Calculation of the ionization energy of superheavy elements using quantum algorithms

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Introduction

- Classical computers can't efficiently simulate large systems (exponential growth of the configuration space).
- Quantum computer is radical solution!
- Modern quantum computers are affected by noise.

Introduction

- Variational Quantum Algorithms are noise resilient.
- In chemical problems, it is often necessary to calculate ionization energies.
- Ionization energy can be obtained as the difference between two separate VQA runs.
- Proposed algorithm for calculating ionization energy is expected to be more robust against noise.

Variational Quantum Eigensolver

The VQE is the hybrid quantum-classical algorithm. It constitutes in minimization of the expectation value

$$E_{\boldsymbol{\theta}} = \frac{\langle \psi(\boldsymbol{\theta}) | \, H \, | \psi(\boldsymbol{\theta}) \rangle}{\langle \psi(\boldsymbol{\theta}) | \psi(\boldsymbol{\theta}) \rangle}, \tag{1}$$

where $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta}) \, |\psi_0\rangle$, $U(\boldsymbol{\theta})$ is parameterized unitary operator, $|\psi_0\rangle$ is initial state.

dUCC-SD ansatz

The chemical-inspired UCC parametrization conserving the number of particles is expressed as

$$|\psi(\boldsymbol{\theta})\rangle = e^{T-T^\dagger}\,|\psi_0\rangle\,, \tag{2}$$

where $T = \sum_{\mu}^{\text{exc}} \theta_\mu \tau_\mu$ is excitation operator, $|\psi_0\rangle$ is Dirac-Fock state.

To convert this ansatz into quantum gates, we use an alternative formulation with the factorized exponents

$$|\psi'(\boldsymbol{\theta})\rangle = \prod_i e^{\theta_{\mu_i}\left(\tau_{\mu_i}-\tau_{\mu_i}^\dagger\right)}\,|\psi_0\rangle\,. \tag{3}$$

Noise model

Calculations were carried out in the presence of

- gate noise,
- statistical noise,
- readout error.

The level of each type of noise is determined by averaged single- $F^{(1q)}$ and two-qubit $F^{(2q)}$ gate fidelities, and the measurement fidelity $F^{(m)}$ as follows

$$p_g^{(1q)} = p_c(1 - F^{(1q)}), \quad p_g^{(2q)} = p_c(1 - F^{(2q)}), \quad p_m = p_c(1 - F^{(m)}), \quad (4)$$

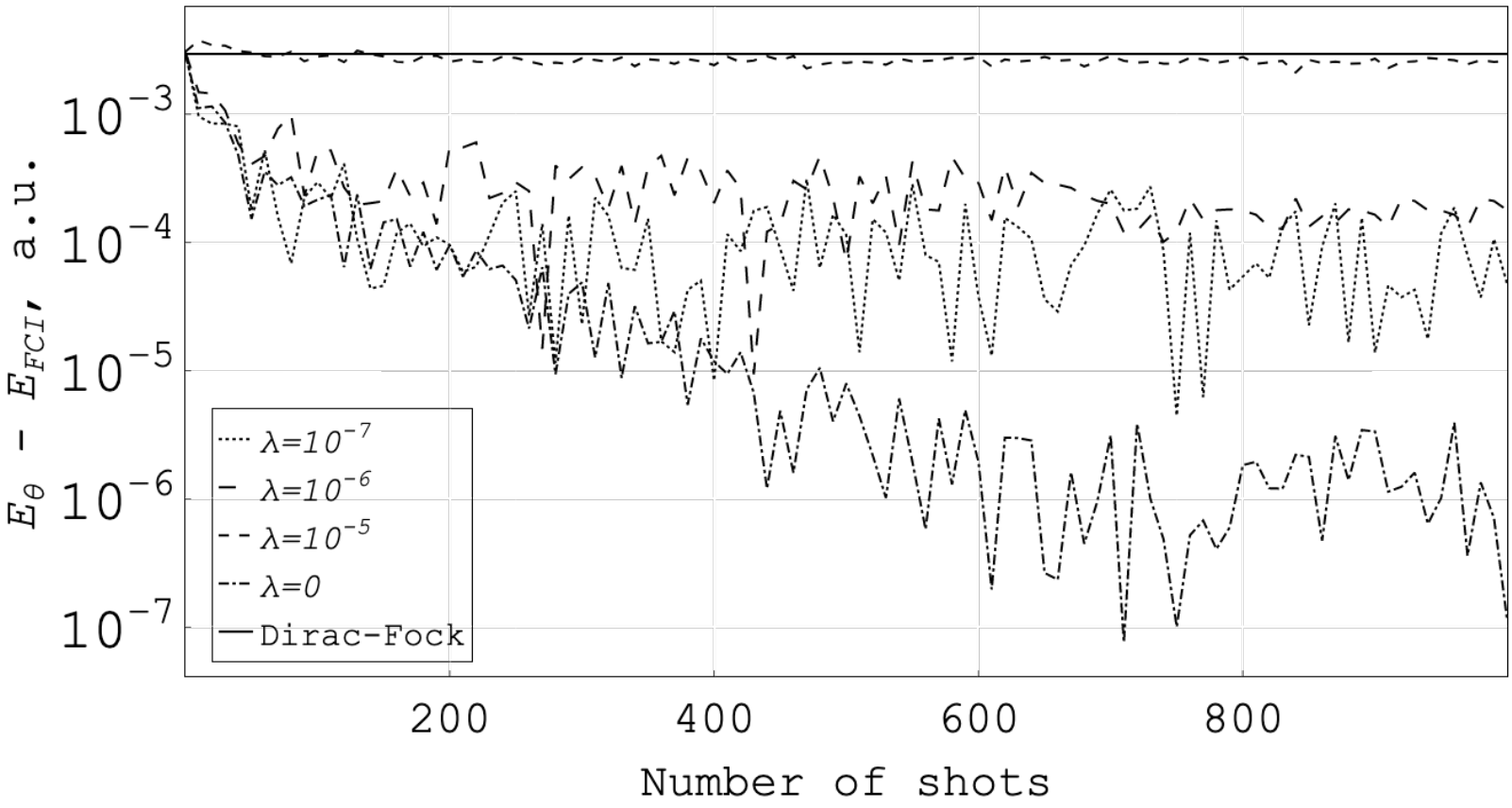
where p_c is the tunable noise level parameter.

Radial orbitals

Basis	Radial orbitals	N_e	N_{orbs}	N_q
A	$\{7s, 7p_{1/2}, 7p_{3/2}\}$	5	8	8

N_e is number of electrons, N_{orbs} is number of radial orbitals, N_q is number of quantum bits.

The ground-state energy of Mc atom



Algorithm for Calculating Ionization Energy

First step of the algorithm constitutes in preparation of the parametrized superposition

$$|\psi_{N,M}(\boldsymbol{\theta})\rangle = \frac{1}{\sqrt{2}} U(\boldsymbol{\theta}) \left(|\psi_N\rangle + |\psi_M\rangle \right), \tag{5}$$

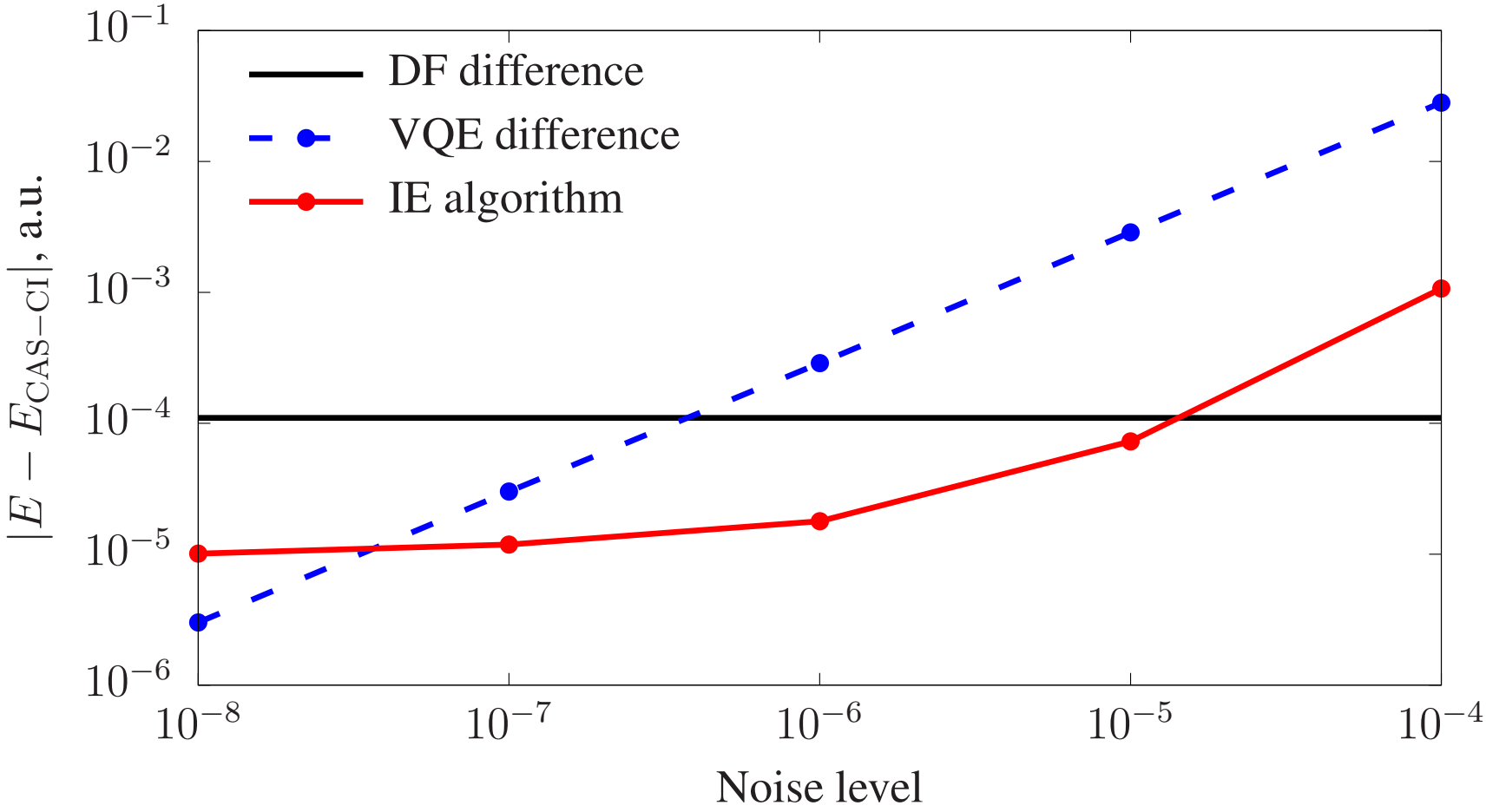
where $|\psi_N\rangle$, $|\psi_M\rangle$ are the Dirac-Fock states of systems with N and M particles respectively, $U(\boldsymbol{\theta})$ is parametrized unitary operator.
In the algorithm we minimize the expectation value

$$E_{\boldsymbol{\theta}} = \langle \psi_{N,M}(\boldsymbol{\theta}) | H | \psi_{N,M}(\boldsymbol{\theta}) \rangle . \tag{6}$$

Finally, we estimate the ionization energy as

$$E_{IE} = \langle \psi_N | U^\dagger(\boldsymbol{\theta}_{\text{opt}}) H U(\boldsymbol{\theta}_{\text{opt}}) | \psi_N \rangle - \langle \psi_M | U^\dagger(\boldsymbol{\theta}_{\text{opt}}) H U(\boldsymbol{\theta}_{\text{opt}}) | \psi_M \rangle . \tag{7}$$

The ionization energy of Mc atom



Conclusions

- The VQE algorithm is highly affected by noise, even for calculations in small basis sets.
- Algorithm for calculating ionization energy was developed.
- The IE algorithm is more robust to noise than the differences of VQE runs.