

Monogamy of entanglement and improved mean-field ansatz for spin lattices

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We consider rather general spin-1/2 lattices with large coordination numbers Z . Based on the monogamy of entanglement and other properties of the concurrence C , we derive rigorous bounds for the entanglement between neighboring spins, such as $C \leq 1/\sqrt{Z}$, which show that C decreases for large Z . In addition, we demonstrate that the concurrence C measures the deviation from mean-field behavior and can only vanish if the mean-field ansatz yields an exact ground state of the Hamiltonian. Motivated by these findings, we propose an improved mean-field ansatz by adding entanglement.

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I. INTRODUCTION

Quantum information theory is not only interesting in view of quantum computers and quantum cryptography but offers important insights into other branches of physics as well. For instance, a deeper understanding of entanglement—which is one of the major differences between classical and quantum physics—can help us to grasp the complexity of quantum many-body problems better. This strategy has already lead to very successful developments, for example, matrix-product states, which have been shown to efficiently approximate ground states of suitable one-dimensional lattice Hamiltonians. For a recent review, see [1]. Unfortunately, transferring this concept to higher-dimensional lattices with a consequently larger coordination number Z is a nontrivial task. Besides tensor-network states [2–4], a step into this direction is the quantum de Finetti theorem [5–7]. In one version, this theorem implies the following statement: If a given state $\hat{\rho}^{(n)}$ of $n \gg 1$ qubits is invariant under permutation of any two of those qubits, then the reduced density matrix of two qubits $\hat{\rho}^{(2)}$ can be approximated by a separable (i.e., nonentangled) state plus $\mathcal{O}(1/n)$ corrections. However, ground states of lattice Hamiltonians typically do not obey the full permutational invariance required for this theorem to hold (unless we have a fully connected lattice where all sites are equally interacting neighbors [8]). In the following, we replace this full permutational invariance by a much smaller subgroup, the lattice isotropy, and derive a similar statement based on the monogamy of entanglement [10,11] and certain properties of the concurrence [12–14].

II. SPIN LATTICE

We consider a general regular, isotropic, and bipartite lattice of spins 1/2 (i.e., qubits) described by the Hamiltonian

$$\hat{H} = \frac{1}{Z} \sum_{\langle \mu, \nu \rangle} \hat{\sigma}_\mu \cdot \mathbf{J} \cdot \hat{\sigma}_\nu + \sum_{\mu} \mathbf{B} \cdot \hat{\sigma}_\mu, \quad (1)$$

where $\hat{\sigma}_\mu = (\hat{\sigma}_\mu^x, \hat{\sigma}_\mu^y, \hat{\sigma}_\mu^z)$ are the usual Pauli matrices acting on the spin at the lattice site μ and $\mathbf{B} = (B_x, B_y, B_z)$ denotes the local field while \mathbf{J} is a 3×3 matrix (tensor) describing the

interactions between neighboring sites μ and ν (denoted by $\langle \mu, \nu \rangle$). Finally, Z is the coordination number (i.e., it counts the number of neighbors ν for each given lattice site μ), and we consider the limit of large Z . The $1/Z$ scaling in front of the \mathbf{J} term is chosen such that the energy per lattice site remains well defined in this limit $Z \rightarrow \infty$.

In general, obtaining the ground state of a Hamiltonian of the form of Eq. (1) can be rather complicated. Here, we shall exploit the properties of entanglement in order to understand the features of this ground state better. Obviously, the knowledge of the reduced density matrices $\hat{\rho}_{\langle \mu, \nu \rangle}$ of neighboring spins μ, ν suffices for calculating the ground-state energy. The entanglement between these sites μ and ν is also completely determined by $\hat{\rho}_{\langle \mu, \nu \rangle}$ and can be measured by the concurrence $C[\hat{\rho}_{\langle \mu, \nu \rangle}]$. This quantity satisfies the monogamy of entanglement; i.e., the one-tangle $\tau_1(\hat{\rho}_\mu) = 4 \det(\hat{\rho}_\mu)$ of a given lattice site μ described by the on-site reduced density matrix $\hat{\rho}_\mu$ yields an upper bound to its entanglement with all neighboring sites ν via [10,11]

$$\tau_1(\hat{\rho}_\mu) = 4 \det(\hat{\rho}_\mu) \geq \sum_{\nu} C^2[\hat{\rho}_{\langle \mu, \nu \rangle}]. \quad (2)$$

Assuming that the ground state obeys the same (discrete) symmetries as the underlying lattice, those matrices $\hat{\rho}_{\langle \mu, \nu \rangle}$ have the same form for all ν . Thus the sum over ν just gives a factor Z and we get the upper bound for the concurrence:

$$C[\hat{\rho}_{\langle \mu, \nu \rangle}] \leq \sqrt{\frac{\tau_1}{Z}} \leq \sqrt{\frac{1}{Z}}, \quad (3)$$

where we have used $\tau_1 \leq 1$ in the last step. As a result, in the limit of large coordination numbers, the entanglement between two spins is suppressed with $1/\sqrt{Z}$ or even stronger (see below). The entanglement between next-nearest neighbors C' can be bound via similar arguments; for example, in a hypercubic lattice in D dimensions (where $Z = 2D$), we get $C' \leq 1/\sqrt{2D(D-1)}$.

III. GROUND-STATE ENERGY

As our next step, we exploit the high symmetry (degeneracy) in the decomposition space for the concurrence (as a quadratic polynomial), which facilitates the decomposition of

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every two-qubit density matrix [12,13]

$$\hat{\rho}_{(\mu\nu)} = \sum_{I=1}^4 p_I |\Psi_{\mu\nu}^I\rangle\langle\Psi_{\mu\nu}^I| \quad (4)$$

into (at most) four pure states $|\Psi_{\mu\nu}^I\rangle$ with the corresponding probabilities p_I such that these states $|\Psi_{\mu\nu}^I\rangle$ have all the same concurrence C . Then the properties of the concurrence enable us to split each state $|\Psi_{\mu\nu}^I\rangle$ into a separable part and an orthogonal entangled part [14]:

$$|\Psi_{\mu\nu}^I\rangle = \sqrt{1-C} |\psi_{\mu}^I\rangle |\psi_{\nu}^I\rangle + \sqrt{C} \hat{U}_{\mu}^I \hat{U}_{\nu}^I |\text{Bell}\rangle_{\mu\nu}, \quad (5)$$

where $|\text{Bell}\rangle$ is one of the maximally entangled Bell states such as $|\text{Bell}\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2} = |\Phi^+\rangle$ while \hat{U}_{μ}^I and \hat{U}_{ν}^I are some local unitary operations which do not change the entanglement. Combining all these results, we get the following estimate for the energy per lattice site:

$$\begin{aligned} \frac{\langle\hat{H}\rangle}{N} &= \sum_{I=1}^4 \frac{p_I}{2} \left[\langle\hat{\sigma}_{\mu}^I\rangle \cdot \mathbf{J} \cdot \langle\hat{\sigma}_{\nu}^I\rangle + \mathbf{B} \cdot (\langle\hat{\sigma}_{\mu}^I\rangle + \langle\hat{\sigma}_{\nu}^I\rangle) \right] \\ &+ \mathcal{O}(\sqrt{C}), \end{aligned} \quad (6)$$

where $\langle\hat{\sigma}_{\mu}^I\rangle = \langle\psi_{\mu}^I|\hat{\sigma}_{\mu}|\psi_{\mu}^I\rangle$ denote local (mean-field) expectation values. The magnitude of the $\mathcal{O}(\sqrt{C})$ corrections can be estimated by the matrix elements of the operators $\hat{\sigma}_{\mu} \cdot \mathbf{J} \cdot \hat{\sigma}_{\nu}$ and $\mathbf{B} \cdot \hat{\sigma}_{\mu}$ between the separable $\langle\psi_{\mu}^I|\langle\psi_{\nu}^I|$ and fully entangled states $\hat{U}_{\mu}^I \hat{U}_{\nu}^I |\text{Bell}\rangle_{\mu\nu}$. Via a global SU(2) rotation $\otimes_{\mu} \hat{V}_{\mu}$, we may diagonalize the matrix \mathbf{J} such that $\hat{\sigma}_{\mu} \cdot \mathbf{J} \cdot \hat{\sigma}_{\nu}$ becomes $J_{xx}\sigma_{\mu}^x\sigma_{\nu}^x + J_{yy}\sigma_{\mu}^y\sigma_{\nu}^y + J_{zz}\sigma_{\mu}^z\sigma_{\nu}^z$. Then we get terms like $J_{xx}\langle\psi_{\mu}^I|\langle\psi_{\nu}^I|\hat{V}_{\mu}^{\dagger}\hat{V}_{\nu}^{\dagger}\sigma_{\mu}^x\sigma_{\nu}^x\hat{V}_{\mu}\hat{V}_{\nu}\hat{U}_{\mu}^I\hat{U}_{\nu}^I|\text{Bell}\rangle_{\mu\nu}$ and analogously for J_{yy} and J_{zz} . Since the maximum overlap between a separable and a Bell state is $1/\sqrt{2}$, the matrix elements of $\hat{\sigma}_{\mu} \cdot \mathbf{J} \cdot \hat{\sigma}_{\nu}$ can be bounded from above by $(|J_{xx}| + |J_{yy}| + |J_{zz}|)/\sqrt{2}$. Similarly, the matrix elements of $\mathbf{B} \cdot \hat{\sigma}_{\mu}$ can be bounded from above by $|\mathbf{B}|/\sqrt{2}$.

Consequently, in the limit of large Z and therefore small C , we may estimate the ground-state energy (per lattice site) by the variational mean-field ansatz:

$$|\Psi_{\text{mf}}\rangle = \bigotimes_{\mu} |\psi_{\mu}\rangle. \quad (7)$$

Inserting this mean-field ansatz and minimizing the energy thus yields an estimate for the exact ground-state energy up to $\mathcal{O}(\sqrt{C})$ corrections. If this variational procedure yields a unique solution $|\psi_{\mu}\rangle = |\psi_0\rangle$, the resulting state $|\psi_0\rangle$ provides a good approximation to the local (on-site) properties of the exact ground state.

IV. ISING MODEL

Let us study this general procedure by means of an explicit example, the quantum Ising model:

$$\hat{H} = -\frac{J}{Z} \sum_{(\mu,\nu)} \hat{\sigma}_{\mu}^x \hat{\sigma}_{\nu}^x - B \sum_{\mu} \hat{\sigma}_{\mu}^z. \quad (8)$$

Up to an irrelevant global phase, the mean-field ansatz (7) can be parametrized via

$$|\psi_{\mu}\rangle = \cos \frac{\vartheta_{\mu}}{2} |\uparrow\rangle + e^{i\varphi_{\mu}} \sin \frac{\vartheta_{\mu}}{2} |\downarrow\rangle, \quad (9)$$

and, after insertion into the Hamiltonian, we get the mean-field energy per lattice site:

$$\begin{aligned} \frac{\langle\hat{H}\rangle_{\text{mf}}}{N} &= -\frac{1}{2} [J \sin \vartheta_{\mu} \cos \varphi_{\mu} \sin \vartheta_{\nu} \cos \varphi_{\nu} \\ &+ B(\cos \vartheta_{\mu} + \cos \vartheta_{\nu})]. \end{aligned} \quad (10)$$

Accordingly, for $B > |J|$, we obtain a unique minimum at $\vartheta_{\mu} = \vartheta_{\nu} = 0$ corresponding to the paramagnetic state $|\Psi_{\text{mf}}\rangle = |\uparrow\uparrow\uparrow\dots\rangle$.

As stated above, this mean-field ansatz $|\psi_{\mu}\rangle = |\uparrow\rangle$ provides a good approximation to the local properties of the exact ground state for large Z and thus small C . To make this statement more precise, let us consider the on-site reduced density matrix of the exact ground state, which can be cast into the most general form:

$$\hat{\rho}_{\mu} = (1-p) |\uparrow\rangle\langle\uparrow| + p |\downarrow\rangle\langle\downarrow| + \alpha |\uparrow\rangle\langle\downarrow| + \alpha^* |\downarrow\rangle\langle\uparrow|. \quad (11)$$

By invoking symmetry arguments, one can even show that α must vanish exactly in the paramagnetic state, but this is not necessary for our purposes. Using the parametrization (9) for the states $|\psi_{\mu}^I\rangle$, a Taylor expansion of Eq. (6) for small $\vartheta_{\mu,v}^I$ yields a bilinear form of the $\vartheta_{\mu,v}^I$ to lowest nontrivial order. Completing the square, we obtain the following inequality:

$$\begin{aligned} \frac{\langle\hat{H}\rangle}{N} &\geq \frac{\langle\hat{H}\rangle_{\text{mf}}}{N} + (B - |J|) \sum_{I=1}^4 \frac{p_I}{4} [(\vartheta_{\mu}^I)^2 + (\vartheta_{\nu}^I)^2] \\ &+ \mathcal{O}(p_I [\vartheta_{\mu,v}^I]^4) + \mathcal{O}(\sqrt{C}), \end{aligned} \quad (12)$$

where $\langle\hat{H}\rangle_{\text{mf}}/N = -B$ is the mean-field energy per lattice site [Eq. (10)]. Obviously, the exact ground-state energy $\langle\hat{H}\rangle/N$ in the above expression must not exceed that of the mean-field ansatz $\langle\hat{H}\rangle_{\text{mf}}/N$, which yields the bound $p_I (\vartheta_{\mu,v}^I)^2 \leq \mathcal{O}(\sqrt{C})$. This implies that the probability p in Eq. (11) scales with $p \leq \mathcal{O}(\sqrt{C})$. Analogously, one can obtain the bound $\alpha \leq \mathcal{O}(\sqrt[4]{C})$ consistent with the properties of $\hat{\rho}_{\mu}$ such as $\det(\hat{\rho}_{\mu}) \geq 0$ or $\text{Tr}\{\hat{\rho}_{\mu}^2\} \leq 1$.

As a result, we find that the one-tangle $\tau_1(\hat{\rho}_{\mu})$ is also suppressed as $\tau_1 \leq \mathcal{O}(\sqrt{C})$. Together with our initial bound $C \leq Z^{-1/2}$ from Eq. (3), we thus get $\tau_1 \leq \mathcal{O}(Z^{-1/4})$. However, inserting this estimate back into Eq. (3), we obtain the improved scaling $C \leq \sqrt{\tau_1/Z} \leq \mathcal{O}(Z^{-5/8})$. Repeatedly iterating this procedure, the scaling exponents eventually converge to

$$C \leq \mathcal{O}(Z^{-2/3}), \quad \tau_1 \leq \mathcal{O}(Z^{-1/3}). \quad (13)$$

On the other hand, the hierarchy of correlations derived in [15,16], for example, suggests that the one-tangle as well as all two-point correlations are suppressed by $1/Z$ in this situation.

Since the maximum two-point correlation cannot be smaller than the concurrence C [17], this would imply an even stronger bound $C \leq \mathcal{O}(Z^{-1})$, but—to the best of our knowledge—

there is no rigorous proof, yet. Of course, the concurrence could be even smaller.

V. IMPROVED MEAN-FIELD ANSATZ

Having found that the concurrence C measures the deviation from the mean-field behavior, let us try to use this insight in order to improve the mean-field ansatz by adding entanglement. Inspired by Eq. (5), we start with the following ansatz for two sites

$$|\Psi_{\mu\nu}\rangle = \mathcal{N}(1 + \hat{\sigma}_\mu \cdot \xi \cdot \hat{\sigma}_\nu) |\uparrow\rangle_\mu |\uparrow\rangle_\nu, \quad (14)$$

where ξ acts as an entangling operation leading to a small but nonzero concurrence and \mathcal{N} is the normalization. For the paramagnetic state $|\Psi_{\text{mf}}\rangle = |\uparrow\uparrow\uparrow\dots\rangle$ of the Ising model, it is sufficient to keep only the relevant operators $\xi\sigma_\mu^x\sigma_\nu^x$ (or $\xi\sigma_\mu^y\sigma_\nu^y$). Applying this procedure to the whole lattice yields the improved mean-field ansatz [18]:

$$|\Psi\rangle_{\text{imf}} = \mathcal{N} \left(\prod_{(\mu,\nu)} \exp\{\xi\hat{\sigma}_\mu^x\hat{\sigma}_\nu^x\} \right) \bigotimes_\mu |\uparrow\rangle_\mu, \quad (15)$$

where $\bigotimes_\mu |\uparrow\rangle_\mu = |\uparrow\uparrow\uparrow\dots\rangle$ is the original mean-field ansatz (without entanglement). Here, we apply this entangling operation to nearest neighbors only, but this can be generalized easily to $\xi_{\mu\nu}\hat{\sigma}_\mu^x\hat{\sigma}_\nu^x$. Using the identity $\exp\{\xi\hat{\sigma}_\mu^x\hat{\sigma}_\nu^x\} = \mathbb{1} \cosh\xi + \hat{\sigma}_\mu^x\hat{\sigma}_\nu^x \sinh\xi$, we get the single-site reduced density matrix:

$$\hat{\rho}_\mu = \frac{1}{2} \left[\mathbb{1} + \left(\frac{\cos(2\Im\xi)}{\cosh(2\Re\xi)} \right)^{Z/2} \hat{\sigma}_\mu^z \right]. \quad (16)$$

The reduced density matrix for nearest neighbors reads

$$\begin{aligned} \hat{\rho}_{(\mu\nu)} &= \frac{1}{4} \left[\mathbb{1} + (\hat{\sigma}_\mu^x\hat{\sigma}_\nu^x - \chi^{2(Z-1)}\hat{\sigma}_\mu^y\hat{\sigma}_\nu^y) \tanh 2\Re\xi \right. \\ &\quad + \chi^{2(Z-1)}\hat{\sigma}_\mu^z\hat{\sigma}_\nu^z + \chi^Z(\hat{\sigma}_\mu^z + \hat{\sigma}_\nu^z) \\ &\quad \left. + \omega^Z(\hat{\sigma}_\mu^x\hat{\sigma}_\nu^y + \hat{\sigma}_\mu^y\hat{\sigma}_\nu^x) \right], \end{aligned} \quad (17)$$

where we have used the following abbreviations:

$$\chi = \frac{\cos(2\Im\xi)}{\cosh(2\Re\xi)}, \quad \omega = \frac{\sin(2\Im\xi)}{\cosh(2\Re\xi)}, \quad (18)$$

containing the real $\Re\xi$ and imaginary part $\Im\xi$ of ξ .

In order to test whether the ansatz (15) is really an improvement, let us consider the energy which reads

$$\frac{\langle \hat{H} \rangle_{\text{imf}}}{N} = -\frac{J}{2} \tanh(2\Re\xi) - B \left(\frac{\cos(2\Im\xi)}{\cosh(2\Re\xi)} \right)^Z. \quad (19)$$

We see that adding entanglement, i.e., increasing ξ , lowers the interaction energy $\propto J$ but increases the on-site term $\propto B$. Furthermore, we find that only the real part of ξ can actually lower the energy, while the imaginary part always leads to an increase. The imaginary part of ξ generates a unitary transformation \hat{U} which cannot lower the energy $\langle \hat{H} \rangle_{\text{imf}}$. As another way to see this, one can apply this unitary transformation \hat{U} to the Hamiltonian (8) instead of the state (15). Obviously, the interaction term $\propto J$ remains invariant under this unitary transformation and thus still yields a zero expectation value, while the expectation value of the local term $\propto B$ can only increase. Consequently, we choose

ξ to be real such that the operation acting on the mean-field state in Eq. (15) is nonunitary (thus the normalization \mathcal{N}). Interestingly, Eq. (15) can then be reinterpreted as an imaginary time evolution operator if we insert the Hamiltonian (8) with $B = 0$ and identify $itJ/Z = \xi$.

As also expected from stationary perturbation type arguments, the minimum energy is reached for a finite value:

$$\xi_{\text{min}} = \frac{J}{4BZ} + \mathcal{O}(1/Z^2). \quad (20)$$

Consistent with the previous observations, the entangling strength ξ decreases for large Z . In addition, because the energy of the improved mean-field ansatz (15) lies below the mean-field value, we know that the concurrence must be nonzero. Let us specify the relevant quantities for this example. The one-tangle obtained from Eq. (16) reads

$$\tau_1 = 1 - \frac{1}{[\cosh(2\xi_{\text{min}})]^{2Z}} = \frac{J^2}{4B^2Z} + \mathcal{O}(1/Z^2). \quad (21)$$

As a result, the concurrence must be suppressed according to $C \leq J/(2BZ) + \mathcal{O}(1/Z^2)$ in view of Eq. (3). To test this bound, let us calculate the concurrence of the state (15). Since the entangling strength ξ scales with $1/Z$ according to Eq. (20), we introduce the scaling variable $\zeta = Z|\xi|$. Then, an expansion into powers of $1/Z$ (for fixed ζ) yields the concurrence [20]:

$$C = 2 \frac{\zeta - \zeta^2}{Z} \Theta(1 - \zeta) + \mathcal{O}(1/Z^2). \quad (22)$$

The positive contribution $+2\zeta/Z$ is basically the concurrence of the pure state (14), up to $\mathcal{O}(1/Z^2)$ corrections. The negative contribution $-2\zeta^2/Z$, on the other hand, stems from the fact that $\hat{\rho}_{(\mu\nu)}$ is a mixed state due to the entanglement with all the other neighboring sites $\lambda \neq \mu, \nu$ which are averaged over when obtaining $\hat{\rho}_{(\mu\nu)}$.

Thus, for small $\zeta \ll 1$, the concurrence C approximately saturates the bound $C \leq J/(2BZ) + \mathcal{O}(1/Z^2)$ from Eq. (3). For larger ζ , on the other hand, the concurrence C lies below this bound, and for $\zeta \geq 1$ it even vanishes—as indicated by the Heaviside step function $\Theta(1 - \zeta)$. For a vanishing concurrence $C = 0$, the arguments above imply that the ansatz (15) cannot yield an improvement over the usual mean-field ansatz (7). However, this does not lead to any inconsistency because this case $\zeta \geq 1$ corresponds to $|\xi| \geq 1/Z$ and therefore $|J| \geq 4B$, which lies already far beyond the (mean-field) critical point at $B = |J|$.

VI. XY MODEL

As another example, let us consider the XY model as described by the Hamiltonian

$$\begin{aligned} \hat{H} &= -\frac{J}{Z} \sum_{\langle\mu,\nu\rangle} \left(\frac{1+\gamma}{2} \hat{\sigma}_\mu^x\hat{\sigma}_\nu^x + \frac{1-\gamma}{2} \hat{\sigma}_\mu^y\hat{\sigma}_\nu^y \right) \\ &\quad - B \sum_\mu \hat{\sigma}_\mu^z, \end{aligned} \quad (23)$$

where $\gamma \in [0,1]$ is the anisotropy parameter. For $\gamma = 1$, we recover the Ising model (8) whereas $\gamma = 0$ yields the isotropic limit. (Away from the isotropic point $\gamma = 0$, the XY model

is in the same universality class as the Ising model.) Using the same variational ansatz (15), the entangling parameter ξ_{\min} yielding the minimum energy is modified by the anisotropy parameter γ via

$$\xi_{\min} = \gamma \frac{J}{4BZ} + \mathcal{O}(1/Z^2). \quad (24)$$

The one-tangle and the concurrence are reduced accordingly. We observe that, for $\gamma > 0$, the improved mean-field ansatz (15) gives an advantage and, consistently, the concurrence is nonzero. In the isotropic case $\gamma = 0$, on the other hand, the mean-field ansatz actually yields the exact ground state in the paramagnetic regime—which is consistent with the vanishing concurrence and $\xi_{\min} = 0$. It has a Berezinskii-Kosterlitz-Thouless transition at $J/B = 1$.

VII. DEGENERATE GROUND STATES

Note that the above arguments require a unique mean-field solution $|\psi_0\rangle$. Let us briefly discuss the cases where this solution is not unique. For $J > |B|$, we are in the symmetry-breaking ferromagnetic regime (on the mean-field level) where the mean-field energy (10) has two minima—one at $\varphi_\mu = \varphi_\nu = 0$ and the other one at $\varphi_\mu = \varphi_\nu = \pi$. For $J \gg |B|$, these two minima move to $\vartheta_\mu = \vartheta_\nu = \pi/2$ corresponding to the states $|\Psi_{\text{mf}}^-\rangle = |\leftarrow\leftarrow\leftarrow\dots\rangle$ and $|\Psi_{\text{mf}}^+\rangle = |\rightarrow\rightarrow\rightarrow\dots\rangle$. Even though the mean-field solution $|\psi_0\rangle$ is not unique in this case, we might select one of the two states as our starting point and carefully proceed in the same way as before. The incoherent average of the results in the two cases corresponds to the mixed state $\hat{\rho} = (|\Psi_{\text{mf}}^+\rangle\langle\Psi_{\text{mf}}^+| + |\Psi_{\text{mf}}^-\rangle\langle\Psi_{\text{mf}}^-|)/2$.

The remaining region of parameter space $J < -|B|$ corresponds to the antiferromagnetic regime (again on the mean-field level) which also breaks the symmetry. In a bipartite lattice, where we do not have to deal with frustration, we could again choose one of the two states as mean-field background and apply the same procedure. In the case of frustration, however, things become more complicated and we cannot find a consistent mean-field background. In this case, the one-tangle could well be of order 1 and thus the concurrence could be much larger, possibly $C = \mathcal{O}(1/\sqrt{Z})$.

Finally, at the critical points $J = \pm B$, we do find a consistent mean-field background, but the estimates after Eq. (12) do not apply anymore, and thus the one-tangle and concurrence could also be larger than they are well inside the paramagnetic phase, for example.

VIII. CONCLUSIONS AND OUTLOOK

We have considered a general regular isotropic spin lattice with local (on-site) terms and nearest-neighbor interactions of Ising type [Eq. (1)]. Assuming that the ground state shares the isotropy of the lattice, monogamy of entanglement [Eq. (2)] implies that the concurrence C between neighboring spins decreases at least as $C \leq 1/\sqrt{Z}$ for large coordination numbers Z . Under certain assumptions (such as a unique mean-field minimum), the bound can be improved to $C \leq \mathcal{O}(Z^{-2/3})$. On the other hand, unless the mean-field ansatz (7) yields an exact ground state of the Hamiltonian (see also [21,22]), the concurrence C is nonzero for nearest neighbors.

In addition, the difference between the exact ground-state energy per lattice site and that of the mean-field ansatz is bounded by $\mathcal{O}(\sqrt{C})$,

$$\frac{\langle\hat{H}\rangle_{\text{mf}}}{N} - \frac{\langle\hat{H}\rangle_{\text{exact}}}{N} \leq (||\mathbf{J}|| + 2|\mathbf{B}|)\sqrt{2C} + \mathcal{O}(C), \quad (25)$$

where $||\mathbf{J}|| = \text{Tr}\{\sqrt{\mathbf{J}^2}\} = |J_{xx}| + |J_{yy}| + |J_{zz}|$, i.e., the nearest-neighbor entanglement C serves as a measure for the deviation from the mean-field solution.

Motivated by these findings, we propose an improved mean-field ansatz (15) by adding a small amount of entanglement. For the Ising model (8) in the paramagnetic regime, we show that this ansatz (15) does indeed yield a better approximation to the ground state and that the one-tangle and the concurrence (22) scale with $1/Z$ in this case, consistent with [15,16]. Even though this is reminiscent of the quantum de Finetti theorem [6], where the corrections do also scale with the inverse of the number n of involved qubits, we would like to stress that the scaling (22) is obtained in a different way (e.g., without assuming full permutational invariance).

As an outlook, one might generalize the improved mean-field ansatz (15) via $\mathcal{N} \exp\{\sum_{\mu\nu} \hat{\sigma}_\mu \cdot \xi_{\mu\nu} \cdot \hat{\sigma}_\nu\} |\Psi_0\rangle$ to situations where the range of $\xi_{\mu\nu}$ is not restricted any more to nearest neighbors only, such that the $\xi_{\mu\nu}$ could add a small amount of long-range entanglement. Also more general states $|\Psi_0\rangle$ such as projected entangled pair states could be considered. As another direction, it would be interesting to generalize our results to states different from the ground state, such as the real-time evolution after a quantum quench, or thermal states, for example. Since thermal states are mixed, one might replace the one-tangle $\tau_1(\hat{\rho}_\mu) = 4 \det(\hat{\rho}_\mu)$ by its convex-roof extension (which is usually smaller), but this quantity does also satisfy the monogamy inequality. Note that the bounds (3) and (6) are only based on the assumption that the state obeys the lattice symmetries. They thus do apply to these cases (real-time evolution after a quantum quench or thermal states) as well. In contrast, the derivation of subsequent bounds such as Eq. (13) is also based on energy minimization arguments [see, e.g., Eq. (12)] and thus only applies to the ground state, but not necessarily to the quantum quench scenario. Even in those cases where the one-tangle in the ground state is suppressed as $\tau_1 = \mathcal{O}(1/Z)$, we would expect that it could increase to $\tau_1 = \mathcal{O}(1)$ during the time evolution after a quantum quench. Hence, the concurrence C [being initially suppressed as $C \leq \mathcal{O}(1/Z)$] could in principle also grow in this situation—as long as it obeys the bound $C \leq 1/\sqrt{Z}$; the precise behavior should be investigated in future studies.

Furthermore, it would be highly desirable to study and extend the various properties of the concurrence (such as the monogamy of entanglement) to further entanglement measures (for extensions of the monogamy for qubits, see [23]) as, e.g., three-particle quantum correlations investigated in [24].

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APPENDIX

In order to illustrate the broad applicability of the improved mean-field ansatz, we briefly discuss a further generalization to the Fermi-Hubbard model, where $\hat{\sigma}_\mu \cdot \mathbf{J} \cdot \hat{\sigma}_\nu$ is replaced by the hopping term $J[\hat{c}_{\mu,\uparrow}^\dagger \hat{c}_{\nu,\uparrow} + \hat{c}_{\mu,\downarrow}^\dagger \hat{c}_{\nu,\downarrow}]$ with fermionic creation and annihilation operators while $\mathbf{B} \cdot \hat{\sigma}_\mu$ corresponds to the interaction term $U\hat{n}_{\mu,\uparrow}\hat{n}_{\mu,\downarrow}$ with $\hat{n}_{\mu,\uparrow} = \hat{c}_{\mu,\uparrow}^\dagger \hat{c}_{\mu,\uparrow}$ and $\hat{n}_{\mu,\downarrow} = \hat{c}_{\mu,\downarrow}^\dagger \hat{c}_{\mu,\downarrow}$. For $U \gg J$, the mean-field ground state $|\Psi_{\text{mf}}\rangle$ in a bipartite lattice at half filling is the Mott insulator state with precisely one fermion per site obeying Néel ordering, i.e., alternating spins (antiferromagnetic).

In analogy to Eq. (14), the linearized corrections to this mean-field ansatz read $\sum_{ij} \hat{A}_{\mu,i} \xi_{\mu\nu,ij} \hat{A}_{\nu,j} |\Psi_{\text{mf}}\rangle$ where the $\hat{A}_{\mu,i}$ form a complete set of on-site operators. If we respect the $U(1)$ symmetry, the term $\hat{A}_{\mu,i} \xi_{\mu\nu,ij} \hat{A}_{\nu,j}$ could

contain products of two, four, six, or eight operators out of $\hat{c}_{\mu,\uparrow}$, $\hat{c}_{\nu,\uparrow}$, $\hat{c}_{\mu,\downarrow}$, $\hat{c}_{\nu,\downarrow}$, and the corresponding raising operators.

As terms containing two operators, we obtain the generators of the well-known particle-hole excitations (which become the doublon-holon excitations in the Mott-Néel state) $\hat{c}_{\mu,\uparrow}^\dagger \hat{c}_{\nu,\uparrow}$ and $\hat{c}_{\mu,\downarrow}^\dagger \hat{c}_{\nu,\downarrow}$, which correspond to a fermionic Bogoliubov transformation. The nontrivial terms with four operators yield the generators for the spin modes $\hat{c}_{\mu,\uparrow}^\dagger \hat{c}_{\nu,\downarrow}^\dagger \hat{c}_{\nu,\uparrow} \hat{c}_{\mu,\downarrow}$ and $\hat{c}_{\nu,\uparrow}^\dagger \hat{c}_{\mu,\downarrow}^\dagger \hat{c}_{\mu,\uparrow} \hat{c}_{\nu,\downarrow}$ while the remaining terms with six and eight operators do not give any new generators after acting on the Mott-Néel state. Thus, the improved mean-field ansatz (15) can be generalized to this case as well and automatically reproduces the relevant particle-hole and spin modes known from other approaches.

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