Strong entanglement of spins inside a quantum domain wall

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Magnetic domain walls (DWs) are widely regarded as classical objects in physics community, even though the concepts of electron spins and spin-spin exchange interaction are quantum mechanical in nature. One intriguing question is whether DWs can survive at the quantum level and acquire the quantum properties such as entanglement. Here we show that spins within a DW are highly entangled in their quantum description. The total magnetization of a magnetic DW is nonzero, which is a manifestation of the global entanglement of the collective spin state. These results significantly deepen our understanding of magnetic DWs and enable the application of DWs in quantum information science. The essential physics can be generalized to skyrmions so that they can also play a role in quantum information processing.

Entanglement is a measure of quantum correlations between two or among more than two quantum particles. It is a natural resource for quantum computing and quantum information processing. Finding/generating, extracting and utilizing this resource is an important task in quantum information science. Entangling tens of particles have been realized experimentally. Remarkably, in superconducting circuits and trapped ions, it is now possible to control and to tune the coupling strength between two spins from ferromagnetic to antiferromagnetic interactions. These developments open intriguing possibilities for studying the quantum properties of magnetic structures, such as DWs, vortices and even skyrmions with a finite number of controllable spins. To initiate this interdisciplinary field, it is essential to connect magnetic structures with the measurable quantities of quantum information, such as purity of spins and global entanglement of the system.

Here we study a quantum magnetic wire with two magnetic domains and a DW in between. We show that all spins in the DW are highly entangled. The net magnetization of DWs does not depend on the nanowire length and it can be well characterized by the global entanglement of the system. In addition, we find that global entanglement of the system is a natural indicator of the phase transition between quantum DWs and domains.

**Results**

**Model of quantum domain walls.** Let us consider the transverse Ising model of $N$ spin-$1/2$ particles on a one dimensional (1D) lattice, subject to boundary fields $h$, the Hamiltonian reads

$$
\mathcal{H} = J \sum_{\langle ij \rangle} \sigma_i^z \cdot \sigma_j^z - g \sum_{i=1}^{N} \sigma_i^z - h(\sigma_1^z + \sigma_N^z),
$$

where $\sigma_i^z$, $\sigma_j^z$ are the Pauli matrices on the $i$-th site, $J$ is the exchange coupling and $g$ is the anisotropy energy. Here $\langle ij \rangle$ denotes nearest neighbor spins. The ground-state energy $E_0$ and the corresponding ground state $|0\rangle$ is calculated using the standard Lanczos algorithm (See Methods for details), which is double checked by the exact diagonalization of the Hamiltonian $\mathcal{H}$ for $N \leq 8$.

In the following, we shall focus on the antiferromagnetic (AFM) coupling ($J > 0$) for an illustration and discussion of our results. The conclusions drawn below can be generalized to the ferromagnetic coupling as well. In an AFM domain, the quantum version of the magnetization order $m_i^z$ and Néel order $n_i^z$ is given by the following expectation values:

$$
m_i^z = \frac{1}{2} \langle 0 | \sigma_i^z + \sigma_{i+1}^z | 0 \rangle, \quad n_i^z = \frac{1}{2} \langle 0 | \sigma_i^z - \sigma_{i+1}^z | 0 \rangle,
$$

where $i = 1, 3, 5, ... N - 1$. Without ambiguity, the number of spins is assumed even and $J = 1.0$ if it is not stated otherwise.

**Domain wall properties.** Let us first look at the numerical results, in the regime with weak anisotropy $g \ll J$. Figure [1] shows the spatial variation of $m_i^z$ and $n_i^z$ for $N = 12$ (triangles), 16 (circles), 20 (squares), respectively. These profiles are similar to those of classical AFM DWs. (1) The Néel order $n_z$ has a typical classical DW profile whose value varies from 1 on the left hand side (LHS) of the chain to $-1$ on the right hand side (RHS). (2) The magnetization order $m_z$ is zero in...
the two domains and reaches its maximum at the DW center. As the system becomes larger, the magnetic moments near the center become smaller, but, by summing all the magnetic moments in the DW, the net magnetization is $m^z = 1/2$, independent of the system size ($N$) as shown in the inset of Fig. 1b.

To further prove the result of $m^z = 1/2$, we look at the structure of a quantum DWs of $N$ spins. The boundary spins are aligned along the $+z$ direction by the external fields. Given $g \ll J$, the AFM exchange interaction dominates the Hamiltonian (1). Thus, the lowest energy states (i.e., ground-state) are those states with only one pair of neighboring spins left alone (sketched as a pair of parallel spins in Fig. 1b) while rest nearest neighboring spins are anti-parallel with each other forming a zero spin singlet state. For $N = 6$, there are five such configurations of same energy as sketched in Fig. 1b. In general, there are $N - 1$ such states of energy $-(N - 3)J$. These states can be further classified into $|\varphi^{S=1}\rangle$ for $S = 1$ and $|\varphi^{S=0}\rangle$ for $S = 0$, $N/2$ for $S = 1$ and the remaining for $S = 0$, where $S$ is the net magnetization of the system. The true ground state under the boundary conditions is the linear combination of this states. The corresponding eigenstate of the Hamiltonian (1) is

$$|0_{th}\rangle = \sum_{i=1}^{N/2} a_i |\varphi^{S=1}_i\rangle + \sum_{i=1}^{N/2-1} b_i |\varphi^{S=0}_i\rangle$$

(3)

where $a_i, b_i$ are the superposition coefficients. By rearranging the basis states such that $S = 1$ and $S = 0$ states are ordered alternatively, the Hamiltonian (1) can be recasted as a tridiagonal-Toeplitz matrix, where the ground state energy is found to be $E_0 = -(N-3)J - 2g \cos(\pi/N)$ with the wave function

$$|0_{th}\rangle = \sqrt{\frac{2}{N}} \left( \sin \frac{\pi}{N}, \sin \frac{2\pi}{N}, ..., \sin \frac{(N-1)\pi}{N} \right),$$

(4)

Note that the anisotropy term $g$ only gives a first-order correction of the ground state energy. As a result, the magnetic moments distribution is given by $m^z_i = (0_{th} | \sigma^z_i + \sigma^z_{i+1} | 0_{th})/2 = u_i$, where $u_i = 2/N \sin^2 \pi i/N$. The net magnetization can be calculated as

$$m^z = \sum_{i=1}^{N/2} u_i = \frac{1}{2},$$

(5)

which does not depend on $N$, in agreement with numerical results. The essential physics is that the ground state is a superposition of total spin $S = 1$ and $S = 0$ configurations with equal contributions ($\sum u_{2i} = \sum u_{2i+1} = 1$) so that the average spin number is always 1/2.

In fact, the above result is also true when the Dzyaloshinskii-Moriya interaction (DMI) $-D\cdot \sum_{i<j} \sigma_i \times \sigma_j$ is added to Hamiltonian (1), where the ground state of the revised Hamiltonian is still solvable analytically. Specifically, for $D = D_0$ ($D > 0$), the ground state is given by,

$$|0_{th}\rangle = \sqrt{\frac{2}{N}} \left( \tau_1 \sin \frac{\pi}{N}, \tau_2 \sin \frac{2\pi}{N}, ..., \tau_{N-1} \sin \frac{(N-1)\pi}{N} \right),$$

(6)

where the prefactor $\tau_1 = 1 - 2 \bmod([i/2], 2)$, $[x]$ is the ceiling function of $x$. Note that $\tau^2 = 1$, the magnetization distribution $m^z = 2/N \sin^2 (\pi i/N)$, is not changed by the DMI. However, the chirality of DW does depend on the sign of $D$. For $D > 0$, the system always prefers a clockwise Néel wall. However, if $D$ reverses the sign, the ground state becomes counter-clockwise. This is consistent with classical case.

**Entanglement.** In quantum information science, the purity of the $i$-th spin is defined as $P_i = \text{tr}(\rho^2_i)$ where $\rho_i$ is the density matrix of the $i$-th spin obtained by tracing all the other spins in the full density matrix $|0\rangle\langle 0|$. It quantifies the distance of a state relative to a pure state; for example, it takes the value 1 for a separable pure state, but 1/2 for a maximally entangled states such as Bell states and Greenberg-Horne-Zeilinger state (GHZ) states.

Figure 2a shows the space distribution of purity as colored rectangles for $N = 12$ (top inset), 16 (middle inset),
and 20 (bottom inset), respectively. Regardless of the system size, the purity takes 1 near the boundary of spin chain and then decreases to form a symmetric dip around the chain center at \(i/N = 1/2\). The magnetization distribution of DWs takes on a peak centered at the dip position and its space dependence is strongly correlated with the purity. Physically, this correlation originates from the antiferromagnetic nature of nearest neighbour interaction. For the spins near the boundary, their directions are strongly bounded by the fixed orientations of the boundary spins and have a larger probability to be in Néel-state-like configurations. Consequently, the magnetization is close to zero and these spins are not entangled near the center are influenced lightly by the boundary with the others (i.e., close to a pure state). The spins of spins close 1/2 at the wire center suggests that the purity of these spins become smaller. The purity of these spins become more uncertain, hence the purity of these spins become smaller. The purity of spins close 1/2 at the wire center suggests that the spins inside the domain walls are highly entangled.

Theoretically, the purity of the \(i\)-th spin is defined by the reduced density operator of the \(i\)-th spin obtained by tracing all the spins except the \(i\)-th spin in density operator \(|0_{th}\rangle\langle 0_{th}|\) as

\[
P_i = \left( \sum_{k=1}^{i-1} u_k \right)^2 + \left( \sum_{k=i}^{N-1} u_k \right)^2 + 2u_i u_{i-1},
\]

where \(i = 1, 2, ..., N\). The third term \(u_i u_{i-1}\) is of the order \(O(1/N^2)\), which is much smaller than the first two terms. Considering \(\sum u_i = 1\), \(P_i\) reaches its minimum value \((1/2)\) at \(i = N/2\), i.e. the chain center, where \(m^2_i = u_i \sin^2(i\pi/N)\) reaches its maximum value.

The correlations of the magnetization distribution and purity distribution can be extended to two dimensions (2D) where rich magnetic structures such as vortices, skyrmions can exist since the physics remain the same. Nevertheless, it is a great challenge to find the ground states in 2D both analytically and numerically. Practically, the correlations also allow us to measure a quantum DW, vortices and even skyrmions by measuring the purity of each spin in a spin chain. The later can be realized by performing state tomography on each system qubit or by a more efficient technique that uses bitwise interactions between the system and identically prepared registers. A typical tomography of the density of states for a clockwise/counter-clockwise DW is shown in Fig. 2a and 2b. The distinguishable distributions of the density matrix allows us to classify clockwise and counter-clockwise DWs.

Furthermore, the direct sum of magnetization recovers the net magnetization of the spin chain while the proper average of the local purity can give the global entanglement \(E_g\) of the spins. The original definition of \(E_g\) is given by Meyer and Wallach and then reformulated in terms of the sum of local purity, i.e.

\[
E_g = \frac{2}{N} \sum_{i=1}^{N} (1 - P_i).
\]

Substituting Eq. (7) into this definition, the leading order of global entanglement is reduced to

\[
E_g = 2 - \frac{2}{N} \sum_{k=1}^{N} \left[ \left( \sum_{i=1}^{k-1} u_i \right)^2 + \left( \sum_{i=k}^{N-1} u_i \right)^2 \right].
\]

The sum increases as \(N\) increases and saturates for \(N > 20\). The limiting value is \(E_g = 2/3 - 5/2\pi^2 \approx 0.41\). This indicates that the spins in a DW is still entangled in
The global entanglement is 
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ical simulation, we fix the exchange coupling and adjust plot the phase diagram of the spin model. In our numerical simulation, we fix the exchange coupling and adjust

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possible to distinguish domain and DW states and the corresponding net magnetization by measuring the global entanglement. Based on this comparison, it becomes

the macroscopic scale \( (N \rightarrow \infty) \). This is quite different from a classic DW that has zero entanglement since all its composite spins have definite orientations.

As a comparison, for a quantum domain state without DWs such as the superposition of two degenerated Néel states,

\[ |0_{\text{h}}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\uparrow\ldots\uparrow\uparrow\rangle + |\uparrow\uparrow\uparrow\ldots\downarrow\downarrow\rangle) \] \hspace{1cm} (10)

The global entanglement is \( E_g = 1 \) while its net magnetization is zero. Based on this comparison, it becomes possible to distinguish domain and DW states and the corresponding net magnetization by measuring the global entanglement of the spin system.

**Phase transition.** To know the size of the phase space where the quantum DWs are stable, it is interesting to plot the phase diagram of the spin model. In our numerical simulation, we fix the exchange coupling and adjust

the anisotropy \( g \) and boundary fields to obtain various ground states in \( h - g \) plane as shown in Fig. 3.

Guided by the red line in Fig. 3b, the ground state changes from a single domain state to a quantum DW at the critical field of \( h_c = J \) for \( g = 0 \). The critical field has a non-trivial dependence on \( g \) and \( h \). For simplicity, we focus on the regime \( g \ll 1 \), where the ground state is mainly determined by the competition of exchange interaction and Zeeman interaction. In this regime, the global entanglement \( (E_g) \) shows an abrupt jump from 1.0 to a smaller value as shown in Fig. 3b and Fig. 3c with \( g = 0.2 \). This abrupt change is due to the distinguishable quantum properties of the domains and DWs. When \( h < h_c \), the exchange interaction dominates the Hamiltonian and the ground state is a superposition of two degenerated Néel states Eq. (10) with \( E_g = 1 \). The numerical value of \( E_g \) is a little smaller than the theoretical value 1, as shown in Fig. 3b, due to the influence of the small anisotropy \( g \) term, which tendency is to align all the spins to \( x \) direction and reduce the entanglement. As the field increases above \( h_c \), the ground state becomes a DW state with finite entanglement 0.41 as discussed previously.

The global entanglement and its first derivative is continuous with \( h \) near the critical field while its second order derivative is discontinuous, as shown in the left inset of Fig. 3c. To verify whether this discontinuity can be a good indicator of the phase transition, we first plot the first derivative of \( E_g \) versus \( h \) in the left inset of Fig. 3c for system size ranging from \( N = 8, 10, 12, 14, 16 \), respectively. Right inset: scaling behavior of the global entanglement around the critical point \( h_c \).

FIG. 3. Phase diagram and the characterization of the phase transition using entanglement. (a) The distribution of net magnetization of the spin chain \((|m^z|)\) in the \( h - g \) phase space. The \( \pm \) signs represent clockwise and counterclockwise DW respectively. \( N = 12 \). (b) Simulated global entanglement \((E_g)\) as a function of boundary field \((h)\). \( g = 0.2 \). Left inset: \( dE_g/dh \) as a function of external field for \( N = 8, 10, 12, 14, 16 \), respectively. Right inset: scaling behavior of the global entanglement around the critical point \( h_c \).

Discussion

We have shown that an AFM DW in a 1D lattice has an intrinsic magnetization of \( 1/2 \) independent of lattice length. The reason is that the ground state is a superposition of \( S = 1 \) states and \( S = 0 \) states of equal amplitude. The global entanglement of such a DW is non-zero and even exists at a macroscopic scale. Moreover, the magnetization profile is closely related to the local purity of spins such that the DW width can be extracted from the purity profile that can be measured through state tomography in quantum information science. The typical energy gap of the ground state and the first excited state in our model is \( 43 \mu eV \) \( (\sim 500 mK) \) for \( N = 20 \). Then the mixture of excited states and ground state can be neglected at a temperature below 500 mK, which leaves a sufficient room to experimentally verify our theoretical prediction.
Since our results are applicable to chiral DWs due to DMI, the main conclusions can be generalized to two dimensional case for magnetic skyrmions. This type of skyrmions has non-zero entanglement that is very different from the classical skyrmions discussed in literature. Further study of the quantum skyrmions may lead to quantum skyrmion spintronics.

Methods
Lanczos algorithm. Our numerical calculation of the ground states of the spin model are based on the Lanczos method. First, a random initial state \( |\psi_0\rangle \) is chosen in the \( 2^N \) dimensional Hilbert space. Then we define a new state \( |\psi_1\rangle \) that is orthogonal to \( |\psi_0\rangle \), realized by subtracting \( \hat{H}|\psi_0\rangle \) over \( |\psi_0\rangle \) i.e.

\[
|\psi_1\rangle = \hat{H}|\psi_0\rangle - a_0|\psi_0\rangle \quad (12)
\]

where \( a_0 = \langle \psi_0 | \hat{H} | \psi_0 \rangle / \langle \psi_0 | \psi_0 \rangle \). Next, we define the state \( |\psi_2\rangle \) that is orthogonal to both \( |\psi_0\rangle \) and \( |\psi_1\rangle \),

\[
|\psi_2\rangle = \hat{H}|\psi_1\rangle - a_1 |\psi_1\rangle - b_0 |\psi_0\rangle \quad (13)
\]

where \( a_1 = \langle \psi_1 | \hat{H} | \psi_1 \rangle / \langle \psi_1 | \psi_1 \rangle \), \( b_0 = \langle \psi_1 | \psi_0 \rangle / \langle \psi_0 | \psi_0 \rangle \). Through iterations, the state \( |\psi_{n+1}\rangle \) is derived as

\[
|\psi_{n+1}\rangle = \hat{H}|\psi_n\rangle - a_n |\psi_n\rangle - b_{n-1} |\psi_{n-1}\rangle \quad (14)
\]

where the coefficients \( a_n = \langle \psi_n | \hat{H} | \psi_n \rangle / \langle \psi_n | \psi_n \rangle \), \( b_{n-1} = \langle \psi_n | \psi_{n-1} \rangle / \langle \psi_{n-1} | \psi_{n-1} \rangle \).

In terms of the mutual orthogonal basis spanned by \( \{|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_n\rangle \} \), the Hamiltonian can be written in the form of a tridiagonal matrix and then diagonalized through the standard subroutine. The ground state energy \( E_n \) is obtained as the smallest eigenvalues of the Hamiltonian. As \( n \) increases, the \( E_n \) will converge to the real ground state energy of the system while the corresponding eigen-vector is the wave function of ground states. The convergence criteria used in the simulations is \( |E_n - E_{n-1}| \leq 10^{-14} \).

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Author contributions
H.Y.Y., M.H.Y. and X.R.W conceived the project. H.Y.Y. performed the numerical and theoretical calculations. All authors analyzed and discussed the results and contributed to the writing of the manuscript.

Additional information
The authors declare no competing financial interests.