1619 \lesssim J_2/J_1 \lesssim 1.317$.

The transition between the Néel and singlet phases occurs at $J_2/J_1 \approx 1/6$. On the scales indicated in Figs. 1(a) and 1(b), the singlet phase appears to be formed at an abrupt first-order discontinuity in the parameters of the MPS ansatz; however, zooming in on the region around this point reveals two continuous transitions (at saddle-point level): the first at $J_2/J_1 \approx 0.1619$, where the translation symmetry is first broken; and the second at $J_2/J_1 = 3 - 2\sqrt{2} \approx 0.1716$, where the singlet state is fully formed (see SM [21] for the analytic details).

This in-plane optimization of the MPS ansatz invites a comparison with Abelian bosonization, which predicts a KT dimerization transition around the same point $J_2/J_1 \approx 1/6$ [4,5,21]. While this picture will be modified by the topological terms, we still expect a universal jump in the spin stiffness ρ (which we derive in the SM [21]). The MPS ansatz (2), on the other hand, furnishes us with an estimate of ρ much more straightforwardly: We simply use the dependence of the energy upon the pitch Δ to evaluate the resistance to inducing

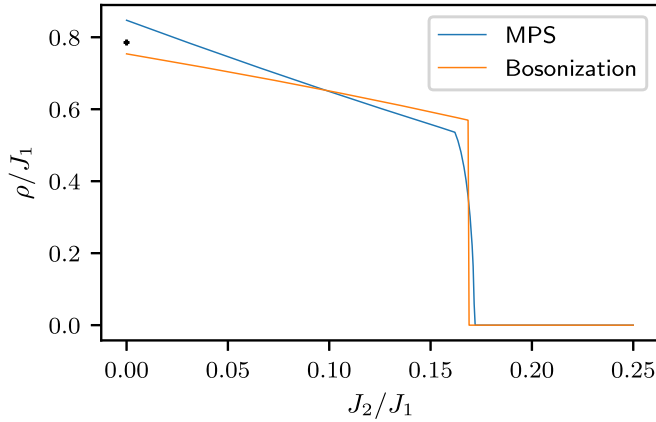


FIG. 2. The spin stiffness ρ as a function of J_2/J_1 across the Néel-dimer transition, obtained from the saddle-point configuration of the MPS ansatz (2) and the bosonized field theory [21]. There is reasonable agreement between the two methods, with both exhibiting the jump at $J_2 = J_2^c$. The black point is the exact (Bethe-ansatz) value, $\pi/4$, at $J_2 = 0$.

a twist in the magnetic order, that is,

$$\rho = \langle N \rangle \left. \frac{\partial^2 E}{\partial \Delta^2} \right|_{\Delta=\pi}, \quad (4)$$

where $\langle N \rangle = \cos(2\psi_A) \cos(2\psi_B)$ is the Néel order parameter. We show the spin stiffness in Fig. 2, and find that, *even at the saddle-point level*, the universal jump associated to the KT transition is visible—though it occurs between the split transitions, rather than discontinuously—and broadly agrees with the field-theoretic estimate [22].

The rest of our treatment focuses on this dimerization transition, for which later work [16–18] went beyond a purely KT treatment and showed the importance of WZ terms in the field theory—they encode the binding of spins to domain walls between singlet covers. We will show in the following that the MPS ansatz captures this physics directly, in the structure of the spin wave function. We note that a higher bond order ansatz would result in better saddle points for the path integral, but we stress that this is not a variational method—the spirit of our approach is to select the lowest bond dimension that captures the qualitative features of the competing orders at the saddle-point level, ensuring both that the path integral is analytically tractable and that the correct critical theory can be constructed in simple perturbative corrections to the saddle-points.

SO(4) order parameter and continuum limit. The first step is to construct a local SO(4) order parameter that treats the Néel and dimer order on an equal footing. In terms of the MPS, the Néel order parameter is

$$N = (-1)^i \langle \hat{\sigma}_i \rangle = \cos(2\psi_i) \cos(2\psi_{i+1}) \hat{n}_i. \quad (5)$$

And, while the singlet states should formally be distinguished by a string order parameter, it suffices here to use a local singlet order parameter

$$D_i = (-1)^i \langle \hat{\sigma}_i^+ \hat{\sigma}_{i+1}^+ + \hat{\sigma}_i^- \hat{\sigma}_{i+1}^- - \hat{\sigma}_{i-1}^+ \hat{\sigma}_i^+ - \hat{\sigma}_{i-1}^- \hat{\sigma}_i^- \rangle, \quad (6)$$

valid when $\hat{n}_i \approx -\hat{n}_{i+1}$, where $\hat{\sigma}^+$ and $\hat{\sigma}^-$ are spin raising and lowering operators in the basis $\{|\hat{n}\rangle, |-\hat{n}\rangle\}$ (these are the usual

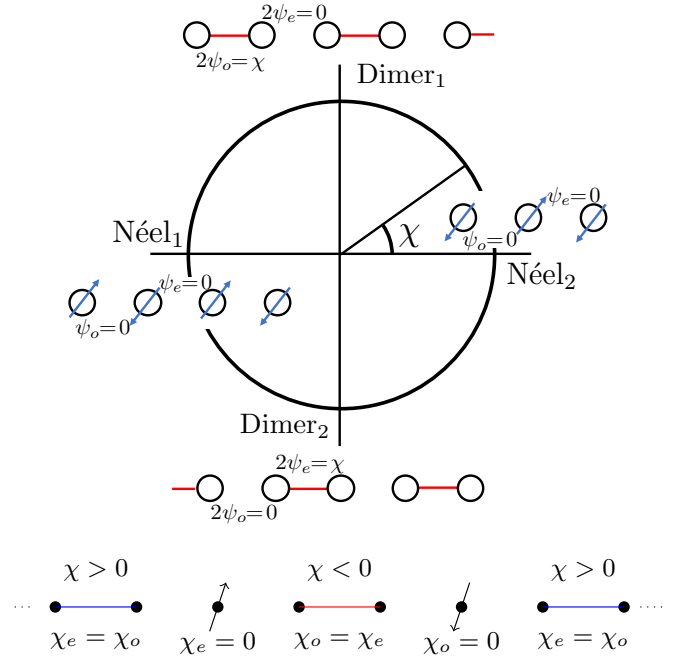


FIG. 3. Order parameter: The parameters of the MPS ansatz (2) must be patched together in order to construct the SO(4) order parameter. The polar angle χ (restricted to the range $\chi \in [-\pi/2, \pi/2]$ to avoid a double cover in the usual way) is introduced so that between $-\pi/2$ and 0 it describes entanglement on even bonds, and between 0 and $\pi/2$ entanglement on the odd bonds. A domain wall in the singlet order produces a free spin, where $\chi = 0$.

raising and lowering operators if $\hat{n} = \hat{z}$). For states given by Eq. (2), this is, explicitly,

$$D_i = (-1)^i [-\sin(2\psi_{i+1}) \cos(\psi_i - \psi_{i+2}) \cos(\psi_i + \psi_{i+2}) + \sin(2\psi_i) \cos(\psi_{i-1} - \psi_{i+1}) \cos(\psi_{i-1} + \psi_{i+1})]. \quad (7)$$

Now, if we allow entanglement on either only even or only odd bonds, we obtain

$$\begin{array}{ll} [\text{even} : \psi_{2i+1} = 0] & [\text{odd} : \psi_{2i} = 0] \\ N_{2i} = \cos(2\psi_{2i}) \hat{n}_{2i} & N_{2i} = \cos(2\psi_{2i+1}) \hat{n}_{2i} \\ N_{2i-1} = -\cos(2\psi_{2i}) \hat{n}_{2i-1} & N_{2i+1} = -\cos(2\psi_{2i+1}) \hat{n}_{2i+1} \\ D_{2i} = \sin(2\psi_{2i}) & D_{2i} = -\sin(2\psi_{2i+1}) \\ D_{2i-1} = \sin(2\psi_{2i}) & D_{2i+1} = -\sin(2\psi_{2i+1}) \end{array} \quad (8)$$

such that in either case $N^2 + D^2 = 1$, and (D, N) forms an SO(4) multiplet [23].

We therefore enforce the constraint in the ansatz that no two consecutive ψ_i are nonzero, and introduce a single angle χ_i which interpolates between the two singlet orders,

$$\begin{aligned} 2\psi_{2i} &= -\chi_{2i} \Theta(-\chi_{2i}) = -\chi_{2i-1} \Theta(-\chi_{2i-1}), \\ 2\psi_{2i+1} &= \chi_{2i} \Theta(\chi_{2i}) = \chi_{2i+1} \Theta(\chi_{2i+1}), \end{aligned} \quad (9)$$

where $\Theta(x)$ is the Heaviside step function. We show how χ rotates between the singlet and Néel orders in Fig. 3.

We note that this order parameter cannot completely characterize the uniform entanglement saddle points; those states directly include significant quantum fluctuations which, in the field theory, are encoded as instantons between the two singlet covers.

Effective action. Now, armed with this joint order parameter, we can construct the field theory as an MPS path integral [6],

$$\mathcal{Z} = \int \mathcal{D}\Psi e^{-S[\Psi]}, \quad S = \int d\tau \langle \Psi | \partial_\tau \Psi \rangle + \mathcal{H}, \quad (10)$$

where $\mathcal{D}\Psi = \mathcal{D}\hat{n}\mathcal{D}\chi\mathcal{D}\xi \cos^2 \chi$ is the functional Haar measure over the restricted MPS ansatz [6]. We note that, despite the enforced staggering of ψ_i , we are still taking advantage of the fact that the MPS path integral captures entanglement in its saddle points (the singlet covers). To derive the kinetic and Hamiltonian terms of the action, we can simply set $\psi_{2i+1} = 0$ (the same continuum limit is recovered if we instead set $\psi_{2i} = 0$), though more care is needed for the topological term. We have the Berry phase

$$\begin{aligned} S_B = \int d\tau \langle \Psi | \partial_\tau \Psi \rangle = iS \int d\tau \left[\sum_i \dot{\phi}_i \cos \theta_i \cos \chi_i \right. \\ \left. + \sum_{2i} \dot{\xi}_{2i} (1 - \cos \chi_{2i}) \right] \end{aligned} \quad (11)$$

(where $S = \frac{1}{2}$), and the Hamiltonian,

$$\begin{aligned} \mathcal{H} = J_1 \sum_{2i} \left[-w_{2i}^x + (1 + w_{2i}^x) \hat{n}_{2i-1} \cdot \hat{n}_{2i} \right. \\ \left. + w_{2i}^z w_{2i+2}^z \hat{n}_{2i} \cdot \hat{n}_{2i+1} \right] \\ + J_2 \sum_{2i} w_{2i}^z w_{2i+2}^z (\hat{n}_{2i} \cdot \hat{n}_{2i+2} + \hat{n}_{2i-1} \cdot \hat{n}_{2i+1}), \end{aligned} \quad (12)$$

where $w^x = \sin \chi \cos \xi$, $w^z = \cos \chi$ are components of an $O(3)$ vector parametrizing the entanglement, and we have set $\psi_{2i+1} = 0$ here and in the ξ term of the Berry phase.

To proceed, we apply Haldane's mapping [24] to the spin degrees of freedom,

$$\hat{n}_i = (-1)^i \hat{m}_i \sqrt{1 - \mathbf{l}_i^2} + \mathbf{l}_i, \quad (13)$$

where $\hat{m}$ is the slowly varying Néel field, and $\mathbf{l}$ captures the fast fluctuations of the magnetization, such that

$$\hat{m}_i^2 = 1, \quad \hat{m}_i \cdot \mathbf{l}_i = 0, \quad \mathbf{l}_i^2 \ll 1. \quad (14)$$

We apply this mapping to the Berry phase (11) and Hamiltonian (12) above, expanding around the saddle points $\chi = \pm\pi/2$ (the singlet covers), and retaining terms up to second order in the fluctuations $\mathbf{l}$ and ξ , and in the derivatives of the slow fields $\hat{m}$ and w . We thus obtain the action (18) of the SO(4) NLSM with a topological term and dimerization potential.

We will give here all of the essential points, and all of the approximations used (see the SM [21] for full details). We begin with the topological term: Inserting Eq. (13) into Eq. (11), we obtain a term

$$\begin{aligned} i\Omega = iS \int d\tau \sum_i (-1)^i \dot{\phi}_i \cos \theta_i \cos \chi_i \\ \sim iS \int d\tau dx \left(\frac{\text{sgn} \chi \cos \chi}{2} - \Theta(\chi) \right) \epsilon^{\mu\nu} \partial_\mu \cos \theta \partial_\nu \phi \end{aligned} \quad (15)$$

(where θ and ϕ are now the angular coordinates of the Néel field $\hat{m}$). This is equal to the Wess-Zumino term identified in Ref. [18] (see also SM [21]),

$$\Omega_{\text{WZ}} = \frac{4\pi S k}{2\pi^2} \int_0^1 d\zeta \int d\tau dx \epsilon_{abcd} u^a \partial_\zeta u^b \partial_\tau u^c \partial_x u^d, \quad (16)$$

where $k \in \mathbb{Z}$ is odd, the factor of $2\pi^2$ in the denominator is the area of S^3 , and $u(\zeta, \tau, x)$ is an arbitrary extension of the field $u(\tau, x) = (\sin \chi, \cos \chi \hat{m}) \equiv (u^0, \mathbf{u})$ satisfying

$$\begin{aligned} u(\zeta = 0, \tau, x) &= (1, 0, 0, 0), \\ u(\zeta = 1, \tau, x) &= u(\tau, x). \end{aligned} \quad (17)$$

The extension allows a coordinate free expression of the WZ term, but Ω and Ω_{WZ} produce the same functional weight for any configuration $u(\tau, x)$ in the path integral.

In the MPS treatment, the internal structure of the ansatz constrains domain walls between different singlet covers to contribute to the overall Berry phase as a free spin; the topological term imposes this same constraint in the field theory.

The kinetic terms follow by integrating out the fast fields, ξ and $\mathbf{l}$. Integrating out ξ is straightforward after expanding Eq. (12) to quadratic order. To integrate out $\mathbf{l}$ we neglect any terms $\sim \cos^2 \chi \mathbf{l}^2$, but otherwise it proceeds as in the standard Haldane mapping [24] (see also SM [21]). We obtain kinetic terms $(\partial_\tau w^z)^2$ and $(w^z)^2 (\partial_\tau \hat{m})^2$, respectively, with the same prefactor $1/(32J_1)$.

To deal with the Hamiltonian, we simply expand in the gradients of $\hat{m}$ and w . We note, however, that fluctuations of $\hat{m}$ are heavily suppressed on the entangled bonds—this means that gradients of $\hat{m}$, like the gradients of w^z , occur over two lattice spacings, not one. Accounting for this fact ensures that both terms, $(\partial_x w^z)^2$ and $(w^z)^2 (\partial_x \hat{m})^2$, appear with the same prefactor, $J_1 - 2J_2$.

Finally, we switch to the standard angular coordinates on S^3 , i.e., we define $\alpha = \pi/2 - \chi$, in terms of which $(w^z)^2 = \sin^2 \alpha$ and $(\partial w^z)^2 \sim (\partial \alpha)^2$. We have then

$$\begin{aligned} S = i\Omega + \int d\tau dx \left[\frac{1}{32J_1} [(\partial_\tau \alpha)^2 + \sin^2 \alpha (\partial_\tau \hat{m})^2] \right. \\ \left. + (J_1 - 2J_2) [(\partial_x \alpha)^2 + \sin^2 \alpha (\partial_x \hat{m})^2] + V(\alpha) \right], \end{aligned} \quad (18)$$

where the dimerization potential is

$$V(\alpha) = -\frac{3J_1}{2} + \frac{J_2}{2} - \frac{J_2}{2} \cos 2\alpha. \quad (19)$$

This form of the action, derived directly from an MPS parametrization of the spin states (2), makes the physics of the transition particularly transparent: If $J_2 < J_2^c$, $V(\alpha)$ is irrelevant, the SO(4) symmetry emerges in the infrared, and the topological term ensures the theory remains gapless; if $J_2 > J_2^c$, $V(\alpha)$ is relevant, and the SO(4) symmetry is broken in favor of dimer order.

Discussion and outlook. In this Letter, we have introduced an MPS ansatz that captures the key physics of the J_1 - J_2 chain, encompassing ferromagnetic, Néel, spiral, and dimer orders. Even at the saddle-point level, it reproduces the essential features of the deconfined Néel-singlet transition at $J_2/J_1 \approx 1/6$, including the universal jump in the spin stiffness (Fig. 2) [25].

From this ansatz, we have directly identified a joint Néel-dimer order parameter, and constructed the field theory from an MPS path integral [6]. While this is, mechanically, somewhat similar to the construction of the field theory of the Heisenberg antiferromagnet ($J_2 = 0$) as a coherent state path integral, the use of MPS-valued fields allows us to recover the correct topological term and NLSM [16–18]. Moreover, the nature of the dimerization transition is remarkably clear in the MPS field theory, where the potential term of an explicit entanglement field flows either to weak or strong coupling.

The MPS resums instantons of the coherent state theory and encodes their topological structure locally in the MPS fields. While this connection has been noted previously [6,26], here we have provided a constructive link: We have shown how the MPS faithfully encodes these topological features, and how this leads directly to the corresponding topological terms in the field theory. It is intriguing to speculate that this connection might be used more generally as a method to resum instantons in favor of a higher bond-dimension MPS path integral—the topological term, after all, arises independently of the Hamiltonian.

The MPS path integral is finding an increasing range of application. It has been used to derive a new treatment of open quantum systems [27], provides a consistent framework unifying the computation of fluctuation corrections around MPS saddle points [28–31], has revealed new connections between classical and quantum chaos [32,33], and with the

present work demonstrates the link between tensor-network and field-theoretical treatments of topological structures in quantum wave functions. Indeed, the effective field theory derived here suggests that the J_1 - J_2 chain has a hitherto unsuspected phase transition [34] between two distinct critical phases: the $O(4)$ nonlinear sigma model with a topological term suggested by Affleck and Haldane [5], and the recent alternative proposal of Zirnbauser [35].

We anticipate that, with a suitable modification of the underlying MPS ansatz to capture the competing orders in a given system, the MPS path integral will provide a generic method to construct field-theoretic descriptions of quantum phase transitions involving a change in the entanglement structure, such as in higher-spin chains [36–39] or ladder structures [40–42]. Moreover, while generic projected entangled pair states (PEPS) are not efficiently contractible [43,44], it may be possible to use sequential circuit ansätze [45] to extend the method to two dimensions and capture deconfined quantum criticality [20].

Acknowledgments. This work was in part supported by the Deutsche Forschungsgemeinschaft under Grant No. SFB 1143 (Project Id. 247310070) and the cluster of excellence ct.qmat (EXC 2147, Project Id. 390858490), by the EPSRC under Grants No. EP/S021582/1 and No. EP/I031014, and by the ERU under ‘Perspectives of a Quantum Digital Transformation’. We acknowledge fruitful discussions in workshops funded by EP/W026872/1.

-
- [1] R. P. Feynman, Difficulties in applying the variational principle to quantum field theories, in *Variational Calculations in Quantum Field Theory* (World Scientific, Singapore, 1987), pp. 28–40.
 - [2] F. Verstraete and J. I. Cirac, Continuous matrix product states for quantum fields, *Phys. Rev. Lett.* **104**, 190405 (2010).
 - [3] J. Haegeman, J. I. Cirac, T. J. Osborne, and F. Verstraete, Calculus of continuous matrix product states, *Phys. Rev. B* **88**, 085118 (2013).
 - [4] F. D. M. Haldane, Spontaneous dimerization in the Heisenberg antiferromagnetic chain with competing interactions, *Phys. Rev. B* **25**, 4925 (1982).
 - [5] I. Affleck and F. D. M. Haldane, Critical theory of quantum spin chains, *Phys. Rev. B* **36**, 5291 (1987).
 - [6] A. G. Green, C. A. Hooley, J. Keeling, and S. H. Simon, Feynman path integrals over entangled states, [arXiv:1607.01778](https://arxiv.org/abs/1607.01778).
 - [7] S. Furukawa, M. Sato, S. Onoda, and A. Furusaki, Ground-state phase diagram of a spin-1/2 frustrated ferromagnetic XXZ chain: Haldane dimer phase and gapped/gapless chiral phases, *Phys. Rev. B* **86**, 094417 (2012).
 - [8] C. K. Majumdar and D. K. Ghosh, On next-nearest-neighbor interaction in linear chain. I, *J. Math. Phys.* **10**, 1388 (1969).
 - [9] C. K. Majumdar and D. K. Ghosh, On next-nearest-neighbor interaction in linear chain. II, *J. Math. Phys.* **10**, 1399 (1969).
 - [10] K. Okamoto and K. Nomura, Fluid-dimer critical point in $S = 1/2$ antiferromagnetic Heisenberg chain with next nearest neighbor interactions, *Phys. Lett. A* **169**, 433 (1992).
 - [11] K. Nomura and K. Okamoto, Critical properties of $S = 1/2$ antiferromagnetic XXZ chain with next-nearest-neighbour interactions, *J. Phys. A: Math. Gen.* **27**, 5773 (1994).
 - [12] S. R. White and I. Affleck, Dimerization and incommensurate spiral spin correlations in the zigzag spin chain: Analogies to the Kondo lattice, *Phys. Rev. B* **54**, 9862 (1996).
 - [13] A. A. Nersisyan, A. O. Gogolin, and F. H. L. Eßler, Incommensurate spin correlations in spin-1/2 frustrated two-leg Heisenberg ladders, *Phys. Rev. Lett.* **81**, 910 (1998).
 - [14] J. Von Delft and H. Schoeller, Bosonization for beginners—re-fermionization for experts, *Ann. Phys.* **510**, 225 (1998).
 - [15] T. Giamarchi, *Quantum Physics in One Dimension* (Clarendon Press, Oxford, UK, 2003), Vol. 121.
 - [16] A. Tanaka and X. Hu, Quantal phases, disorder effects, and superconductivity in spin-Peierls systems, *Phys. Rev. Lett.* **88**, 127004 (2002).
 - [17] A. Tanaka and X. Hu, Many-body spin Berry phases emerging from the π -flux state: Competition between antiferromagnetism and the valence-bond-solid state, *Phys. Rev. Lett.* **95**, 036402 (2005).
 - [18] T. Senthil and M. P. A. Fisher, Competing orders, nonlinear sigma models, and topological terms in quantum magnets, *Phys. Rev. B* **74**, 064405 (2006).
 - [19] F. D. M. Haldane, $O(3)$ nonlinear σ model and the topological distinction between integer and half-integer spin antiferromagnets in two dimensions, *Phys. Rev. Lett.* **61**, 1029 (1988).

- [20] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Deconfined quantum critical points, *Science* **303**, 1490 (2004).
- [21] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevResearch.7.L012037> for a more detailed analysis of the saddle points of the MPS ansatz; an estimate for the spin stiffness from Abelian bosonization; the dynamical gauge fixing of the spin coherent states; and a more detailed account of the derivation of the NLSM from the MPS path integral, including how the coordinate and WZ forms of the topological term are equivalent.
- [22] Optimizing over the full bond-order two MPS manifold produces a better variational state, but the point of the MPS ansatz (2) is that it can be manipulated analytically—allowing it to connect to the field theory.
- [23] Note that $\sin(2\psi)$ and $\cos(2\psi)$ are swapped compared to the usual polar decomposition of an $SO(4)$ multiplet.
- [24] A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer, Berlin, 2012).
- [25] Indeed, if one restricts to helimagnetic phases with uniform entanglement and the pure singlet covers, then the transition is first order at exactly $J_2/J_1 = 1/6$.
- [26] P. J. D. Crowley, T. Đurić, W. Vinci, P. A. Warburton, and A. G. Green, Quantum and classical dynamics in adiabatic computation, *Phys. Rev. A* **90**, 042317 (2014).
- [27] F. Azad, A. Hallam, J. Morley, and A. G. Green, Phase transitions in the classical simulability of open quantum systems, *Sci. Rep.* **13**, 8866 (2023).
- [28] S. Wouters, N. Nakatani, D. Van Neck, and G. K.-L. Chan, Thouless theorem for matrix product states and subsequent post density matrix renormalization group methods, *Phys. Rev. B* **88**, 075122 (2013).
- [29] L. Vanderstraeten, J. Haegeman, and F. Verstraete, Simulating excitation spectra with projected entangled-pair states, *Phys. Rev. B* **99**, 165121 (2019).
- [30] M. Van Damme, R. Vanhove, J. Haegeman, F. Verstraete, and L. Vanderstraeten, Efficient MPS methods for extracting spectral information on rings and cylinders, *Phys. Rev. B* **104**, 115142 (2021).
- [31] S. Leontica and A. G. Green, Zero-point energy of tensor fluctuations on the MPS manifold, [arXiv:2410.22411](https://arxiv.org/abs/2410.22411).
- [32] A. Hallam, J. G. Morley, and A. G. Green, The Lyapunov spectra of quantum thermalisation, *Nat. Commun.* **10**, 2708 (2019).
- [33] S. Leontica and A. G. Green, Entanglement growth from squeezing on the MPS manifold, [arXiv:2401.13740](https://arxiv.org/abs/2401.13740).
- [34] A. J. McRoberts, C. Hooley, and A. G. Green, The J_1 - J_2 spin chain and the $O(3)$ non-linear sigma model at $\theta = \pi$, [arXiv:2411.08095](https://arxiv.org/abs/2411.08095).
- [35] M. R. Zirnbauer, On the infrared limit of the $O(3)$ nonlinear σ -model at $\theta = \pi$, [arXiv:2408.12215](https://arxiv.org/abs/2408.12215).
- [36] Y. Xian, Spontaneous trimerization of spin-1 chains, *J. Phys.: Condens. Matter* **5**, 7489 (1993).
- [37] N. Chepiga, I. Affleck, and F. Mila, Dimerization transitions in spin-1 chains, *Phys. Rev. B* **93**, 241108(R) (2016).
- [38] T. Yamaguchi, S.-L. Drechsler, Y. Ohta, and S. Nishimoto, Variety of order-by-disorder phases in the asymmetric J_1 - J_2 zigzag ladder: From the delta chain to the J_1 - J_2 chain, *Phys. Rev. B* **101**, 104407 (2020).
- [39] S. Reja and S. Nishimoto, Topological phases in half-integer higher spin J_1 - J_2 Heisenberg chains, *Phys. Rev. B* **110**, 054436 (2024).
- [40] D. G. Shelton, A. A. Nersesyan, and A. M. Tsvelik, Antiferromagnetic spin ladders: Crossover between spin $S = 1/2$ and $S = 1$ chains, *Phys. Rev. B* **53**, 8521 (1996).
- [41] G.-H. Liu, H.-L. Wang, and G.-S. Tian, Existence of dimerized phases in frustrated spin ladder models, *Phys. Rev. B* **77**, 214418 (2008).
- [42] C. A. Lamas and J. M. Matera, Dimerized ground states in spin- S frustrated systems, *Phys. Rev. B* **92**, 115111 (2015).
- [43] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Computational complexity of projected entangled pair states, *Phys. Rev. Lett.* **98**, 140506 (2007).
- [44] N. Schuch, I. Cirac, and F. Verstraete, Computational difficulty of finding matrix product ground states, *Phys. Rev. Lett.* **100**, 250501 (2008).
- [45] M.-C. Banuls, D. Pérez-García, M. M. Wolf, F. Verstraete, and J. I. Cirac, Sequentially generated states for the study of two-dimensional systems, *Phys. Rev. A* **77**, 052306 (2008).