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High-performance density matrix simulator for testing VQE methods using iteratively-grown ansätze

The electronic structure problem is a potential use case for NISQ computers, and Variational Quantum Eigensolver (VQE) algorithms are the leading contender for near-term molecular energy calculations. VQEs use sequences of parameterised unitary matrices known as ansätze to generate a trial state, which is optimised via the Rayleigh-Ritz variational principle to obtain an estimate for the expectation value of a given Hamiltonian. To improve VQE viability, we require ansätze with short circuit depths (and hence greater noise resilience) with minimal variational parameters (for ease of optimisation), which retain the ability to access the entire Hilbert space. Iterative methods, such as Adaptive Derivative-Assembled Pseudo-Trotter ansätz Variational Quantum Eigensolver (ADAPT-VQE), dynamically construct problem-specific ansätze by repeatedly appending the best unitary from a pool according to some decision rule (such as energy gradient maximisation). Recently, the Qubit-Excitation-Based ADAPT-VQE scheme has been proposed, wherein the pool of fermionic excitation evolutions is replaced by one of qubit excitation evolutions, and the decision rule is modified. This has been shown to reduce CNOT depth compared to ADAPT-VQE, potentially improving noise resilience. We have developed a fast, exact density matrix VQE simulator, with depolarising noise channels, to test this claim and compare the noise resilience of different VQE methods. The simulator has been verified by comparison to existing work, and extended to cover realistic noise models and noise mitigation strategies.