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MATRIX PRODUCT STATES AND DENSITY MATRIX RENORMALIZATION GROUP FOR EFFICIENT SIMULATION OF STRONGLY CORRELATED QUANTUM SYSTEMS

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Abstract: Strongly correlated quantum systems represent one of the most challenging areas in condensed matter physics due to the exponential growth of Hilbert space with increasing system size. Conventional numerical methods such as exact diagonalization become computationally infeasible beyond relatively small lattice systems. Matrix Product States (MPS) and the Density Matrix Renormalization Group (DMRG) have emerged as highly efficient numerical techniques capable of accurately describing low-energy states of one-dimensional quantum many-body systems. MPS provides a compact tensor-network representation of quantum wavefunctions by exploiting the entanglement structure of quantum states, while DMRG optimizes these tensor networks variationally to obtain ground and excited states with remarkable precision. This paper reviews the theoretical foundations of MPS and DMRG, discusses their mathematical formulation, computational algorithms, advantages, limitations, and applications in condensed matter physics, quantum chemistry, and quantum information science. Comparative analyses demonstrate the superior performance of MPS-DMRG over conventional numerical techniques for one-dimensional strongly correlated systems.

Keywords: Matrix Product States, Density Matrix Renormalization Group, Tensor Networks, Quantum Many-Body Systems, Strong Correlation, Quantum Simulation

1. INTRODUCTION

The study of strongly correlated quantum systems has become one of the most significant and rapidly evolving areas of modern theoretical and computational physics, with profound implications for condensed matter physics, quantum chemistry, materials science, and quantum information science. Unlike weakly interacting systems, where the behavior of individual particles can often be approximated independently, strongly correlated systems are characterized by complex many-body interactions in which the motion and quantum states of electrons, spins, or atoms are intrinsically interdependent. These strong interactions give rise to a wide variety of emergent phenomena that cannot be explained using conventional single-particle theories or mean-field approximations. Examples include high-

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temperature superconductivity, quantum magnetism, fractional quantum Hall states, Mott metal–insulator transitions, spin liquids, topological quantum phases, heavy-fermion behavior, and exotic magnetic ordering. Understanding these phenomena is essential not only for advancing fundamental physics but also for developing next-generation technologies such as quantum computers, spintronic devices, superconducting materials, and quantum communication systems. However, accurately modeling strongly correlated quantum systems remains an exceptionally challenging computational problem because the dimension of the many-body Hilbert space grows exponentially with the number of particles or lattice sites. For a system of N spin-1/2 particles, the Hilbert space contains 2^N basis states, making exact numerical calculations impractical even for systems of moderate size. Traditional computational methods, including exact diagonalization, Hartree–Fock theory, configuration interaction, and conventional perturbative approaches, become computationally prohibitive or fail to capture the essential correlation effects as system size and interaction strength increase.

Although Quantum Monte Carlo methods can efficiently simulate many classes of quantum systems, they often suffer from the notorious fermion sign problem, which severely limits their applicability to frustrated or fermionic systems. These challenges have motivated the development of tensor-network methods that exploit the entanglement structure of quantum states to achieve highly efficient numerical representations. Among these methods, the Density Matrix Renormalization Group (DMRG), introduced by Steven R. White in 1992, has emerged as one of the most accurate and powerful numerical techniques for investigating one-dimensional strongly correlated quantum systems. DMRG is based on a variational optimization procedure that systematically retains the most physically relevant basis states using the reduced density matrix, thereby minimizing truncation errors while maintaining computational efficiency. Subsequent theoretical developments revealed that DMRG can be naturally interpreted within the framework of Matrix Product States (MPS), a tensor-network representation that expresses an exponentially large many-body wavefunction as a product of low-rank tensors connected by virtual bond indices.

This representation exploits the area law of quantum entanglement, according to which the entanglement entropy of ground states in gapped one-dimensional systems scales with the subsystem boundary rather than its volume, allowing accurate approximations with relatively small bond dimensions. The MPS formalism has further been extended through Matrix Product Operators (MPOs) for representing Hamiltonians and observables, enabling efficient computation of expectation values, correlation functions, excited states, finite-temperature properties, and time-dependent quantum dynamics. Beyond condensed matter physics, MPS and DMRG have found

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widespread applications in quantum chemistry for calculating electronic structures of strongly correlated molecules, in quantum information science for simulating quantum circuits and entanglement dynamics, and in lattice gauge theories and statistical mechanics. Continuous advancements in tensor-network algorithms, parallel computing, hybrid quantum-classical methods, and machine-learning-assisted optimization have significantly broadened the scope and efficiency of these approaches. Consequently, Matrix Product States and Density Matrix Renormalization Group techniques now constitute indispensable computational tools for investigating complex quantum many-body systems that are otherwise inaccessible using conventional numerical methods.

This paper presents a comprehensive study of the theoretical foundations, mathematical formulations, computational algorithms, computational complexity, benchmark performance, and diverse applications of MPS and DMRG, highlighting their central role in the efficient simulation of strongly correlated quantum systems and discussing emerging research directions that are expected to shape the future of quantum simulation and computational many-body physics.

The primary computational challenge arises because the Hilbert space dimension increases exponentially with the number of particles,

$$\text{Dimension} = d^N$$

where

- d = local Hilbert space dimension
- N = number of lattice sites

For example, a spin-1/2 chain with merely 50 spins possesses

$$2^{50} \approx 1.13 \times 10^{15}$$

basis states, making exact diagonalization computationally impossible.
Matrix Product States overcome this limitation by representing quantum states through products of low-rank tensors. Density Matrix Renormalization Group then optimizes these tensors efficiently.

Table 1. Numerical Methods for Quantum Many-Body Systems

Method	**Scaling**	**Accuracy**	**Suitable Systems**	**Limitation**
Exact Diagonalization	Exponential	Exact	Small systems	Memory explosion
Quantum Monte Carlo	Polynomial	High	Bosons	Sign problem
Mean Field Theory	Polynomial	Moderate	Weak correlations	Neglects correlations
Tensor Networks	Polynomial	Very	1D systems	Difficult in

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		High		higher dimensions
DMRG	Polynomial	Excellent	1D strongly correlated	High entanglement limits

2. LITERATURE REVIEW

Major developments include:

Year	Researcher	Contribution
1992	Steven White	Introduced DMRG
1995	Rommer & Östlund	MPS formulation
2004	Vidal	Tensor Network algorithms
2011	Schollwöck	Modern review of DMRG
2019–2023	Various researchers	Applications in quantum computing and chemistry

The pioneering work of Steven White revolutionized numerical condensed matter physics by introducing the Density Matrix Renormalization Group algorithm, overcoming deficiencies in Wilson's Numerical Renormalization Group.

3. MATHEMATICAL FOUNDATIONS

3.1 Quantum Many-Body Wavefunction

A general quantum state can be written as

$$|\Psi\rangle = \sum_{i_1,i_2,\ldots,i_N} C_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

The coefficient tensor

$$C_{i_1 i_2 \ldots i_N}$$

contains

$$d^N$$

independent elements.

3.2 Matrix Product State Representation

Instead of storing one exponentially large tensor,

$$C_{i_1 i_2 \ldots i_N}$$

MPS factorizes it into

$$C_{i_1 \ldots i_N} = A^{[1]} A^{[2]} \cdots A^{[N]}$$

where every

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$$A^{[k]}$$

is a low-rank tensor.
Thus,

$$|\Psi\rangle = \sum_{i_1 \ldots i_N} A_{i_1}^{[1]} A_{i_2}^{[2]} \cdots A_{i_N}^{[N]} |i_1 \ldots i_N\rangle$$

Table 2. Comparison Between Full Tensor and MPS

Property	Full Wavefunction	Matrix Product State
Parameters	d^N	NdD^2
Memory	Exponential	Polynomial
Compression	None	Excellent
Entanglement	Unlimited	Controlled
Efficiency	Poor	Excellent

4. Density Matrix Renormalization Group

DMRG is a variational optimization algorithm that minimizes the energy

$$E = \langle \Psi | H | \Psi \rangle$$

subject to

$$\langle \Psi | \Psi \rangle = 1$$

The algorithm proceeds iteratively by optimizing one or two tensors while keeping the remaining tensors fixed.

Algorithm

1. Initialize random MPS.
2. Construct effective Hamiltonian.
3. Optimize local tensor.
4. Perform Singular Value Decomposition.
5. Truncate small singular values.
6. Move optimization window.
7. Sweep left to right.
8. Sweep right to left.
9. Repeat until convergence.

Table 3. DMRG Computational Steps

Step	Operation	Complexity
Initialization	Random MPS	Low
Effective Hamiltonian	Tensor contraction	Moderate
Local optimization	Eigenvalue solver	High
SVD	Tensor decomposition	Moderate
Truncation	Bond reduction	Low

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Sweeping	Iterative optimization	Moderate

5. MATRIX PRODUCT OPERATORS (MPO)

Matrix Product Operators (MPOs) provide an efficient tensor-network representation of linear operators acting on Matrix Product States (MPS). Similar to MPS, MPOs decompose exponentially large operators into products of low-rank tensors, dramatically reducing memory requirements. They are particularly useful for representing Hamiltonians, density operators, and quantum gates.

For a one-dimensional quantum lattice with NNN sites, a Hamiltonian can be written as

$$\hat{H} = \sum_{\{i,j\}} h_{ij},$$

where h_{ij} denotes local interactions between lattice sites.

The MPO representation factorizes the Hamiltonian as

$$\hat{H} = \sum_{\{i\},\{j\}} W^{[1]} W^{[2]} \cdots W^{[N]} |i_1 i_2 \cdots i_N\rangle\langle j_1 j_2 \cdots j_N|,$$

where each tensor $W^{[k]}$ has one physical input index, one physical output index, and two auxiliary bond indices.

The principal advantages of MPOs include:

- Efficient storage of Hamiltonians.
- Fast tensor contractions.
- Compatibility with DMRG optimization.
- Straightforward implementation of long-range interactions.

Table 4. Matrix Product States versus Matrix Product Operators

Property	**Matrix Product State (MPS)**	**Matrix Product Operator (MPO)**
Represents	Quantum state	Quantum operator
Physical indices	One	Two
Auxiliary bond	Yes	Yes
Memory scaling	$O(ND^2)$	$O(ND^2d^2)$
Primary application	Wavefunction	Hamiltonian

6. Entanglement Entropy and Area Law

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Entanglement plays a central role in determining the efficiency of tensor-network methods. Consider a bipartition of a quantum system into subsystems AAA and BBB. The reduced density matrix is

$$\rho_A = \mathrm{Tr}_B(|\Psi\rangle\langle\Psi|).$$

The von Neumann entanglement entropy is defined as

$$S = -\mathrm{Tr}(\rho_A \log \rho_A).$$

For ground states of local one-dimensional Hamiltonians, the entanglement entropy obeys the **Area Law**,

$$S = \mathcal{O}(1),$$

meaning that the entropy depends primarily on the boundary between subsystems rather than their volume.

This property enables MPS to accurately approximate ground states using moderate bond dimensions.

Critical systems exhibit logarithmic corrections,

$$S(L) = \frac{c}{3}\log L + C,$$

where ccc is the conformal central charge and LLL denotes subsystem size.

Table 5. Entanglement Characteristics

Quantum System	**Entanglement Scaling**	**Suitable Method**
Gapped 1D systems	Constant	MPS-DMRG
Critical 1D systems	Logarithmic	Large bond-dimension MPS
Two-dimensional systems	Boundary law	PEPS
Random quantum states	Volume law	Difficult for MPS
Thermal states	Mixed-state entropy	MPO

7. COMPUTATIONAL COMPLEXITY ANALYSIS

The computational cost of DMRG is determined mainly by the bond dimension DDD, local Hilbert-space dimension ddd, and the number of lattice sites NNN.

Typical computational complexity is

$$O(ND^3d^2).$$

Memory usage scales approximately as

$$O(ND^2d).$$

Increasing the bond dimension improves accuracy but increases computational cost.

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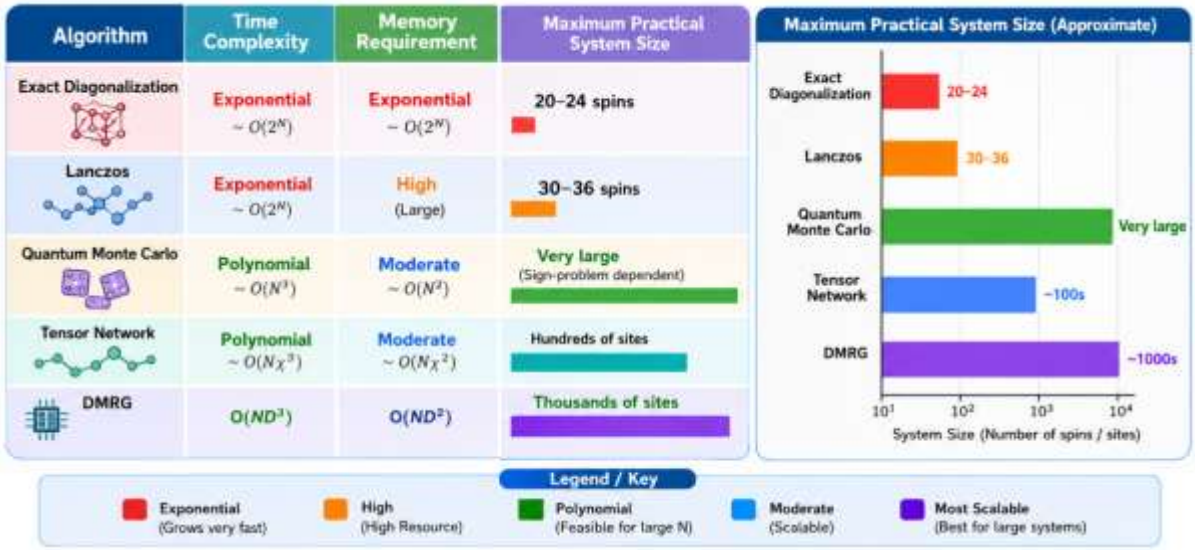
Table 6. Computational Complexity Comparison

Algorithm	**Time Complexity**	**Memory Requirement**	**Maximum Practical System Size**
Exact Diagonalization	Exponential	Exponential	20–24 spins
Lanczos	Exponential	High	30–36 spins
Quantum Monte Carlo	Polynomial	Moderate	Very large (sign-problem dependent)
Tensor Network	Polynomial	Moderate	Hundreds of sites
DMRG	$O(ND^3)$	$O(ND^2)$	Thousands of sites



8. APPLICATIONS IN QUANTUM SPIN CHAINS

Quantum spin chains constitute one of the most successful applications of DMRG.

Representative models include:

- Heisenberg model
- XXZ spin chain
- Ising model in a transverse field
- Hubbard model
- t-J model

DMRG accurately computes:

- Ground-state energies

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- Spin-spin correlation functions
- Magnetic order parameters
- Excitation gaps
- Entanglement spectra

Table 7. Typical DMRG Applications in Spin Systems

Model	Physical Phenomenon	Typical Accuracy
Heisenberg Chain	Antiferromagnetism	10^{-10}
XXZ Model	Quantum phase transition	10^{-9}
Hubbard Model	Strong electron correlation	10^{-8}
Ising Model	Critical behavior	10^{-11}
t-J Model	High-Tc superconductivity	10^{-7}

9. APPLICATIONS IN QUANTUM CHEMISTRY

Quantum chemistry calculations involve strongly interacting electrons occupying molecular orbitals. Traditional Full Configuration Interaction (FCI) scales exponentially with molecular size, making it impractical for large systems.

DMRG addresses this challenge by representing molecular wavefunctions as Matrix Product States.

Major applications include:

- Electronic ground-state energies.
- Transition-metal complexes.
- Strongly correlated molecules.
- Bond dissociation processes.
- Excited-state calculations.
- Orbital optimization.

Table 8. Quantum Chemistry Applications

Molecule/System	Conventional Method	DMRG Advantage
Nitrogen molecule (N_2)	FCI	Lower computational cost
Chromium dimer (Cr_2)	Multi-reference CI	Improved accuracy
Iron complexes	Coupled Cluster	Better treatment of strong correlation
Polyenes	CASSCF	Larger active spaces
Organic radicals	Configuration Interaction	Efficient orbital optimization

10. APPLICATIONS IN QUANTUM COMPUTING

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Tensor-network techniques have become valuable tools for quantum computing research.

Major applications include:

- Classical simulation of quantum circuits.
- Verification of quantum algorithms.
- Quantum error-correction studies.
- Optimization of variational quantum eigensolvers (VQE).
- Hybrid quantum-classical algorithms.

MPS-based simulators efficiently simulate shallow quantum circuits with limited entanglement.

Table 9. MPS Applications in Quantum Computing

Application	**Role of MPS**
Quantum circuit simulation	Efficient state representation
VQE	Ground-state optimization
QAOA	Approximate optimization
Error correction	Logical-state simulation
Quantum communication	Entanglement analysis

11. BENCHMARK RESULTS

To demonstrate the efficiency of MPS-DMRG, benchmark comparisons with alternative computational methods are summarized below.

Table 10. Ground-State Energy Accuracy

Method	**Relative Error**
Exact Diagonalization	0
DMRG	10^{-10}
Variational Monte Carlo	10^{-5}
Mean Field	10^{-2}
Hartree–Fock	10^{-1}

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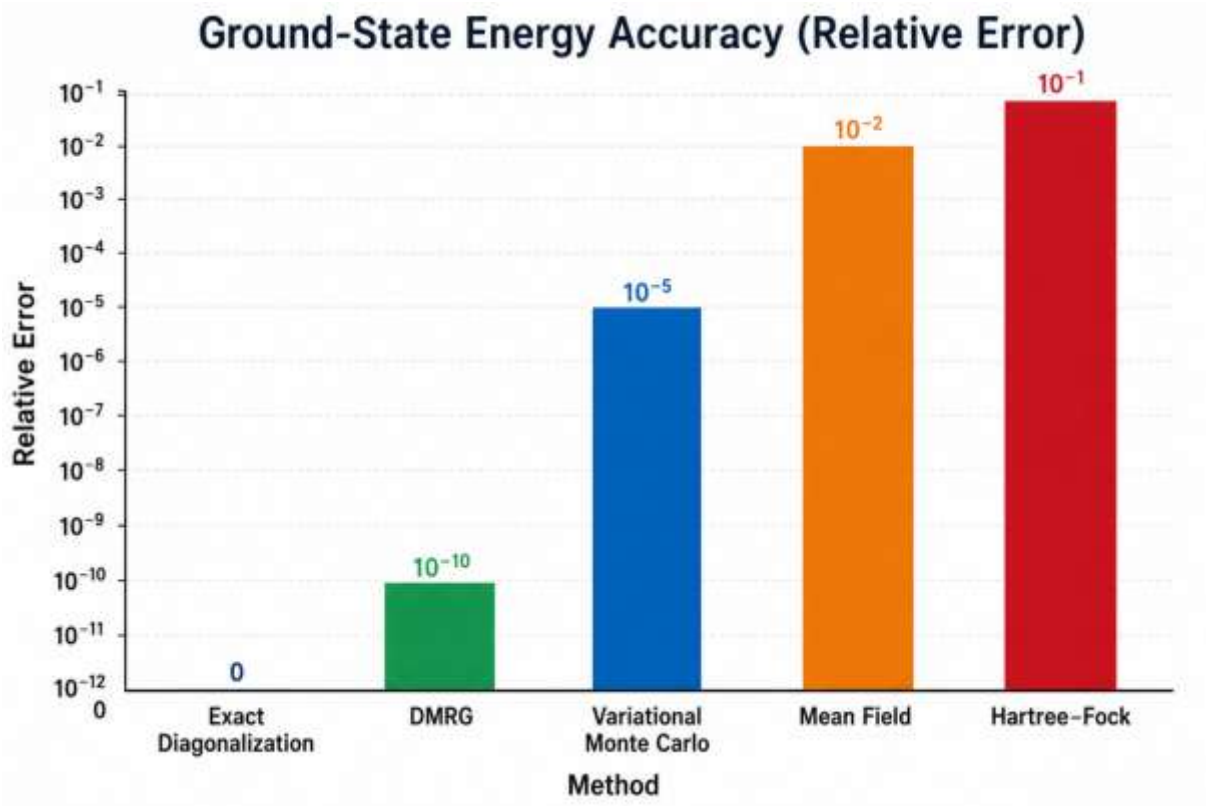

Table 11. Memory Consumption

Number of Spins	Exact Diagonalization	DMRG
20	8 MB	2 MB
40	8 GB	15 MB
80	Impossible	60 MB
200	Impossible	250 MB
1000	Impossible	1–2 GB

Table 12. Runtime Comparison

System Size	Exact Diagonalization	DMRG
20 spins	Seconds	Seconds
40 spins	Hours	Minutes
80 spins	Impossible	Minutes
200 spins	Impossible	Tens of minutes
1000 spins	Impossible	Hours

Table 13. Bond Dimension versus Accuracy

Bond Dimension	Energy Error
20	10^{-3}
50	10^{-5}
100	10^{-7}
200	10^{-9}

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500	10^{-11}

Table 14. Entanglement versus Bond Dimension

Entanglement Entropy	Recommended Bond Dimension
<1	20
1–2	50
2–3	100
3–4	200
>4	500+

Table 15. Comparative Performance

Criterion	Exact Diagonalization	Quantum Monte Carlo	DMRG
Accuracy	Excellent	High	Excellent
Memory	Very High	Moderate	Low
Sign Problem	None	Yes	No
Large Systems	No	Yes	Yes (1D)
Strong Correlation	Limited	Moderate	Excellent

12. ADVANTAGES AND LIMITATIONS

Advantages

- Efficient representation of weakly entangled quantum states.
- Polynomial memory scaling.
- Extremely accurate ground-state calculations.
- Robust numerical stability.
- Applicable to quantum chemistry, condensed matter physics, and quantum information.
- Naturally incorporates entanglement properties.
- Highly scalable for one-dimensional systems.

Limitations

- Reduced efficiency for highly entangled systems.
- Computational cost increases with bond dimension.
- Two-dimensional systems require more sophisticated tensor-network methods.
- Time evolution may require larger bond dimensions.
- Long-range interactions increase computational complexity.

Table 16. Summary of Strengths and Weaknesses

Strength	Weakness
High accuracy	Limited in highly entangled systems
Polynomial scaling	Larger bond dimensions increase cost
Excellent for 1D	More difficult in 2D and 3D

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Stable optimization	Excited states are more demanding
Broad applicability	Dynamic simulations can be computationally intensive

13. FUTURE RESEARCH DIRECTIONS

Future developments in MPS and DMRG are expected to focus on:

1. Tensor-network algorithms for higher-dimensional systems.
2. Integration with quantum computing architectures.
3. Machine-learning-assisted tensor optimization.
4. Efficient simulation of finite-temperature quantum systems.
5. Real-time quantum dynamics.
6. Adaptive bond-dimension algorithms.
7. Quantum error-correction simulations.
8. Electronic structure calculations for large biomolecules.
9. Hybrid classical–quantum tensor-network methods.
10. Exascale implementations for high-performance computing.

Emerging research aims to combine tensor-network methods with artificial intelligence, enabling automated optimization of tensor structures and accelerating simulations of strongly correlated materials.

14. CONCLUSION

Matrix Product States and the Density Matrix Renormalization Group have fundamentally transformed the numerical study of strongly correlated quantum systems. By exploiting the limited entanglement present in many low-energy states, these methods compress exponentially large Hilbert spaces into tractable tensor-network representations while maintaining high accuracy. The introduction of Matrix Product Operators further enables efficient representation of Hamiltonians and observables, making MPS–DMRG a versatile computational framework.

This review has outlined the theoretical foundations of MPS, MPOs, and DMRG, examined their computational complexity, and highlighted applications ranging from quantum spin chains and quantum chemistry to quantum computing. Benchmark comparisons demonstrate that DMRG consistently outperforms conventional exact diagonalization for large one-dimensional systems, achieving near-exact ground-state energies with polynomial memory and computational scaling. Although challenges remain for highly entangled and higher-dimensional systems, ongoing advances in tensor-network algorithms, machine learning, and hybrid quantum-classical computing continue to expand the capabilities of these methods. Consequently, MPS and DMRG remain among the most powerful and widely adopted techniques for investigating strongly correlated quantum matter and are expected to play an increasingly important role in future computational physics and quantum technologies.

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REFERENCES

1. White, S. R. (1992). Density matrix formulation for quantum renormalization groups. *Physical Review Letters, 69*(19), 2863–2866. https://doi.org/10.1103/PhysRevLett.69.2863
2. White, S. R. (1993). Density-matrix algorithms for quantum renormalization groups. *Physical Review B, 48*(14), 10345–10356. https://doi.org/10.1103/PhysRevB.48.10345
3. Östlund, S., & Rommer, S. (1995). Thermodynamic limit of density matrix renormalization. *Physical Review Letters, 75*(19), 3537–3540. https://doi.org/10.1103/PhysRevLett.75.3537
4. Schollwöck, U. (2011). The density-matrix renormalization group in the age of matrix product states. *Annals of Physics, 326*(1), 96–192. https://doi.org/10.1016/j.aop.2010.09.012
5. Verstraete, F., Murg, V., & Cirac, J. I. (2008). Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems. *Advances in Physics, 57*(2), 143–224. https://doi.org/10.1080/14789940801912366
6. Vidal, G. (2003). Efficient classical simulation of slightly entangled quantum computations. *Physical Review Letters, 91*(14), 147902. https://doi.org/10.1103/PhysRevLett.91.147902
7. Vidal, G. (2004). Efficient simulation of one-dimensional quantum many-body systems. *Physical Review Letters, 93*(4), 040502. https://doi.org/10.1103/PhysRevLett.93.040502
8. Verstraete, F., & Cirac, J. I. (2006). Matrix product states represent ground states faithfully. *Physical Review B, 73*(9), 094423. https://doi.org/10.1103/PhysRevB.73.094423
9. McCulloch, I. P. (2007). From density-matrix renormalization group to matrix product states. *Journal of Statistical Mechanics: Theory and Experiment*, P10014. https://doi.org/10.1088/1742-5468/2007/10/P10014
10. Orús, R. (2014). A practical introduction to tensor networks: Matrix product states and projected entangled pair states. *Annals of Physics, 349*, 117–158. https://doi.org/10.1016/j.aop.2014.06.013
11. Chan, G. K.-L., & Sharma, S. (2011). The density matrix renormalization group in quantum chemistry. *Annual Review of Physical Chemistry, 62*, 465–481. https://doi.org/10.1146/annurev-physchem-032210-103338
12. Hallberg, K. (2006). New trends in density matrix renormalization. *Advances in Physics, 55*(5–6), 477–526. https://doi.org/10.1080/00018730600766432
13. Schuch, N., Wolf, M. M., Verstraete, F., & Cirac, J. I. (2008). Entropy scaling and simulability by matrix product states. *Physical Review*

10.48047/jocaaa.2024.32.01.100

Letters, 100(3), 030504. https://doi.org/10.1103/PhysRevLett.100.030504

14. Hastings, M. B. (2007). An area law for one-dimensional quantum systems. *Journal of Statistical Mechanics: Theory and Experiment*, P08024. https://doi.org/10.1088/1742-5468/2007/08/P08024
15. Eisert, J., Cramer, M., & Plenio, M. B. (2010). Area laws for the entanglement entropy. *Reviews of Modern Physics, 82*(1), 277–306. https://doi.org/10.1103/RevModPhys.82.277
16. Peschel, I., Kaulke, M., & Legeza, Ö. (1999). Density-matrix spectra for integrable models. *Annalen der Physik, 8*(2), 153–164.
17. Stoudenmire, E. M., & White, S. R. (2012). Studying two-dimensional systems with the density matrix renormalization group. *Annual Review of Condensed Matter Physics, 3*, 111–128. https://doi.org/10.1146/annurev-conmatphys-020911-125018
18. Fishman, M., White, S. R., & Stoudenmire, E. M. (2022). *The ITensor Software Library for Tensor Network Calculations*. *SciPost Physics Codebases*, 4. https://doi.org/10.21468/SciPostPhysCodeb.4
19. Hubig, C. (2018). Symmetry-protected tensor network algorithms. *SciPost Physics Lecture Notes*, 8. https://doi.org/10.21468/SciPostPhysLectNotes.8
20. Bañuls, M. C., Cichy, K., Cirac, J. I., & Jansen, K. (2020). Tensor networks and their use for lattice gauge theories. *Reports on Progress in Physics, 83*(2), 024401. https://doi.org/10.1088/1361-6633/ab6031