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Variational Quantum Eigensolver with Mutual Variance-Hamiltonian Optimization

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The zero-energy variance principle can be exploited in variational quantum eigensolvers for solving general eigenstates but its capacity for obtaining a specified eigenstate, such as ground state, is limited as all eigenstates are of zero energy variance. We propose a variance-based variational quantum eigensolver for solving the ground state by searching in an enlarged space of wavefunction and Hamiltonian. With a mutual variance-Hamiltonian optimization procedure, the Hamiltonian is iteratively updated to guild the state towards to the ground state of the target Hamiltonian by minimizing the energy variance in each iteration. We demonstrate the performance and properties of the algorithm with numeral simulations. Our work suggests an avenue for utilizing guided Hamiltonian in hybrid quantum-classical algorithms.

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Quantum computing provides a promising avenue for simulating quantum systems,[1–8] in which solving eigenstates is a basic task for many applications. Among those quantum eigensolvers,[9–20] variational quantum eigensolver (VQE) has received intensive studies in recent years,[12–17,19,20] as it is suitable for implementing on near-term intermediate-scale quantum computers.[21] This is because VQE can leverage up the power of parameterized quantum circuit to represent an exponentially large wave function on quantum processors, where the parameters can be obtained by hybrid quantum-classical optimization.

The variational quantum eigensolver is built on the variational principle and it is important to set a cost function, by minimizing which the target eigenstate can be found through hybrid quantum-classical optimization. Conventionally, VQE uses the energy as a cost function.[12] As the variational energy is bounded below by the ground-state energy, VQE based on minimizing the energy can be used for solving the ground state problem. To solve excited states, the cost function can be modified as a linear combination of energies of orthogonal states as for the subspace-search VQE,[19] or with a penalty term such that enforcing an excited state has a lowest cost.[20]

Alternatively, one may use the energy variance as the cost function, which is bounded below by zero.[22–24] As an eigenstate always has zero energy variance, VQE based on minimizing the variance can be used for solving an arbitrary eigenstate.[23,24] Nevertheless, it fails to tell us different eigenstates apart and consequently it is hard to solve a specified eigenstate,[24] such as ground state or low-lying excited states that are interested for many applications.

In this Letter, we aim to solve the ground state of quantum systems with the variance-based variational quantum eigensolver. We construct a cost function in which both the wavefunction and the Hamiltonian are parameterized. By a mutual variance-Hamiltonian optimization, the Hamiltonian will flow from an initial Hamiltonian to the target Hamiltonian. Consequently, the initial state will be evolved into the ground state of the target Hamiltonian. The performance and properties of the algorithm are investigated with numeral simulations. Beyond enriching a family of variance-based VQE, our work also shows the potential of exploiting a space of Hamiltonian for solving a given Hamiltonian by quantum computing.

Variational Quantum Eigensolver. To start, let us consider a Hamiltonian $H = \sum_{i=1}^{N} c_i L_i$, where each L_i is a product of Pauli operators. By introducing $\boldsymbol{c} = (c_1, c_2, \ldots, c_N)^{\mathrm{T}}$ and $\boldsymbol{L} = (L_1, L_2, \ldots, L_N)^{\mathrm{T}}$, the Hamiltonian can be written as $H = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{L}$. To solve an eigenstate of H variationally on a quantum computer, one shall parameterize the eigenstate with an ansatz $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|\psi_0\rangle$, where $U(\boldsymbol{\theta})$ is a parameterized unitary operator and $|\psi_0\rangle$ is a reference state.

The traditional VQE algorithm finds $\boldsymbol{\theta}$ by minimizing the variational energy,[12] $\mathcal{E}(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$. We call it energy VQE. As the variational energy is bounded below by the ground-state energy, energy VQE is suitable for solving the ground state. Alternatively, one can use the energy variance as a cost function of VQE,[24] which we call it the variance VQE. The variational energy variance is defined as

$$\Delta(\boldsymbol{\theta}) \equiv \langle H^2\rangle_{\boldsymbol{\theta}} - \langle H\rangle_{\boldsymbol{\theta}}^2 \geq 0, \tag{1}$$

where $\langle *\rangle_{\boldsymbol{\theta}} = \langle\psi(\boldsymbol{\theta})| * |\psi(\boldsymbol{\theta})\rangle$. It is convenient to introduce a covariance matrix defined as[25–27] $\mathcal{G}_{ij}(\boldsymbol{\theta}) = \langle L_i L_j\rangle_{\boldsymbol{\theta}} - \langle L_i\rangle_{\boldsymbol{\theta}}\langle L_j\rangle_{\boldsymbol{\theta}}$. The energy variance can then be expressed as $\Delta(\boldsymbol{\theta}) = \boldsymbol{c}^{\mathrm{T}}\mathcal{G}(\boldsymbol{\theta})\boldsymbol{c}$.

By minimizing $\Delta(\boldsymbol{\theta})$, one can find some eigenstates for

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H. Notably, variance VQE can self-verify an eigenstate by checking the energy variance to be zero.[28] However, the issue of variance VQE is that it cannot guarantee a solution of a specified eigenstate,[24] such as the ground state or low-lying excited states interested for physics, as all eigenstates have zero energy variance.

Hamiltonian-Guided Variance VQE (HG-VVQE). How to exploit the properties of variance to find the ground state of the Hamiltonian? It is inspiring to recall the quantum adiabatic algorithm (QAA)[29] and its variational version.[30,31] In order to solve the ground state of the target Hamiltonian H, the QAA first constructs a simple initial Hamiltonian H_0 whose ground state is easy to prepare. Subsequently, an adiabatic evolution path from H_0 to H is designed such that the initial state will be evolved into the ground state of H. Moreover, the energy VQE can be incorporated to accelerate QAA by minimizing the energy of intermediate Hamiltonian in the evolution path, enforcing that the ground state is always maintained until the target Hamiltonian.

Similarly, we may construct a variance VQE guided with a sequence of Hamiltonian which is tuned towards to the target Hamiltonian. An essential difference from the variational QAA is that the evolution path of Hamiltonian does not require to be given beforehand. Instead, one can parameterize the Hamiltonian as $H(\boldsymbol{c}') = \boldsymbol{c}'^{\mathrm{T}} L$ and the flow of $\boldsymbol{c}'$ to $\boldsymbol{c}$ of the Hamiltonian will be determined in the optimization process. For this reason we construct the cost function

$$\mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta}) = \boldsymbol{c}'^{\mathrm{T}} \mathcal{G}(\boldsymbol{\theta}) \boldsymbol{c}' + \lambda |\boldsymbol{c} - \boldsymbol{c}'|^2. \tag{2}$$

The first term measures the energy variance and the second term characterizes a distance between the parameterized Hamiltonian $H(\boldsymbol{c}')$ and the target Hamiltonian $H(\boldsymbol{c})$. The hyperparameter λ adjusts the ratio between two terms. The cost function $\mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta})$ involves an enlarged space of both wavefunction and Hamiltonian, and it is minimized to zero for an eigenstate of the Hamiltonian $H(\boldsymbol{c})$.

Mutual Variance-Hamiltonian Optimization. Minimization of $\mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta})$ in general can not promise a solution of ground state of $H(\boldsymbol{c})$. To reach for a ground state, one can refer to an optimization process in a wavefunction–Hamiltonian space.[32] A scheme of such optimization, termed as variance-Hamiltonian optimization, is described in the algorithmic chart 1 given in Table 1 and is illustrated in Fig. 1.

Table 1. Algorithmic chart 1.

Algorithm 1 variance-Hamiltonian optimization
Require: $\psi(\boldsymbol{\theta}_0)$, $\boldsymbol{c}'_0$
Ensure: $\psi(\boldsymbol{\theta}_i)$
function VHO ($\psi(\boldsymbol{\theta}_0)$, $\boldsymbol{c}'_0$)
repeat
$\boldsymbol{c}'_i = \mathrm{argmin}_{\boldsymbol{c}'}\ \mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta}_{i-1})$
$\boldsymbol{\theta}_i = \mathrm{argmin}_{\boldsymbol{\theta}}\ \mathcal{C}(\boldsymbol{c}'_{i-1}, \boldsymbol{\theta})$
until $\boldsymbol{c}'_i = \boldsymbol{c}$
end function

Initially, the Hamiltonian is parameterized with $\boldsymbol{c}'_0$ whose ground state can be easily prepared. To fit for the VQE framework, the ground state can be generated by a variational quantum circuit with specified parameter.

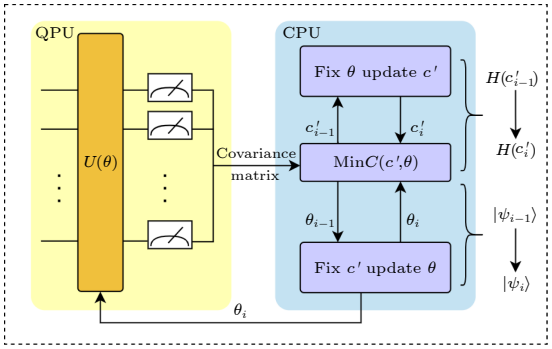

Fig. 1. Illustration of the HG-VVQE algorithm with a mutual variance-Hamiltonian optimization, where the parameter of wavefunction $\boldsymbol{\theta}$ and parameter of Hamiltonian $\boldsymbol{c}'$ are alternatively updated.

The optimization process alternatively updates the Hamiltonian and the wavefunction, which corresponds to updating the parameters $\boldsymbol{c}'$ and $\boldsymbol{\theta}$, respectively. (1) In the Hamiltonian-updating stage where $\boldsymbol{\theta}$ is fixed, the cost function is a quadratic function of $\boldsymbol{c}'$, which can be minimized with the least-square method. (2) In the wavefunction-searching stage where $\boldsymbol{c}'$ is fixed, only the variance term in the cost function depends on $\boldsymbol{\theta}$ and the task is reduced to variance VQE for the Hamiltonian $H(\boldsymbol{c}')$. Minimization of variance can be performed using the gradient descent method,[14,33]

$$\boldsymbol{\theta}_i = \boldsymbol{\theta}_{i-1} - \eta \frac{\partial \mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta}_{i-1})}{\partial \boldsymbol{\theta}} = \boldsymbol{\theta}_{i-1} - \eta \boldsymbol{c}'^{\mathrm{T}} \frac{\partial \mathcal{G}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \boldsymbol{c}',$$

with η representing the step size. Here, gradient of each element of the covariant matrix $\mathcal{G}(\boldsymbol{\theta})$ should be evaluated exactly with the shift rule[34,35] or approximately using a differential scheme. It is known that gradient-based optimization for variational quantum algorithm may meet the barren plateau problem.[36] For HG-VVQE, we find the same issue of barren plateau with the ansatz in Eq. (4) (see the Supplementary Material,[37] which includes Refs. [38,39]).

It is stressed that the presence of the second term in $\mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta})$ guarantees a flow of Hamiltonian towards $H(\boldsymbol{c})$. Moreover, the hyperparameter λ can adjust the evolution speed of the Hamiltonian as an analog of QAA. For $\lambda \to 0$, the evolution speed is very small, reminding of the adiabatic limit. This benefits to a solution of the ground state but the algorithm can be slow. In practice, a proper choice of λ is necessary. In addition, the optimization of variance for each intermediate Hamiltonian $H(\boldsymbol{c}')$ can be terminated once the variance is smaller than a given threshold, which will be investigated later.

Model Hamiltonian and Ansatz. For the demonstration, we take a fully connected transverse-field Ising model as a model Hamiltonian. Since the HG-VVQE is closely related to the adiabatic quantum algorithm in the spirit that it evolves easy-prepared ground state of an initial Hamiltonian gradually to the ground state of the target Hamiltonian, it is expected that HG-VVQE can be applied to general Hamiltonian, once one can start with an initial Hamiltonian with easily prepared ground state. The

Hamiltonian of N qubits is described as follows:

$$H(\boldsymbol{c}) = -\sum_{i\neq j} g_{ij} Z_i Z_j - \sum_i h_i X_i. \tag{3}$$

Without loss of generality, the coefficients h_i are positive. The initial Hamiltonian for HG-VVQE can be chosen as $H_0 = -\sum_i h_i X_i$ and its ground state is $|\psi_0\rangle = |+\rangle^{\otimes N}$.

The wavefunction ansatz $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|\psi_0\rangle$ is constructed such that the parameterized unitary operator $U(\boldsymbol{\theta} = 0)$ becomes an identity. A choice of such $U(\boldsymbol{\theta})$ can be given in the following (also see Ref. [40]). The parameterized quantum circuit involves p blocks, each block including one layer single-qubit rotations and one layer two-qubit rotations (with a parameter set $\boldsymbol{\theta} = (\alpha, \beta)$),

$$U(\boldsymbol{\theta}) = \prod_{l=1}^{p} e^{-iH_x(\beta_l)} e^{-iH_{zz}(\alpha_l)}. \tag{4}$$

Here $H_x(\beta_l) = \sum_i \beta_{l,i} h_i X_i$ and $H_{zz}(\alpha_l) = \sum_{ij} \alpha_{l,i} g_{ij} Z_i Z_j$, with $\lambda_{l,i}$, $\zeta_{l,i}$, and $\alpha_{l,i}$ being the parameters at the l-th block. The ansatz is inspired from the Hamiltonian variational ansatz [41] but with more parameters and thus can be more expressive. We call it the multi-angle HVA. Though not universal, multi-angle HVA may suffice for investigating the ground state $H(\boldsymbol{c})$ as suggested by numeral simulations. Moreover, the expressivity increases with a larger p.

Numeral Simulation Results. The performance of HG-VVQE and its properties are demonstrated by numeral simulations on classical computers with an open-source package *Qibo*. [42] We use $N = 4$ for the model and $p = 3$ for the ansatz. The initial parameter of the wavefunction ansatz is set as 0.01 for all elements of $\boldsymbol{\theta}$. Both VVQE and HG-VVQE use the same multi-angle HVA for comparison. By numerical simulation, a comparison between the HG-VVQE and VVQE is presented in Fig. 2. As can be seen, the HG-VVQE can find the ground state of the Hamiltonian, where the VVQE obtains an excited state.

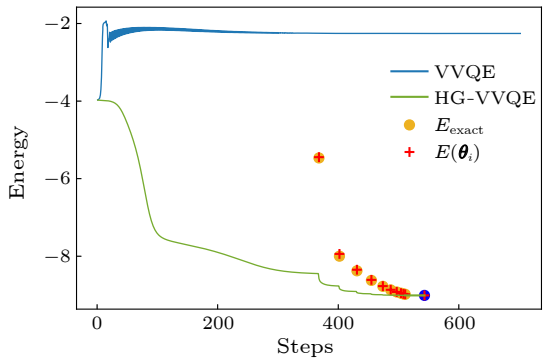

Fig. 2. Comparison of evolutions of energy in the process of optimization for the HG-VVQE and the VVQE. For intermediate Hamiltonian $H(\boldsymbol{c}')$, E_{exact} is the ground-state energy by exact diagonalization and $E(\boldsymbol{\theta}_i)$ is energy obtained by the wavefunction-searching process of HG-VVQE. The blue dot is the ground-state energy of $H(\boldsymbol{c})$.

The advantage of HG-VVQE over VVQE in solving the ground state can be understood in a language of landscape for the cost function $\mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta})$. For VVQE, the landscape of energy variance can have many global minimums of zero, which all correspond to eigenstates. With an initial parameter $\boldsymbol{\theta}_0$, it is difficult to find an optimization method that the ground state can be singled out from those global minimums. However, for HG-VVQE, one can connect the ground state of the target Hamiltonian with the ground state of an initial Hamiltonian in the landscape. The mutual variance-Hamiltonian optimization is designed to find such a connection path.

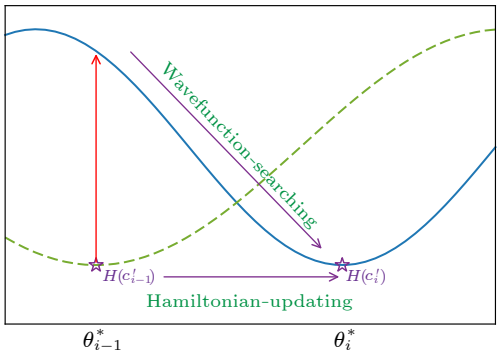

Fig. 3. Schematic diagram of landscape changes due to Hamiltonian-updating. The purple arrow marks a rising of the cost function after the Hamiltonian is updated.

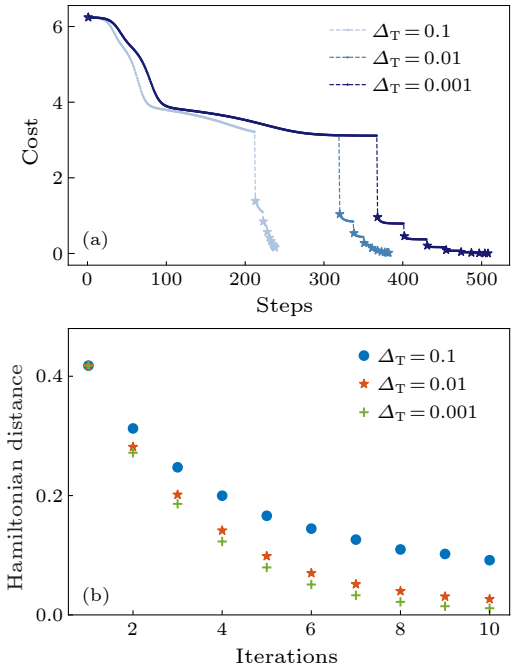

Fig. 4. Variance threshold Δ_T as the terminate criteria. (a) The trajectory of the cost function during the optimization process with different Δ_T. The asterisk marks the update of the Hamiltonian. (b) Optimization of HG-VVQE with different Δ_T. In all simulations, the hyperparameter $\lambda = 1$, and the gradient descent $\eta = 0.008$.

To explain how the desired ground state can be found, a picture of the optimization process is given in Fig. 3. The landscape of $\mathcal{C}(\boldsymbol{c}', \boldsymbol{\theta})$ can be cut into slices, and each slice is a landscape of variance at a fixed $\boldsymbol{c}'$. For a parameter $\boldsymbol{\theta}^*_{i-1}$ corresponding to the ground state of $H(\boldsymbol{c}'_{i-1})$, the slice is switched into the landscape of $H(\boldsymbol{c}'_i)$ when the Hamiltonian is updated to $H(\boldsymbol{c}'_i)$. Consequently, once the differ-

ence of Hamiltonian is small, $\boldsymbol{\theta}^*_{i-1}$ still stands in the same trap of landscape as $\boldsymbol{\theta}^*_i$, which corresponds to the ground state of $H(\boldsymbol{c}'_i)$. As a result, $\boldsymbol{\theta}^*_{i-1}$ will be optimized into $H(\boldsymbol{c}'_i)$ in the wavefunction-searching process. The above procedure is repeated until the slice ends at $\boldsymbol{c}$. It should be pointed out that the path of Hamiltonian-updating is obtained automatically in the optimization process rather than by design beforehand. Moreover, the path is related to the hyperparameter λ in the cost function and the termination criteria in the wavefunction-searching process, as will be revealed later.

Termination Criterion. In the wavefunction-searching stage, the variance should be minimized with regard to $\boldsymbol{\theta}$ by fixing $\boldsymbol{c}'$. However, it is unnecessary to minimize the variance to zero for the intermediate Hamiltonian which should be time-consuming. Instead, one can use a termination criterion, e.g., the optimization stops once the variance is smaller than a threshold. As the variance is bounded blow by zero, we can always choose a small value of threshold. This is unlike the situation of energy-VQE where the exact ground-state energy is unknown in prior.

We investigate how the convergence of the cost function and the flow of Hamiltonian are effected by the termination criterion. According to Fig. 4(b), under varied thresholds of variance, the speed of Hamiltonian flow tends to be faster for a small threshold. However, the wavefunction-searching stage will require more steps of gradient descents for a small threshold Δ_{T} [see Fig. 4(a)], which is not favorable since it is demanding for quantum resources. Rather, we can select a reasonable large threshold.

Role of Hyperparameter λ. As mentioned above, the hyperparameter λ accounts for the speed of Hamiltonian-updating which is important for reaching the ground state. It is expected that a large (smaller) λ leads to faster (slower) Hamiltonian-updating. Under varied λ, Fig. 5 shows a flow of $H(\boldsymbol{c}')$ to $H(\boldsymbol{c})$ characterized by the distance between Hamiltonian with the optimization iterations. As expected, the larger the λ is, the quicker the Hamiltonian flows to $H(\boldsymbol{c})$.

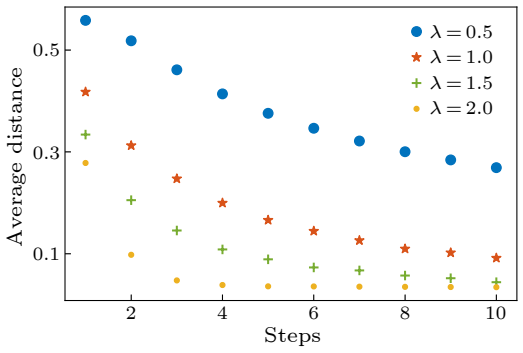

Fig. 5. Changes of Hamiltonian distances in the optimization under different hyperparameters λ.

We also compare the performances of HG-VVQE at different $\lambda = 0.5, 1.0, 1.5, 2.0$. As shown in Table 2, the required steps of optimization is reduced when increasing λ from 0.5 to 1.5, while the ground state is still reached. However, for $\lambda = 2$ an excited state is obtained. This suggests that a proper large λ should be chosen so that the goal of obtaining the ground state can be realized without loss of efficiency. On the other hand, one may exploit a larger λ for solving some low-lying excited states. The value of λ in the optimization process may also be adjusted. As the mechanism shall rely on properties of the landscape, we can leave it for further investigation.

Table 2. Parameter settings and numerical results under different hyperparameters λ.

λ	Step size	Step count	Cost function	Energy
0.5	0.006	1536	9.668×10^{-5}	−9.011
1.0	0.006	566	9.689×10^{-5}	−9.011
1.5	0.006	447	9.517×10^{-5}	−9.011
2.0	0.006	13658	9.996×10^{-5}	−2.256

In summary, we have proposed a variance-based variational quantum eigensolver for solving ground state of a quantum system. By the mutual variance-Hamiltonian optimization, an evolution path of Hamiltonian can be found, guided by which the initial state will flow to the ground state of the target Hamiltonian. We have demonstrated the algorithm with numeral simulations and have investigated its properties. Our work advocates an exploiting of a family of Hamiltonian for solving a given Hamiltonian on a quantum computer.

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Supplementary material for: Variational quantum eigensolver with mutual variance-Hamiltonian optimization

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The hybrid quantum-classical optimization for minimizing the cost function at the wavefunction-searching stage requires to calculate gradients of the energy variance. However, the optimization can be difficulty due to barren plateaus, which states that the gradients can vanish exponentially with the increasing of qubit number or circuit depth for general random circuits such as the hardware efficient ansatz [1]. The issue of barren plateaus is related both to the type of cost function [2] as well as the architecture of parameterized quantum circuits [3]. In this paper, we adopt energy variance instead of energy in the cost function. Moreover, the ansatz inspired by the Hamiltonian variational ansatz (HVA), called as multi-angle HVA, is designed specifically for solving the fully-connected Ising model. In this regard, it is necessary to explore whether the issue of barren plateaus still exist.

For this, we compare variances of gradients for cost function of both energy and energy variance under the multi-angle HVA (Fig. s1 (a)) and the hardware efficient ansatz (Fig. s1 (b)), respectively. The hardware efficient ansatz is universal, whose each block consisted two layers of one-qubit rotations and one layer two-qubit entangled gates. The gradients at larger size and deeper depth are calculated. A random sampling method is adopted to evaluate the variance of gradients, where one tenth of the total number of input parameters is randomly sampled each time and the sampling is repeated 20 times. As seen in Fig. s1, variances of gradients under both ansatzs and for both energy and energy variance decrease exponentially with the increasing of qubits. This indicates that the multi-angle HVA in our paper share the same issue of barren plateaus as the hardware efficient ansatz. To solve the barren plateaus problem, one should refer to more specific ansatz. In addition, it is observed in Fig. s1 (a) that the vanishing of gradients with the circuit depth is not obvious for both energy and energy variance, which indicates that the multi-angle HVA may reduce the vanishing of gradients for deep quantum circuit.

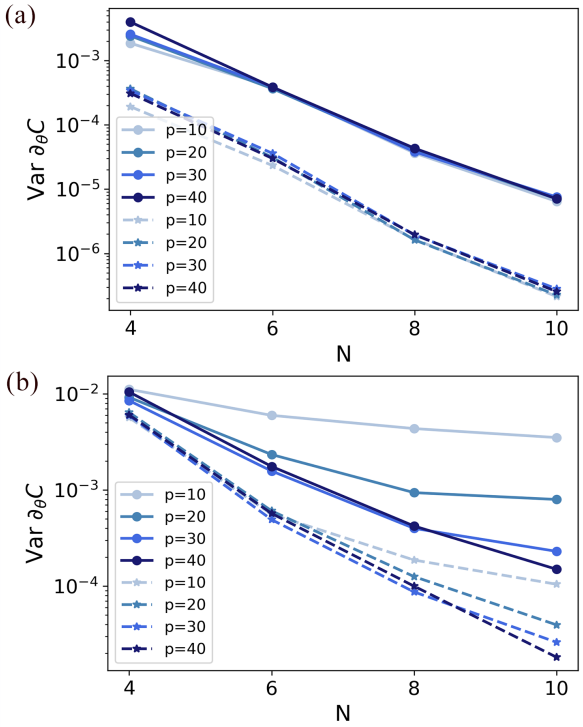

Fig. s1. Variance of gradients evaluated by random sampling for both VQE(solid line) and HG-VVQE(dashed line). The fully connected transverse-field Ising model is adopted. (a) The multi-angle Hamiltonian variational ansatz used in the paper. (b) Hardware efficient ansatz.

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