


Singularity in entanglement negativity across finite-temperature phase transitions

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Phase transitions at a finite (i.e., nonzero) temperature are typically dominated by classical correlations, in contrast to zero temperature transitions where quantum mechanics plays an essential role. Therefore, it is natural to ask if there are any signatures of a finite-temperature phase transition in measures that are sensitive only to quantum correlations. Here we study one such measure, namely, entanglement negativity, across finite-temperature phase transitions in several exactly solvable Hamiltonians and find that it is a singular function of temperature across the transition. Our results also lead to a mean-field argument that shows that negativity can distinguish spontaneous symmetry breaking with local order parameter at finite temperature from that in the ground state. Along the way, we prove certain general results which simplify the calculation of negativity for commuting projector Hamiltonians and as an aside, we also calculate the entanglement of formation exactly in an interacting model.

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Interacting quantum systems with competing interactions can exhibit phase transitions at both zero and nonzero temperatures. Heuristically, the zero temperature phase transitions result due to quantum fluctuations while the finite-temperature phase transitions typically result from thermal fluctuations [1]. As an example, consider the 2 + 1-D transverse field Ising model on a square lattice: $H = - \sum_{\langle i,j \rangle} Z_i Z_j - h \sum_i X_i$. Here the critical exponents associated with the zero temperature phase transition belong to the three-dimensional Ising universality while those for the finite-temperature phase transition belong to the two-dimensional Ising universality [1,2]. That is, at any nonzero temperature, the universal critical exponents are identical to those corresponding to the purely classical Hamiltonian $H = - \sum_{\langle i,j \rangle} Z_i Z_j$. Given this observation, it is natural to ask are there any singular correlations at a finite-temperature transition that are intrinsically quantum mechanical? For a pure state, von Neumann entanglement entropy is a good measure of quantum correlations, but since we are interested in finite-temperature transitions, we need to consider measures of mixed state entanglement. With this motivation, in this paper we will introduce certain quantum models which exhibit finite-temperature transitions, and we will analytically study mixed state entanglement measures in these models, with a particular focus on entanglement negativity [3].

One way to motivate mixed state entanglement measures is via the notion of ‘separable’ states—these are states that can be prepared from any other state using only local operations and classical communications (LOCC) and therefore are not entangled. A bipartite mixed state is separable if it can be written as $\rho = \sum_i p_i \rho_{A,i} \otimes \rho_{B,i}$ where $p_i > 0$ while $\rho_{A,i}, \rho_{B,i}$ are valid density matrices [4,5]. For *pure* states, the von Neumann entropy $S = -\text{tr}(\rho_A \log(\rho_A))$, where ρ_A is the reduced density matrix on Hilbert space A , is a faithful

measure of quantum correlations. However, S is rather ineffective at capturing mixed state quantum correlations. For example, even a thermal density matrix corresponding to a purely *classical* Hamiltonian will have a rather substantial von Neumann entropy S that equals the thermal entropy for region A . Several measures of mixed state entanglement have been proposed (see, e.g., Ref. [6] for an overview) including entanglement of formation, entanglement of distillation, entanglement of purification, squashed entanglement, and entanglement negativity. As yet, all of these measures, with the exception of entanglement negativity, require optimizing a function over all possible quantum states, making their calculation rather challenging (see, e.g., Ref. [7]). Therefore, below we will primarily focus on the entanglement negativity with one exception; for a specific many-body model we will also calculate the entanglement of formation.

The entanglement negativity (henceforth, just ‘negativity’ for brevity) is defined as follows [3,8]: Given a bipartite density matrix ρ acting on the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, one first performs a partial transpose *only* on the Hilbert space \mathcal{H}_B to obtain a matrix ρ^{T_B} . Explicitly, if $\rho = \sum_{A,B,A',B'} \rho_{AB,A'B'} |A\rangle|B\rangle\langle A'|\langle B'|$, then $\rho^{T_B} =$

$\sum_{A,B,A',B'} \rho_{AB,A'B'} |A\rangle|B'\rangle\langle A'|\langle B|$. The matrix ρ^{T_B} is Hermitian but

is not necessarily positive semidefinite. The negativity E_N is defined as $E_N = \log(\|\rho^{T_B}\|_1)$. As shown in Ref. [9] it is an entanglement monotone despite not being convex. The utility of negativity becomes apparent when one notices that it is zero for separable mixed states [3,5,10–12]. This is because for separable states, ρ^{T_B} is a valid density matrix, and therefore, $\|\rho^{T_B}\|_1 = 1$. The main drawback of negativity is that it can be zero even for nonseparable states [13]. Heuristically, this means that although negativity is insensitive to classical correlations, it does not capture *all* quantum correlations. As a proper entanglement measure for mixed states, negativity has been studied in various contexts including fermionic systems

[14,15], disordered systems [16], gapped one-dimensional models [17], and one-dimensional conformal field theories [18]. It has also been applied to study the quantum dynamics in integrable systems [19].

Since we will also briefly discuss entanglement of formation, denoted as E_F , let us also recall its definition. E_F for a bipartite mixed state ρ_{AB} is defined as follows [20]: decomposing ρ_{AB} as a convex sum of pure states, $\rho_{AB} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ where $p_i > 0$ with $\sum_i p_i = 1$, E_F is given by $E_F = \inf \sum_i p_i S(\text{Tr}_B |\psi_i\rangle\langle\psi_i|)$ where S is the von Neumann entropy. Therefore, E_F is the least possible entanglement of any ensemble of pure states that realizes a given mixed state. In contrast to negativity, E_F is zero if and only if a state is separable.

To begin with, we note one feature of negativity shared by all Hamiltonians considered here, as well as in several other lattice models (see, e.g., Refs. [21–25]) and continuum field theories [26,27]: above a certain temperature, the negativity for the corresponding thermal (Gibbs) state becomes exactly zero. This temperature is called ‘sudden death temperature’ denoted as T_d . One of the central questions we will ask is the following. Consider an interacting system which exhibits spontaneous symmetry breaking below a critical temperature T_c . Assuming that negativity E_N is nonzero in the vicinity of the transition (i.e., the condition $T_d > T_c$ is satisfied), is E_N a singular function of the tuning parameter (e.g., the temperature) across the transition?

We now state our main result. We find that in all models considered in this paper, whenever negativity is nonzero in the vicinity of the transition, it is always singular across the transition. This result is at variance with expectations from Ref. [23] where numerical calculations on finite sized systems for the 2 + 1-D quantum Ising model suggested that negativity is analytic across the corresponding T_c . We will return to a comparison with Ref. [23] after discussing our results.

II. MEAN-FIELD MODELS

As a starting point, consider a single site mean-field Hamiltonian for the transverse field Ising model: $H_{1\text{ site}}^{MF} = -mzZ - hX$, where z is the coordination number. The corresponding thermal state is indeed separable, which might lead one to expect that perhaps negativity is always an analytic function across finite-temperature transitions. However, a single site mean field is too crude an approximation: Within such a mean-field approximation, even the ground state is unentangled and shows no singularity in the quantum entanglement across a $T = 0$ quantum phase transition (QPT), in contrast to the known exact results (see, e.g., Refs. [28–30]). To improve upon this, we next consider a *two-site* mean-field theory:

$$H_{2\text{ sites}}^{MF} = -m(z-1)(Z_1 + Z_2) - Z_1 Z_2 - h(X_1 + X_2) \quad (1)$$

and study the negativity for a bipartition that runs across the two sites. A straightforward calculation shows that whenever $T_d > T_c$, the critical temperature for the phase transition, the negativity is a singular function of the temperature across the transition, see Fig. 1. Incidentally, since an analytical expression for entanglement of formation E_F is available for any state acting on two qubits [31], we calculate E_F as well for

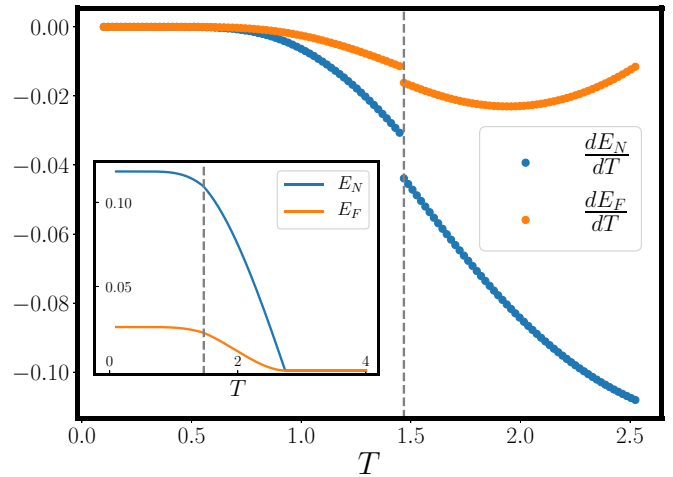


FIG. 1. The derivative of entanglement negativity $\frac{dE_N}{dT}$ and the derivative of entanglement of formation $\frac{dE_F}{dT}$ corresponding to the thermal state for a two site mean-field theory of the transverse field Ising model, Eq. (1) with $h = 3.8$ and $z = 4$. Inset: E_N and E_F for the two site mean-field theory for the same problem. The vertical dashed gray line in both plots indicates the location of the critical temperature.

this mean-field model and find that it is also singular across the transition (Fig. 1).

III. A NONLOCAL COMMUTING PROJECTOR MODEL

Motivated by the two-site mean-field result and the models studied in Ref. [32], we next consider a Hamiltonian which exhibits a finite-temperature transition and where negativity is calculable exactly in the thermodynamic limit. The model is defined on a one-dimensional lattice with L sites where each lattice site has four qubits:

$$H = -\frac{1}{4L} \left(\sum_i (Z_{i1}Z_{i2} + Z_{i3}Z_{i4}) \right)^2 - g_z \sum_i Z_{i1}Z_{i2}Z_{i3}Z_{i4} - g_x \sum_i (X_{i1}X_{i2} + X_{i3}X_{i4}). \quad (2)$$

The most notable feature of this Hamiltonian is that it is a sum of commuting terms, and it supports a finite-temperature transition where the Ising symmetry corresponding to $Z_{i1}Z_{i2} \rightarrow -Z_{i1}Z_{i2}$, $Z_{i3}Z_{i4} \rightarrow -Z_{i3}Z_{i4}$ gets spontaneously broken. The first term in the Hamiltonian makes it nonlocal and leads to a finite-temperature Ising transition in the mean-field universality class. Defining the order parameter $m = \langle Z_{i1}Z_{i2} \rangle = \langle Z_{i3}Z_{i4} \rangle$, one finds that in the thermodynamic limit, the critical temperature is given by the solution of the equation $2\beta = 1 + e^{-2\beta g_z}$ while the order parameter m is determined via $\frac{\sinh(2\beta m)}{\cosh(2\beta m) + e^{-2\beta g_z}} = m$ which implies that close to T_c , $m = a\sqrt{T_c - T}$, as expected. Next, we calculate the negativity of this model for the bipartition that runs across the four qubits on a chosen site, i.e., $A = \{i_\alpha, i < 0, \alpha = 1, 2, 3, 4\} \cup \{i = 0, \alpha = 1, 3\}$ and $B = \bar{A}$ where we have chosen the cut across the site 0 for convention. One finds that for all $T \geq T_c$, and for $0 \leq (T_c - T)/T_c \ll 1$, the negativity is given by

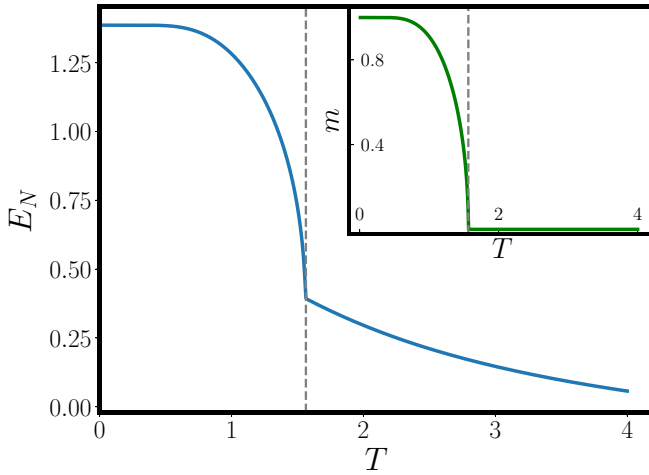


FIG. 2. Negativity as a function of temperature for the nonlocal commuting projector model, Eq. (2), for $g_x = 2$, $g_z = 1$. Inset: Temperature dependence of the magnetization. The vertical dashed gray line in both plots indicates the location of the critical temperature.

$E_N = \log(1 + F)$, where

$$F = \frac{e^{\beta g_z} \sinh(2\beta g_x) \cosh(2\beta m) - e^{-\beta g_z} \cosh(2\beta g_x)}{2(\cosh(\beta g_x))^2 (e^{\beta g_z} \cosh(2\beta m) + e^{-\beta g_z})} \quad (3)$$

assuming $F > 0$ (see Appendix B 1 for derivation); otherwise negativity is zero which also yields an expression for T_d by setting $F = 0$. Since the critical temperature T_c depends only on g_z , one can always tune g_x , so that the sudden death temperature is higher than T_c . Since m is a singular function of temperature so is negativity. In fact E_N simply inherits the cusp singularity of m across the phase transition, i.e., $\frac{dE_N}{dT}|_{T=T_c^-} \neq \frac{dE_N}{dT}|_{T=T_c^+}$, see Fig. 2 which also shows the temperature dependence of negativity for all temperatures including $T < T_c$.

One drawback of the model just discussed is that it is nonlocal and relatedly exhibits mean-field scaling exponents. Therefore, it would be worthwhile to study negativity in thermal states of local Hamiltonians that host a finite-temperature transition.

IV. LOCAL COMMUTING PROJECTOR MODELS

A. A general result regarding negativity

Before considering local models, we notice a property specific to commuting projector models that will simplify our subsequent discussion. Let's decompose a commuting projector Hamiltonian as $H = H_A + H_B + H_{AB}$ so that H_A (H_B) denotes the interaction between spins in A (B) and H_{AB} denotes the interaction between A and B . We further denote the Hilbert space of spins of region A (B) that interact with B (A) by ∂A (∂B), and define $A' = A - \partial A$, $B' = B - \partial B$, i.e., spins strictly in the 'bulk' of A (B). Given a thermal density matrix $\rho = e^{-\beta H}/Z$, one can show that (see Appendix A 3 for derivation)

$$\|\rho^{T_B}\|_1 = \|\bar{\rho}_{\partial A, \partial B}\|_1, \quad (4)$$

where $\bar{\rho}_{\partial A, \partial B}$ is a density matrix defined on $\partial A \cup \partial B$: $\bar{\rho}_{\partial A, \partial B} = \frac{1}{Z} (e^{-\beta H_{AB}})^{T_{AB}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}$. This property results from the fact that partial transpose affects operators only at the boundary (i.e., only in the factor $e^{-\beta H_{AB}}$ in the expression for ρ), and furthermore one can always find a basis in which H_A , H_B , and $(e^{-\beta H_{AB}})^{T_{AB}}$ can all be simultaneously diagonalized. If we further assume that

$$\{e^{-\beta H_{AB}}\}^{T_{AB}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)} = \{e^{-\beta H_{AB}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}\}^{T_{AB}}, \quad (5)$$

then one can show that the negativity between A and B is exactly the same as the negativity between ∂A and ∂B :

$$\|\rho^{T_B}\|_1 = \|\bar{\rho}_{\partial A, \partial B}\|_1, \quad (6)$$

where $\rho_{\partial A, \partial B} = \frac{1}{Z} \text{Tr}_{A', B'} e^{-\beta H} = \frac{1}{Z} e^{-\beta H_{AB}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}$ is the reduced density matrix for the boundary spins. Note that the assumption Eq. (5) fails only if there exist constraints between commuting operators. For instance, given a two-dimensional (2D) toric code on a torus [33], the product of all plaquette (star) operators is an identity operator. Consequently, $\text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}$ generates the plaquette and star operators supported on the bipartition boundary, and Eq. (5) does not hold true. If one instead considers the 2D toric code on a plane, no constraint among different commuting operators exists, and Eqs. (5) and (6) are correct. For the models considered in this paper, Eq. (6) continues to hold, and we will report results on models which violate this assumption elsewhere.

B. An explicit calculation of negativity

With the aforementioned property specific to commuting projector Hamiltonian, we now turn our attention to the negativity in a local Hamiltonian defined on a square lattice, with two species of spins, a and b , on each lattice site:

$$H = - \sum_{\langle ij \rangle} Z_{ia} Z_{ib} Z_{ja} Z_{jb} - g \sum_i X_{ia} X_{ib}. \quad (7)$$

This model exhibits a finite-temperature phase transition in the 2D Ising universality class, and due to the commuting projector property, the corresponding T_c is exactly the same as the Onsager's solution [34] to the classical Ising model on the square lattice, $H = - \sum_{\langle i, j \rangle} s_i s_j$, irrespective of the value of g . Let us first consider the negativity between one spin on a single site, say, 'a' spin on site 0, and the rest of the system. Since all local commuting operators are independent, to calculate the negativity, we only need the reduced density matrix for spins at the boundary [as stated in Eq. (6)], which in this case are the spins on sites 0 and four neighbors of site 0. For simplicity, we present the result of the negativity only for a specific range of g , namely, $e^{-3\beta} < \tanh(\beta g) < e^{-4\beta}$ where the calculation is technically simpler, see Appendix B 2 for details. This is sufficient to illustrate the singular nature of negativity across the finite-temperature transition hinted above. One finds that the negativity E_N is given by:

$$E_N = \log\{1 - 4A[\cosh(\beta g)e^{-4\beta} - \sinh(\beta g)e^{4\beta}](1 + 4c_1 + 2c_2 + c_3)\}, \quad (8)$$

where $A^{-1} = 2^5 \cosh(\beta g)(\cosh[4](\beta) + (c_1 + \frac{1}{2}c_2) \sinh[2](2\beta) + c_3 \sinh[4](\beta))$ and $\{c_i | i = 1, 2, 3\}$ are given by the expectation values of certain local operators measured by the bulk density matrix $\rho_{\text{bulk}} \sim \exp(-\beta(H_A + H_B))$ so that they are all singular functions of the tuning parameters g, T across the critical point. Inheriting the singularity of c_i , the negativity between the single spin and the rest of the system is also singular. Note that there is no symmetry reason for the singularity to cancel out in the particular combination of c_i 's that enter the expression for A . To confirm this, we calculated the coefficients c_i within the mean field approximation and checked that E_N is indeed singular across the transition (see Appendix B 2).

C. A general argument for singularity in negativity

By exploiting the general result in Eq. (4), we can now argue rather generally that negativity will be singular across a phase transition in a commuting projector Hamiltonian for an arbitrary bipartition scheme. To begin with, we write the bulk Hamiltonian as $H_A + H_B = -\sum_m \alpha_m P_m$, where $\{P_m\}$ is the set of local commuting operators supported only on A or B . For brevity of the discussion, P_m is chosen from the Pauli group and is thus a tensor product of Pauli matrices over sites with $P_m^2 = 1$. To utilize the result from Eq. (4), we first calculate the following:

$$\begin{aligned} & \frac{1}{Z} \text{Tr}_{A',B'} e^{-\beta(H_A + H_B)} \\ &= \frac{1}{Z} \text{Tr}_{A',B'} \prod_m (\cosh(\beta \alpha_m) + P_m \sinh(\beta \alpha_m)) \\ &= \frac{1}{Z} \left[\prod_m \cosh(\beta \alpha_m) \right] \sum_{\{\tau_m\}} \text{Tr}_{A',B'} \left[\prod_m (P_m \tanh(\beta \alpha_m))^{\tau_m} \right], \end{aligned} \quad (9)$$

where $\tau_m \in \{0, 1\}$ indicates whether P_m is present or not. Due to the presence of the trace over the bulk region, among all possible $\prod_m P_m^{\tau_m}$, only those operators acting on the bulk trivially survive, which we call $\{Q_k\}$. Also note that Q_k can be expressed as tensor products of local commuting operators $\{O'_m\}$ supported on the boundary region $\partial A \cup \partial B$. Therefore, Eq. (4) gives

$$\|\rho^{T_B}\|_1 = \left\| (e^{-\beta H_{AB}})^{T_{\partial B}} \sum_k c_k Q_k \right\|_1. \quad (10)$$

The coefficients c_k are proportional to the expectation value of Q_k with respect to the bulk density matrix ρ_{bulk} and are therefore a singular function of the tuning parameter across T_c , similar to the coefficients c_1, c_2, c_3 discussed above for the case of a single site negativity appearing in Eq. (8). Since the matrix inside the one-norm from Eq. (10) consists of commuting operators O'_m , its eigenvalues can be obtained by treating them as numbers. Therefore, it follows that the negativity is

$$E_N = \log \left(\sum_k c_k f_k \right), \quad (11)$$

where $f_k = g \sum_{\{O'_m\}} |(e^{-\beta H_{AB}})^{T_B}| Q_k$. Here the factor g takes care of the possible degeneracy from transforming the trace in Hilbert space to summing commuting operators, i.e., $\text{Tr}_{\partial A, \partial B} = g \sum_{O'_m}$. Also, the summation over O'_m should take care of the potential constraints for O'_m . For instance, given a three-dimensional toric code, summing each plaquette operator cannot be treated independently since the product of six plaquette operators on a cubic unit cell is an identity operator.

A key observation from Eq. (11) is that, in contrast to c_k , the coefficients f_k are determined only by the matrix defined on the boundary spins via the above expression and are oblivious to the bulk criticality. Therefore, the negativity inherits the singularity associated with the bulk criticality due to its dependence on coefficients c_k .

V. QUANTUM SPHERICAL MODEL

Finally, we consider a completely different class of models which are also exactly solvable and in which one again finds that the negativity is singular across the phase transition. In particular, consider the quantum spherical model [35]:

$$H = \frac{1}{2} g \sum_{i=1}^N p_i^2 - \frac{1}{2N} \sum_{i,j=1}^N x_i x_j + \mu \left[\sum_{i=1}^N x_i^2 - \frac{N}{4} \right], \quad (12)$$

where x_i and p_j satisfy the canonical commutation relation $[x_i, p_j] = i\delta_{ij}$, while the constraint $\langle \sum_{i=1}^N x_i^2 \rangle = \frac{N}{4}$ is imposed only on average via the Lagrange multiplier μ . The above model shows a phase transition associated with spontaneous breaking of the Ising symmetry $x_i \rightarrow -x_i$ at temperature β_c^{-1} determined via $\sqrt{g_c} = \frac{1}{2} \tanh(\frac{1}{2}\beta_c \sqrt{g_c})$. In the ordered phase, μ is pinned to $1/2$. The negativity of this model can be calculated analytically using the correlation matrix technique of Ref. [36]. Dividing the system into two equal halves, one finds that (see Appendix B 3) the negativity $E_N = \text{Max}\{0, -\frac{1}{2} \log(\nu)\}$ where $\nu = \frac{2}{\beta \sqrt{g}} \coth(\frac{1}{2}\beta \sqrt{g})$ in the ordered phase, while $\nu = \frac{1}{2} \sqrt{\frac{2\mu-1}{g}} \coth(\frac{1}{2}\beta \sqrt{(2\mu-1)g})$ in the disordered phase where the chemical potential is given by the equation $\sqrt{\frac{2g}{\mu}} = \tanh(\frac{1}{2}\beta \sqrt{2g\mu})$. Using these equations, one finds that the first derivative of the negativity across the phase transition is discontinuous: $\frac{\partial E_N}{\partial g} |_{g_c^+} = \frac{1}{2g_c} + \frac{\beta_c^2}{24} (1 - \frac{8}{4+\beta_c-4\beta_c g_c})$ while $\frac{\partial E_N}{\partial g} |_{g_c^-} = \frac{4+\beta_c-4\beta_c g_c}{16g_c}$. As shown in Fig. 3, the first derivative of E_N clearly exhibits a discontinuity at the thermal critical point.

VI. EXACT CALCULATION OF ENTANGLEMENT OF FORMATION IN COMMUTING PROJECTOR MODELS

The models introduced in this paper allowed for a rather straightforward evaluation of negativity while illustrating non-trivial features. It is natural to wonder whether one can calculate any other measures of mixed state entanglement for similar models. To that end, we now present a result on the entanglement of formation E_F , a quantity which is generally rather hard to calculate since it requires optimization over all

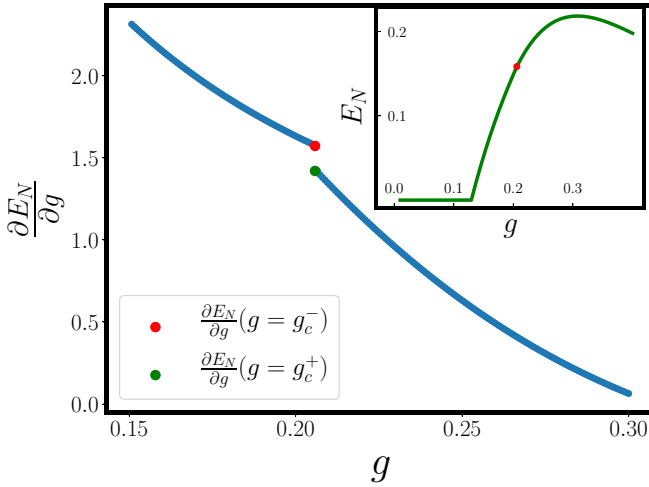


FIG. 3. First derivative of the negativity as a function of the parameter g [see Eq. (12)] at $T = 0.15$ for the spherical model. The inset shows the negativity as a function of g , where the red dot labels the critical point.

possible states. Consider the following Hamiltonian which is closely related to the Hamiltonians in Eqs. (2) and (7):

$$H = -\frac{1}{2L} \left(\sum_{i=1}^L Z_{i1} Z_{i2} \right)^2 - g \sum_{i=1}^L X_{i1} X_{i2}. \quad (13)$$

This Hamiltonian exhibits a finite-temperature phase transition at $T_c = 1$. For defining the entanglement of formation E_F , similar to our earlier discussion, we choose a bipartition for the subsystem A and its complement B that cuts through the two spins 1 and 2 on a chosen site s . For such a bipartition scheme, we prove that in the thermodynamic limit ($L \rightarrow \infty$), E_F between A and B is exactly given by that between two spins in the mean-field density matrix defined as $\rho_{MF} \propto e^{-\beta H_s}$, where $H_s = -m Z_{s1} Z_{s2} - g X_{s1} X_{s2}$ and m satisfies the mean-field equation $\tanh(\beta m) = m$. Using the exact result by Wothers on E_F for two qubits [31], this yields an analytical expression for E_F .

Our strategy is to find an upper bound and a lower bound on E_F that happen to match each other. Here we briefly outline the proof (see Appendix C for details). For calculating an upper bound, we perform an Hubbard-Stratonovich transformation to decompose the density matrix ρ :

$$\rho = \frac{1}{Z} e^{-\beta H} = \frac{1}{Z} \sqrt{\frac{\beta L}{2\pi}} \int dm e^{-\frac{1}{2} \beta L m^2 - \beta \sum_{i=1}^L H_i(m)}, \quad (14)$$

where a local Hamiltonian $H_i(m)$ for the i site of two spins is defined as $H_i(m) = -m Z_{i1} Z_{i2} - g X_{i1} X_{i2}$. By decomposing the matrix $e^{-\beta H_i(m)} = \sum_{k_i} w_{k_i}^i(m) |k_i(m)\rangle \langle k_i(m)|$, one can upper bound the entanglement of formation $E_F(A, B)$ between A, B in ρ by the entanglement of formation $E_F(s1, s2)$ between two spins $s1, s2$ in the mean-field density matrix $\rho_{MF} \propto e^{-\beta H_s}$:

$$E_F(A, B) \leq E_F(s1, s2). \quad (15)$$

For the lower bound, since any entanglement measure is nonincreasing under a partial trace [37], $E_F(A, B)$ is bounded

by the entanglement of formation between two spins at site s from below. By calculating the reduced density matrix on site s , we show that

$$E_F(s1, s2) \leq E_F(A, B). \quad (16)$$

Combining Eqs. (15) and (16), we complete the proof. Unfortunately, in this model, the entanglement of formation exhibits a sudden death temperature which is lower than T_c for all values of g , and therefore, E_F is zero in the vicinity of the transition.

VII. DISCUSSION AND SUMMARY

So far we have shown that finite-temperature transitions in quantum systems can show singular features in entanglement negativity, despite the fact that the universal critical exponents associated with these transitions are still given by classical statistical mechanics. Therefore, it is legitimate to ask whether negativity can at all distinguish the spontaneous symmetry breaking at finite temperature with spontaneous symmetry breaking at zero temperature? The answer is in the affirmative. For concreteness, again consider the exactly solvable model in Eq. (2) although the argument is rather general. Below T_c , and in the absence of an infinitesimal symmetry breaking field, the partition function gets equal contribution from both positive and negative values of the order parameter. On the other hand, in the thermodynamic limit, and in the presence of an infinitesimal symmetry breaking field, only one of the two sectors contribute, and therefore, the thermal entropy with and without field satisfies $S(h=0) - S(h=0^+) = \log(2)$. This is why the spontaneous symmetry breaking at a finite temperature is an example of ergodicity breaking [38] or relatedly, a ‘self-correcting classical memory’ [39]. Since this is a classical phenomenon, a faithful measure of quantum correlations should be insensitive to it. One may now explicitly calculate the negativity with and without infinitesimal symmetry breaking field for the Hamiltonian in Eq. (2) and show that $E_N(h=0) = E_N(h=0^+)$ (see Appendix B 1). Schematically, at a mean-field level, $\rho(h=0) = (\rho(m^*) + \rho(-m^*))/2$ where m^* is the mean-field value of the order parameter, and therefore $|\rho^{T_B}|_1(h=0) = (|\rho(m^*)^{T_B}|_1 + |\rho(-m^*)^{T_B}|_1)/2 = |\rho(m^*)^{T_B}|_1 = |\rho^{T_B}|_1(h=0^+)$. In strong contrast, for spontaneous symmetry breaking at $T=0$, when $h=0$, the ground state wave function (and not the density matrix) is a sum of the ground state wave functions corresponding to positive and negative order parameters (a ‘cat state’) while at $h=0^+$, only one of the two sectors contribute. Therefore, all measures of quantum entanglement, including von Neumann entanglement entropy and in particular negativity satisfy $E_N(h=0) - E_N(h=0^+) = \log(2)$.

To summarize, we analytically demonstrated that negativity is singular across finite-temperature phase transitions for several models. This may seem counterintuitive since the universal properties associated with transitions are controlled by a purely classical Hamiltonian with the same symmetries. One way to resolve this apparent tension is to note that negativity is sensitive to short-distance quantum correlations close to the bipartition boundary. Since even local properties, such as magnetization or energy density, are singular across

the transition, one expects that the area law associated with negativity will generically pick up a singular contribution as well. In contrast to our results, Ref. [23], based on small scale numerics ($L \lesssim 10$ sites), concluded that negativity for the 2 + 1-D quantum Ising model has no singularity across the finite-temperature transition. Although we don't have any analytical results for the negativity of the 2 + 1-D quantum Ising model, for the general reasons just mentioned, we suspect that negativity will be singular in this model as well. As is evident from the insets of Figs. 1 and 3, it can be rather hard to detect the singularity in negativity unless one has access to an analytical expression or precise numerical data on very large system sizes. We hope that our results will prompt further in-depth numerical and field-theoretic calculations of entanglement negativity in systems that exhibit finite-temperature transitions.

The singularity in negativity for the local models discussed in this paper is somewhat analogous to the singular area-law contribution at a zero-temperature QPT discussed in Ref. [29]. At the same time, the absence of finite-temperature topological order [40] in our models suggests that unlike the zero temperature case, there is no additional subleading $O(1)$ constant. If so, then one might be able to cancel out the singular contribution completely via an appropriate subtraction scheme, perhaps similar to that in Ref. [41]. Relatedly, it would be also interesting to find models where the singularity associated with negativity cannot be canceled out in any subtraction scheme and is therefore related only to universal, long-distance quantum correlations. On a more practical front, it would be interesting to devise models where the singularity in negativity can be measured experimentally, using quantum state tomography [42], or via swap-based methods on multiple copies of a system [43–45].

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APPENDIX A: GENERAL RESULTS REGARDING COMMUTING PROJECTOR HAMILTONIANS

1. Partial Transposition Preserves the Set of Eigenvectors

Consider a commuting projector Hamiltonian $H = H_A + H_B + H_{AB}$, where H_A and H_B denote the part of H with support only in real space region A and B , and H_{AB} denotes the interaction between A and B . Define $\{O_m\}$ as the set of local commuting operators, a commuting projector Hamiltonian can be written as $H = \sum_m c_m O_m$. The thermal density matrix, $\rho = e^{-\beta H} / Z$ with $Z = \text{Tr} e^{-\beta H}$, can be expanded as: $\rho = \sum_\alpha d_\alpha Q_\alpha$, where each $\{Q_\alpha\}$ is a tensor product of operators from the set $\{O_m\}$. Since all operators in H commute, H , ρ , and $\{O_m\}$ share the same eigenvectors. Under the partial transpose over the Hilbert space in B , one obtains $\rho^{T_B} = \sum_\alpha d_\alpha Q_\alpha^{T_B}$. If Q_α only acts on A or B , then $Q_\alpha^{T_B} = Q_\alpha$. Only

when the support of Q_α involves A and B simultaneously is it possible for Q_α to receive a minus sign under partial transpose. This implies that the operators basis for ρ^{T_B} is still $\{Q_\alpha\}$, and thus the eigenvectors of ρ^{T_B} are exactly the same as those of ρ , and the eigenvalues of ρ^{T_B} can be obtained by replacing $\{O_m\}$ by their eigenvalues. In the argument above we implicitly assumed that all matrix elements of $\{Q_\alpha\}$ are real in the basis where we perform a partial transpose. If there exists complex matrix elements instead, $\{Q_\alpha\}$ might get a minus sign even when $\{Q_\alpha\}$ acts only on A or B . Nevertheless, one can check that ρ^{T_B} is still generated by tensor products of $\{O_m\}$, and therefore the conclusion remains the same.

2. Partial Trace Preserves the Set of Eigenvectors

Here we show that for commuting projector Hamiltonians, the thermal density matrix ρ and the reduced density matrix ρ_A obtained by tracing out all the degrees of freedom in B share the same set of eigenvectors. As discussed above, $\rho = \sum_\alpha d_\alpha Q_\alpha$, where $\{Q_\alpha\}$ collects all possible operators from the product of commuting operators $\{O_m\}$. By tracing out all the degrees of freedom in B for ρ , basis operators in $\{Q_\alpha\}$ which act nontrivially on B vanish. This implies that the operator basis of reduced density matrix ρ_A is generated by those operators in $\{Q_\alpha\}$ which act on B trivially, and thus ρ_A commutes with all local commuting operators.

3. Bipartite Negativity from a Density Matrix on Boundary

Here we show that the negativity between two spatial regions of a thermal density matrix of a commuting projector Hamiltonian is given by the negativity of a density matrix localized on the boundary of the bipartition. Following the notation in the main text, we define $\partial A(\partial B)$ as the collection of spins on the boundary of $A(B)$ that interacts with $B(A)$, and define $A'(B')$ as the collection of spins in the bulk of $A(B)$ that only couples to spins in $A(B)$. The set of local commuting operators $\{O_m\}$ in the Hamiltonian can be written as $\{O_m\} = \{O_m^\partial\} \cup \{O_m^A\} \cup \{O_m^B\}$ with O_m^∂ supported on both ∂A , ∂B and $O_m^A(O_m^B)$ supported on $A(B)$. We decompose a Hamiltonian as $H = H_A + H_B + H_{AB}$, so that $H_A(H_B)$ involving $O_m^A(O_m^B)$ denotes the interaction between the spins in $A(B)$, and H_{AB} involving O_m^∂ denotes the interaction between the boundary spins in $\partial A \cup \partial B$. For simplicity, we also assume that the system is time reversal invariant, so that for $\rho = e^{-\beta H} / Z$, the partial transpose over the Hilbert space in B acts nontrivially only on H_{AB} :

$$\rho^{T_B} = \frac{1}{Z} (e^{-\beta H_{AB}})^{T_{\partial B}} e^{-\beta(H_A + H_B)}. \quad (\text{A1})$$

The one-norm of ρ^{T_B} can be obtained via the replica trick

$$\begin{aligned} \|\rho^{T_B}\|_1 &= \lim_{n_e \rightarrow 1} \text{Tr}(\rho^{T_B})^{n_e} \\ &= \lim_{n_e \rightarrow 1} \frac{1}{Z^{n_e}} \text{Tr}_{\partial A, \partial B} \{ [(e^{-\beta H_{AB}})^{T_{\partial B}}]^{n_e} \text{Tr}_{A', B'} \rho e^{-n_e \beta(H_A + H_B)} \}, \end{aligned} \quad (\text{A2})$$

where n_e is first treated as an even integer, but is analytically continued to 1 at the end. Since the argument inside the

trace $\text{Tr}_{\partial A, \partial B}$ involves only commuting operators, we have $\text{Tr}_{\partial A, \partial B} = g \sum_{\{O_m\}}$, where the prefactor g accounts for degeneracy and the prime above the summation symbol restricts the summation over only O_m supported on $\partial A \cup \partial B$. Therefore,

$$\|\rho^{T_B}\|_1 = \frac{g}{Z} \sum_{\{O_m\}} \{ |(e^{-\beta H_{AB}})^{T_{\partial B}} | \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)} \}. \quad (\text{A3})$$

This result implies that one can equivalently start from a density matrix $\bar{\rho}_{\partial A, \partial B} = \frac{1}{Z} (e^{-\beta H_{AB}})^{T_{\partial B}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}$, and show that

$$\|\rho^{T_B}\|_1 = \|\bar{\rho}_{\partial A, \partial B}\|_1. \quad (\text{A4})$$

Suppose that $\text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}$ does not involve local commuting operators across the bipartition boundary, i.e., operators in $\{O_m^\partial\}$, then

$$\{e^{-\beta H_{AB}}\}^{T_{\partial B}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)} = \{e^{-\beta H_{AB}} \text{Tr}_{A', B'} e^{-\beta(H_A + H_B)}\}^{T_{\partial B}}. \quad (\text{A5})$$

This result implies that

$$\|\rho^{T_B}\|_1 = \|\rho_{\partial A, \partial B}^{T_{\partial B}}\|_1, \quad (\text{A6})$$

where $\rho_{\partial A, \partial B}$ is the reduced density matrix from ρ on $\partial A \cup \partial B$: $\rho_{\partial A, \partial B} = \text{Tr}_{A', B'} \rho$. In other words, the negativity of two spatial regions is given by the negativity between boundary spins. In fact with a similar calculation, one can show that the above results [Eq. (A4), Eq. (A6)] also hold true for any commuting projector Hamiltonian without time reversal symmetry.

APPENDIX B: CALCULATIONAL DETAILS OF NEGATIVITY FOR VARIOUS MODELS DISCUSSED IN THE MAIN TEXT

1. Infinite-Range Commuting Projector Hamiltonian

Consider a one-dimensional lattice of size L where each lattice site has four qubits, the model Hamiltonian is

$$H = -\frac{1}{4L} \left(\sum_{i=1}^L (Z_{i1}Z_{i2} + Z_{i3}Z_{i4}) \right)^2 - g_z \sum_{i=1}^L Z_{i1}Z_{i2}Z_{i3}Z_{i4} - g_x \sum_{i=1}^L (X_{i1}X_{i2} + X_{i3}X_{i4}). \quad (\text{B1})$$

The density matrix at inverse temperature β is $\rho = \frac{1}{Z} e^{-\beta H}$ with $Z = \text{Tr} e^{-\beta H}$. Since every local term commutes, we can perform Hubbard-Stratonovich transformation for $e^{-\beta H}$:

$$e^{-\beta H} = \sqrt{\frac{\beta L}{\pi}} \int dm e^{-\beta L m^2 - \beta \sum_{i=1}^L H_i(m)}, \quad (\text{B2})$$

where a local Hamiltonian $H_i(m)$ for the i site of four spins is defined as:

$$H_i(m) = -m(Z_{i1}Z_{i2} + Z_{i3}Z_{i4}) - g_z Z_{i1}Z_{i2}Z_{i3}Z_{i4} - g_x (X_{i1}X_{i2} + X_{i3}X_{i4}). \quad (\text{B3})$$

Equation (B2) implies that all sites are separable since ρ manifestly takes the form $\rho = \sum_k p_k \rho_k^1 \otimes \cdots \otimes \rho_k^L$ where

$p_k \geq 0$, ρ_k^i is a local density matrix on the i th site. As a result, to have nonzero negativity, an entanglement cut should be made across one of the sites (say the s th site) such that four spins on the s th site are not in the same subsystem. In the following calculation, A comprises all the lattice sites with site index $i < s$ and two spins labeled by 1,3 on the s th site while B comprises all the lattice sites with site index $i > s$ and two spins labeled by 2,4 on the s th site. The negativity E_N can be calculated via a replica trick:

$$E_N = \log \|\rho^{T_B}\|_1 = \lim_{n_e \rightarrow 1} \frac{\text{Tr} [((e^{-\beta H})^{T_B})^{n_e}]}{\text{Tr} [e^{-\beta H}]}. \quad (\text{B4})$$

Notice that n_e is an even number as performing trace, but analytic continuation $n_e \rightarrow 1$ is taken in the end. First we calculate the thermal partition function:

$$Z = \text{Tr} e^{-\beta H} = \left(\frac{\beta L}{\pi} \right)^{\frac{1}{2}} \int dm e^{-\beta L m^2} \text{Tr} e^{-\beta \sum_{i=1}^L H_i(m)} = \left(\frac{\beta L}{\pi} \right)^{\frac{1}{2}} \int dm e^{-\beta L f(m)} \quad (\text{B5})$$

where

$$f(m) = m^2 - \log [e^{\beta g_z} \cosh(2\beta m) + e^{-\beta g_z}] - \log [8 \cosh[2](\beta g_x)]. \quad (\text{B6})$$

The integral over m is dominated by the saddle point m^* , which satisfies $\frac{\partial f(m)}{\partial m} |_{m^*} = 0$:

$$\frac{\sinh(2\beta m^*)}{\cosh(2\beta m^*) + e^{-2\beta g_z}} = m^*. \quad (\text{B7})$$

The critical behavior of m^* can be determined by expanding Eq. (B7) to $O(m^{*3})$:

$$\frac{2\beta m^*}{1+w} + \frac{4(w-2)}{3(1+w)^2} \beta^2 m^{*3} = m^*, \quad (\text{B8})$$

where $w(\beta) \equiv e^{-2\beta g_z}$. Define $\beta_c \equiv \frac{1+w(\beta_c)}{2}$, for $\beta > \beta_c$, we can have nonzero solution for $m^* = \pm m_0$:

$$m_0 = \sqrt{\frac{3\beta_c(\beta - \beta_c)}{\beta^3(3 - 2\beta_c)}} \sim \sqrt{T_c - T} \quad (\text{B9})$$

while for $\beta < \beta_c$, $m^* = 0$ is the only allowed solution. Notice that the critical inverse temperature β_c is determined by solving the transcendental equation:

$$2\beta_c = 1 + e^{-2\beta_c g_z}. \quad (\text{B10})$$

On the other hand, for the calculation of $\text{Tr} [((e^{-\beta H})^{T_B})^{n_e}]$, since each site is separable, taking partial transpose over B amounts to only taking the partial transpose on the two spins labeled by 2,4 on the s th site:

$$[e^{-\beta H}]^{T_B} = \sqrt{\frac{\beta L}{\pi}} \int dm e^{-\beta L m^2 - \beta \sum_{i \neq s} H_i(m)} [e^{-\beta H_s(m)}]^{T_B}. \quad (\text{B11})$$

By introducing n_e replicas, we have

$$\begin{aligned} \text{Tr}[(e^{-\beta H})^{T_B}]^{n_e} &= \left(\frac{\beta L}{\pi}\right)^{\frac{n_e}{2}} \int \prod_{a=1}^{n_e} dm_a e^{-\beta L \sum_{a=1}^{n_e} m_a^2} \text{Tr}_{i \neq s} \{e^{-\beta \sum_{a=1}^{n_e} \sum_{i \neq s} H_i(m_a)}\} \text{Tr}_s \left\{ \prod_{a=1}^{n_e} [e^{-\beta H_s(m_a)}]^{T_B} \right\} \\ &= \left(\frac{\beta L}{\pi}\right)^{\frac{n_e}{2}} \int \prod_{a=1}^{n_e} dm_a e^{-\beta L F_{n_e}(\{m_a\})} \frac{\text{Tr}_s \left\{ \prod_{a=1}^{n_e} [e^{-\beta H_s(m_a)}]^{T_B} \right\}}{\text{Tr}_s \left\{ \prod_{a=1}^{n_e} e^{-\beta H_s(m_a)} \right\}}, \end{aligned} \quad (\text{B12})$$

where

$$\beta F_{n_e}(\{m_a\}) = \sum_{a=1}^{n_e} m_a^2 - \log \left[e^{\beta n_e g_z} \cosh \left(2\beta \sum_{a=1}^{n_e} m_a \right) + e^{-\beta n_e g_z} \right] - \log[8 \cosh[2](\beta n_e g_x)]. \quad (\text{B13})$$

This multidimensional integral is again dominated by saddle points $\{m_a^* | a = 1, 2, \dots, n_e\}$, which can be obtained from $\frac{\partial F_{n_e}(\{m_a\})}{\partial m_a} \Big|_{m_a^*} = 0$:

$$\frac{\sinh(2\beta \sum_{a=1}^{n_e} m_a^*)}{\cosh(2\beta \sum_{a=1}^{n_e} m_a^*) + e^{-2\beta n_e g_z}} = m_a^* \quad \forall a. \quad (\text{B14})$$

Assuming replica symmetry is preserved, we have $m_{n_e}^* = m_a^* \forall a$ with

$$\frac{\sinh(2n_e \beta m_{n_e}^*)}{\cosh(2n_e \beta m_{n_e}^*) + e^{-2\beta n_e g_z}} = m_{n_e}^*. \quad (\text{B15})$$

As $n_e \rightarrow 1$, the above equation is exactly the saddle point equation for the thermal partition function [Eq. (B7)]. This implies $\lim_{n_e \rightarrow 1} m_{n_e}^* = m^*$. By plugging Eq. (B5) and Eq. (B12) into Eq. (B4), one finds

$$\|\rho^{T_B}\|_1 = \frac{\int dm e^{-\beta L f(m, g_z, g_x)} \|\rho_s^{T_B}(m)\|_1}{\int dm e^{-\beta L f(m, g_z, g_x)}}, \quad (\text{B16})$$

where

$$\rho_s(m) \equiv \frac{e^{-\beta H_s(m)}}{\text{Tr}_s \{e^{-\beta H_s(m)}\}}. \quad (\text{B17})$$

For $T > T_c$, there is a unique saddle point m^* , and

$$\|\rho^{T_B}\|_1 = \|\rho_s^{T_B}(m^*)\|_1 \frac{\int dm e^{-\beta L f(m, g_z, g_x)}}{\int dm e^{-\beta L f(m, g_z, g_x)}} = \|\rho_s^{T_B}(m^*)\|_1. \quad (\text{B18})$$

For $T < T_c$, there are two saddle points $m^* = \pm m_0$, and thus we arrive at

$$\|\rho^{T_B}\|_1 = \frac{\|\rho_s^{T_B}(m_0)\|_1 \int_{\text{around } m_0} dm e^{-\beta L f(m, g_z, g_x)} + \|\rho_s^{T_B}(-m_0)\|_1 \int_{\text{around } -m_0} dm e^{-\beta L f(m, g_z, g_x)}}{\int_{\text{around } m_0} dm e^{-\beta L f(m, g_z, g_x)} + \int_{\text{around } -m_0} dm e^{-\beta L f(m, g_z, g_x)}}. \quad (\text{B19})$$

Since $\|\rho_s^{T_B}(m_0)\|_1 = \|\rho_s^{T_B}(-m_0)\|_1$, we have

$$\|\rho^{T_B}\|_1 = \|\rho_s^{T_B}(m^*)\|_1. \quad (\text{B20})$$

This result implies that to calculate the bipartite negativity between A and B , it is sufficient to calculate the reduced density matrix for the s th site (ρ_s) where we made an entanglement cut. Incidentally, the above calculation explicitly demonstrates the claim $E_N(h=0) = E_N(h=0^+)$ mentioned in the main text where $E_N(h=0)$ is the negativity in the absence of an infinitesimal symmetry breaking field (so that it receives contribution from both m_0 and $-m_0$) while $E_N(h=0^+)$ is the negativity in the presence of such a field so that it receives contribution only from one saddle point (say, m_0). From now on, we suppress lattice site index s in the calculation since only four qubits on a single site is relevant. Meanwhile, m will replace m^* as the mean-field order parameter for brevity. The local density matrix is

$$\rho_s = \frac{1}{Z_s} e^{-\beta H_s} = \frac{1}{Z_s} e^{\beta m(Z_1 Z_2 + Z_3 Z_4) + \beta g_z Z_1 Z_2 Z_3 Z_4 + \beta g_x (X_1 X_2 + X_3 X_4)}, \quad (\text{B21})$$

where the partition function Z_s is

$$Z_s = \text{Tr} e^{-\beta H_s} = 8(\cosh(\beta g_x))^2 (e^{\beta g_z} \cosh(2\beta m) + e^{-\beta g_z}). \quad (\text{B22})$$

By taking partial transpose over $\{2, 4\} \in B$, we have

$$\begin{aligned} (e^{-\beta H_s})^{T_{24}} &= e^{\beta g_z Z_1 Z_2 Z_3 Z_4} [(\cosh(\beta g_x))^2 e^{\beta m(Z_1 Z_2 + Z_3 Z_4)} + (\sinh(\beta g_x))^2 e^{-\beta m(Z_1 Z_2 + Z_3 Z_4)} X_1 X_2 X_3 X_4] \\ &\quad + \frac{1}{2} \sinh(2\beta g_x) e^{-\beta g_z Z_1 Z_2 Z_3 Z_4} [e^{\beta m(-Z_1 Z_2 + Z_3 Z_4)} X_1 X_2 + e^{\beta m(Z_1 Z_2 - Z_3 Z_4)} X_3 X_4]. \end{aligned} \quad (\text{B23})$$

Due to the simple form of $(e^{-\beta H_s})^{T_{24}}$, we are able to obtain all the eigenvalues of $\rho_s^{T_{24}}$ and exploit the following formula to calculate the negativity:

$$E_N = \log \left[\sum_i |v_i| \right] = \log \left[1 - 2 \sum_{v_i < 0} v_i \right], \quad (\text{B24})$$

where $\{v_i\}$ denotes eigenvalues of $\rho_s^{T_{24}}$. Since $Z_1 Z_2, Z_3 Z_4, X_1 X_2, X_3 X_4$ commute with each other, the corresponding eigenvalues of these operators $z_{12}, z_{34}, x_{12}, x_{34} = \pm 1$ completely specify an eigenvector of $(e^{-\beta H_s})^{T_{24}}$, which takes the following form

$$|\psi\rangle = \frac{1}{2}(|s_1, s_2\rangle \pm |-s_1, -s_2\rangle) \otimes (|s_3, s_4\rangle \pm |-s_3, -s_4\rangle), \quad (\text{B25})$$

with $s_i = \pm 1$ for $i = 1, 2, 3, 4$. With this observation, the eigenvalues of $(e^{-\beta H_s})^{T_{24}}$ can be obtained by replacing operators by their eigenvalues:

$$\begin{aligned} \lambda(z_{12}, z_{34}, x_{12}, x_{34}) &= e^{\beta g_z z_{12} z_{34}} [(\cosh(\beta g_x))^2 e^{\beta m(z_{12} + z_{34})} + (\sinh(\beta g_x))^2 e^{-\beta m(z_{12} + z_{34})} x_{12} x_{34}] \\ &+ \frac{1}{2} \sinh(2\beta g_x) e^{-\beta g_z z_{12} z_{34}} [e^{\beta m(-z_{12} + z_{34})} x_{12} + e^{\beta m(z_{12} - z_{34})} x_{34}]. \end{aligned} \quad (\text{B26})$$

For $T > T_c, m = 0$, one finds

$$\lambda(z_{12}, z_{34}, x_{12}, x_{34}) = e^{\beta g_z z_{12} z_{34}} [(\cosh(\beta g_x))^2 + (\sinh(\beta g_x))^2 z_{12} z_{34}] + \frac{1}{2} \sinh(2\beta g_x) e^{-\beta g_z z_{12} z_{34}} [x_{12} + x_{34}]. \quad (\text{B27})$$

When

$$\begin{aligned} z_{12} &= 1, z_{34} = -1, x_{12} = -1, x_{34} = -1 \\ z_{12} &= -1, z_{34} = 1, x_{12} = -1, x_{34} = -1, \end{aligned} \quad (\text{B28})$$

we can have negative λ :

$$\lambda = e^{-\beta g_z} \cosh(2\beta g_x) - e^{\beta g_z} \sinh(2\beta g_x). \quad (\text{B29})$$

Thus, for $T > T_c$, the twofold degenerate negative eigenvalue of $\rho_s^{T_{24}}$ is

$$v = \frac{e^{-\beta g_z} \cosh(2\beta g_x) - e^{\beta g_z} \sinh(2\beta g_x)}{16(\cosh(\beta g_x))^2 \cosh(\beta g_z)}, \quad (\text{B30})$$

and the negativity can be obtained by using Eq. (B24):

$$E_N = \log \left[1 + \max \left\{ 0, \frac{e^{\beta g_z} \sinh(2\beta g_x) - e^{-\beta g_z} \cosh(2\beta g_x)}{4(\cosh(\beta g_x))^2 \cosh(\beta g_z)} \right\} \right]. \quad (\text{B31})$$

Note that at T_c , one requires

$$e^{-2\beta_c g_z} < \tanh(2\beta_c g_x) \quad (\text{B32})$$

to have nonzero negativity. This is always achievable by tuning g_x since β_c is only determined by g_z . For $T < T_c$, depending on the values of m , there could be more choices of $(z_{12}, z_{34}, x_{12}, x_{34})$ that can give negative eigenvalues of $\rho_s^{T_{24}}$. For simplicity, we consider $T \rightarrow T_c^-$, where $m \sim \sqrt{T_c - T} \rightarrow 0^+$, and only the configurations in Eq. (B28) can possibly give negative eigenvalues. This is sufficient for our purpose since we only concern the possibly nonanalytic behavior of the negativity. Therefore, as $T \rightarrow T_c^-$, the twofold degenerate negative eigenvalue of $\rho_s^{T_{24}}$ is

$$v = \frac{e^{-\beta g_z} \cosh(2\beta g_x) - e^{\beta g_z} \sinh(2\beta g_x) \cosh(2\beta m)}{8(\cosh(\beta g_x))^2 (e^{\beta g_z} \cosh(2\beta m) + e^{-\beta g_z})}. \quad (\text{B33})$$

Finally, the negativity valid for $T > T_c^-$ is given by

$$E_N = \log \left[1 + \max \left\{ 0, \frac{e^{\beta g_z} \sinh(2\beta g_x) \cosh(2\beta m) - e^{-\beta g_z} \cosh(2\beta g_x)}{2(\cosh(\beta g_x))^2 (e^{\beta g_z} \cosh(2\beta m) + e^{-\beta g_z})} \right\} \right] \quad (\text{B34})$$

Due to the singular behavior of $m(T)$:

$$m = \begin{cases} a\sqrt{T_c - T} & \text{for } T \rightarrow T_c^- \\ 0 & \text{for } T > T_c, \end{cases} \quad (\text{B35})$$

the negativity E_N is also a singular function across T_c .

2. Two-dimensional Commuting Projector Hamiltonian

Consider a two-dimensional lattice, where each site has two spins labeled by ‘a’ and ‘b’ respectively, the model Hamiltonian is

$$H = - \sum_{(ij)} \tilde{z}_i \tilde{z}_j - g \sum_i \tilde{x}_i, \quad (\text{B36})$$

where $\tilde{z}_i \equiv Z_{ia} Z_{ib}$, $\tilde{x}_i \equiv X_{ia} X_{ib}$. Consider a thermal density matrix $\rho_T \sim \exp -\beta H$, here we present the calculation of the negativity between one spin on a single site, say, ‘a’ spin in site 0 (subsystem A), and its complement (subsystem B). As discussed above, to calculate the negativity, we only need the reduced density matrix for spins at the boundary which in this case are the spins at site 0 and its neighboring sites (labelled as 1,2,3,4 clockwise). The corresponding reduced density matrix on these five sites is

$$\rho = A' e^{-\beta g(\tilde{x}_1 + \tilde{x}_2 + \tilde{x}_3 + \tilde{x}_4)} [\cosh(\beta g) e^{\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} + \sinh(\beta g) e^{\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} \tilde{x}_0] \\ [1 + c_1(\tilde{z}_1 \tilde{z}_2 + \tilde{z}_2 \tilde{z}_3 + \tilde{z}_3 \tilde{z}_4 + \tilde{z}_4 \tilde{z}_1) + c_2(\tilde{z}_1 \tilde{z}_3 + \tilde{z}_2 \tilde{z}_4) + c_3 \tilde{z}_1 \tilde{z}_2 \tilde{z}_3 \tilde{z}_4]. \quad (\text{B37})$$

Here A' is determined by demanding $\text{Tr} \rho = 1$ and $c_1 = \langle \tilde{z}_j \tilde{z}_{j+1} \rangle$; $c_2 = \langle \tilde{z}_j \tilde{z}_{j+2} \rangle$; $c_3 = \langle \tilde{z}_1 \tilde{z}_2 \tilde{z}_3 \tilde{z}_4 \rangle$, where the expectation values are taken with respect to the bulk thermal density matrix $\rho_{\text{bulk}} \sim \exp -\beta(H_A + H_B)$. In fact, due to the property of commuting local terms, c_i can be obtained by considering the thermal state of a bulk classical Hamiltonian, i.e., $g = 0$, with one spin per site, and one just needs to replace the composite operator \tilde{z}_i by a Pauli Z operator at site i (i.e., Z_i). For instance,

$$c_1 = \langle \tilde{z}_j \tilde{z}_{j+1} \rangle = \frac{\text{Tr} \tilde{z}_j \tilde{z}_{j+1} e^{\beta \sum_{(ij)} \tilde{z}_i \tilde{z}_j + \beta g \sum_i \tilde{x}_i}}{\text{Tr} e^{\beta \sum_{(ij)} \tilde{z}_i \tilde{z}_j + \beta g \sum_i \tilde{x}_i}} = \frac{\text{Tr} Z_j Z_{j+1} e^{\beta \sum_{(ij)} Z_i Z_j}}{\text{Tr} e^{\beta \sum_{(ij)} Z_i Z_j}}. \quad (\text{B38})$$

Under the partial transposition over B , the density matrix is

$$\rho^{T_B} = A' e^{-\beta g(\tilde{x}_1 + \tilde{x}_2 + \tilde{x}_3 + \tilde{x}_4)} [\cosh(\beta g) e^{\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} + \sinh(\beta g) e^{-\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} \tilde{x}_0] \\ [1 + c_1(\tilde{z}_1 \tilde{z}_2 + \tilde{z}_2 \tilde{z}_3 + \tilde{z}_3 \tilde{z}_4 + \tilde{z}_4 \tilde{z}_1) + c_2(\tilde{z}_1 \tilde{z}_3 + \tilde{z}_2 \tilde{z}_4) + c_3 \tilde{z}_1 \tilde{z}_2 \tilde{z}_3 \tilde{z}_4]. \quad (\text{B39})$$

The eigenvalues of ρ^{T_B} can be obtained by just replacing \tilde{x}_i, \tilde{z}_i by ± 1 . In fact, $e^{-\beta g(\tilde{x}_1 + \tilde{x}_2 + \tilde{x}_3 + \tilde{x}_4)}$ is irrelevant since it just provides a multiplicative factor when summing negative eigenvalues, which got canceled out by the normalization factor. Effectively, it is sufficient to consider the eigenvalues

$$\lambda = A [\cosh(\beta g) e^{\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} + \sinh(\beta g) e^{-\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} \tilde{x}_0] \\ [1 + c_1(\tilde{z}_1 \tilde{z}_2 + \tilde{z}_2 \tilde{z}_3 + \tilde{z}_3 \tilde{z}_4 + \tilde{z}_4 \tilde{z}_1) + c_2(\tilde{z}_1 \tilde{z}_3 + \tilde{z}_2 \tilde{z}_4) + c_3 \tilde{z}_1 \tilde{z}_2 \tilde{z}_3 \tilde{z}_4], \quad (\text{B40})$$

where \tilde{x}_0 and each \tilde{z}_i takes ± 1 , which gives $2^6 = 64$ eigenvalues, and A is chosen such that the sum of these 64 eigenvalues remains unity. $[1 + c_1 \dots]$ part is always non-negative since it is obtained by performing partial trace for a density matrix (positive semidefinite). As a result, λ can be negative only when $\tilde{x}_0 = -1$ and $e^{2\beta \tilde{z}_0(\tilde{z}_1 + \tilde{z}_2 + \tilde{z}_3 + \tilde{z}_4)} < \tanh(\beta g)$. For a given g , there are many choices of \tilde{z}_i that can result in negative eigenvalues. As our purpose is to check whether the negativity picks up a singularity at a thermal critical point, it is sufficient to restrict g in a range such that only a few eigenvalues are negative. We set g in the range $e^{-8\beta} < \tanh(\beta g) < e^{-4\beta}$, and there are only two negative eigenvalues given by

$$\tilde{z}_0 = 1, \quad \tilde{z}_1 = \tilde{z}_2 = \tilde{z}_3 = \tilde{z}_4 = -1 \\ \tilde{z}_0 = -1, \quad \tilde{z}_1 = \tilde{z}_2 = \tilde{z}_3 = \tilde{z}_4 = 1. \quad (\text{B41})$$

Finally, as

$$e^{-8\beta} < \tanh(\beta g) < e^{-4\beta}, \quad (\text{B42})$$

we obtain the expression of the negativity:

$$E_N = \log\{1 - 4A[\cosh(\beta g) e^{-4\beta} - \sinh(\beta g) e^{4\beta}](1 + 4c_1 + 2c_2 + c_3)\}. \quad (\text{B43})$$

$$A^{-1} = 2^5 \cosh(\beta g) [\cosh[4](\beta) + (c_1 + \frac{1}{2}c_2) \sinh[2](2\beta) + c_3 \sinh[4](\beta)] \quad (\text{B44})$$

Due to the singularity of c_i at the thermal critical point, the negativity E_N is expected to be singular. To confirm this intuition, we now adopt a mean-field approach to calculate the coefficient c_1, c_2, c_3 . The exact nature of singularities associated with c_i for

our model would of course be determined by the critical exponents of the 2D Ising model. As shown in Eq. (B38), c_i is exactly given by the corresponding classical Hamiltonian with one spin per site. As a result, we consider the mean-field Hamiltonian

$$H = -(3m + Z_0)(Z_1 + Z_2 + Z_3 + Z_4), \quad (\text{B45})$$

we determine m from $m = \langle Z_i \rangle = \text{Tr} \rho Z_i$ for $i = 1$ to 4, where ρ is a density matrix associated with H . It is straightforward to obtain the mean-field equation for m :

$$m = \frac{\cosh[4](\beta(3m + 1)) \tanh(\beta(3m + 1)) + \cosh[4](\beta(3m - 1)) \tanh(\beta(3m - 1))}{\cosh[4](\beta(3m + 1)) + \cosh[4](\beta(3m - 1))}. \quad (\text{B46})$$

T_c can be determined from this equation, and it is straightforward to show that $m = 0$ as $T \rightarrow T_c^+$, and $m \sim \sqrt{T_c - T}$ as $T \rightarrow T_c^-$. Finally, c_1, c_2, c_3 can be obtained:

$$\begin{aligned} c_1 = c_2 = \langle Z_1 Z_2 \rangle &= \frac{\cosh[2](\beta(3m + 1)) \sinh[2](\beta(3m + 1)) + \cosh[2](\beta(3m - 1)) \sinh[2](\beta(3m - 1))}{\cosh[4](\beta(3m + 1)) + \cosh[4](\beta(3m - 1))} \\ c_3 = \langle Z_1 Z_2 Z_3 Z_4 \rangle &= \frac{\sinh[4](\beta(3m + 1)) + \sinh[4](\beta(3m - 1))}{\cosh[4](\beta(3m + 1)) + \cosh[4](\beta(3m - 1))}. \end{aligned} \quad (\text{B47})$$

Plug the coefficients into Eq. (B43), and expand it for small m ,

$$E_N = \log \left\{ 1 - 4[\cosh(\beta g)e^{-4\beta} - \sinh(\beta g)e^{4\beta}] \left\{ \frac{16 \cosh(4\beta)}{1 + 4 \cosh(4\beta + \cosh(8\beta))} + \frac{1728\beta^2[1 + 6 \cosh(4\beta) + \cosh(8\beta)]m^2}{[1 + 4 \cosh(4\beta + \cosh(8\beta))]^2} \right\} \right\}. \quad (\text{B48})$$

There the negativity E_N is manifestly singular at T_c due to the singularity from m .

3. Quantum Spherical Model

Consider the Hamiltonian for a quantum spherical model: $H = \frac{1}{2}g \sum_{i=1}^N p_i^2 - \frac{1}{2N} \sum_{i,j=1}^N x_i x_j + \mu[\sum_{i=1}^N x_i^2 - \frac{N}{4}]$ where $[x_i, p_j] = i\delta_{ij}$. μ is chosen so that $\langle \sum_{i=1}^N x_i^2 \rangle = \frac{N}{4}$ where the expectation value is taken with respect to the thermal density matrix. Define $x_k = \frac{1}{\sqrt{N}} \sum_j e^{ikj} x_j$, $p_k = \frac{1}{\sqrt{N}} \sum_j e^{ikj} p_j$ and introduce a_k, a_k^\dagger : $p_k = -i\sqrt{\frac{\omega_k}{2g}}(a_k - a_{-k}^\dagger)$, $x_k = \sqrt{\frac{g}{2\omega_k}}(a_k + a_{-k}^\dagger)$ the Hamiltonian can be diagonalized:

$$H = \sum_k \omega_k (a_k^\dagger a_k + \frac{1}{2}) - \frac{\mu}{4} N, \quad (\text{B49})$$

where the single particle energy ω_k is

$$\omega_k = \begin{cases} \omega_0 = \sqrt{2g(\mu - \frac{1}{2})} & \text{for } k = 0 \\ \omega_1 = \sqrt{2g\mu} & \text{for } k \neq 0. \end{cases} \quad (\text{B50})$$

Note that in order to have a stable theory, $\mu \geq \frac{1}{2}$. From Eq. (B49), the free energy density f can be calculated:

$$f = \frac{1}{N\beta} \log [2 \sinh(\frac{1}{2}\beta\omega_0)] + \frac{N-1}{N\beta} \log [2 \sinh(\frac{1}{2}\beta\omega_1)] - \mu/4. \quad (\text{B51})$$

μ is determined from $\langle \sum_{i=1}^N x_i^2 \rangle = \frac{N}{4}$, which is equivalent to $\frac{\partial f}{\partial \mu} = 0$:

$$\frac{1}{2N} \sqrt{\frac{g}{2(\mu - \frac{1}{2})}} \coth(\frac{1}{2}\beta\sqrt{2g(\mu - \frac{1}{2})}) + \frac{N-1}{2N} \sqrt{\frac{g}{2\mu}} \coth(\frac{1}{2}\beta\sqrt{2g\mu}) = \frac{1}{4}. \quad (\text{B52})$$

In the thermodynamic limit $N \rightarrow \infty$, μ is a singular function of β, g . For $2\sqrt{g} \coth(\frac{1}{2}\beta\sqrt{g}) > 1$, the system is in a disordered phase, with μ determined from

$$\sqrt{\frac{g}{2\mu}} \coth(\frac{1}{2}\beta\sqrt{2g\mu}) = \frac{1}{2}, \quad (\text{B53})$$

while the condition $2\sqrt{g} \coth(\frac{1}{2}\beta\sqrt{g}) < 1$ gives the ordered phase, and μ is pinned to $\frac{1}{2}$. Here we briefly describe the covariance matrix formalism for calculating the negativity of a Gaussian state ρ for N degrees of freedom. First we calculate the covariance matrix in displacements $(\gamma_x)_{ij} = \langle \{x_i - \bar{x}_i, x_j - \bar{x}_j\} \rangle$ and the covariance matrix in momenta $(\gamma_p)_{ij} = \langle \{p_i - \bar{p}_i, p_j - \bar{p}_j\} \rangle$, where $\bar{x}_i = \text{tr} \rho x_i$, $\bar{p}_i = \text{tr} \rho p_i$, and $\{A, B\} = AB + BA$ is the anticommutator. Define the subsystem A composed by degrees of freedom for site $i = 1, 2, \dots, N_A$ and the complement B composed by the rest of sites, we calculate $\tilde{\gamma} = \gamma_x R \gamma_p R$, where R is diagonal

matrix with 1 for the first N_A diagonal entries and -1 for the rest of the diagonal entries. By diagonalizing $\tilde{\gamma}$, we obtain its eigenvalues $\{v_i | i = 1, 2, \dots, N\}$, from which the negativity E_N can be calculated

$$E_N(\rho) = \sum_{i=1}^N \max\{0, -\frac{1}{2} \log v_i\}. \quad (\text{B54})$$

For the thermal state of the spherical model, a straightforward calculation shows that

$$\begin{aligned} (\gamma_x)_{ij} &= 2\langle x_i x_j \rangle = m_x + \delta_{ij} d_x \\ (\gamma_p)_{ij} &= 2\langle p_i p_j \rangle = m_p + \delta_{ij} d_p, \end{aligned} \quad (\text{B55})$$

with

$$\begin{aligned} m_x &\equiv \frac{1}{N} \left[\sqrt{\frac{g}{2\mu-1}} \coth\left(\frac{1}{2}\beta\sqrt{(2\mu-1)g}\right) - \sqrt{\frac{g}{2\mu}} \coth\left(\frac{1}{2}\beta\sqrt{2\mu g}\right) \right] \\ d_x &\equiv \sqrt{\frac{g}{2\mu}} \coth\left(\frac{1}{2}\beta\sqrt{2\mu g}\right) \\ m_p &\equiv \frac{1}{N} \left[\sqrt{\frac{2\mu-1}{g}} \coth\left(\frac{1}{2}\beta\sqrt{(2\mu-1)g}\right) - \sqrt{\frac{2\mu}{g}} \coth\left(\frac{1}{2}\beta\sqrt{2\mu g}\right) \right] \\ d_p &\equiv \sqrt{\frac{2\mu}{g}} \coth\left(\frac{1}{2}\beta\sqrt{2\mu g}\right). \end{aligned} \quad (\text{B56})$$

Thus we have

$$\tilde{\gamma} = \gamma_x R \gamma_p R = d_x d_p \mathbb{1}_N + m_x d_p J_N + m_p d_x \begin{pmatrix} J_{N/2} & -J_{N/2} \\ -J_{N/2} & J_{N/2} \end{pmatrix} \quad (\text{B57})$$

where we define J_N as an $N \times N$ all-ones matrix. All three matrices on the right-hand side commute with each other so they can be diagonalized with the same set of eigenvectors. Since both the second and the third matrix are rank-1 matrix, it is easy to calculate the eigenvalues. Finally, the eigenvalues of $\tilde{\gamma}$ are

$$v_k = \begin{cases} d_x d_p = [\coth(\frac{1}{2}\beta\sqrt{2\mu g})]^2 & \text{for } k = 1, 2, \dots, N-2 \\ d_x d_p + N m_x d_p = \sqrt{\frac{2\mu}{2\mu-1}} \coth(\frac{1}{2}\beta\sqrt{(2\mu-1)g}) \coth(\frac{1}{2}\beta\sqrt{2\mu g}) & \text{for } k = N-1 \\ d_x d_p + N m_p d_x = \sqrt{\frac{2\mu-1}{2\mu}} \coth(\frac{1}{2}\beta\sqrt{(2\mu-1)g}) \coth(\frac{1}{2}\beta\sqrt{2\mu g}) & \text{for } k = N \end{cases} \quad (\text{B58})$$

One can check that $v_k > 1$ for $k = 1, 2, \dots, N-1$ for all values of parameters in the model, and only v_N can be less than 1 to contribute to the entanglement negativity:

$$E_N = \text{Max}\{0, -\frac{1}{2} \log v\} \quad (\text{B59})$$

where

$$v \equiv v_N = \sqrt{\frac{2\mu-1}{2\mu}} \coth\left[\frac{1}{2}\beta\sqrt{(2\mu-1)g}\right] \coth\left[\frac{1}{2}\beta\sqrt{2\mu g}\right]. \quad (\text{B60})$$

By using Eq. (B53) in the disordered phase, and $\mu = \frac{1}{2}$ in the ordered phase, v can be further simplified:

$$v = \begin{cases} \frac{2}{\beta\sqrt{g}} \coth\left(\frac{1}{2}\beta\sqrt{g}\right) & \text{for ordered phase} \\ \frac{1}{2} \sqrt{\frac{2\mu-1}{g}} \coth\left(\frac{1}{2}\beta\sqrt{(2\mu-1)g}\right) & \text{for disordered phase.} \end{cases} \quad (\text{B61})$$

To study the singularity of E_N at the critical point, we calculate the first derivative of E_N with respect to g to observe its discontinuity at a critical point:

$$\begin{aligned} \frac{\partial E_N}{\partial g} \Big|_{g_c^+} &= \frac{1}{2g_c} + \frac{\beta_c^2}{24} \left(1 - \frac{8}{4 + \beta_c - 4\beta_c g_c} \right) \\ \frac{\partial E_N}{\partial g} \Big|_{g_c^-} &= \frac{4 + \beta_c - 4\beta_c g_c}{16g_c}. \end{aligned} \quad (\text{B62})$$

APPENDIX C: ENTANGLEMENT OF FORMATION IN AN INFINITE-RANGE COMMUTING PROJECTOR HAMILTONIAN

To begin with, we recall the definition of the entanglement of formation: A density matrix ρ acting on a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ can be decomposed as a convex sum of pure states

$$\rho = \sum_k P_k |k\rangle \langle k|, \quad (C1)$$

and for each $|k\rangle$, we can calculate the reduced density matrix on A : $\rho_k^A = \text{Tr}_B |k\rangle \langle k|$, from which the entanglement entropy $S_A(|k\rangle)$ is obtained: $S_A(|k\rangle) = -\text{Tr}_A \rho_k^A \log \rho_k^A$. The entanglement of formation $E_F(A, B)$ is defined as

$$E_F(A, B) = \min \sum_k P_k S_A(|k\rangle), \quad (C2)$$

where minimization over all possible pure state decomposition is taken. Here we provide a model, where the entanglement of formation can be calculated analytically by showing its upper and lower bound coincide in the thermodynamic limit. Consider a one-dimensional lattice of size L where each lattice site has two qubits, the model Hamiltonian is

$$H = -\frac{1}{2L} \left(\sum_{i=1}^L Z_{i1} Z_{i2} \right)^2 - g \sum_{i=1}^L X_{i1} X_{i2}. \quad (C3)$$

The density matrix at inverse temperature β is $\rho = \frac{1}{Z} e^{-\beta H}$ with $Z = \text{Tr} e^{-\beta H}$. We make an entanglement cut across one of the sites (say the s th site) such that the two spins on the s th site are not in the same subsystem. In the following calculation, A comprises all the lattice sites with site index $i < s$ and the spin labeled by 1 on the s th site while B comprises all the lattice sites with site index $i > s$ and the spin labeled by 2 on the s th site. For such a bipartition scheme, we prove that the entanglement of formation E_F between A and B is exactly that from a mean-field density matrix for just two spins, where a closed form expression for E_F is available. Our strategy is to find an upper bound and a lower bound on E_F that happen to match each other.

1. Upper Bound

Entanglement of formation E_F requires a minimization scheme over all possible pure state decompositions. By considering a particular way of decomposition, we thus give an upper bound for E_F . First we perform the Hubbard-Stratonovich transformation for ρ :

$$\rho = \frac{1}{Z} e^{-\beta H} = \frac{1}{Z} \sqrt{\frac{\beta L}{2\pi}} \int dm e^{-\frac{1}{2}\beta L m^2 - \beta \sum_{i=1}^L H_i(m)}, \quad (C4)$$

where a local Hamiltonian $H_i(m)$ for the i site of two spins is defined as:

$$H_i(m) = -m Z_{i1} Z_{i2} - g X_{i1} X_{i2}. \quad (C5)$$

Each $e^{-\beta H_i(m)}$ can be decomposed: $e^{-\beta H_i(m)} = \sum_{k_i} w_{k_i}^i(m) |k_i(m)\rangle \langle k_i(m)|$. As a result,

$$\rho = \sum_{\{k_i\}} \int dm \frac{1}{Z} \sqrt{\frac{\beta L}{2\pi}} e^{-\frac{1}{2}\beta L m^2} \left(\prod_i w_{k_i}^i(m) \right) |k_1, \dots, k_L\rangle \langle k_1, \dots, k_L|. \quad (C6)$$

The entanglement entropy between A and B in $|k_1, \dots, k_L\rangle \langle k_1, \dots, k_L|$ is given by the entanglement entropy between just two spins at site s due to the product state structure for different sites. Therefore,

$$E_F(A, B) \leq \min_{\{k_i\}} \sum_{\{k_i\}} \int dm \frac{1}{Z} \sqrt{\frac{\beta L}{2\pi}} e^{-\frac{1}{2}\beta L m^2} \left(\prod_i w_{k_i}^i(m) \right) S_{s1}(|k_s(m)\rangle), \quad (C7)$$

where $S_{s1}(|k_s(m)\rangle)$ is the entanglement entropy between spins at s_1 and s_2 in the state $|k_s(m)\rangle$, and the minimum is taken among all possible pure state decomposition of $e^{-\beta H_i(m)}$. Since $S_{s1}(|k_s\rangle)$ is independent of how we decompose $e^{-\beta H_i}$ for $i \neq s$. The summation over $k_i \forall i \neq s$ can be performed on $w_{k_i}^i$:

$$\sum_{\{k_i | i \neq s\}} \prod_{i \neq s} w_{k_i}^i = (\text{Tr}_i e^{-\beta H_i(m)})^{L-1} = e^{-\beta(L-1)f(m)}, \quad (C8)$$

where $f(m)$ is a mean-field free energy density. Consequently,

$$E_F(A, B) \leq \min_{k_s} \frac{\int dm e^{-\beta L f(m)} \sum_{k_s} \frac{1}{Z_s} w_{k_s}^s(m) S_{s1}(|k_s(m)\rangle)}{\int dm e^{-\beta L f(m)}}, \quad (C9)$$

with $Z_s \equiv \text{Tr}_s e^{-\beta H_s(m)}$. In the $L \rightarrow \infty$ limit, the argument inside the summation over k_s is dominated only by saddle points, and thus

$$E_F(A, B) \leq \min_{k_s} \sum \frac{1}{Z_s} w_{k_s}^s(m^*) S_{s1}(|k_s(m^*)|), \quad (\text{C10})$$

where m^* is a saddle point obtained by minimizing $f(m)$. Define the mean field density matrix on a single site of two spins:

$$\rho_s(m^*) = \frac{1}{Z_s} e^{-\beta H_s(m^*)}, \quad (\text{C11})$$

we show

$$E_F(A, B) \leq E_F(s1, s2), \quad (\text{C12})$$

i.e., the entanglement of formation between A and B is upper bounded by the entanglement of formation between two spins in the mean field density matrix.

2. Lower Bound

As a bona fide entanglement measure, entanglement of formation is nonincreasing under a partial trace. This implies that $E_F(a, b) \leq E_F(A, B)$, where a and b denote a subsystem in A and B , respectively. Here we choose two spins at the sites s as a and b . A calculation shows that the reduced density matrix at site s is

$$\rho_s = \frac{1}{Z} \text{Tr}_{i \neq s} e^{-\beta H} = \frac{\int dme^{-\beta L f(m)} \frac{1}{Z_s} e^{-\beta H_s(m)}}{\int dme^{-\beta f(m)}} = \frac{\int dme^{-\beta L f(m)} \rho_s(m)}{\int dme^{-\beta f(m)}} \quad (\text{C13})$$

where $f(m) = -\frac{1}{\beta} \log Z_s = -\frac{1}{\beta} \log \text{Tr}_s e^{-\beta H_s(m)}$ is the free energy density. In $L \rightarrow \infty$ limit, ρ_s is exactly given by $\rho_s(m^*)$ where the saddle point m^* is the location of the global minimum of $f(m)$. One way to see this is to expand ρ_s in a complete operator basis on site s and show that expectation value of any operator on site s is precisely given by $\rho_s(m^*)$. This calculation shows that

$$E_F(s1, s2) \leq E_F(A, B). \quad (\text{C14})$$

By combining Eq. (C12) and Eq. (C14), one finds that the bipartite entanglement of formation between A and B is exactly that between two spins in the mean field density matrix which can be calculated analytically using the result of Ref. [31].

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