Constructing tensor network wavefunction for a generic two-dimensional quantum phase transition via thermofield double states

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The most important feature of two-dimensional quantum Rokhsar-Kivelson (RK) type models is that their ground state wavefunction norms can be mapped into the partition functions of two-dimensional statistical models so that the quantum phase transitions become the thermal phase transitions of the corresponding statistical models. For a generic quantum critical point, we generalize the framework of RK wavefunctions by introducing the concept of the thermofield double (TFD) state, which is a purification of the equilibrium density operator. Moreover, by expressing the TFD state in terms of the projected entangled pair state, its \(N\)-order of Rényi entropy results in a three-dimensional statistical model in Euclidian spacetime, describing the generic quantum phase transitions. Using the toric code model with two parallel magnetic fields as an example, we explain these ideas and derive the partition function of the three-dimensional \(Z_2\) lattice gauge-Higgs model, where the phase transitions are characterized by the three-dimensional universality classes.

Introduction. -Recently quantum spin liquids, topological phases of matter, and their quantum phase transitions have been attracted enormous research interest, and there has been a very active development of tensor network states to study these correlated quantum many-body phenomena.\(^{[1-4]}\). Since the ground states and low-energy excited states of two-dimensional (2D) quantum systems with local interactions are only weak entangled, the entanglement entropy of a region scales with its area\(^{[5,6]}\). Then infinite projected entangled-pair states (iPEPS) or tensor network states\(^{[7-10]}\) has become a powerful theoretical tool to characterize those correlated quantum many-body phases in the thermodynamic limit\(^{[11,12]}\). However, there still exists an open problem about how well the iPEPS can describe two-dimensional quantum critical states emerging at the quantum critical points\(^{[13,14]}\).

Since the norm of the iPEPS can be related to a partition function of classical statistical models, the zero-temperature quantum phase transitions can be mapped to the temperature-driven classical phase transitions\(^{[15-18]}\), and there is a class of exact 2D critical iPEPS with a small value of bond dimension, describing the ground states of the generalized Rokhsar-Kivelson (RK) Hamiltonians at their critical point\(^{[19,21]}\). However, a generic 2D quantum phase transition should be described by the partition function of a 3D classical statistical model in the Euclidian space, where an extra dimension corresponds to the "imaginary time" to represent thermal fluctuations at the critical point. And the emerging critical properties of the 2D quantum model belong to the same universality class as that of the 3D classical system. Therefore, the most important question is to establish a general framework connecting the tensor network wavefunction for a 2D quantum system to a 3D classical partition function, and to find out the necessary conditions under which the general framework can be applied.

In this paper, we generalize the RK wavefunctions to the framework of the so-call thermofield double (TFD) states\(^{[22]}\), which are defined in an enlarged Hilbert space \(\mathcal{H}_P \otimes \mathcal{H}_F\) consisting of the physical space \(\mathcal{H}_P\) and a fictitious space \(\mathcal{H}_F\). The TFD state is a purification of a mixed density operator in thermal equilibrium, and the thermal fluctuations is encoded in the form of quantum entanglement between the physical and fictitious parts. For a class of 2D quantum systems, their model Hamiltonians can be divided into two noncommutative parts \(\hat{H} = \hat{H}^{(1)} + \hat{H}^{(2)}\) and each part is a sum of the commuting local terms. We can introduce a tensor network TFD state with variational parameters, and then a reduced TFD density operator can be obtained by integrating out the fictitious degrees of freedom. We prove that the \(N\)-th order Rényi entropy gives rise to the partition function of 3D statistical models in the Euclidian space, where the imaginary time dimension is discretized into \(N\) layers. In the large \(N\) limit, we expect that the phase transitions of the 3D statistical models characterize the quantum phase transitions in the 2D quantum model. As an example, we carefully study the toric code model in two parallel fields\(^{[23,24]}\). By constructing a variational tensor network TFD state, we successfully derive the partition function of the 3D lattice gauge-Higgs model\(^{[25,27]}\), which can be used to describe the topological quantum phase transitions out of the toric code phase.

General framework. -From a 2D classical Hamiltonian \(E(\sigma_1, \cdots, \sigma_n)\) with spin variables \(\{\sigma_i\}\), the RK-type wavefunction with a parameter \(\beta\) is defined by

\[
|\psi(\beta)\rangle = \sum_\sigma e^{-\beta E(\sigma)/2} |\sigma\rangle.
\]

where \(|\sigma\rangle = |\sigma_1, \cdots, \sigma_n\rangle\) and \(\{\sigma\}\) is a set of completely orthogonal basis. The wavefunction norm precisely corresponds to the partition function of a classical model with \(\beta\) as the inverse temperature:

\[
Z(\beta) = \langle \psi(\beta) | \psi(\beta) \rangle = \sum_\sigma \exp[-\beta E(\sigma)].
\]
With such a quantum-classical mapping, all equal-time correlation functions of local observable operators are mapped into the correlation functions of the classical partition function. Then the quantum phase transitions in the RK wavefunction are described by the partition function of a 2D classical model.

When we consider a 2D quantum Hamiltonian $\hat{H}(\sigma_1, \cdots, \sigma_n)$ with spin operators $\{\sigma_i\}$, a generic quantum wavefunction can be expressed as

$$\Psi(\beta) = \sum_\sigma e^{-\beta \hat{H}(\sigma_1, \cdots, \sigma_n)/2} |\sigma\rangle. \quad (3)$$

When $\beta \to \infty$, the wavefunction $|\Psi(\infty)\rangle$ approaches to the ground state of $\hat{H}$. Unlike the RK-type wavefunctions, the norm of the wavefunction $\langle \Psi(\beta) | \Psi(\beta) \rangle$ is significantly different from the partition function of the quantum Hamiltonian $Z(\beta) = tr e^{-\beta \hat{H}}$. The former sums over both diagonal and off-diagonal matrix elements of the density operator $e^{-\beta \hat{H}}$, the latter is just a sum of diagonal matrix elements. So the derived partition function becomes a ground state projector, leading to a product state $|\Psi(\beta)\rangle = \prod_\sigma e^{-\alpha_\sigma \hat{H}_\sigma(\beta)/2} |\sigma\rangle_F$, where $\alpha_\sigma$ are variational parameters. Then we can express the corresponding TFD state as

$$\tilde{\Psi}(\alpha_1, \alpha_2) = \sum_\sigma e^{-\alpha_1 \hat{H}_1(\beta)/2} e^{-\alpha_2 \hat{H}_2(\beta)/2} |\sigma\rangle_F, \quad (7)$$

where $\alpha_1, \alpha_2$ are variational parameters. Then we express the corresponding TFD state as

$$\tilde{\Psi}(\alpha_1, \alpha_2) = \sum_{\sigma, \tilde{\sigma}} (e^{-\alpha_1 \hat{H}_1(\beta)/2} e^{-\alpha_2 \hat{H}_2(\beta)/2})_{\tilde{\sigma}} |\sigma\rangle_F \otimes |\tilde{\sigma}\rangle_F, \quad (8)$$

and those coefficients can be easily written as the products of local Boltzmann weights

$$(e^{-\alpha_1 \hat{H}_1(\beta)/2} e^{-\alpha_2 \hat{H}_2(\beta)/2})_{\tilde{\sigma}} = \sum_s \prod_v \exp (-\epsilon^{s_v}_v \epsilon^{s_v}_v (\alpha_1, \alpha_2)), \quad (9)$$

where the auxiliary degrees of freedom $s = s_1, \cdots, s_m$ have been introduced and $\epsilon^{s_v}_v, \epsilon^{s_v}_v, \epsilon^{s_v}_v$ are the sets of spin variables belonging to the vertex $v$. When the local Boltzmann weights are replaced by local tensors, the TFD state wavefunction becomes an iPEPS with physical degrees of freedom $\tilde{\sigma}, \sigma$. From Eq. 4, after integrating out the fictitious degrees of freedom, we obtain a reduced TFD density operator

$$\rho = tr_F |\tilde{\Psi}\rangle \langle \tilde{\Psi}| = e^{-\alpha_1 \hat{H}_1(\beta)/2} e^{-\alpha_2 \hat{H}_2(\beta)/2} e^{-\alpha_1 \hat{H}_1(\beta)/2}. \quad (10)$$

In order to construct the partition function of a 3D statistical model for the critical iPEPS, we stack $N$ copies of $\rho$ and contract all degrees of freedom including those at the top of the $N$-th layer and those at the first layer. Then we identify $Z_N = tr \rho^N_{\text{PEPS}}$ as a partition function in the Euclidian spacetime. Actually the usual $N$-th order Rényi entropy is given by

$$S_N = \log tr \rho^N_{\text{PEPS}}. \quad (11)$$

So the derived partition function $Z_N$ can be explicitly written in terms of the local tensors of the iPEPS,
and the partition function of a 2D quantum system is transformed into that of a 3D classical one, which can be simulated with the classical resources. If the intra-layer interactions in the spatial directions have the same form as the inter-layer interactions in the imaginary time direction, the isotropic 3D model at the critical point has an emergent Lorentz symmetry and the dynamical critical exponent \( z = 1 \).

**Toric code model in two parallel fields.** - To illustrate the above general theory, we consider the toric code model defined on a square lattice

\[
H_{TC} = -\sum_v A_v - \sum_p B_p, \tag{12}
\]

\[
A_v = -\sum_v \prod_{\langle ij \rangle \in v} \sigma_{ij}^x, \quad B_p = -\sum_p \prod_{\langle ij \rangle \in p} \sigma_{ij}^z,
\]

where the vertex and plaquette terms \( A_v \) and \( B_p \) involve four Pauli spin-1/2 operators located on the bonds between sites \( i \) and \( j \). \( A_v = -1 \) is associated with an electric charge excitation, while \( B_p = -1 \) is associated with a magnetic flux excitation. The ground states can be projected out by the projectors of the subspaces:

\[
|\Psi_{m TC}^v\rangle = \prod_v (1 + A_v) |\uparrow\rangle^{\otimes L}, \quad |\Psi_{TC}^p\rangle = \prod_p (1 + B_p) |\uparrow\rangle^{\otimes L},
\]

where \( |\uparrow\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2} \) and \( L \) is the bond number. On a manifold with the trivial topology, the ground state is non-degenerate, \( |\Psi_{TC}^p\rangle = |\Psi_{m TC}^v\rangle \).

It is useful to represent the ground states as iPEPS. When auxiliary degrees of freedom \( s_j = \pm 1 \) on each site is introduced, the off-diagonal projector can be expressed as a projected entangled pair operator (PEPO)

\[
\prod_v (1 + A_v) = \sum_{s \sigma} \prod_{\langle ij \rangle \in v} \frac{1 + s_i s_j \sigma_{ij}^x \bar{\sigma}_{ij}}{2} |\sigma\rangle\langle \bar{\sigma}|,
\]

corresponding to a double-line PEPO on the dual lattice in Fig. 1(a), while the diagonal projector is just a single line PEPO on the dual lattice

\[
\prod_p (1 + B_p) = \sum_{\sigma} \prod_{\langle ij \rangle \in p} \left[ 1 + \prod_{\langle ij \rangle \in \hat{v}} \sigma_{ij} \right] |\sigma\rangle\langle \sigma|,
\]

with \( \hat{v} = p \) as a vertex of the dual lattice, as shown in Fig. 1(b).

In order to study topological quantum phase transitions out of the topological phase, two different parallel fields are introduced into the toric code model

\[
H = H_{TC} - b_x \sum_{\langle ij \rangle} \sigma_{ij}^x - b_z \sum_{\langle ij \rangle} \sigma_{ij}^z. \tag{13}
\]

This generalized toric code model cannot be exactly solved, because the eigenvalues of \( A_v \) and \( B_p \) are no longer good quantum numbers. According to our general proposal, a good variational wavefunction can be expressed as

\[
|\Psi (h_x, a, h_z, b)\rangle = |\Psi_{x A} T_{x B} |\uparrow\rangle^{\otimes L},
\]

\[
T_{x A} = \prod_{\langle ij \rangle} (1 + h_x \sigma_{ij}^x) \prod_v (1 + a A_v), \quad T_{x B} = \prod_{\langle ij \rangle} (1 + h_z \sigma_{ij}^z) \prod_p (1 + b B_p), \tag{14}
\]

with the parameters \( h_x, h_z, a, b \in [0,1] \). When \( a = 0, b = 1 \), this wavefunction is reduced to the deformed wavefunction[16], whose norm can be mapped into the partition function of the 2D classical Ashkin-Teller model[17]. When \( h_z = 0 \), this variational wavefunction has been previously used to consider the topological phase transitions of the toric code phase[20].

To represent the general variational wavefunction as the tensor networks, the off-diagonal and diagonal deformation operators are written as PEPOs

\[
T_{x A} \propto \sum_{s \sigma} \exp \left[ J_A \sum_i s_i + J_x \sum_{\langle ij \rangle} s_i s_j \sigma_{ij} \sigma_{ij} \right] |\sigma\rangle\langle \sigma|,
\]

\[
T_{x B} \propto \sum_{\sigma} \exp \left[ J_x \sum_{\langle ij \rangle} \sigma_{ij} + J_B \sum_{\langle ij \rangle} \prod_{\langle kl \rangle \in p} \bar{\sigma}_{ij} \right] |\sigma\rangle\langle \sigma|.
\]

where \( 2J_A = -\log a, J_x = \tanh^{-1} h_z, 2J_x = -\log h_x, J_B = \tanh^{-1} b \). Then \( T = T_{x A} T_{x B} \) is a triple-line PEPO as displayed in Fig. 1(c)

\[
\mathbb{T} \propto \sum_{s \sigma \bar{\sigma}} \exp \left( J_A \sum_i s_i + J_x \sum_{\langle ij \rangle} s_i s_j \sigma_{ij} \right. \left. + J_z \sum_{\langle ij \rangle} \sigma_{ij} + J_B \sum_{\langle ij \rangle} \prod_{\langle kl \rangle \in p} \bar{\sigma}_{ij} \right) |\sigma\rangle\langle \bar{\sigma}|. \tag{15}
\]
Acting $T$ on the reference state $|+\rangle^\otimes L$ gives rise to the triple-line PEPS $|\tilde{\Psi}(h_x,a,h_z,b)\rangle$, displayed in Fig. 1(d).

With the operator $T$, the corresponding TFDM state can be expressed as

$$|\tilde{\Psi}(h_x,a,h_z,b)\rangle = \sum_\sigma T|\sigma\rangle_F \otimes |\sigma\rangle_F.$$  

(16)

Then a reduced density matrix can be obtained by tracing out the degrees of freedom of the fictitious space:

$$\rho = \text{tr}_F |\tilde{\Psi}(h_x,a,h_z,b)\rangle \langle\tilde{\Psi}(h_x,a,h_z,b)| \equiv TT^\dagger.$$  

(17)

Actually $T_{x,A}$ can be regarded as a similar transformation, so we can further simplified the reduced density operator as

$$\rho \sim T(J_A, J_x, J_z, J_B).$$  

(18)

with the modified parameters

$$J_A = \frac{1}{2} \log \frac{1 + a^2}{2a}, \quad J_x = 2 \tanh^{-1} h_z,$$

$$J_z = \frac{1}{2} \log \frac{1 + h_x^2}{2h_x}, \quad J_B = 2 \tanh^{-1} b.$$  

According to the general framework, the partition function of a 3D classical model can be constructed from the Rényi entropy:

$$Z_N = \text{tr}_R \rho^N \propto \text{tr}_{T^N} (J_A, J_x, J_z, J_B).$$  

(19)

By ignoring the unimportant coefficients, the explicit form of the partition function can be written as

$$Z_N = \sum_{\sigma^{[1]}, \sigma^{[2]}, \ldots, \sigma^{[N]}_{x=1}} \prod_{ij} \left[ \tilde{J}_A \sum_i \sigma_i^{[r+\frac{1}{2}]} + \tilde{J}_z \sum_{(ij)} \sigma_{ij}^{[r]} + \tilde{J}_x \sum_{(ij)} \sigma_{ij}^{[r+\frac{1}{2}]} + \tilde{J}_B \sum_{(ij)\in p} \prod_{(ij)\in p} \sigma_{ij}^{[r+1]} \right],$$

where we have substituted the labels $\sigma_{ij}^{[r]}, \sigma_{ij}^{[r+\frac{1}{2}], i_{ij}^{[r+\frac{1}{2}]}}$ for the labels $\sigma_{ij}, \sigma_{ij}, s_{ij}$. The partition function $Z_N$ is defined in the 3D Euclidean spacetime in the large $N$ limit, the entanglement structure between different layers is displayed in Fig. 2

When the isotropic inter-layer and intra-layer interactions are required, we have to restrict the variational parameters as

$$\tilde{J}_A = \tilde{J}_z = 2 \tanh^{-1} h_z \equiv K,$$

$$\tilde{J}_x = \tilde{J}_B = \frac{1}{2} \log \frac{1 + h_x^2}{2h_x} \equiv K_p,$$

and the number of the varying parameters are reduced. Then the obtained partition function can be simplified as

$$Z_N = \sum_{\sigma} \exp \left[ K \sum_{(ij)} \sigma_{ij} + K_p \sum_{(ij)\in p} \prod_{(ij)\in p} \sigma_{ij} \right].$$  

(20)

and a 3D Ising type of phase transition occurs at a critical value of $K_p$. On the other hand, along the $h_z$ axis, $K_p = \frac{1}{2} \log \frac{1 + h_x^2}{2h_x}$ is extremely large and the corresponding partition function can be written

$$Z_N = \sum_{\sigma} \prod_{p} \left( 1 + \prod_{(ij)\in p} \sigma_{ij} \right) \exp \left[ K \sum_{(ij)} \sigma_{ij} \right].$$  

(21)

When new spin variables $\mu_i$ are introduced on the cubic lattice sites $i$, the spin variables $\sigma_{ij}$ on the bond between the sites $i$ and $j$ can be represented by the new variables $[3]:$ $\sigma_{ij} = \mu_i \mu_j,$ and the partition function of a 3D Ising model is thus obtained

$$Z_N = \sum_{\mu} \exp \left[ K \sum_{(ij)} \mu_i \mu_j \right],$$  

(22)

which is a 3D Ising spin model on a cubic lattice. There is a ferromagnetic-paramagnetic phase transition at a critical value of $K$. 

FIG. 2: The entanglement between two neighbouring layers in a three-dimensional tensor network structure.
Moreover, when $h_x = h_z$, $K$ and $K_p$ satisfies the self-dual condition of the Ising gauge-Higgs model\[33]\: $2K = -\log \tanh K_p$, $2K_p = -\log \tanh K$. In Fig. 3 (b), we displays the phase diagram of this 3D classical model derived from the numerical Monte Carlo calculations\[25, 27, 34\], and the similar phase diagram has been also obtained from higher-order perturbation expansion\[24\]. Actually the phase diagram is symmetric about the self-dual line $h_x = h_z$, and the continuous phase transition between the toric code phase and Higgs (confining) belongs to the 3D Ising universality class. There is a first-order transition line along the self-dual line, but it ends at a critical point. In addition, the three transition lines just meet at a tri-critical point.

**Conclusion and Outlook.** -We have generalized the framework of RK wavefunctions using the TFD states. Compared with the RK wavefunctions, the TFD states contain the information of both equal and unequal time correlation functions. The partition function describing general quantum phase transitions can be extracted from the Rényi entropy of the TFD state ansatz and it is further interpreted as a 3D classical model by using the PEPS representation of the TFD state. These ideas are illustrated by mapping the general deformed toric code wavefunction into the 3D classical $\mathbb{Z}_2$ gauge-Higgs model. Moreover, our framework might be useful for studying the thermodynamical properties of quantum critical points. We notice the PEPS method has been used to numerically study generic quantum critical points\[35, 36\], which is beyond the RK type wavefunction with non-generic conformal quantum critical points\[19\]. The static critical exponents have been accurately extracted with the finite correlation scaling method\[37\]. However, the information of dynamical exponents is not included in the PEPS. This might be improved by taking the TFD states into consideration.

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