Calculation of the moscovium atom using quantum algorithms

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27.05.2024

Introduction

Classical computer:

- Classical computers can't efficiently simulate large systems, because of exponential growth of the configuration space with increasing the number of particles.

Quantum computer:

- Quantum computers can have an exponential advantage over classical computers by using the effects of quantum mechanics.
- Modern quantum computers are affected by noise caused by decoherence and inaccuracies in the execution of quantum gates.

Jordan-Wigner encoding

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s, \tag{1}$$

where H – electronic Hamiltonian of interest, h_{pq}, h_{pqrs} – one- and two-electron overlap integrals, $a_p^\dagger$, a_p – creation and annihilation operators.

$$|f_{N_{\text{orbs}}-1} \dots f_0\rangle \to |q_{N_{\text{orbs}}-1}\rangle \otimes \dots |q_0\rangle\,, \tag{2}$$

where $f_j, q_j \in \{0, 1\}$, state of each qubit $|q_j\rangle$ stores f_j, the occupation number of orbital j.
In Jordan-Wigner encoding

$$H = \sum_i \gamma_i P_i, \tag{3}$$

where $P_i \in \{I, \sigma^x, \sigma^y, \sigma^z\}^{\otimes N_{\text{orbs}}}$ – tensor product of Pauli operators.

Variational Quantum Eigensolver

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

$$E_{\boldsymbol{\theta}} = \frac{\langle \psi(\boldsymbol{\theta}) | H | \psi(\boldsymbol{\theta}) \rangle}{\langle \psi(\boldsymbol{\theta}) | \psi(\boldsymbol{\theta}) \rangle}, \tag{4}$$

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

dUCC-SD ansatz

In the UCC approach with single and double excitations, the generic state is expressed as

$$|\psi_{\mathrm{UCC-SD}}\rangle = e^{T-T^\dagger}\,|\psi\rangle\,, \tag{5}$$

where $T = \sum_{\mu}^{\mathrm{exc}} t_\mu \tau_\mu$ – excitation operator, $|\psi\rangle$ – Dirac-Fock state.

$$\tau_\mu \equiv a_{ij\ldots}^{ab\ldots} = a_a^\dagger a_b^\dagger \ldots a_j a_i, \tag{6}$$

where μ denotes indices $i, j, \ldots$ and $a, b, \ldots$, which label occupied and virtual orbitals of the reference state, respectively.

$$|\psi_{\mathrm{dUCC-SD}}\rangle = \prod_i e^{t_{\mu_i}\left(\tau_{\mu_i} - \tau_{\mu_i}^\dagger\right)}\,|\psi\rangle\,. \tag{7}$$

Hardware-efficient ansatz

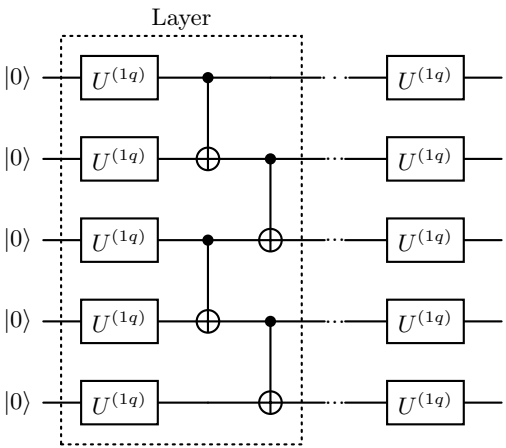
Hardware-efficient (HE) has the form

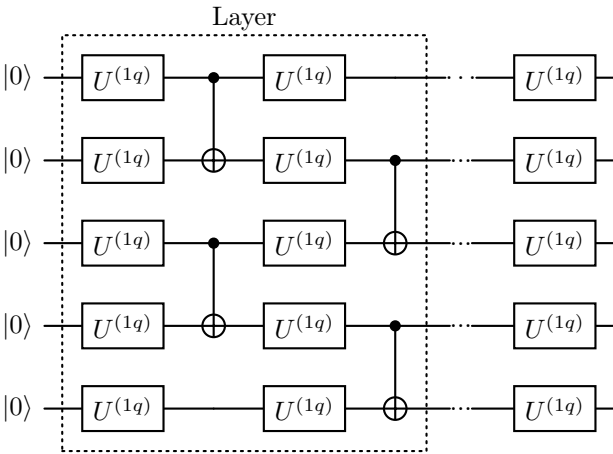
$$U_{\mathrm{HE}}(\boldsymbol{\theta}) = \prod_{q=1}^{N_q} U_q^{(1q)}(\boldsymbol{\theta}_{L+1q}) \times U_{\mathrm{ent}} \prod_{q=1}^{N_q} U_q^{(1q)}(\boldsymbol{\theta}_{Lq}) \times \cdots \times \underbrace{U_{\mathrm{ent}} \prod_{q=1}^{N_q} U_q^{(1q)}(\boldsymbol{\theta}_{1q})}_{\text{layer}}, \tag{8}$$

where N_q – number of qubits, $U_q^{(1q)}(\boldsymbol{\theta}_{lq})$ – single-qubit rotation gate, U_{ent} – non-parameterized entangling operator.
Initial state can be defined as follows:

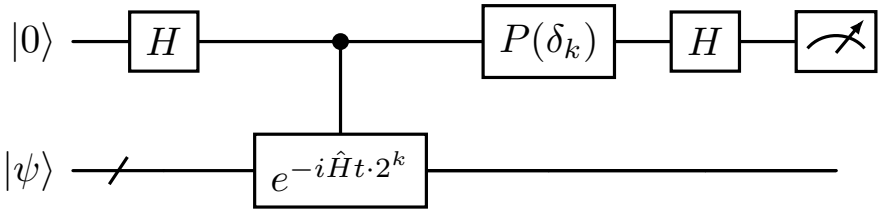
$$|\psi\rangle = |\mathbf{0}\rangle = |0\rangle^{\otimes N_q}. \tag{9}$$

Hardware-efficient ansatz





Iterative Quantum Phase Estimation



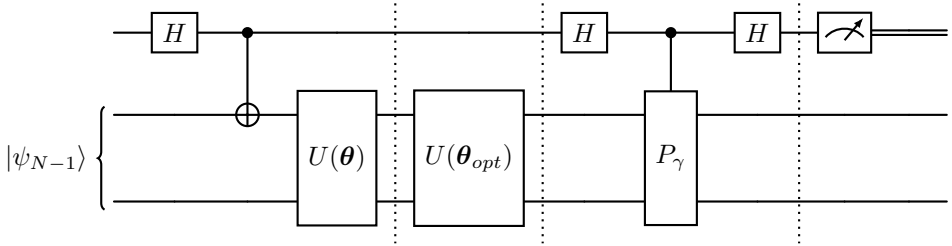
Suzuki-Trotter decomposition

$$e^{-iHt} = \left(e^{-i\sum\limits_n \gamma_n P_n \tau}\right)^{N_t} = \left(e^{-iH'\tau}\right)^{N_t} + O(t\tau), \tag{10}$$

where $\tau = t/N_t$, N_t – Trotterization depth, H' can be defined as follows

$$e^{-iH't} = \prod_n e^{-i\gamma_n P_n \tau}. \tag{11}$$

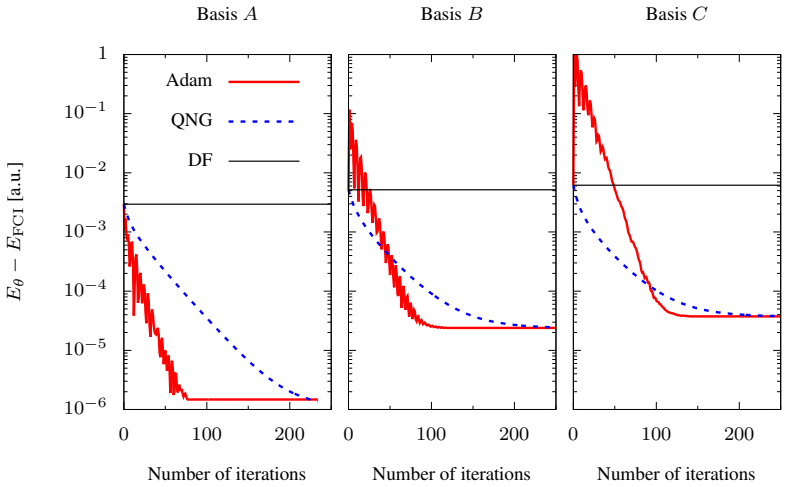
Algorithm for the direct calculation of the ionization energy



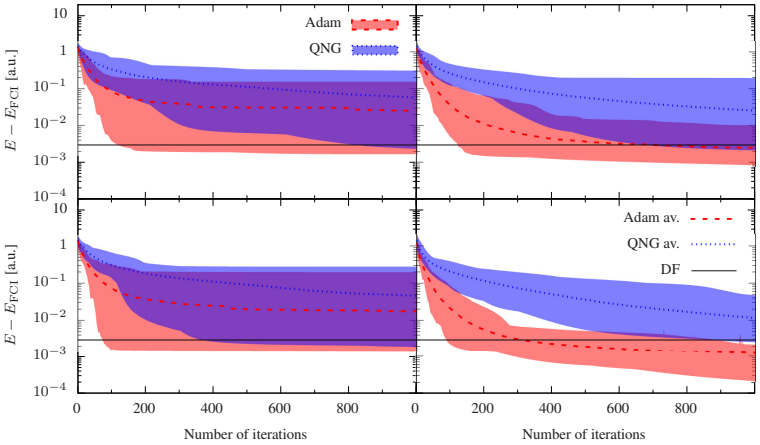
Radial orbitals

Basis	Radial orbitals	N_e	N_{orbs}	N_q
A	$\{7s, 7p_{1/2}, 7p_{3/2}\}$	5	8	6
B	$+\{8s, 8p_{1/2}, 8p_{3/2}\}$	5	16	14
C	$+\{6d_{3/2}, 6d_{5/2}\}$	15	26	24

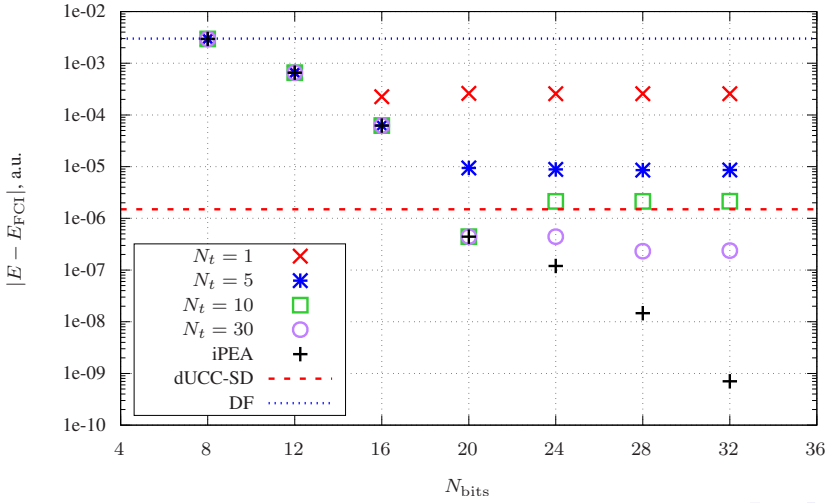
The difference between the expectation value of the VQE obtained with the use of the dUCC-SD ansatz and E_{FCI}



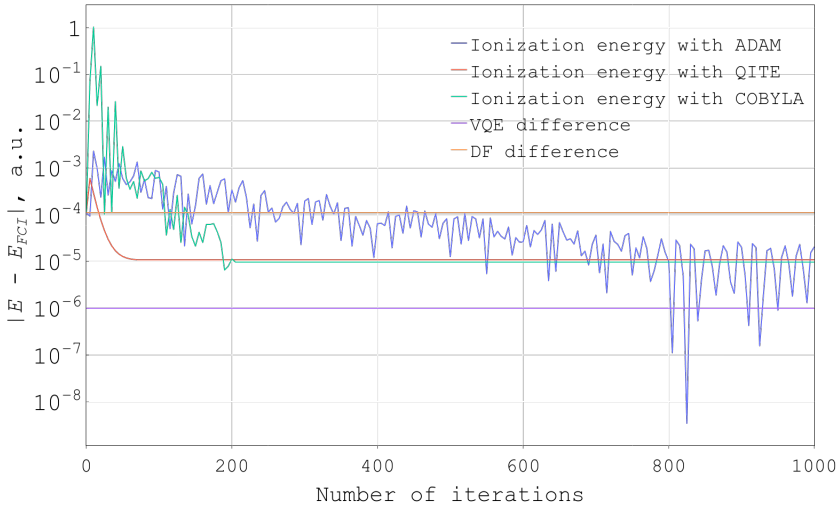
The difference between the expectation value of the VQE obtained with the use of the HE ansatz and E_{FCI}



The difference between the exact ground-state energy E_{FCI} and the energy obtained by iPEA



Ionization energy with use of dUCC-SD ansatz



Conclusions

- Hardware-Efficient ansatz doesn't allow to significantly improve the accuracy of the Dirac-Fock approximation.
- dUCC-SD allows one to obtain energy with the high precision in the relatively small number of optimization steps.
- Number of required gates for iPEA is several orders of magnitude larger than the number of gates required for the construction of the dUCC-SD ansatz.
- The algorithm of the ionization energy calculation implemented using simulator of quantum computer without noise allows obtaining a sufficiently accurate solution.