Letter

Advancing hybrid quantum-classical algorithms via mean operators

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Hybrid quantum-classical algorithms have been suggested to control the quantum entanglement of many-body systems in noisy intermediate-scale quantum technology, and yet their applicability is limited by the numbers of qubits and quantum operations. Here, we propose a mean-operator theory which overcomes limitations by combining the advantages of hybrid algorithms and standard mean-field theory. We demonstrate that an introduction of a mean operator prepares an entangled target many-body state with a significantly reduced number of quantum operations. We also show that a class of mean operators is expressed as time-evolution operators, which indicates that our theory is directly applicable to quantum simulations with Rydberg atoms and trapped ions.

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Introduction. Remarkable quantum entanglement phenomena have been uncovered by experimental advances in quantum science and technology. Systems with about 50 qubits have been manipulated, and quantum entanglement has achieved computational tasks well beyond classical computations known as quantum supremacy [1,2]. Recently, enormously entangled many-body states such as topologically ordered states have been realized in a 31-qubit superconducting quantum processor [3] and a 219-atom programmable quantum simulator of Rydberg atom arrays [4]. Signatures of fractionalized particles also have been reported in systems with about an Avogadro number of electrons [5–8], which manifests a massive entanglement of many-body systems.

Theoretical efforts also have been made to utilize quantum entanglement, and variational hybrid quantum-classical algorithms such as the quantum-approximate-optimization algorithm (QAOA) have been proposed [9,10]. The main idea is to employ classical computations to complement expensive quantum operations and design a variational circuit to prepare a target quantum state. The applicability of the algorithm has already been demonstrated in trapped-ion experiments [11–13]. However, the numbers of qubits and quantum operations are seriously limited in noisy intermediate-scale quantum (NISQ) technology. Recent theoretical works even found a fundamental limitation of QAOA where a deep circuit proportional to the system size is necessary to achieve a nontrivial quantum state [14,15]. Thus, a theory which reduces the number of quantum operations and applies to a system with an arbitrary number of qubits is in great demand.

In this Letter, we provide a variational theory which overcomes the limitations by combining the advantages of hybrid algorithms and standard mean-field theory (MFT), referred to as the mean-operator theory (MOT). Our main strategy is to allow an operator with a judicious guess, called a mean operator, to capture the essential characteristics of an entangled many-body state such as symmetry properties and entanglement patterns. Then, the conventional QAOA is performed to refine a variational state quantitatively as illustrated in Fig. 1. The mean operator plays a similar role of a mean-field order parameter in standard MFT. To find an explicit form of a mean operator, it is particularly useful to employ intuitions from quantum many-body states in condensed matter such as symmetry and entanglement properties.

We demonstrate that our theory significantly reduces the number of quantum operations to prepare target states and is even applicable to spatial dimensions higher than two. Furthermore, a class of mean operators may be realized as time-evolution operators because they are chosen to be unitary operators, and thus our theory may be directly applicable to experiments of near-term quantum simulations including Rydberg atoms and trapped ions. Our theory may also serve as a theoretical tool to investigate general quantum many-body problems outperforming conventional mean-field type methods.

Mean-operator theory. The MOT adopts the variational method of quantum mechanics and an ansatz state of a system with a symmetry group $\mathbb{G}$,

$$|\Psi;\{\alpha,\beta\}_p,\{\phi\}\rangle = \hat{S}(\{\alpha,\beta\}_p)\cdot\hat{M}(\{\phi\})\cdot\prod_j|+\rangle_j, \quad (1)$$

consists of three main objects: (1) $\hat{M}(\{\phi\})$ is the mean operator with a set of parameters $\{\phi\}$, which is nontrivial under $\mathbb{G}$ for a generic ϕ; (2) $\hat{S}(\{\alpha,\beta\}_p)$ is the symmetric operator with a set of parameters $\{\alpha,\beta\}_p$, which is trivial under $\mathbb{G}$; and (3) $\prod_j|+\rangle_j$ is the symmetric product state with a site index j, where $|+\rangle_j$ is trivial under $\mathbb{G}$.

Here, p is an integer determining the complexity and accuracy of the ansatz and is referred to as the depth level

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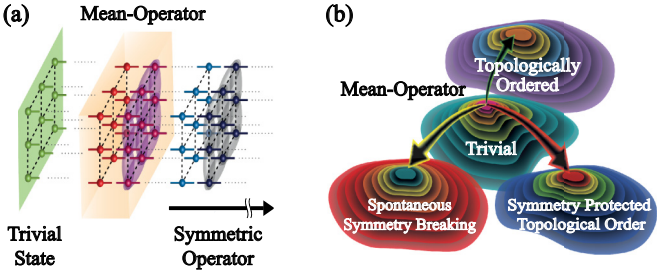

FIG. 1. (a) Construction of a variational state by an acting mean operator and symmetric operator on a trivial state. (b) The mean operators directly access nontrivial phases such as symmetry-breaking, and symmetry-protected topological and/or topologically ordered phases. The symmetric operator increases quantum entanglement, and its action is analogous to a standard hybrid quantum-classical algorithm such as QAOA.

of MOT. In this Letter, we assume translational symmetry and that the representation of $\mathbb{G}$ is decomposed into the on-site unitary. By minimizing the energy expectation value of a Hamiltonian H, $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$, a better approximated ground state is obtained with more parameters. Thus, our tasks boil down to evaluating the ground state energies with constructed $|\Psi;\{\alpha,\beta\}_p,\{\phi\}\rangle$ where the canonical tensor network representation [16] is extensively utilized for numerical evaluations [see Supplemental Material (SM) [17] for details].

A symmetric operator $\hat{S}(\{\alpha,\beta\}_p)$ employs hybrid quantum-classical algorithms such as QAOA [10] and refines a variational state quantitatively. As usual, the total Hamiltonian is decomposed as $H=H_1+H_2$, where H_1 and H_2 do not commute each other, and the symmetric operator may be written as $\hat{S}(\{\alpha,\beta\}_p)=\prod_{a=1}^{p}e^{-i\alpha_a H_1}e^{-i\beta_a H_2}$ with parameters (α_a,β_a) with a certain depth p. By construction, H_1 and H_2 are symmetric under $\mathbb{G}$.

A mean operator $\hat{M}(\{\phi\})$ significantly reduces the number of quantum operations to access nontrivial states, including topological or symmetry-broken states. The nontrivial property under $\mathbb{G}$ allows us to explore a much wider region in the Hilbert space effectively than the standard QAOA. In particular, there exists a special subset of $\{\phi_s\}$ which makes the variational state $\hat{M}(\{\phi_s\})\prod_j|+\rangle_j$ both entangled and symmetric. It is obvious that the state is hard to be constructed by using the conventional QAOA. In what follows, we apply our MOT to three different cases. The MOT has similarities to mean-field theory in statistical mechanics in the sense that we choose a variational ansatz. While real variables are chosen for a mean-field theory in statistical mechanics, we choose quantum operators for our MOT. We note that some recent works also employ the idea of mean-field theory to quantum simulation [18].

Case 1: Spontaneously symmetry-broken state. Let us first consider spontaneous symmetry breaking. To be specific, we consider the transverse-field Ising model [19,20] with a dimensionless coupling constant g,

$$H_1(g)=-(1-g)\sum_{\langle i,j\rangle}Z_iZ_j-g\sum_j X_j, \tag{2}$$

where Pauli matrices X_j, Y_j, Z_j at site j on a hypercubic lattice are used. For the sake of simplicity, we employ the Hartree unit ($\hbar=1$) unless indicated otherwise. The Hamiltonian enjoys $\mathbb{Z}_2$ symmetry with $\{I,\prod_j X_j\}$. The identity operator I is introduced, and the symmetric product state $\prod_j|+\rangle_j$ with $X_j|+\rangle_j=|+\rangle_j$ is the ground state of $H_1(\infty)$.

The conventional MFT starts by introducing a mean-field Hamiltonian,

$$\begin{aligned}H_{1,\mathrm{MF}}(g)&=\sum_j -2d(1-g)mZ_j-gX_j+d(1-g)m^2\\&=\sum_j[f_1(g,d,m)e^{-i\phi Y_j}X_je^{+i\phi Y_j}+f_2(g,d,m)],\end{aligned}$$

where $f_1(g,d,m)=-\sqrt{g^2+4(1-g)^2d^2m^2}$, $f_2(g,d,m)=d(1-g)m^2$. The order parameter and energy density are $m(\phi)=\langle G_{\mathrm{MF}}|Z_j|G_{\mathrm{MF}}\rangle$ and $\varepsilon(\phi)\equiv\langle G_{\mathrm{MF}}|H|G_{\mathrm{MF}}\rangle/N$ with a total site number N. Solving the MF Hamiltonian, its ground state $|G_{\mathrm{MF}}\rangle$ is

$$|G_{\mathrm{MF}}\rangle=e^{-i\phi_0\sum_j Y_j}\prod_j|+\rangle_j,\quad \tan(2\phi_0)=\frac{2(1-g)dm}{g}.$$

Minimizing the energy density determines the order parameter, $m^{(0)}=\pm\sqrt{1-\frac{g^2}{4(1-g)^2d^2}}$, in spatial dimension d, which gives a critical coupling constant, $g_c^{(0)}=\frac{2d}{1+2d}$. The MFT results can be connected to MOT by choosing the operators

$$\hat{M}(\phi)=e^{-i\phi\sum_j Y_j},\quad \hat{S}=I,$$

which manifest the equivalence between MFT and the depth-zero ($p=0$) MOT. Hence, we consider the operators

$$\begin{aligned}\hat{M}_1(\phi)&=e^{-i\sum_j\phi Y_j},\\ \hat{S}_1(\{\alpha,\beta\}_p)&=\prod_{a=1}^{p}e^{-i\alpha_a\sum_j X_j}e^{-i\beta_a\sum_{\langle i,j\rangle}Z_iZ_j}.\end{aligned} \tag{3}$$

Applying $\hat{S}_1$ with a nonzero p, systematic improvements are achieved by employing the tensor network representation. The trivial product state $\prod_j|+\rangle_j$ can be recast as a bond dimension $D=1$ tensor network state regardless of the spatial dimension. Similarly, the tensor product of the local unitary gates, e.g., the mean operator $\hat{M}_1(\phi)=\prod_i e^{-i\phi Y_i}$, is also represented as a $D=1$ tensor network operator. On the other hand, the product of the two-site or multisite unitary gates requires a bond dimension larger than 1, which indicates the generation of quantum entanglement. Details on the computation of ε and m are provided in SM [17]. Figure 2 presents the order parameter obtained by MOT for $d=1$, 2, and 3, of which the critical points are significantly improved with the nonzero depth.

A few remarks are in order. First, the $p=0$ calculations are equivalent to the ones of the standard MFT. In other words, our MOT may be understood as a general extension of MFT, and its systematic improvement is achieved by introducing the symmetric operator. Second, the $p=0$ calculation does not capture any quantum entanglement because both the mean operator and the trivial state are of the product forms. We emphasize that the mechanism of the improvement in MOT is the entangled nature of the exchange interaction term in

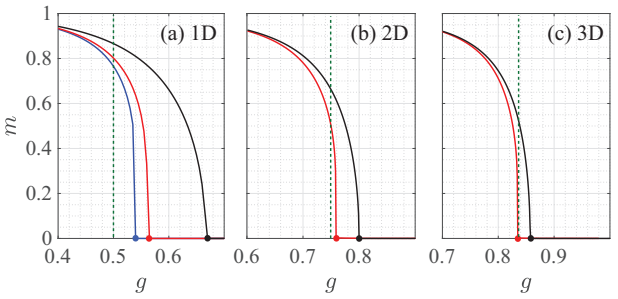

FIG. 2. Magnetization obtained by MOT in a (a) one-dimensional (1D), (b) two-dimensional (2D), and (c) three-dimensional (3D) transverse-field Ising model, $H_1(g)$. Here, the green dotted lines stand for the exact critical points, i.e., $g_c^{\text{exact}} = 0.5$, 0.7527, and 0.8376 in 1D, 2D, and 3D, respectively. The depth-two MOT in 1D finds $g_c^{(2)} \simeq 0.54$, and the depth-one MOT finds $g_c^{(1)} \simeq 0.759$ and $g_c^{(1)} \simeq 0.836$ for 2D and 3D, respectively.

$\hat{S}_1$. Third, our discussions may be easily generalized to a system with a larger group structure where MFT is well developed. Knowledge of the MFT may be used to choose a mean operator.

Case 2: Symmetry-protected topological state. Our MOT is applicable to topological states. One prime example is a symmetry-protected topological (SPT) ground state of the cluster model under a transverse magnetic field in one spatial dimension [20],

$$H_2(g) = -(1-g)\sum_{j=1}^{L-2} Z_j X_{j+1} Z_{j+2} - g\sum_{j=1}^{L} X_j. \tag{4}$$

The $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry with $\{I, \prod_e X_j, \prod_o X_j, \prod_{e,o} X_j\}$ exists, where the subscripts e and o for even and odd sites. A trivial product state is $\prod_j |+\rangle_j$ with $X_j|+\rangle_j = |+\rangle_j$, which is the ground state of $H_2(g=1)$.

We choose the operators,

$$\hat{M}_2(\phi_1, \phi_2) = e^{-i\phi_2 \sum_j Z_j Z_{j+1}} e^{-i\phi_1 \sum_j Z_j},$$

$$\hat{S}_2(\{\alpha, \beta\}_p) = \prod_{a=1}^{p} e^{-i\beta_a \sum_j Z_j X_{j+1} Z_{j+1}} e^{-i\alpha_a \sum_j X_j},$$

and the zero depth level ($p = 0$) calculation gives the ground state energy,

$$\varepsilon^{(0)}(\phi_1, \phi_2) = (1-g) C_{2\phi_1} S_{2\phi_2}^2 - g C_{2\phi_1} C_{2\phi_2}^2. \tag{5}$$

Minimizing the energy density, a quantum phase transition is obtained at $g_c^{(0)} = 1/2$, which is the same as the exact one [21]. The trivial product state with ($\phi_1 = \phi_2 = 0$) appears as the ground states in $1/2 < g < 1$, while an entangled state with ($\phi_1 = \pi/2, \phi_2 = \pm\pi/4$) optimizes the model below $g < 1/2$. We stress that the mean operator $\hat{M}_2(\phi_1, \phi_2)$ is *entangled* because it cannot be written as a product of local operators unless $\phi_2 = 0$. The higher-order term $Z_j Z_{j+1}$ is essential and becomes the source of anomalous symmetry action at the boundaries.

We present the entanglement spectra of our variational ground states with $p = 1$ in Fig. 3(a), where all levels exhibit fourfold degeneracy below the critical value $g_c \simeq 0.56$ while fourfold degeneracy disappears above g_c [22]. Note that the

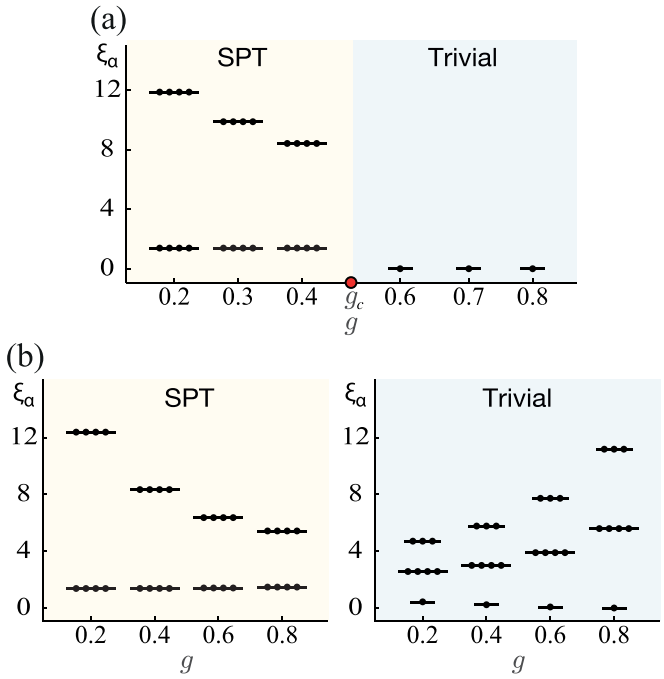

FIG. 3. (a) Entanglement spectrum, $\varepsilon_\alpha = e^{-\xi_\alpha}$, of $H_2(g)$ obtained by the depth-one MOT with four variational parameters. The topological phase transition at g_c is well captured by the number of degeneracy of the spectrum, where the fourfold degeneracy for $g < g_c$ is a characteristic of the SPT phase. (b) Entanglement spectra of the depth-two QAOA states with four variational parameters. The initial states are chosen to be the ground states of $H_2(g=0)$ (left) and $H_2(g=1)$ (right), respectively. Numerical calculations are performed with 20 qubits, and a periodic boundary condition is imposed.

number of variational parameters is four. The tensor network representations of $\hat{M}_2(\phi_1, \phi_2)$ and $\hat{S}_2(\{\alpha, \beta\}_p)$ are constructed and used to evaluate the ground state energy of $H_2(g)$.

To demonstrate the advantages of our MOT, we perform conventional QAOA calculations and illustrate their entanglement spectra in Fig. 3(b). To use four variational parameters, the conventional depth-two QAOA is performed with different initial states. In the left (right) figure, the ground state of $H_2(g)$ with $g = 0$ ($g = 1$) is chosen as the initial state, respectively. The absence of quantum phase transitions is manifest, indicating that the MOT outperforms the conventional QAOA.

Note that the mean operator breaks $\mathbb{G}$ for generic values of (ϕ_1, ϕ_2), but the one with $(\pi/2, \pi/4)$ produces a symmetric state. Therefore, the ground state with the mean operator becomes not only entangled but also symmetric under $\mathbb{G}$. This is equivalent to the well-known fact that a SPT state cannot be obtained by acting local symmetric transformations on a trivial state.

Case 3: Competition physics. One significant advantage of our MOT is the expressive power to describe both symmetry-broken and topological states, which allows us to access intriguing phenomena such as competition physics between spontaneously symmetry-broken and topological states.

As a proof of principle, we consider the Levin-Gu model [23] with a ferromagnetic exchange interaction term and a transverse-field term with two parameters (g, λ) on a

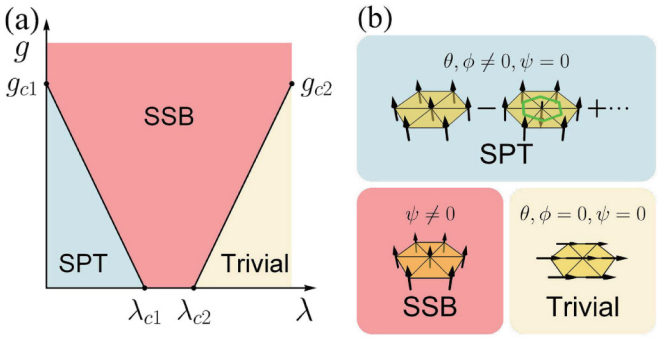

FIG. 4. Competition between symmetry-protected topological and spontaneously symmetry-broken (SSB) states. (a) The depth-zero MOT phase diagram of $H_3(\lambda, g)$. The critical values are $\lambda_{c1} = 0.4$, $\lambda_{c2} = 0.6$, $g_{c1} = g_{c2} = 1/6$. The trivial and SPT states are characterized by $(\theta, \phi, \psi) = (0, 0, 0)$, $(-\pi/8, \pi/24, 0)$, respectively, and the spontaneously symmetry-broken state is characterized by $\psi \neq 0$. (b) Illustration of the wave functions of the three states.

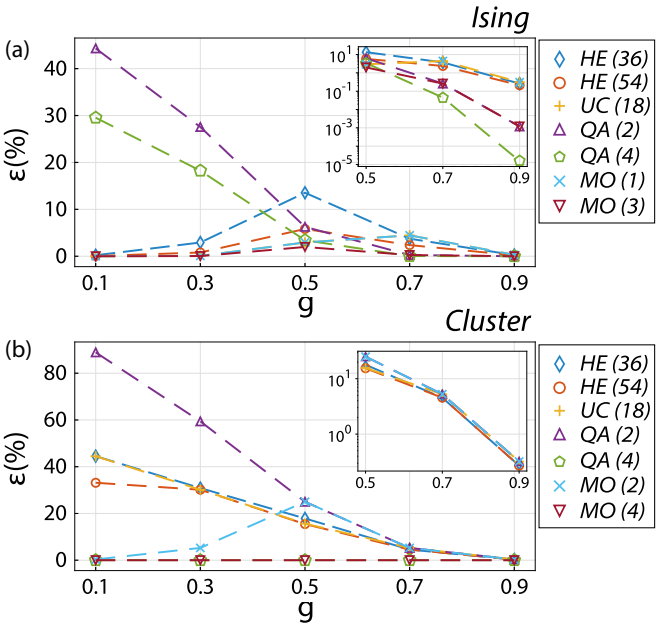

FIG. 5. Errors of the ground state energy with different ansatzes. (a) Transverse field Ising model with six qubits. (b) The cluster model with six qubits. The insets are results for g between 0.5 and 0.9, plotted on a log-linear scale. The insets do not display outcomes for QAOA with depth-2 and MOT with depth-1 for the cluster model, as they are capable of producing a precise ground state.

triangular lattice,

$$H_3(\lambda, g) = (1 - \lambda)H_{\mathrm{LG}} + gH_{\mathrm{ex}} + \lambda H_{\mathrm{PM}}. \tag{6}$$

The Levin-Gu Hamiltonian, trivial paramagnetic Hamiltonian, and the ferromagnetic exchange Hamiltonians are

$$H_{\mathrm{LG}} = -\sum_j B_j, \quad H_{\mathrm{ex}} = -\sum_{\langle jk \rangle} Z_j Z_k, \quad H_{\mathrm{PM}} = -\sum_j X_j,$$

with the dressed qubit term, $B_j = -X_j \prod_{\langle jkl \rangle} i^{(\frac{1-Z_k Z_l}{2})}$, where $\langle jkl \rangle$ are the three nearest-neighbor sites around the site j. The Hamiltonian enjoys $\mathbb{Z}_2$ symmetry, $\{I, \prod_j X_j\}$, and a trivial product state is $\prod_j |+\rangle_j$ with $X_j|+\rangle_j = |+\rangle_j$, which is the ground state of $H(\infty, g)$ for a finite g. Note that each term of the three Hamiltonians captures the physics of symmetry-protected topological, spontaneously symmetry-broken, and trivial states, respectively.

We choose the mean operator,

$$\hat{M}_3(\theta, \phi, \psi) = \prod_{\langle jkl \rangle} e^{-i\theta Z_j Z_k Z_l - i\phi(Z_j + Z_k + Z_l)} e^{-i\psi \sum_j Y_j}.$$

Each operator associated with the three parameters (θ, ϕ, ψ) breaks $\mathbb{Z}_2$ symmetry generically. The term with θ is made of three adjacent qubits, describing nontrivial entanglement between adjacent qubits. For simplicity, a symmetric operator is set to be the identity in this work. It is straightforward to increase the depth, which may be used in the properties of a refined many-body wave function. For example, one can show that the behaviors of the strange correlator [24] persist around the depth-zero calculations perturbatively.

Varying with (θ, ϕ, ψ), we find three different phases in the λ-g plane, as shown in Fig. 4. We stress that the spontaneously symmetry-broken state exists even without the exchange interaction ($g = 0$), and its region becomes larger with a bigger g. This clearly shows competition physics between symmetry-protected topological and spontaneously symmetry-broken states. It is an intriguing open question whether the spontaneously symmetry-broken state survives for calculations with a nonzero depth, which we leave for future work. Also, another scenario associated with a stripe order has been recently suggested [25], which may also be interesting to test in the future.

Our model has a nontrivial duality ($\lambda \leftrightarrow 1 - \lambda$), which makes the phase boundary symmetric in the λ-g plane (see SM [17]). The quantum phase transitions between spontaneously symmetry-broken and symmetry-protected topological states and the ones between spontaneously symmetry-broken and trivial states are continuous, and we argue that both of them are in the Ising universality class based on the duality. Though they are in the same universality class in the thermodynamic limit, it is interesting how their edge modes behave differently at the transitions.

Advantages of MOT. We stress two advantages of MOT. First, our MOT is more efficient in finding ground states than other protocols such as a hardware-efficient ansatz (HE), unitary coupled clustered ansatz (UC), and QAOA. To demonstrate the efficiency, we utilize the two canonical Hamiltonians, $H_1(g)$ and $H_2(g)$ with six qubits, and evaluate the error of the ground state energy value,

$$\varepsilon(g) \equiv \left| \frac{E_N(g) - E_G(g)}{E_G(g)} \right| \times 100, \tag{7}$$

where $E_G(g)$ is the exact eigenvalue from the exact diagonalization with six qubits and $E_N(g)$ is an estimated value of each numerical method. The number of free parameters for each method is specified by a number within parentheses. As shown in Fig. 5, it is clear that MOT calculations show the best energy estimation with small numbers of parameters for

all values of g. For the transverse-field Ising model, MOT with three parameters, MOT(3), outperforms a hardware-efficient ansatz with 54 parameters. Similarly, MOT(4) captures the exact ground state energy for the cluster model while UC(18) and HE(54) show larger errors. Thus, we argue that our MOT calculations are generically better than the other methods to find the minimum energy.

Second, the expressive power of the hybrid algorithm can be enhanced significantly by utilizing the mean operator. We investigate the probability of an overlap between random states and the MOT/QAOA ansatz and find that the quantum circuit can represent a much wider range of quantum states by inserting the mean operator (see SM [17]). Our result indicates that the MOT ansatz may have superior expressive power to other protocols.

Discussion. Our MOT overcomes the fundamental limitations of QAOA and enables us to prepare a target state with a shallow circuit. A mean operator captures the essential characteristics of the target state, and thus finding a mean operator is at the heart of MOT. Intuitions from condensed matter theory such as symmetry and entanglement properties can be particularly useful, as shown in the above cases where the nontrivial property under a given symmetry and the degree of entanglement of an operator are two important factors. An investigation of a class of mean operators may provide an alternative way to classify quantum many-body states.

Our MOT is applicable to near-term quantum simulations. Hybrid algorithms have already been demonstrated in one-dimensional trapped-ion problems [13], and their possibilities in a few qubits have been proposed [14,26]. Since our MOT is a natural extension of a hybrid algorithm, we believe that applications of MOT are plausible and powerful, especially in 2D and 3D. A realization of a mean operator may be a key step to simulate an entangled many-body state in a shallow quantum circuit.

We anticipate that our MOT can be extended and applied in a variety of ways. For instance, one can introduce the spatial fluctuations of the mean operator that may provide insight into quantum field theories. Furthermore, a mean operator may be extended to be nonunitary, and then the MOT can access topologically ordered states, similar to the recent realization of a toric code state [3] (see also SM [17]). Our MOT may be implemented for studying exotic interacting systems, including fractons [27] and non-Fermi-liquid states, which we leave for future work.

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