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Nonvariational imaginary-time evolution for first-quantized molecular systems

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While the variational quantum eigensolver (VQE) is widely used today, the imaginary-time evolution (ITE) on a quantum computer is a promising formalism for obtaining the ground state of a quantum system. We proposed recently an algorithm for finding the optimal molecular geometries [1] based on the the probabilistic ITE (PITE) [2] for a first-quantized molecular system. We discuss the applicability of the scheme by focusing on the computational cost. The scheme exhibits quantum advantage with respect to electronic and nuclear degrees of freedom when employing the multi-step PITE [3].

[1] Kosugi, Nishi, and Matsushita, npj Quantum Inf. **9**, 112 (2023)
[2] Kosugi, Nishiya, Nishi, and Matsushita, Phys. Rev. Research **4**, 033121 (2022)
[3] Nishi, Kosugi, Nishiya, and Matsushita, arXiv:2308.03605

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