

A Neural-Guided Variational Quantum Algorithm for Efficient Sign Structure Learning in Hybrid Architectures

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ABSTRACT

Variational quantum algorithms hold great promise for unlocking the power of near-term quantum processors, yet they are frequently hindered by high measurement costs, barren plateaus, and challenging optimization landscapes. Here, we introduce sVQNHE, a neural-guided variational quantum algorithm that decouples amplitude and sign learning across classical and quantum modules, respectively. Our approach employs shallow quantum circuits composed of commuting diagonal gates to efficiently model quantum phase information, while a classical neural network learns the amplitude distribution and guides circuit optimization in a bidirectional feedback loop. This hybrid quantum-classical synergy not only reduces measurement costs but also achieves high expressivity with limited quantum resources and improves the convergence rate of the variational optimization. We demonstrate the advancements brought by sVQNHE through extensive numerical experiments (including realistic noisy simulations and sampling-based simulations). For the 6-qubit J1-J2 model — a prototypical system with a severe sign problem for Monte Carlo-based methods — it reduces the mean absolute error by 98.9% and suppresses variance by 99.6% relative to a baseline neural network, while requiring nearly 19x fewer optimization steps than a standard hardware-efficient VQE. Furthermore, for MaxCut problems on 45-vertex Erdős–Rényi graphs, sVQNHE improves solution quality by 19% and quantum resource efficiency by 85%. Importantly, this framework is designed to be scalable and robust against hardware noise and finite-sampling uncertainty, making it well-suited for both current NISQ processors and future high-quality quantum computers. Our results highlight a promising path forward for efficiently tackling complex many-body and combinatorial optimization problems by fully exploiting the synergy between classical and quantum resources in the NISQ era and beyond.

Introduction

Quantum computing promises transformative advances in a variety of applications, from combinatorial optimization to ground-state preparation and dynamical simulation of many-body systems^{1,2}. However, large-scale quantum circuits remain challenging to implement due to hardware limitations, gate errors, and limited qubit coherence³. One of the most urgent goals in the noisy intermediate-scale quantum (NISQ) era, and the subsequent early fault-tolerant era⁴ (Early FTQC), is to maximize computational utility within these constraints by employing shallow circuits and error-mitigated designs⁵.

Among the many strategies proposed to enable practical applications under these conditions, hybrid quantum–classical algorithms, particularly variational quantum algorithms (VQAs)^{6–8}, stand out. VQAs combine parameterized quantum circuits (PQC) with classical optimization routines, using quantum circuits as ansatzes to solve problems that can be formulated within a variational framework. Despite initial enthusiasm, standard VQAs face at least three critical challenges. First, optimization challenges, such as barren plateaus^{9–13}, where gradients vanish exponentially with circuit depth or system size, severely limit

trainability. Second, measurement costs scale poorly with both qubit count and circuit parameters, placing heavy demands on quantum resources. Third, even hardware-efficient circuit designs may require long depths to represent certain wavefunctions, but decoherence makes such computations unreliable in practice¹⁴.

Meanwhile, deep learning has demonstrated remarkable capabilities in learning complex functions and high-dimensional structures from large datasets. In fact, neural networks (NNs) have set new standards for computational efficiency in tasks like quantum simulation^{15–19}, which are also commonly associated with quantum computing. A natural question then arises: can quantum resources enhance NN-based variational methods and help push the computational boundary of what is achievable with current and near-future hardware? Previous works have extensively investigated and documented that NNs can efficiently model the wavefunction amplitudes (i.e., essentially the probability distribution), but struggle to capture intricate sign or phase structures in many-body systems^{3,19–23}. On the other hand, modeling the phase structure of an arbitrary wavefunction can be well approximated with some variations of parameterized Instantaneous Quantum Polynomial (IQP) circuit^{24–29}. This observation motivates one way to combine PQC with NN to jointly model complex wavefunction within a hybrid variational framework. Importantly, such models may exhibit potential quantum advantage if continuous variable IQP (CV-IQP) operations exist for a single iteration^{30,31}.

Numerous efforts have explored the combination of quantum computing with deep learning in various settings^{32–34}. An especially relevant example is the variational quantum-neural hybrid eigensolver (VQNHE)³⁵ algorithm, previously developed by one of us and collaborators. This method uses a neural network to post-process quantum states prepared by a shallow circuit, forming a hybrid quantum-neural ansatz that efficiently expands the accessible quantum state space. However, VQNHE still faces limitations in trainability and incurs non-trivial measurement overhead.

In light of these developments and challenges, we revisit how best to harness both quantum and classical resources within a variational framework, one that maximizes hybrid advantages while mitigating their downsides. To this end, we propose sign-VQNHE (sVQNHE), a hybrid algorithm that comprehensively assuages all the major challenges facing mainstream VQAs: expressiveness, measurement cost, trainability, and robustness (see Table 1). In short, the key innovations of sVQNHE lie in its principled separation of quantum and classical roles: the diagonal layers of the quantum circuit are tasked to model the phase structure (with much reduced measurement costs), while a non-negative neural network only has to learn the amplitude (or effectively, the probability) distribution for improved numerical stability. These components are coupled through an iterative amplitude-transfer mechanism that maps the neural state onto a shallow and classically simulatable quantum layer. Compared to the original VQNHE, this re-design of the hybrid quantum-neural framework not only optimizes expressivity with shallow circuits and substantially improves the measurement costs and the gradient-based convergence rate, but also inherently mitigates sampling noise and decoherence, yielding more robust solutions under realistic conditions (see Results).

During the iterative, bidirectional feedback optimization loop (to train the PQC and NN parameters), if a single diagonal quantum layer cannot fully capture the target wavefunction’s sign structure, we extend the circuit depth by adding a layer of classically simulatable gates along with a new diagonal layer. The classical gate layer approximates the amplitude function learned by the NN by solving a tractable optimization problem, allowing the NN to guide amplitude refinement and assist in layer-wise circuit optimization without encountering barren plateaus. Importantly, because only the parameters of commuting diagonal gates are optimized on the quantum device, the required number of quantum measurements is dramatically reduced compared to the conventional non-commuting circuit ansatzes. In practice, at the last layer of the iterative, bidirectional feedback optimization procedure, one can choose to relax the constraint and allow the neural network to output complex values, thereby enhancing the expressiveness of the hybrid quantum-neural ansatz. Finally, our new algorithm improves the convergence behavior of the original VQNHE by incorporating a stable layer-by-layer training strategy that suppresses numerical instabilities.

This newly proposed iterative and bidirectional feedback loop enables efficient training, expressive state representations, and significant reductions in circuit depth and measurement cost. Our numerical experiments validate these advantages. For instance, in the 6-qubit J1–J2 model, sVQNHE reduces mean absolute error by 98.9% and variance by 99.6% relative to a baseline NN, while achieving nearly 19× faster convergence compared to a hardware-efficient VQE using similar quantum resources. In solving the MaxCut problem on 45-node Erdős–Rényi graphs, sVQNHE improves solution quality by 19% and quantum resource efficiency by 85% over a brickwork ansatz VQE baseline³⁶.

In summary, sVQNHE offers a scalable and practical path forward for tackling complex many-body quantum simulations and large-scale combinatorial optimization problems by fully leveraging the synergy between classical and quantum computation. As both quantum hardware and neural network models continue to advance, we anticipate that hybrid frameworks like sVQNHE will play an increasingly important role in achieving real-world quantum utility.

Challenge	Problem Description	sVQNHE Solution
Representation	NN-based Variational Monte Carlo struggles to model complex phase structure	Delegate the quantum circuit to learn phase structure
Measurement	VQE: $\mathcal{O}(2dn^{k'})$, commuting gates compress groups to $\mathcal{O}(n^{k'})$ ($k' < k$) VQNHE: $\mathcal{O}(2dn^k)$, n qubit, $\mathcal{O}(n^k)$ operators, d parameter	Commuting gates enable simultaneous measurements, reducing cost to $\mathcal{O}(n^k)$
Optimization	VQE: barren plateau in deep circuits VQNHE: potential numerical instability	Neural-guided layer-wise optimization with gradual amplitude transfer
Noise	VQE: affected by hardware noise and finite sampling noise VQNHE: NN mitigates errors but amplifies sampling noise	Gradual amplitude transfer reduces sampling noise, NN mitigates errors

Table 1. Key challenges in existing algorithms and sVQNHE’s mitigation strategies

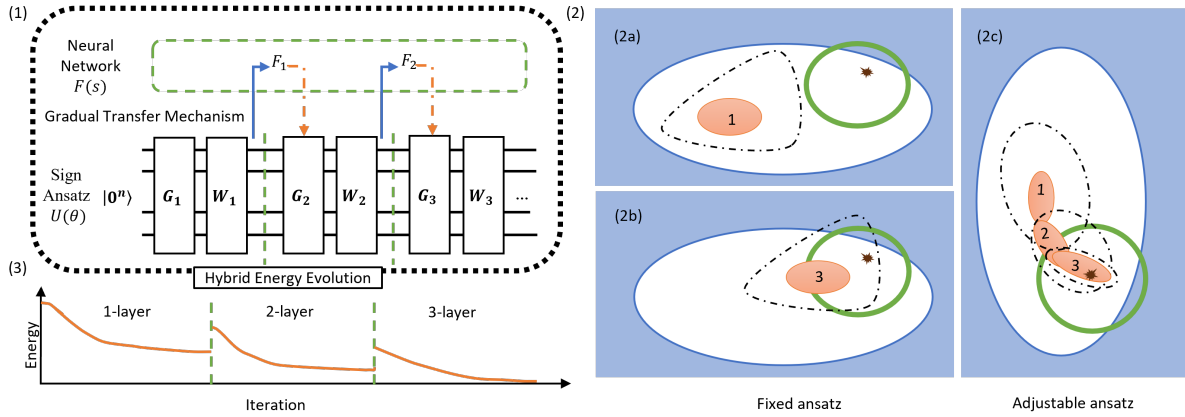


Figure 1. (1) The algorithm seamlessly integrates quantum circuits with neural networks. The quantum circuits interleaves diagonal layers ($W_1 \cdots W_n$) with shallow, simutable layers ($G_1 \cdots G_n$). Parameters of the G layers are optimized classically using a gradual transfer mechanism, while those of the W layers are adjusted via the parameter shift rule on the actual hardware. Leveraging the commuting properties of the diagonal layers, the number of measurements needed to compute gradients for the d parameters of W drops from $\mathcal{O}(2d)$ to $\mathcal{O}(1)$. (2) Illustration of sVQNHE’s advantages: the star represents the optimal solution, the green circle represents the initial solution space that is easy to explore by the NN, the orange region represents the solution space accessible to the PQC, and the black circle represents the coverage of the hybrid quantum-classical scheme. Among them, (2a) describes the suboptimal situation, that is, PQC cannot connect the classical region with the optimal solution, and the hybrid scheme is difficult to cover the optimal solution; (2b) shows the potential quantum advantage; (2c) describes the transition strategy from (2a) to (2b) through parameter adjustment. (3) Illustration of the energy optimization process using the hierarchical optimization scheme. When entering the next layer, the local optimal solution will be jumped out due to the newly introduced parameters.

Results

Theoretical Framework of sVQNHE

We introduce sVQNHE, a hybrid quantum-classical variational algorithm designed to address key limitations of conventional VQAs, including high measurement cost, barren plateaus, limited expressive power with shallow circuits, and noise-induced errors. This framework builds on the original VQNHE approach by introducing a layer-wise, phase-amplitude decoupling strategy²⁴ (see Fig. 1) that enhances trainability, scalability, and sampling robustness.

To elucidate the algorithm, we begin by summarizing the redesign of the quantum circuit and classical NN ansatzes. The overall (unnormalized) ansatz takes the form:

$$|\psi\rangle = F \prod_{i=0}^{L-1} W_i G_i |0\rangle, \quad (1)$$

where F denotes a post-processing operator defined by a classical NN. The following paragraphs explain the design of the hybrid ansatz and the associated bidirectional optimization strategy. Finally, the algorithm is summarized in Alg. 1.

Quantum Circuit for Phase Structure Learning. The quantum circuit ansatz consists of alternating layers of parameterized gates: (G_i, W_i) . G_i are classically simulatable and non-diagonal layers (e.g., R_y gates), primarily responsible for shaping the amplitude structure. G_1 is usually taken to be a layer of Hadamard gates to create a uniform superposition. W_i are diagonal gates (e.g., R_z and R_{zz}) designed to encode the phase structure of the wavefunction. These layers are added iteratively when greater expressivity is needed, and their parameters are optimized in a layer-wise fashion.

Classical Neural Network for Amplitude Modeling. The classical neural network is constrained to produce non-negative outputs, and is used to model the amplitude $F = \sum_s f(s) |s\rangle \langle s|$ of the quantum state in the computational basis. With the phase information delegated to the quantum circuit, the NN is focused on learning the probability distribution. Prior works have shown that classical neural networks are highly effective at this task, particularly for systems with smooth or structured amplitude landscapes^{20,21,24}.

Bidirectional Feedback Loop: Decoupling Amplitude and Phase. At each iteration i , a new block of parameterized quantum layers (G_i, W_i) is added to the circuit. The process follows two key steps. (1) Forward Initialization Step: The classical NN operator F from the previous iteration is approximated by the shallow quantum layer G_i , via a tractable classical optimization procedure as detailed in the Method section. This ensures that G_i inherits the amplitude structure previously learned by the NN. (2) Hybrid Optimization: Once G_i is initialized, the neural operator F is reset and jointly optimized with the parameters of the new diagonal gate layer W_i , as done in the original VQNHE algorithm. This hybrid optimization simultaneously refines both the amplitude (F) and sign structure (W_i) in a tightly coupled quantum-classical feedback loop.

Algorithm 1 sVQNHE Hybrid Algorithm

Require: n -qubit system, target Hamiltonian $H = \sum_i c_i P_i$

Ensure: Optimized energy value E_{final}

Initialization

- 1: Initialize quantum state $|\psi_0\rangle \leftarrow |0\rangle^{\otimes n}$
- 2: Initialize classical neural network parameters
- 3: Define diagonal operator $F_1 \leftarrow \sum_s f(s) |s\rangle \langle s|$ ▷ $f(s)$: NN-predicted amplitude
- 4: Set $G_1 \leftarrow H^{\otimes n}$ ▷ Uniform superposition

Joint Optimization

- 5: **while** $\neg$ converged **do** ▷ Global convergence
- 6: **for** $l \leftarrow 1$ **to** L **do** ▷ Layer-wise optimization
- 7: **if** $l > 1$ **then**
- 8: Update θ^{st} to minimize $\|G_l - F_{l-1}\|$ ▷ Gradual Transfer Mechanism, see Method for detail
- 9: **end if**
- 10: $E_l \leftarrow 0$ ▷ Reset layer energy

Hybrid Energy Estimation

- 11: **repeat**
 - 12: Apply operator: $|\psi_l\rangle \leftarrow W_l(\theta^{wt}) G_l(\theta^{st}) |\psi_{l-1}\rangle$
 - 13: Construct hybrid state: $|\psi_{l,f}\rangle \leftarrow F_l |\psi_l\rangle$
 - 14: **for each** Pauli term $P_i \in H$ **do**
 - 15: Compute $E_{P_i} \leftarrow \frac{\langle \psi_{l,f} | P_i | \psi_{l,f} \rangle}{\langle \psi_{l,f} | \psi_{l,f} \rangle}$
 - 16: Accumulate energy: $E_l \leftarrow E_l + c_i \cdot E_{P_i}$
 - 17: **end for**
 - 18: Update NN parameters for F_l
 - 19: Update parameters: θ^{wt} ▷ Measurement Strategy, see Method for detail
 - 20: **until** $|\Delta E_l| < \epsilon_{\text{conv}}$ ▷ Energy convergence
 - 21: **end repeat**
 - 22: Check global convergence ▷ Track E_l across layers
 - 23: **end while**
 - 24: **return** E_L ▷ Final optimized energy
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Adaptive Hybrid Ansatz with Controlled Expressivity

Conventional variational algorithms, such as the VQE and the QAOA, typically rely on predefined circuit ansatzes^{37,38}. These ansatzes, often inspired by physical principles like Trotterized dynamics in QAOA, impose a static architecture that can limit their effectiveness. For example, if the ansatz fails to capture the complex entanglement or sign structure of the target ground state, the optimization may converge to suboptimal local minima. To address this, adaptive methods like adapt-VQE^{10,39} iteratively construct the ansatz by selecting gates from a predefined pool. However, these approaches encounter significant hurdles: the gate pool may not include operations capable of generating sufficient entanglement, thus constraining expressiveness, and the iterative gate selection process requires a large number of quantum measurements, making it impractical for large-scale systems.

In contrast, VQNHE and sVQNHE employ a hybrid quantum-classical ansatz that effectively leverages both quantum and classical resources to represent a quantum state. This approach significantly expands the accessible quantum states with shallow quantum circuits. Nevertheless, the original VQNHE still assumes a fixed ansatz approach, which could clearly be optimized to further reduce circuit depth. To this end, sVQNHE adopts a neural-guided framework to systematically extend the circuit's depth along with controlled expressiveness. Its shallow quantum layers G_l are sequentially determined under the gradual guidance of a classical neural network.

A key feature of sVQNHE is its ability to achieve high expressiveness and stable convergence even with simple layers of G_l . For instance, take G_l to be a layer of R_y rotations on each qubit, can already enhance the ansatz's flexibility. This capability is rigorously supported by Theorem 1 (Expressiveness of the Quantum Circuit Ansatz), which analyzes the Lie algebra generated by specific sets of operators^{12,40-43}. Consider the generator set $\mathcal{G}_1 = \{Z_{D_{2j}} \mid j = 1, 2, \dots, \lfloor \frac{m}{2} \rfloor\} \cup \{Y_i \mid i = 1, 2, \dots, n\}$, where Y_i are Pauli Y operators on individual qubits, and $Z_{D_{2j}}$ are Pauli Z operators on specific qubit subsets. The theorem proves that the corresponding Lie algebra is $\mathfrak{g}_1 = \mathfrak{su}(2^{n-1}) \oplus \mathfrak{su}(2^{n-1})$, a highly expressive structure with a dimension far exceeding that of alternative generator sets (e.g., $\mathcal{G}_2$). This large Lie algebra indicates that even layers primarily composed of R_y gates, can explore a vast state space, enhancing the ansatz's ability to approximate complex quantum states efficiently.

Moreover, the design of the quantum layers G_l in sVQNHE is guided by structural constraints that ensure computational efficiency and scalability. Proposition 1 (Commuting Block Structure) provides a critical insight: if a block diagonal matrix $M = M_{1,1} \oplus \dots \oplus M_{m,m}$ has distinct eigenvalues across its blocks, any matrix commuting with M must preserve the same block structure. In the context of sVQNHE, this proposition informs the construction of G_l layers. By respecting this commuting block structure, sVQNHE can increase circuit depth in a controlled manner, isolating commuting blocks (e.g., W_i).

Unlike rigid ansatzes (e.g., QAOA's Trotterized structure) or gate-pool-dependent methods (e.g., adapt-VQE), sVQNHE avoids both architectural rigidity and measurement bottlenecks, achieves higher expressivity with less quantum resource demands.

Efficient Measurement and Trainability via Diagonal Gates and Neural Guidance

Traditional variational quantum algorithms face two intertwined challenges that limit scalability: high measurement costs and the emergence of barren plateaus. The first challenge arises from the need to estimate gradients by measuring non-commutative operators, a process requiring $\mathcal{O}(2d)$ measurements for d trainable parameters. In large systems with $\text{poly}(n)$ operators, this results in a prohibitive $\mathcal{O}(2d \cdot \text{poly}(n))$ measurement overhead, which becomes computationally intractable as circuits scale. The second challenge, barren plateaus, manifests as exponentially vanishing gradients in high-dimensional parameter spaces, rendering optimization ineffective. These issues are exacerbated in deep circuits and systems with many qubits, where the parameter landscape grows increasingly complex and gradients vanish rapidly due to the curse of dimensionality.

The sVQNHE framework addresses these limitations through two synergistic innovations. First, it employs commuting diagonal gates, such as R_z and R_{zz} rotations, which enable simultaneous measurement of expectation values in one basis. This compresses the per-operator measurement cost to $\mathcal{O}(1)$, reducing the total overhead to $\mathcal{O}(\text{poly}(n))$ for $\text{poly}(n)$ operators (see details in the method section). This stands in stark contrast to the multiplicative $\mathcal{O}(2d \cdot \text{poly}(n))$ scaling of traditional VQNHE and conventional VQAs, allowing sVQNHE to tackle large-scale problems efficiently.

Secondly, our framework incorporates layer-wise neural guidance to decompose the optimization process into manageable subproblems, addressing a critical limitation of traditional layer-wise VQAs⁴⁴. In conventional layer-wise VQAs, the absence of a global perspective on the optimization landscape renders sequential layer optimization prone to converging at local minima. In contrast, the sVQNHE framework employs a classical neural network to guide the optimization of each quantum layer, producing a hybrid state $|\psi_{l,f}\rangle$ that is more expressive than the state $|\psi_l\rangle$ obtained from hierarchical quantum circuits alone. This neural guidance not only helps avoid suboptimal local minima but also focuses parameter updates on one specific block each time, such as W_l at the l -th iteration. This approach ensures that gradients remain measurable even in deep circuits, since the effective parameter space at each optimization step can always be restricted to a minuscule fraction of the full deep circuit. Together, these strategies circumvent the dual bottlenecks of measurement overhead and barren plateaus, establishing a scalable

pathway for variational quantum algorithms in practical applications.

Sampling Noise Robustness

Under the finite sampling conditions, the mixture energy estimate in VQNHE requires normalization to counteract the non-unitary transformation induced by the neural network module F . The variance of the energy estimate $\hat{E}_{P_i}$ is governed by:

$$\text{Var}(\hat{E}_{P_i}) = \text{Var}(\langle \psi_{L,f} | P_i | \psi_{L,f} \rangle) \cdot \text{Var}(g^{-1}(s, L)), \quad (2)$$

where $g(s, L) = \frac{1}{n_s} \sum_{s_i} f^2(s_i)$, and $s_1, \dots, s_{n_s}$ are i.i.d. samples drawn from the distribution $|\langle s | \psi_L \rangle|^2$. The expectation and variance of $g(s, L)$ are $\mathbb{E}[g(s, L)] = \mathbb{E}[f^2(s)]$ and $\text{Var}(g(s, L)) = \frac{1}{n_s} \text{Var}[f^2(s)]$, where $s \sim |\langle s | \psi_L \rangle|^2$. This normalization process amplifies the sampling noise in the mixture energy estimate compared to the standard VQE, as quantified by $\text{Var}(g^{-1}(s, L)) > 1$. Notably, when the number of layer $L = 1$ is fixed, this formulation form simplifies to that of the original VQNHE algorithm.

The sVQNHE algorithm introduces a layer-adaptive gradual transmission mechanism. As the quantum circuit depth L increases, the algorithm shifts computational responsibility to the quantum component, progressively diminishing the weighting effect of $f(s)$ across configurations s . This mechanism ensures:

$$\text{Var}_{s \sim |\langle s | \psi_L \rangle|^2} (f^2(s)) \xrightarrow{L \uparrow} 0. \quad (3)$$

For sufficiently large L , $\text{Var}_{s \sim |\langle s | \psi_L \rangle|^2} (f^2(s)) < 1$. By the uniform convergence of the series,

$$\text{Var}(g^{-1}(s, L)) = \sum_i \mu_i \text{Var}_{s \sim |\langle s | \psi_L \rangle|^2} [f^2(s)], \quad (4)$$

with $\mu_i > 0$. This variance asymptotically approaches zero as $L \rightarrow \infty$. In our numerical experiment, as illustrated in Figures 3 and 4, the coefficient of variation of energy $\text{CV} \propto \sqrt{\text{Var}(g^{-1}(s, L))}$ decays with L , suggesting that the algorithm has better noise immunity under actual sampling constraints as L increase. In summary, we eliminate a source of numerical instability (which subsequently affects the convergence rate) of the original VQNHE.

Experimental Results

To rigorously validate the accuracy and efficiency of our proposed algorithm for the ground-state preparation of a given Hamiltonian, we conducted systematic evaluations across four canonical manybody problems: the 1D J1-J2 model, the 2D Heisenberg model, the Transverse Field Ising Model (TFIM), and the Classical Ising model. These models were chosen to represent diverse physical systems with varying degrees of sign problem severity and ground-state complexity. We employed three methodologies, sVQNHE, VQE, and NNs, to benchmark their performance. Additionally, we integrated the encoding scheme proposed in Ref.³⁶ to demonstrate the superiority of sVQNHE over conventional VQAs (such as QAOA and VQE) in solving the MaxCut problem, a prototypical combinatorial optimization task.

Our experiments included a 6-qubit 1D J1-J2 model with $J_1/J_2 = 0.6$, a configuration known to exhibit a highly non-trivial ground-state phase structure⁴⁵. This model serves as a representative case for systems with intricate sign signatures. We also tested a 9-qubit 2D Heisenberg model with periodic boundary conditions, which is known to incur severe sign-related challenges for numerical methods⁴⁶. For comparison, we analyzed a 9-qubit 1D TFIM (solvable via Jordan-Wigner transform) and two 1D Ising models (6 and 12 qubits). Both TFIM and Ising models we chose are Sign-problem-free systems. Nevertheless, they still present non-trivial challenges in different ways. For example, they are relevant to the qubit-formulated combinatorial optimization problems. We evaluated our algorithm under four scenarios to assess its theoretical advantages and practical robustness:

- **Ideal Simulation:** Quantified intrinsic accuracy, variability, and scalability under ideal conditions.
- **Real-World Simulation:** Assessed robustness under realistic quantum conditions, combining depolarization-based gate errors (two-qubit: 0.005; single-qubit: 0.0013) with bitstring-sampling-based estimation of observables and gradients.
- **Scalability Under Finite Sampling:** Demonstrated that sVQNHE's advantage over existing methods³⁶ can be sustained with system size.

We emphasize that the results of all the so-called "non-ideal" experiments are based on the original sampling data (of bitstrings) from noisy quantum circuits, without implementing any quantum error mitigation procedures. As sVQNHE possesses an inherent and robust error mitigating capability⁴⁷ due to the fact that the hybrid quantum-neural ansatz can be directly tuned with the classical NN module during the noisy optimization process.

1. Ideal Simulation

We conducted a systematic evaluation of the performance of sVQNHE and other methods (VQNHE, VQE, NN, QAOA) focusing on accuracy, variability, and measurement efficiency. All the calculations were done in statevector-type exact numerical computations. For consistency, sVQNHE and VQNHE utilized the same non-negative real neural network component (MLP), while the NN method employed a real MLP with identical parameters and structure. The quantum components of sVQNHE and VQNHE were our single-layer sign ansatz and a hardware-efficient ansatz with a similar number of parameters, respectively. In Table 2, these are denoted as sign-NN and hea-NN, respectively. The VQE method used a hardware-efficient ansatz with varying layers, such as HEA2 for two layers. Similarly, the QAOA method was tested with different layers, for instance, QAOA10 for ten layers. All methods initialized quantum circuit parameters using independent uniform distributions $U(-2\pi, 2\pi)$, optimized for the same number of steps, and averaged the estimated energy from 20 random initial points. The baseline algorithm in Table 2 is NN.

Simulating Frustrated Many-Body Systems

For the 1D J1-J2 model, which features a non-trivial ground state, the sVQNHE method (sign-NN) demonstrated significant improvements over the NN method, the VQE method (HEA2), and the VQNHE method (hea-NN). Specifically, Table 2 shows that after 2000 optimization steps, the sign-NN method reduced the mean absolute error (MAE) by 98.9% and the variance by 99.6% for the 6-qubit J1-J2 model compared to the NN method. Additionally, Figure 2 illustrates the scaling results (from 6 qubits to 12 qubits) of sign-NN and NN with the same number of optimization steps to achieve the minimum error. The advantage of sign-NN increases with the number of qubits. In contrast, while hea-NN also reduced the MAE by 75.1% compared to NN, its variance was larger than that of NN (variance: hea-NN > NN > sign-NN). Furthermore, due to the non-commutative structure of hea, the measurement amount for sign-NN was significantly smaller than that for hea-NN under similar parameter amounts. These three points—improved accuracy, reduced variance, and reduced measurement amount—demonstrate the superiority of sVQNHE over the original VQNHE algorithm. Regarding convergence speed, sign-NN significantly outperformed HEA2. To achieve the same error threshold, HEA2 required 12.6 times more optimization steps on average than sign-NN. In the most efficient cases, HEA2 needed 1676 steps to reach the same accuracy, while sign-NN only required 89 steps. Additionally, the probability of the sign-NN successfully reaching the target accuracy was 12 times higher than that of HEA2, highlighting its excellent reliability and efficiency (for details, please refer to the supplementary material). Similar results were observed in the Heisenberg model, further verifying the capability of sVQNHE to handle systems affected by the sign problem.

Model	Method	R_{MAE}	R_{Var}
6-qubit 1D J1-J2	sign-NN	-0.989	-0.996
	hea-NN	-0.751	1.955
	HEA2	-0.916	-0.132
9-qubit 2D Heisenberg	HEA1	-0.331	0.554
	hea-NN	-0.119	33.793
	sign-NN	-0.872	-0.832
9-qubit 1D TFIM	HEA1	-0.290	0.019
	sign-NN	-0.640	-0.728
9-qubit 1D Ising	HEA1	0.129	0.909
	QAOA5	20.674	15.583
	QAOA10	1.205	11.835
	sign-NN	-0.416	-0.455
12-qubit 1D Ising	HEA1	6.822	10.002
	QAOA10	77.012	80.404
	sign-NN	-0.811	-0.979

Table 2. Performance Analysis of sVQNHE Algorithm. Here, the range of R_{MAE} and R_{Var} is $(-1, +\infty)$. The closer to -1 , the better (see Equations (12) and (13) in the Method section for details). The baseline algorithm NN model is a real Multi-Layer Perceptron (MLP). HEA1 and HEA2 represent VQE methods employing 1-layer and 2-layer Hardware-Efficient Ansatz, respectively. QAOA5 and QAOA10 represent the QAOA method with layers 5 and 10, respectively. The Sign Ansatz employs R_{zz} gates to connect all edges of the corresponding physical model.

Simulating Sign-Problem-Free Many-Body Systems

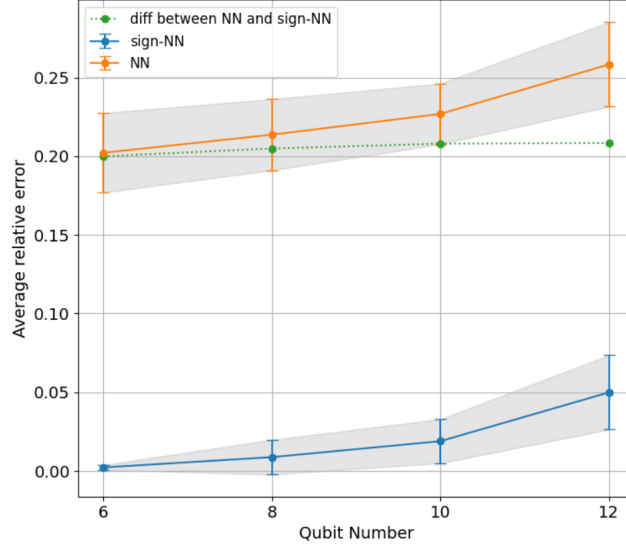


Figure 2. Scaling test for the 1D J1-J2 model. The x-axis shows the number of qubits, while the y-axis displays the average relative error from the sVQNHE method (sign-NN, blue line) and the NN method (NN, orange line) after 20 runs of 2000 steps each. The green line illustrates the difference in average relative error between the NN and sign-NN methods as the qubit count increases. Shaded regions represent the relative error bar scaled by 0.5.

Although the above results highlight the advantages of sVQNHE in sign-frustrated quantum models, the same architectural design is effective even in sign-free systems, where phase modeling is trivial for the ground state itself, but the ability to explore a broader Hilbert space (as defined by the PQC-generated phase structures) turns out to be beneficial for the optimization convergence in the numerical investigated presented in this subsection. More precisely, please see the last three rows of Table 2.

In our numerical experiments on the Ising model, the sign-NN approach demonstrates substantial improvements over the NN in both error reduction and variance compression. At 9 qubits, sign-NN achieves a 41.6% reduction in MAE compared to NN, indicating a significant enhancement in accuracy. This advantage becomes even more pronounced at 12 qubits, where sign-NN reduces MAE by 81.1% relative to NN, showcasing its superior scalability with increasing system size. Similarly, in terms of variance, sign-NN outperforms NN by reducing variance by 45.5% at 9 qubits. This gap widens dramatically at 12 qubits, with sign-NN achieving a 97.9% reduction in variance compared to NN, highlighting its ability to deliver consistent and reliable results as the system scales. When benchmarked against the QAOA in the 9-qubit Ising model, sign-NN maintains its performance edge. A 5-layer QAOA configuration requires a comparable number of per-iteration measurements to sign-NN but yields a higher MAE, indicating lower accuracy. Extending QAOA to 10 layers improves its accuracy, yet it still falls short of sign-NN’s performance. This trend persists and becomes more evident at 12 qubits, where sign-NN’s scalability further amplifies its advantage over QAOA. The consistency of these results extends to the TFIM. The superior performance of sign-NN can be attributed to its carefully designed ansatz, optimized with neural network guidance. Unlike QAOA, which uses R_x gates and constrains all Z- and X-related gates within a layer to share a single parameter, the Sign Ansatz employs R_{zz} and R_y gates with independent parameters. This design, as supported by Theorem 1, generates a higher-dimensional Lie algebra ($\mathfrak{g}_1$) compared to QAOA’s ($\mathfrak{g}_2$), enabling sign-NN to explore a broader unitary space through multi-qubit Z-phase adjustments. The phase-focusing architecture of the Sign Ansatz, which leverages multi-qubit Z-gates to refine phase information, allows for efficient navigation of high-dimensional solution spaces. When combined with neural network optimization, this approach achieves high accuracy and low variance at a reduced computational cost, making sVQNHE particularly well-suited for large-scale quantum optimization problems.

2. Real-World Simulation

Next, we consider how robustly sVQNHE performs when there exists both gate errors (for e.g. depolarization channels) and uncertainty induced by the finite sampling of bitstrings instead of statevector calculations as in the previous section. We evaluated sVQNHE against VQE, adopting two distinct optimization strategies, layered-VQE (layerwise optimization) and standard-VQE (joint optimization of all parameters), using an identical ansatz circuit. sVQNHE employed non-negative real neural networks, while both VQE methods utilized the same Sign Ansatz without NN augmentation. For all VQE schemes, the resource consumption was saved by measurement based on commuting groups. All simulations capped iterations at 400.

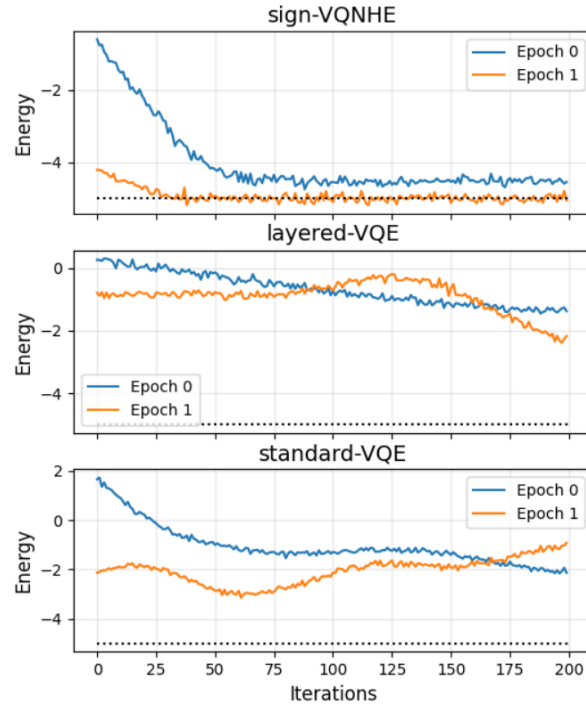


Figure 3. Performance evaluation of sVQNHE and VQE variants under a 3-qubit 1D Heisenberg Hamiltonian. Energy (y-axis) versus iteration count (x-axis), with the ground state energy marked by a black dashed line. For sVQNHE and layered-VQE (layered optimization), blue and orange lines correspond to the first and second evolutionary layers, respectively, where each layer introduces new variational parameters. For standard-VQE (overall optimization), the lines reflect energy progression across sequential steps under fixed parameterization. For sVQNHE, coefficients of variation after stabilization (final 50 iterations per layer) are $cv_1 = 0.01618$ and $cv_2 = 0.015912$, indicating a reduction in variability in the second layer.

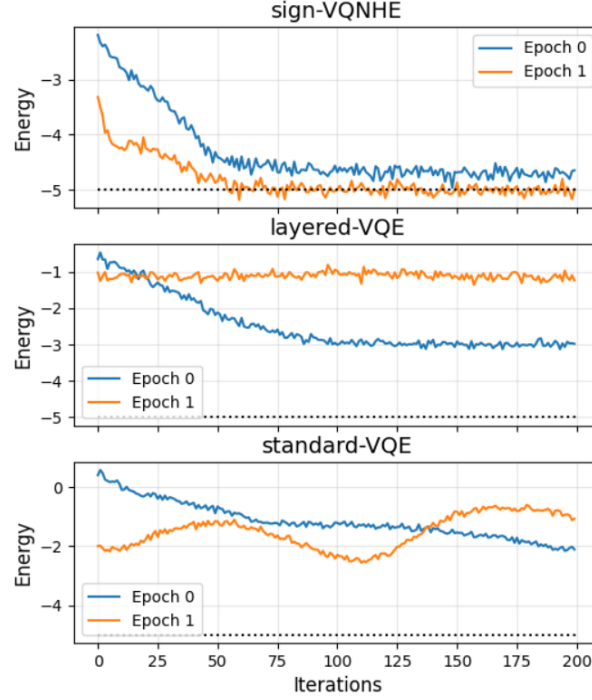


Figure 4. Energy convergence of sVQNHE and VQE variants under a noisy 3-qubit 1D Heisenberg Hamiltonian. Iteration count (x-axis) versus energy (y-axis). The solid black dashed line marks the ground state energy value. For layered optimization (sVQNHE, layered-VQE), blue and orange lines denote first- and second-layer parameter updates, respectively; standard-VQE (overall optimization) reflects sequential parameter refinement. For sVQNHE, coefficients of variation after stabilization (final 50 iterations per layer) are $cv_1 = 0.01534$ and $cv_2 = 0.01487$, indicating a reduction in variability in the second layer.

As shown in Figures 3 and 4, sVQNHE consistently achieved faster convergence than VQE, both with and without device noise. While layered optimization inherently reduces computational resource demands, mitigates noise sensitivity via shallower circuits, and often accelerates convergence, it is not applicable to the general VQE framework due to premature convergence to local optimal solutions. Specifically, the 1-layer Sign Ansatz fails as a viable initial parameterization for VQE’s layered optimization, as evidenced by the divergent performance of layer-VQE and standard VQE in our tests. However, integrating NNs into the Sign Ansatz (as in sVQNHE) circumvents this limitation, enabling effective layered optimization by delegating partial modeling duty to the neural network. Post-convergence analysis of sVQNHE revealed that the coefficient of variation (CV) for the second optimization layer remained lower than that of the first layer across all noise conditions. This validates the efficacy of our gradual transfer mechanism, which systematically refines solutions while maintaining stability under noise.

3. Scaling Under Sampling Errors

Finally, we investigate whether the observed advantage of sVQNHE can be sustained as the system size increases under the real-world setting of extracting PQC state by sampling bitstrings on quantum circuits. An example is provided in Figure 5. We evaluate the solution quality and measurement cost of the MaxCut problem on Erdős–Rényi random graphs with an edge connection probability of 0.3 as the graph size increases. To establish this advantage, we compare sVQNHE against the Sign Ansatz VQE (sign-VQE) and the recently proposed brickwork-VQE³⁶, all evaluated under the same polynomial encoding model. This model encodes the m binary variables of the MaxCut problem into the Pauli correlations across k qubits, enabling the representation of $m = O(n^k)$ variables with only n qubits, where $k > 1$ is an integer. Unlike the direct encoding schemes like QAOA, which require m qubits—one per variable—this approach achieves polynomial compression in the qubit count. The desired solution of the combinatorial problem is now encoded in terms of a non-classical Hamiltonian. The compression ratio depends on the polynomial order k , allowing us to tackle larger MaxCut instances with fewer qubits. All methods are evaluated under a unified encoding framework with $k = 2$ to ensure fairness.

To evaluate solution quality across varying scales, we conducted experiments with 1,200 measurement shots, averaging results over multiple trials. As shown in Figure 5(Left), scaling sVQNHE parameters—through enhancements in the NN component or other optimizations—consistently widens its performance gap over competing methods. Specifically, sVQNHE, which employs NN-guided hierarchical optimization and NN post-processing, significantly outperforms sign-VQE and

brickwork-VQE. Sign-VQE adopts the final PQC structure from sVQNHE (a two-layer sign ansatz with two diagonal and two non-diagonal layers) but omits the NN-guided optimization and post-processing used in sVQNHE. Brickwork-VQE, in contrast, utilizes a VQE with a brickwork ansatz, as detailed in³⁶. Figure 5(Left) reveals that, without NN guidance and post-processing (sign-VQE vs. brickwork-VQE), the sign ansatz shows no clear advantage over the brickwork ansatz, with comparable solution quality and similar measurement costs. However, sVQNHE’s hybrid approach - integrating hierarchical optimization guided by NN and NN post-processing to Sign Ansatz - yields a marked improvement. For instance, the performance gap between sVQNHE and baseline methods increases by approximately 6% $\approx (0.96 - 0.90)/0.90$ for 9-vertex graphs and 19% $\approx (1 - 0.84)/0.84$ for 45-vertex graphs when using parameter set 2. Additionally, Figure 5(Right) shows that sVQNHE significantly reduces single-step measurement consumption compared to both sign-VQE and brickwork-VQE. With parameter set 2, it achieves 86% $\approx (72 - 10)/72$ and 85% $\approx (306 - 46)/306$ improvements in quantum resource efficiency for 9- and 45-vertex systems, respectively. Additionally, in the Supplementary Information, we provide a preliminary comparison of resource consumption for larger instances, further highlighting sVQNHE’s advantages in scalability and efficiency under large-scale conditions. This underscores its potential for large-scale quantum applications.

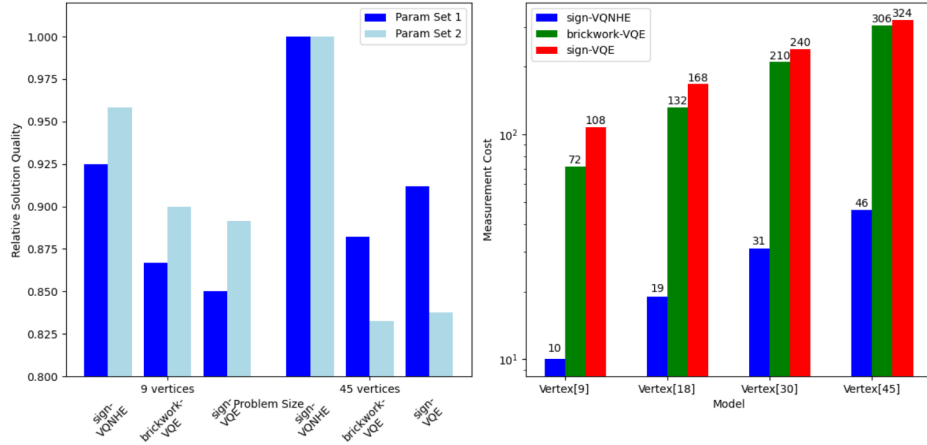


Figure 5. Scaling test of sVQNHE using the MaxCut problem as an example. (Left) The relative solution quality for the MaxCut problem, comparing parameter sets 1 and 2 across different problem sizes. The methods sign-VQNHE, brickwork-VQE, and sign-VQE correspond to the sVQNHE method with a 2-layer sign ansatz, the VQE method with brickwork ansatz, and the VQE method with 2-layer sign ansatz, respectively. The depth of brickwork ansatz is determined according to the reference³⁶, that is, the circuit depth is sublinearly related to the number of vertices in the graph. For sign-VQE, the ansatz is the same as the circuit finally generated by the corresponding sVQNHE scheme finally generated, utilizing a two-layer sign ansatz with two diagonal and two non-diagonal layers. The value range of relative solution quality is $[0, 1]$. The closer to 1, the better the performance is compared with other algorithms (see Equation (14) in the Method section for details). For example, in the case of 45 vertices, the quality of the solution of sVQNHE is relatively optimal regardless of whether the parameter set is 1 or 2. (Right) The single-step measurement consumption for the same problem sizes. Parameter set 2 features an increased number of parameters in the NN component and doubles the number of iterations compared to parameter set 1. The circuit depth in the brickwork architecture scales sub-linearly with the number of vertices.

Discussion

We present sVQNHE, a hybrid quantum-classical framework that strategically optimizes the roles of quantum and classical resources. Compared to the original VQNHE, our approach significantly improves measurement efficiency, substantially suppresses the numerical instability of the neural network, and enhances overall convergence.

Notably, sVQNHE leverages commuting diagonal gates to encode quantum sign structures, allowing efficient gradient estimation with far fewer measurements. The classical neural network is tasked with learning wavefunction amplitudes and guiding parameter updates, effectively sidestepping the barren plateau issue commonly seen in deep quantum circuits. This division of labor enables a layer-wise optimization strategy that remains stable even under noise and sampling limitations.

Our numerical simulations demonstrate compelling improvements across a broad class of computational problems. In the 6-qubit J1-J2 model, the sVQNHE method with a single-layer assumption achieves more than 7-fold the average accuracy and 19-fold the convergence speed of the 2-layer hardware-efficient VQE. Compared with the baseline NN, the average accuracy is improved by nearly two orders of magnitude. In sign-free models such as the TFIM and Ising chains, sVQNHE consistently

outperforms QAOA and VQE, achieving broader expressivity and better scalability. For combinatorial optimization, such as MaxCut on 45-node graphs, sVQNHE improves solution quality by 19% and quantum resource efficiency by 85% compared to brickwork ansatz-based VQE.

Taken together, these results highlight sVQNHE's broad applicability, efficiency, and scalability. By tightly integrating neural networks with quantum circuits along with a revised role that each component plays in the new algorithm, sVQNHE offers a practical path toward quantum utility on NISQ and early fault-tolerant devices. Looking ahead, this framework can be further extended by incorporating advanced machine learning models and better measurement strategies, and applied to a wider class of many-body simulation and large-scale optimization problems. Extending sVQNHE to tackle PQC-based quantum machine learning is also conceptually straightforward. As quantum hardware continues to evolve, we expect sVQNHE to remain a strong candidate for bridging theoretical capabilities with real-world impact.

Methods

The Hamiltonian of J1-J2 Model and Heisenberg Model

For the 2D Heisenberg models are constructed with non-periodic boundary conditions, whose Hamiltonian can be written as,

$$H = h_i \sum_i Z^i + J_{ij} \sum_{edges} X^i X^j + Y^i Y^j + Z^i Z^j. \quad (5)$$

In our numerical simulation, we use the coefficient setting of $(h_i, J_{i,j})$ to be $(1, 0.4)$ in 9-qubit 2D Heisenberg model and $(1, 1)$ in 3-qubit Heisenberg model.

For the Hamiltonian of the n-qubit 1D J1-J2 spin model with non-periodic boundary conditions, it can be written as

$$H = \sum_{i=1}^{n-1} J_1 (X^i X^{i+1} + Y^i Y^{i+1} + Z^i Z^{i+1}) + \sum_{i=1}^{n-2} J_2 (X^i X^{i+2} + Y^i Y^{i+2} + Z^i Z^{i+2}). \quad (6)$$

In our numerical simulation, we use the coefficients $J_1 = 1$ and $J_2 = 0.6$, since for the $J_2 > 0.5$ the sign problem is non-trivial for the J1-J2 model.

Detail of the Theoretical Framework

Theorem 1 (*Expressiveness of the Quantum Circuit Ansatz*)^{12,40–43} Let $\mathfrak{g}_1$ and $\mathfrak{g}_2$ be the Lie algebras corresponding to the generators $\mathcal{G}_1$ and $\mathcal{G}_2$, respectively, where:

$$\mathcal{G}_1 = \{Z_{D_{2j}} \mid j = 1, 2, \dots, \lfloor \frac{m}{2} \rfloor\} \cup \{Y_i \mid i = 1, 2, \dots, n\},$$

$$\mathcal{G}_2 = \left\{ \sum Z_{D_{2j}} \mid j = 1, 2, \dots, \lfloor \frac{m}{2} \rfloor \right\} \cup \left\{ \sum X_i \mid i = 1, 2, \dots, n \right\},$$

where $m \in \{2, 3, \dots, n\}$, X_i and Y_i are the Pauli strings with Pauli X and Pauli Y operators at the i th position, respectively, D_{2j} is the set of all $2j$ -combinations from the set $\{1, 2, \dots, n\}$, and $Z_{D_{2j}}$ is the Pauli string with the Pauli Z operator on the set of positions D_{2j} . Then, the following statements hold:

- $\mathfrak{g}_1 = \mathfrak{su}(2^{n-1}) \oplus \mathfrak{su}(2^{n-1})$.
- $\dim(\mathfrak{g}_2) < \dim(\mathfrak{g}_1)$.

Proposition 1 (*Commuting Block Structure*) Let M be a block diagonal matrix $M = M_{1,1} \oplus \dots \oplus M_{m,m}$ with distinct eigenvalues across blocks. Then, any matrix commuting with M must share its block structure.

Gradual transfer mechanism

Our algorithm enforces strict classical-to-quantum information transfer by iteratively aligning the classically simulable G_l (shallow quantum circuit blocks) with the classical part F_{l-1} . This can be performed by different schemes, such as:

1. Frobenius norm minimization (global): Minimize the full matrix distance: $\|G_l - F_{l-1}\|_F^2$.
2. Test state projection consistency (local): For a set of Haar-random test states $\{|\psi_{\text{test}}^k\rangle\}$, enforce consistency in the projected probability distribution

$$P_G^k(s) = |\langle s | G_l | \psi_{\text{test}}^k \rangle|^2, \quad P_F^k(s) = |\langle s | F_{l-1} | \psi_{\text{test}}^k \rangle|^2 \quad (7)$$

by minimize expected KL divergence $\mathbb{E}_k [\text{KL}(P_G^k \| P_F^k)] \rightarrow 0$. This test state sampling provides a weaker but practical consistency condition, avoiding direct optimization of G_l .

Measurement Strategy and Cost

In our layered optimization strategy, we focus on performing measurements for any given layer. To estimate the measurement cost of the Sign Ansatz, we use the parameter shift rule mentioned in Equation (8) to compute the gradient of each parameter in the circuit. The parameter shift rule is defined as follows:

$$\nabla_{\theta} f(x; \theta) = \frac{1}{2} [f(x; \theta + \frac{\pi}{2}) - f(x; \theta - \frac{\pi}{2})]. \quad (8)$$

To maximize the efficiency of executing the parameter shift rule, we exploit the commutative property of $W(\theta^W)$. During iterative parameter updates, this approach simplifies the process: we only need to add the corresponding quantum gate after circuit W for each updated parameter. Specifically, for the parameters in $W(\theta^W) = W_1(\theta_1^W) \cdots W_{n_W}(\theta_{n_W}^W)$, we have

$$\frac{\partial E_{P_i}(\theta^W)}{\partial \theta_k^W} = \frac{1}{2} (E_{P_i}(\theta_k^W + \frac{\pi}{2}) - E_{P_i}(\theta_k^W - \frac{\pi}{2})). \quad (9)$$

Since W_k and F are all commutative, and $E_{P_i}(\theta^W) = \langle \psi_0 | W^\dagger(\theta^W) F^\dagger P_i F W(\theta^W) | \psi_0 \rangle$, we have

$$\begin{aligned} E_{P_i}(\theta_k^W \pm \frac{\pi}{2}) \\ = \langle \psi_0 | W^\dagger(\theta^W) F^\dagger W_k^\dagger(\pm \frac{\pi}{2}) P_i W_k(\pm \frac{\pi}{2}) F W(\theta^W) | \psi_0 \rangle. \end{aligned} \quad (10)$$

Equation (9) and (10) imply that to obtain the gradient of θ^W , we only need to add the measurement of Pauli string $L_i = W_k^\dagger(\frac{\pi}{2}) P_i W_k(\frac{\pi}{2})$.

Note that any measurement of $Z \in L_i$ can be done by adding a factor $\prod_{i \in \text{ind}_Z} (1 - s_i)$ to the coefficient $(1 - 2s_0)$, where ind_Z is the position of Z in L_i and s_i is the Boolean value of the i index, so only changes in X and Y in L_i will cause the number of measurements to increase. Let P_i be a Pauli string containing exactly $|p_1|$ Pauli X or Y operators. Let W_k be the rotation gate corresponding to Z_p with $|p_2|$ operators. Since the transformations between X and Y can occur between L_i and P_i only if $|p_1 \cap p_2|$ is odd or $|p_1 \cap p_2| = |p_2|$, then for a Hamiltonian with $|p_1| \leq 2$, such as the 1D J1-J2 model, the total amount of measurement we need is $O(m_H)$, where m_H is the number of Pauli strings P_i in H . Here, p_1 and p_2 are non-empty subsets of the power set of all positions of the n qubit system.

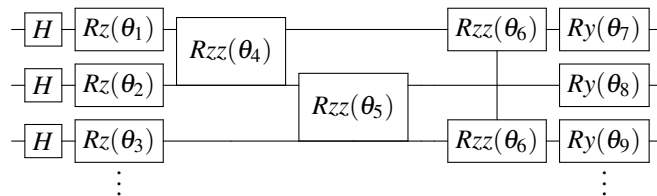
In summary, due to the commutation properties of the Sign Ansatz, our algorithm requires fewer measurements compared to general algorithms that rely on parameterized quantum circuits. For instance, considering the 1D J1-J2 model presented below (11), if $|p| \geq 2$ in the Sign Ansatz, the total number of measurements in a single iteration of our algorithm is equal to $3(n_1 + n_2) + 1$, where n_1 is the number of $\langle i, j \rangle$, and n_2 is the number of $\langle\langle i, j \rangle\rangle$.

$$H = J_1 \sum_{\langle i, j \rangle} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \Delta_1 \sigma_i^z \sigma_j^z) + J_2 \sum_{\langle\langle i, j \rangle\rangle} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \Delta_2 \sigma_i^z \sigma_j^z) + B_H \sum_i \sigma_i^z. \quad (11)$$

Here $\sigma^{x,y,z}$ are the Pauli matrices, Δ_1 and Δ_2 are the anisotropy parameters for nearest-neighbor and next-nearest-neighbor interactions, and B_H is the strength of an external magnetic field. $\langle i, j \rangle$ and $\langle\langle i, j \rangle\rangle$ denote sums over nearest-neighbor and next-nearest-neighbor spin pairs, respectively.

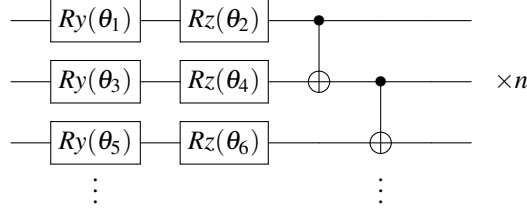
The details of our numerical simulation

We use TensorCircuit⁴⁸ to efficiently obtain all the quantum circuits and the neural network numerical results with the following Ansatz setting, and the details of the VQNHE algorithm are in the [TensorCircuit Demo](#).



The Sign Ansatz design equivalents for the sampling and noise versions of the numerical results with finite shots are detailed as follows. A combination of YM , YP , C_z , and R_z gates equivalently replaces the R_{zz} gate. Similarly, the R_y gate is equivalently replaced by a combination of XP , XM , and R_z gates. Here, YM and YP denote positive and negative rotations by $\frac{\pi}{4}$ around the Y -axis of the Bloch sphere, respectively, while XM and XP denote positive and negative rotations by $\frac{\pi}{4}$ around the X -axis of the

Bloch sphere, respectively. The two-qubit gates used in our cases connect the edges of the model (1D J1-J2 model and 2D Heisenberg model).



In the design of Hardware Efficient Ansatz, where the *CNOT* is only connecting the two nearest qubits (2D Heisenberg Model), n is the number of repetitions. Note that after repeating the above block n times, one more layer of R_y and one more layer of R_z are added. For example, for HEA2 used in this paper, there are three R_y layers, three R_z layers, and two *CNOT* layers. Similarly, the *CNOT* gate in the numerical simulation of the finite-shot version is equivalently replaced by a combination of YM , YP , and C_z gates.

Metrics

In the experiment, we use the following metrics to evaluate the performance of the method:

- Mean absolute error ratio R_{MAE} :

$$R_{MAE} = \frac{MAE_1 - MAE_0}{MAE_0}. \quad (12)$$

The metric R_{MAE} represents the relative reduction in mean absolute error (MAE) of different algorithms compared to the baseline algorithm (NN) with the same number of iterations. Here MAE_0 represents the MAE of the baseline algorithm (NN) being compared. The smaller the R_{MAE} value, the better the compared algorithm is relative to NN.

- Variance ratio R_{Var} :

$$R_{Var} = \frac{Var_1 - Var_0}{Var_0}. \quad (13)$$

The metric R_{Var} represents the relative reduction in the variance of different algorithms compared to the baseline algorithm (NN) given the same number of iterations. Among them, Var_0 represents the variance of the baseline algorithm (NN) being compared. The smaller the R_{Var} value, the more stable the compared algorithm is relative to NN, and the smaller the variability of the results.

- Estimated approximation ratio R_e for the MaxCut problem:

$$R_e = \frac{MaxCut_{algo}}{MaxCut_{max}}. \quad (14)$$

The metric R_e provides an estimated approximation ratio based on the best-known result for the MaxCut problem, which measures the relative solution quality. Here, $MaxCut_{max}$ represents the maximum MaxCut value achieved across all evaluated algorithms, while $MaxCut_{algo}$ denotes the MaxCut value obtained by the specific algorithm under assessment. A value of R_e approaching 100% indicates superior performance relative to the other algorithms compared.

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Code and data availability

The source code and data associated with this project are publicly available. They can be accessed at the following GitHub repository: <https://github.com/renmengzhen/sVQNHE>

Supplementary

Optimizing Quantum Resources with Sign Ansatz VQNHE

In this section, we evaluate the quantum resource efficiency of the sVQNHE framework against the Hardware Efficient Ansatz VQE. First, we test different ansatz on the 9-qubit 2D Heisenberg model with the initial state $|++ \dots ++\rangle$. The results are shown in Figure 6, it can be seen that sVQNHE uses very few quantum resources to converge to the desired accuracy compared

to both neural networks and VQE, which implies that the sVQNHE reaches the desired accuracy with fewer quantum resources compared to VQE in the number of circuits, and the number of parameters. Besides, since the zero quantum resource results indicate that without the assistance of Sign Ansatz the neural network itself cannot reach good accuracy, we can secondly claim that this framework can greatly improve the expressiveness of the neural network with limited quantum resources. In addition, we also verified the quantum resource efficiency of sVQNHE relative to VQE on the J1-J2 model. The results are shown in the Table 3.

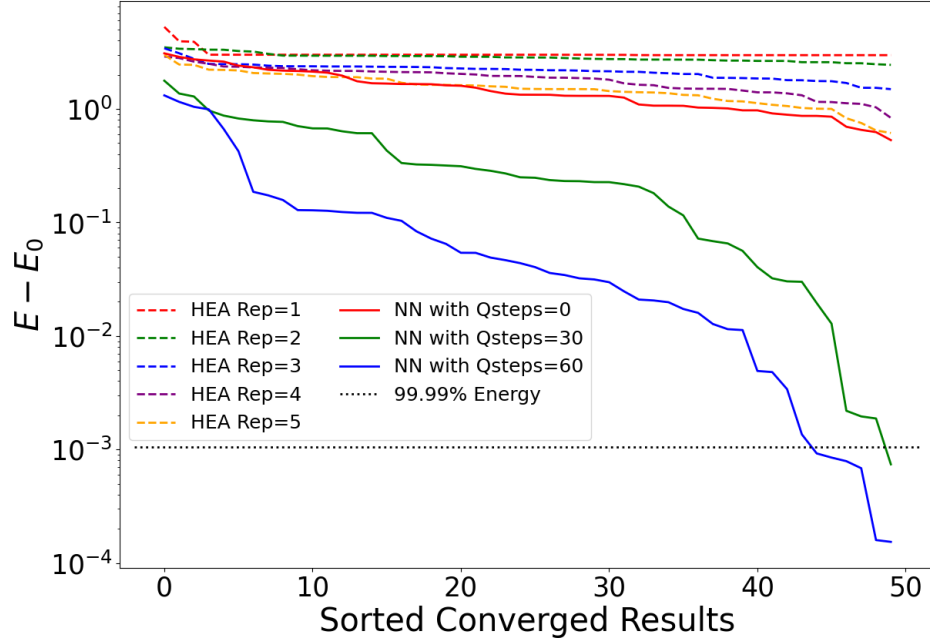


Figure 6. 9-qubit Heisenberg Model Result. The x-axis shows sorted results by the converged energy with different random initial parameters. The y-axis is the energy difference from the ground state. The red, green, and blue dashed lines are responding to Hardware Efficient Ansatz with repetitions equal to 1, 2, and 3, and the solid line is Complex MLP(3,3) with Sign Ansatz, where the total number of parameters in the neural network is 317. Both of them start from the initial state $|+\dots+\rangle$. The dotted line 99.99% Energy is 0.0001 times the ground state energy.

Table 3. Convergence Efficiency Comparison for the 6 qubit J1-J2 Model

Method	Average Optimization Steps	Success Probability (%)	Summary
sVQNHE	132.67	60	faster convergence with higher reliability
VQE (2-layer HEA)	1676.00	5	more steps and has a lower success rate

Explanation: This table compares the convergence efficiency of sVQNHE and VQE (with a 2-layer hardware-efficient ansatz) for the 6-qubit J1-J2 model. The metrics include the average number of optimization steps required to reach 99.45% of the ground state energy and the probability of success. sVQNHE outperforms VQE by requiring fewer steps (132.67 vs. 1676) and achieving a higher success rate (60% vs. 5%), demonstrating superior efficiency in quantum resource utilization.

Sampling Efficiency Verification

This section presents a compelling argument for performing sampling from the quantum circuit component rather than the classical neural network component that describes the amplitude. Our objective is to verify the computational advantages in the main text argument. As illustrated in Figure 7, we compare the convergence curve of our model with that shown in Figures 3 and 4 of the main text. The key difference is that the set of bitstrings s here is obtained by sampling from the classical neural network component. Compared to the results in Figures 3 and 4 of the main text, we observe that performing sampling from the quantum circuit component is better; fewer shots can yield more stable iterations and faster convergence. This suggests that

our quantum circuit can effectively sample from complex probability distributions that are intractable for classical computers, thereby providing a high-quality solution space that closer approximates the true solution space.

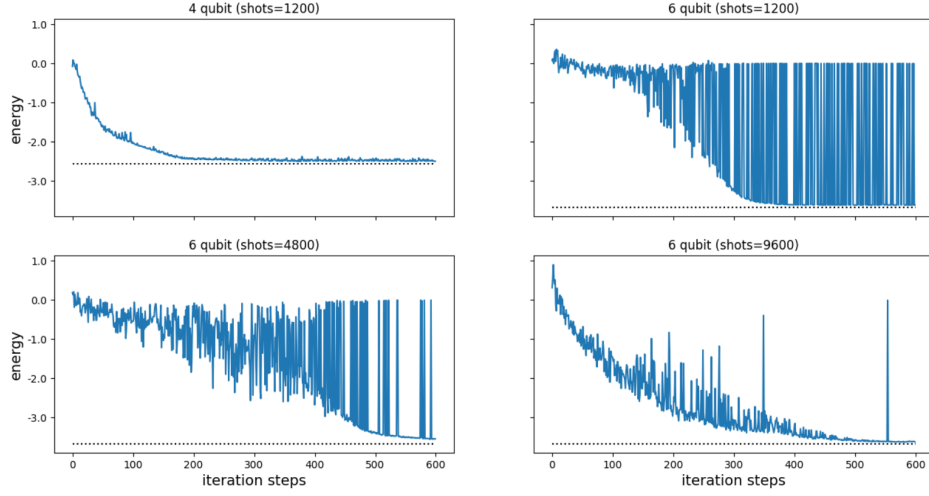


Figure 7. Sampling Efficiency Verification under 2D Heisenberg Hamiltonian. The figure illustrates the results obtained under varying numbers of qubits and shots. Sampling is conducted from the classical neural network component. The x-axis denotes the number of iterations, while the y-axis represents the energy. The solid dotted line indicates the ground state energy value of the corresponding model.

Preliminary Resource Consumption Analysis for Larger Instances

Table 4. Resource Comparison for Larger Instances

Qubits	Encoding	Vertices	brickwork-VQE measurement cost	Comparison	sVQNHE measurement cost
17	2	408	3000	>	409
	3	2040	24150	>	4081
30	2	1305	9612	>	1306
	3	12180	141246	>	24361

Explanation: This table compares the measurement costs of sVQNHE and brickwork-VQE under 2nd and 3rd order polynomial encodings for 17 and 30 qubits. The vertex count represents the maximum number of graph vertices for the maxcut problem corresponding to each qubit count and encoding scheme. Measurement cost reflects the number of measurement circuits required per iteration. sVQNHE consistently requires fewer circuits, demonstrating superior efficiency in quantum resource utilization.

In this section, we compare the measurement requirements for a single iteration of the brickwork-VQE and sVQNHE schemes under 2nd and 3rd order polynomial encodings³⁶, with equal shots per operator. As shown in the Table. 4, the savings in measurements, defined as the reduction when using sVQNHE compared to brickwork-VQE, scale linearly with the number of vertices in the graph. While this scaling is linear, the absolute savings become significantly large for graphs with many vertices, resulting in a substantial efficiency advantage for sVQNHE in large-scale quantum systems.