Augmenting Density Matrix Renormalization Group with Matchgates and Clifford Circuits

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(Received 14 January 2026; accepted manuscript online 3 March 2026)

Matchgates and Clifford circuits are two types of quantum circuits which can be efficiently simulated classically, though the underlying reasons are quite different. Matchgates are essentially the single particle basis transformations in the Majorana fermion representation, which can be easily handled classically, while the Clifford circuits can be efficiently simulated using the tableau method according to the Gottesman–Knill theorem. In this work, we propose a new wave-function ansatz in which matrix product states (MPS) are augmented with the combination of Matchgates and Clifford circuits (dubbed MCA-MPS) to take advantage of the representing power of all of them. Moreover, the optimization of MCA-MPS can be efficiently implemented within the density matrix renormalization group method. Our benchmark results on one-dimensional hydrogen chain show that MCA-MPS can improve the accuracy of the ground-state calculation by several orders of magnitude over MPS with the same bond dimension. This new method provides us a useful approach to study quantum many-body systems. The MCA-MPS ansatz also expands our understanding of classically simulatable quantum many-body states.

DOI: 10.1088/0256-307X/43/4/040708 CSTR: 32039.14.0256-307X.43.4.040708

1. Introduction. The classical simulation of strongly correlated quantum many-body systems is one of the most important tasks in the study of condensed matter physics. Over the past decades, many different types of many-body methods were proposed,[1–7] which can effectively handle different categories of quantum systems. Tensor network state is one representative of them and stems from the famous density matrix renormalization group (DMRG) method.[8] DMRG is now the workhorse for one-dimensional (1D) quantum many-body systems because the underlying wave-function ansatz, matrix product states (MPS),[9] can capture the entanglement structure of 1D quantum systems. DMRG has difficulty handling higher-dimensional quantum systems, and new ansatzes have been proposed by generalizing MPS to higher dimensions (such as PEPS,[10] PESS,[11] MERA,[12,13] and so on[5,6]) to encode the area law of entanglement entropy[14] in quantum many-body systems. Nevertheless, DMRG is still widely used in the study of quasi-1D systems because of its low computational cost and the ability to obtain accurate ground state by pushing the bond dimension to large numbers. There are also attempts to enhance the representional power of MPS by augmenting it with disentanglers while retaining its favorable computational cost.[15]

The developments in the field of quantum computing and quantum information[16] have identified special quantum circuits that can be efficiently simulated classically. Clifford circuits[17] and matchgates[18] are two types of classically simulatable quantum circuits. In the Majorana fermion representation, Matchgates are essentially the evolution of Gaussian states,[19] which can be efficiently handled classically. Clifford circuits, composed solely of Clifford gates (Hadamard gate, the phase gate S, and the controlled-NOT gate), can be efficiently simulated using the tableau method according to the Gottesman–Knill theorem.[17,20,21] Giving that MPS, matchgates and Clifford circuits can efficiently describe different types of quantum states (low-entangled states, stabilizer states, and Gaussian states respectively), it is tempting to combine them to construct a more powerful ansatz.

In Ref. [22], the Clifford circuits-augmented matrix product states (CAMPS) method was proposed (also see Refs. [23,24]), in which MPS are augmented with Clifford circuits. To solve the ground state of a quantum system using CAMPS, the MPS need only to deal with the so-called non-stabilizerness entanglement entropy,[25] because the Clifford circuits account for the stabilizer contribution, resulting in significantly higher accuracy than that of MPS with the same bond dimension. The opti-

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mization of both the MPS and the Clifford circuits can be efficiently implemented by a slight modification of the DMRG method. Later on, CAMPS were also generalized to the study of time evolution [26,27] and the calculation of finite-temperature properties. [28] It was also applied to fermionic models [29] by mapping the fermionic degrees of freedom to spin-1/2 degrees of freedom via the Jordan–Wigner transformation. With CAMPS, it was further found that dualities (like the Kramer–Wannier self-duality) in certain 1D quantum systems can be represented by Clifford circuits. [30,31]

Matchgates were first proposed in Ref. [18] and have been proven to be classically simulatable. Later, it was realized that circuits built from matchgates are essentially transformations describing the evolution of Gaussian states, [19] a fact known to enable classical simulability. In this regard, studies of combining matchgates with MPS have a long history, taking the form of single-particle basis transformations. [32,33]

In this work, we propose a new ansatz in which the MPS are augmented with both matchgates and Clifford circuits (dubbed MCA-MPS). The representational power of combining matchgates and Clifford circuits was previously studied in Ref. [34]. It is known that Clifford circuits can describe quantum states with large entanglement [35] (and correlation), but they are not universal for quantum computation. Clifford circuits can describe only stabilizer states. The distance between a given quantum state and a stabilizer state is usually called magic or non-stabilizerness, and many quantities have been proposed to quantify it. [36–41] Quantum states described by matchgates are Gaussian states, which exhibit no two-body correlations but can possess large magic. [42] In this sense, the combination of Clifford circuits and matchgates can complement each other to enhance representational power. It is known that MPS can describe "general" low-entangled states. Given these facts, MCA-MPS, which take advantage of the representing ability of all ingredients in it, should be a powerful ansatz. We show that the optimization of the MPS, matchgates, and Clifford circuits within MCA-MPS can be efficiently implemented via a slight modification of the DMRG method. We also benchmark MCA-MPS on the 1D hydrogen chain and the two-dimensional hydrogen lattice [see Supplementary Materials (SM)]. The results show that MCA-MPS significantly improve the accuracy of the ground-state energy by several orders of magnitude compared with that of MPS having the same bond dimension.

2. Methods. To synergistically leverage the distinct representational capabilities of MPS, matchgates, and Clifford circuits, we introduce the new MCA-MPS ansatz. Its structure, depicted in Fig. 1, is defined as

$$|\text{MCA-MPS}\rangle = CG|\text{MPS}\rangle\,, \tag{1}$$

where $|\text{MPS}\rangle$ represents a standard matrix product state efficiently capturing low-entanglement states, G denotes matchgate circuits, and C denotes Clifford circuits. Here, the matchgate and Clifford circuits act as disentanglers applied to the original $|\text{MPS}\rangle$, yielding the final ansatz $|\text{MCA-MPS}\rangle$. Matchgate circuits G implement $SO(2N)$ transformations within the Majorana fermion representation [19] ($\gamma_i \to O_{ij}\gamma_j$, with $O \in SO(2N)$ and γ_i the Majorana operators). This component enables efficient representation of Gaussian states. The subsequent Clifford circuits C further enhance the ansatz by applying Pauli-basis transformations.

The MCA-MPS ansatz is variationally optimized using a modified DMRG algorithm via a sequential procedure. First, the component of MPS is initialized and refined through standard DMRG optimization to yield a suitable initial state. Subsequently, the matchgate circuits G are introduced and optimized to reduce entanglement entropy and further minimize the ground-state energy (see Ref. [43] for details). Physically, this matchgate optimization is equivalent to an adaptive single-particle basis rotation. Following this, the Clifford circuits C are applied and optimized to achieve additional energy and entanglement reduction (see Ref. [22] for details). These optimization steps are integrated within the DMRG framework. Both matchgate and Clifford circuit optimization can be

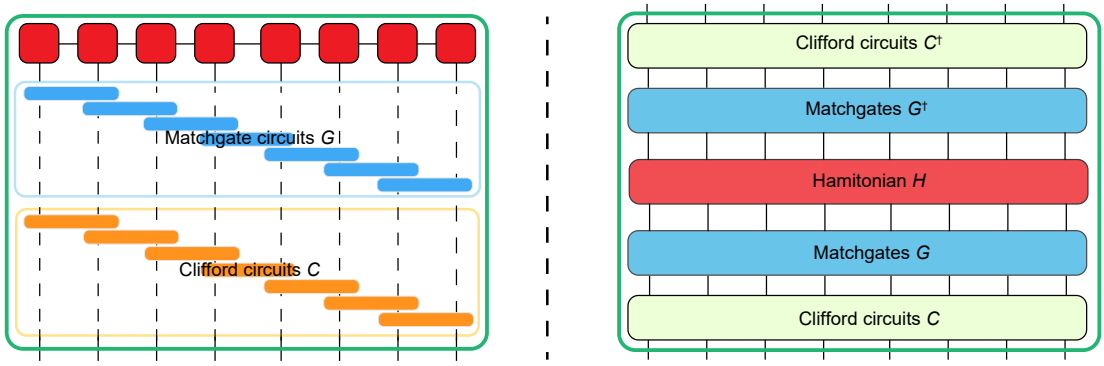

Fig. 1. Schematic illustration of the MCA-MPS. Left: The structure of the MCA-MPS ansatz, $|\text{MCA-MPS}\rangle = CG|\text{MPS}\rangle$, depicting the sequential application of matchgate circuits G and Clifford circuits C to the matrix product state $|\text{MPS}\rangle$, which corresponds to the Hamiltonian H. Note that we consider only $|\text{MCA-MPS}\rangle$ states that are less entangled than $|\text{MPS}\rangle$. Right: The equivalent Hamiltonian transformation, where the original Hamiltonian H is transformed into an effective Hamiltonian $H_{\text{MCA-MPS}} = CGHG^\dagger C^\dagger$ via successive application of matchgates and Clifford circuits.

performed after the eigenstate is obtained for the effective Hamiltonian in DMRG and before truncation is carried out via singular value decomposition.[22] The optimization of Clifford circuits is conducted in the Pauli basis. Matchgate circuit optimization can proceed in either the Pauli or fermionic basis. If the fermionic basis is employed for matchgate optimization, a Jordan–Wigner transformation is used to map fermionic operators to spin operators prior to optimizing the Clifford circuits.

In the MCA-MPS framework, $|\text{MPS}\rangle$ is associated with the original Hamiltonian H, while the final ansatz $|\text{MCA-MPS}\rangle$ corresponds to the transformed effective Hamiltonian $H_{\text{MCA-MPS}}$,

$$H_{\text{MCA-MPS}} = CGHG^{\dagger}C^{\dagger} = \sum_i a_i P_i \,, \tag{2}$$

where P_i is a Pauli string and a_i is the corresponding coefficient. We highlight the critical importance of the operational sequence when combining matchgates and Clifford circuits. We use common two-body interactions as an example in the following discussion. While matchgates can change the number of Pauli strings in the Hamiltonian's expansion, they are limited to generating a specific subset of at most $O(N^4)$ Pauli strings (with N the number of orbitals or single-particle basis), because the effect of a matchgate can be represented as $\gamma_i \to O_{ij}\gamma_j$, where matrix $O \in SO(2N)$ and the γ_i are Majorana operators.[19] Clifford circuits, in contrast, inter-convert Pauli strings while conserving the Hamiltonian's term count. The optimal strategy involves an initial matchgate application to transform the Hamiltonian into a structure characterized by $O(N^4)$ terms. Subsequently, Clifford circuits operate on this structured Hamiltonian, transforming these $O(N^4)$ terms to further optimize the ground-state representation. Inverting this order is detrimental: initial Clifford transformations, though preserving the number of Pauli strings, do not generally conserve the interaction form in the Majorana fermion representation. This can convert two-body interactions into complex many-body interactions, rendering subsequent matchgate application increasing the number of interaction terms in the transformed Hamiltonian.

3. Model. We test the MCA-MPS method on the 1D hydrogen chain[44] with 12 atoms (H_{12}) at an equal bond distance $R = 1$ Å in the minimal atomic basis (STO-3G, with $N = 24$ and total electron number $N_e = 12$). We use restricted Hartree–Fock (RHF) orbitals to test our algorithm. The deliberate use of RHF orbitals, rather than local atomic orbitals, is to illustrate the power of MCA-MPS: because RHF orbitals are delocalized and thus more entangled, traditional DMRG calculations become more challenging. The second-quantized Hamiltonian for *ab initio* DMRG[45–48] takes the form:

$$H = \sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i,j,k,l,\alpha,\beta} V_{ijkl} c^{\dagger}_{i\alpha} c^{\dagger}_{j\beta} c_{k\beta} c_{l\alpha}, \tag{3}$$

where t_{ij} and V_{ijkl} are molecular integrals and $c^{(\dagger)}_{i\sigma}$ are fermionic annihilation (creation) operators. For simplicity, we consider only particle-number-conserving matchgates (equivalent to orbital transformations) in this work.

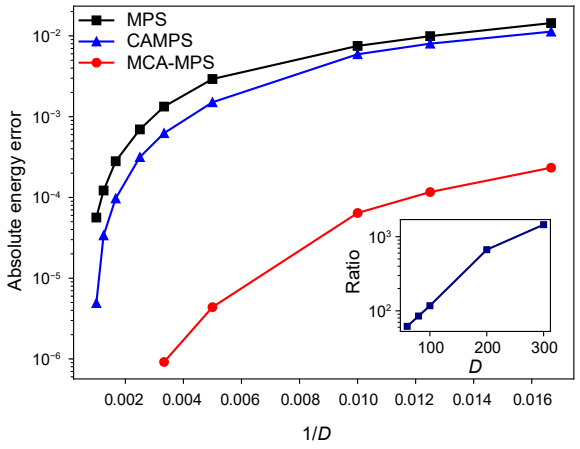

Fig. 2. Ground-state energy error (in the unit of Hartree) for the 1D hydrogen chain H_{12} (with restricted Hartree–Fock orbital) relative to exact energy, plotted against bond dimension D. Results are shown for both MPS, CAMPS, and MCA-MPS. Errors are defined as $|E_{\text{exact}} - E_{\text{MPS}}|$, $|E_{\text{exact}} - E_{\text{CAMPS}}|$, and $|E_{\text{exact}} - E_{\text{MCA-MPS}}|$ respectively. The inset displays the ratio of the MPS error over to that of MCA-MPS, quantifying the improvement achieved by MCA-MPS over standard MPS at the same bond dimension. We find that MCA-MPS achieves several orders-of-magnitude improvement, and this improvement becomes more dramatic with increasing bond dimension.

In the optimization of matchgates, each spatial orbital is treated as one site in the DMRG calculation (with local dimension $d = 4$ and bond dimension $D = 50$). In the optimization of Clifford circuits, spin-up and spin-down orbitals are treated as two independent sites (each with local dimension $d = 2$), making the application of Clifford circuits straightforward.[29]

4. Results. The exact ground-state energy for the hydrogen chain H_{12} in the given basis is -6.452816 Hartree. In Fig. 2, we compare the ground-state energy errors (in the unit of Hartree) obtained with MPS, CAMPS, and MCA-MPS. The errors are defined as $|E_{\text{exact}} - E_{\text{MPS}}|$, $|E_{\text{exact}} - E_{\text{CAMPS}}|$, and $|E_{\text{exact}} - E_{\text{MCA-MPS}}|$, respectively. As shown in Fig. 2, the MCA-MPS method yields substantially more accurate ground-state energies than both the MPS and CAMPS methods. The error for MCA-MPS is consistently several orders of magnitude smaller. We also observe that the ratio of the MPS error to the MCA-MPS error increases with bond dimension D, as depicted in the inset of Fig. 2. This ratio reaches approximately 100 at $D = 100$ and grows to over 1000 at $D = 300$, underscoring the powerful synergy of matchgates and Clifford circuits in enhancing the accuracy of ground-state energy calculations.

Figure 3 illustrates the entanglement entropy (for a mid-chain bipartition) of the 1D H_{12} system for the MPS, CAMPS, and MCA-MPS methods. For MPS, the entanglement entropy steadily increases with bond dimension D, and for CAMPS it also increases at small D. Conversely, the MCA-MPS exhibits a significantly lower entanglement entropy that shows little dependence on D. This significant reduction and rapid saturation of entanglement

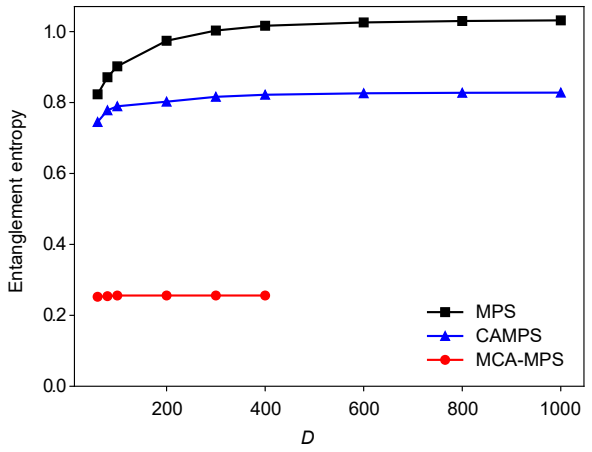

Fig. 3. Entanglement entropy of the 1D hydrogen chain H_{12} for MPS, CAMPS, and MCA-MPS. The entropy is computed for a bipartition of the system into two equal halves and plotted as a function of bond dimension D. We find that the entanglement entropy converges at small bond dimensions in MCA-MPS. The entanglement entropy in MCA-MPS is reduced by a factor of approximately 4 relative to that of MPS, consistent with the significant improvement in ground-state energy accuracy shown in Fig. 2.

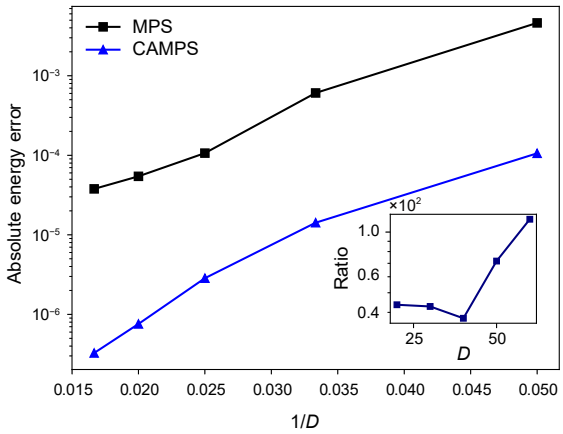

Fig. 4. Similar to Fig. 2: energy error (in the unit of Hartree) for the 1D hydrogen chain H_{12} relative to the exact energy, but for optimized atomic orbital (OAO) orbitals. For OAO orbitals, matchgates offer no improvement; thus, only results for MPS and CAMPS are shown. Errors are defined as $|E_{\text{exact}} - E_{\text{MPS}}|$ and $|E_{\text{exact}} - E_{\text{CAMPS}}|$, respectively. The inset displays the ratio of these errors, quantifying the improvement achieved by CAMPS over standard MPS at the same bond dimension. We find that CAMPS achieve several orders-of-magnitude improvement, and this improvement becomes more dramatic with increasing bond dimension. We also observe a turning point in the inset, beyond which the improvement of CAMPS increases rapidly with bond dimension D. This feature suggests that, at sufficiently large D, CAMPS captures the key underlying entanglement structure.

entropy in MCA-MPS suggest that matchgates and Clifford circuits efficiently capture the dominant entanglement features, leaving a less entangled state for the subsequent MPS representation. This leads to a more compact and efficient description of the system's overall entanglement. The dramatic reduction in entanglement entropy is consistent with the significant improvement in ground-state energy accuracy shown in Fig. 2.

We emphasize that the choice of orbitals critically impacts the performance of the matchgate and Clifford components in our MCA-MPS ansatz. With orthonormalized atomic orbitals, for example, the matchgate component offers no improvement beyond MPS, whereas the Clifford component still provides a significant error reduction (Fig. 4). This underscores the necessity of combining both types of circuits to ensure optimal performance across general cases (see SM for results on 2D systems).

As analyzed above and in the SM, the sequential optimization reveals a strong synergy: Clifford circuits continue to lower the energy significantly even after matchgate optimization converges, confirming that they optimize the ground state from different angles. We can also perform a global optimization of matchgate and Clifford circuits, in which Clifford circuit optimization is applied to the orbitals at intermediate steps of the matchgate optimization. This joint optimization method, in principle, could locate the global minimum, since the orbitals converged from matchgate optimization are not necessarily the best orbital for subsequent Clifford circuit optimization (see SM for detailed results).

5. Discussion. In this work, we present benchmark results for the MCA-MPS method on the 1D hydrogen chain instead of simpler lattice models because the interaction term in the original Hamiltonian of the 1D hydrogen chain (or general molecular systems) is dense (i.e., it scales as N^4 with N the number of total orbitals or single-particle basis). As discussed, transforming the Hamiltonian with particle-number-conserving matchgates is equivalent to a unitary transformation of the single-particle orbitals; which transform local interactions, like those in the Hubbard model, to long-range ones, significantly increasing computational complexity. In contrast, transformation with Clifford circuits does not increase the number of terms in the Hamiltonian. Therefore, to apply MCA-MPS to lattice models like Hubbard model, one needs to find ways to reduce the number of terms in the matchgate-transformed Hamiltonian. In this work, the optimization of matchgate and Clifford circuits are implemented separately. It is also possible to find ways to optimize them simultaneously or iteratively to improve the accuracy. It will be interesting to also implement basis truncation [49] in MCA-MPS to study systems with large basis set. We only consider $U(1)$ symmetry preserved matchgates in this work, it is also possible to release this constraint to gain further improvement in certain cases.

6. Conclusion and Perspectives. We develop a new wavefunction ansatz, called MCA-MPS, in which MPS are augmented with both matchgates and Clifford circuits. We also show the optimization of all the MPS, Clifford circuits, and the matchgates in MCA-MPS can be effectively implemented by a minor modification of the DMRG method. Our benchmark results on the 1D hydrogen chain and two dimensional lattice systems show that the MCA-MPS method significantly improves the accuracy of the

ground-state energy by several orders of magnitude compared to MPS with the same bond dimension. This approach provides a useful tool for studying quantum many-body systems. The MCA-MPS ansatz also expands our understanding of classically simulatable quantum many-body states. In the future, it will be interesting to explore the combination of other classical many-body methods with different types of classically simulatable quantum circuits.

Note Added. Upon completing our work, we became aware of similar works,[50,51] where the combination of Clifford circuits, matchgates, and MPS are also discussed.

Acknowledgements. MQ acknowledges the support from the National Key Research and Development Program of MOST of China (Grant No. 2022YFA1405400), the National Natural Science Foundation of China (Grant Nos. 12274290 and 12522406), and the Innovation Program for Quantum Science and Technology (Grant No. 2021ZD0301902). ZL acknowledges the support from the Quantum Science and Technology-National Science and Technology Major Project (Grant No. 2023ZD0300200) and the Fundamental Research Funds for the Central Universities.

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