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A Study of Entanglement and Ansatz Expressivity for the Transverse-Field Ising Model using VQE

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The Variational Quantum Eigensolver (VQE) is a leading hybrid quantum-classical algorithm for simulating many-body systems in the NISQ era. However, its effectiveness relies not only on accessing ground-state energies but also on preparing accurate eigenvectors, and the latter is particularly challenging in degenerate and strongly entangled regimes. We investigate this problem using the transverse-field Ising model (TFIM) with periodic boundary conditions in one, two, and three dimensions, employing up to 27 qubits. We adopt two ansatzes - the physics-inspired Hamiltonian Variational Ansatz (HVA) and the hardware-efficient EfficientSU2 from Qiskit. We benchmark them using energy variance, entanglement entropy, spin correlations, and magnetization. We find that while entanglement entropy is well reproduced in 1D, higher-dimensional systems demand deeper circuits and longer optimization. EfficientSU2 provides smoother optimization and performs well in low-entanglement regimes but underestimates critical correlations. In contrast, HVA circuits capture the entangled ground-state structure near criticality, though with more rugged optimization landscapes. We further show that VQE offers complementary insights into entanglement scaling in 3D TFIM by directly accessing the reduced density matrix and von Neumann entropy—an advantage over Quantum Monte Carlo methods, which are limited to Rényi entropy. These results demonstrate practical benchmarks for ansatz-design as well as highlight entanglement and correlation measures as diagnostics for reliable variational simulations of lattice models.

Parallel Session (for talks only)

Quantum computing and quantum information

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