Calculation of the moscovium atom using quantum algorithms

Durova A. V., Zaytsev V. A., Maltsev I. A., Groshev M. E., Shabaev V. M.

St. Petersburg State University, St. Petersburg, Russia

15.05.2024

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

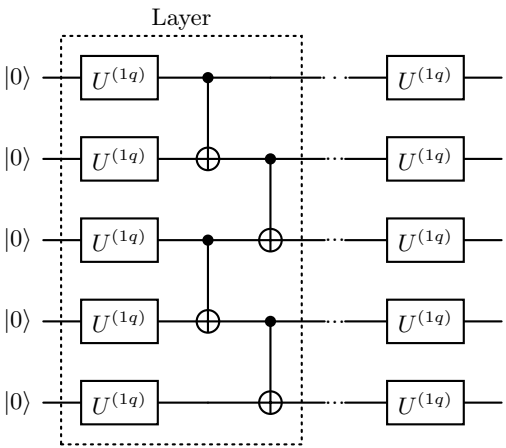
Hardware-efficient (HE) has the form

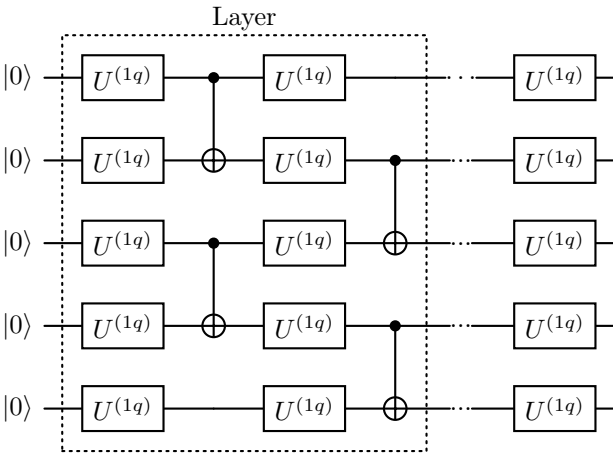
$$U_{\mathrm{HE}}(\boldsymbol{\theta}) = \prod_{q=1}^{N_q} U_q^{(1q)}(\boldsymbol{\theta}_{L+1q}) \times U_{\mathrm{ent}} \prod_{q=1}^{N_q} U_q^{(1q)}(\boldsymbol{\theta}_{Lq}) \times \cdots \times \underbrace{U_{\mathrm{ent}} \prod_{q=1}^{N_q} U_q^{(1q)}(\boldsymbol{\theta}_{1q})}_{\text{layer}}, \tag{8}$$

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:

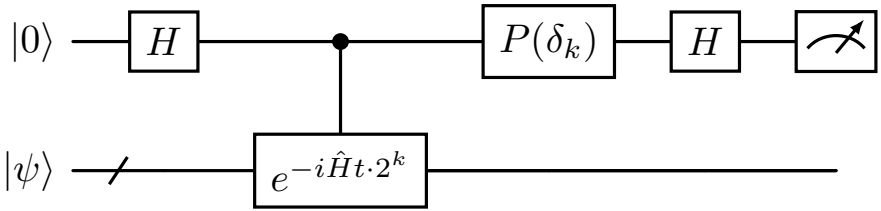
$$|\psi\rangle = |\mathbf{0}\rangle = |0\rangle^{\otimes N_q}. \tag{9}$$

Hardware-efficient ansatz





Iterative Quantum Phase Estimation



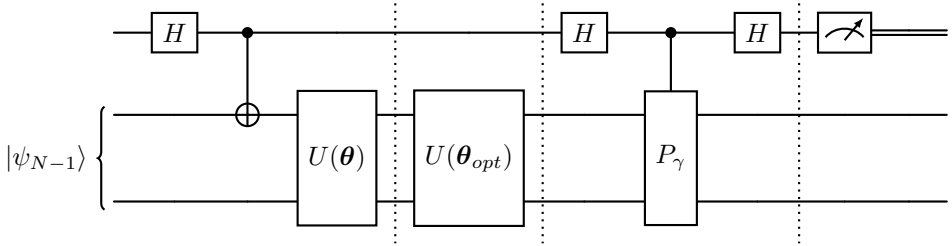
Suzuki-Trotter decomposition

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

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

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

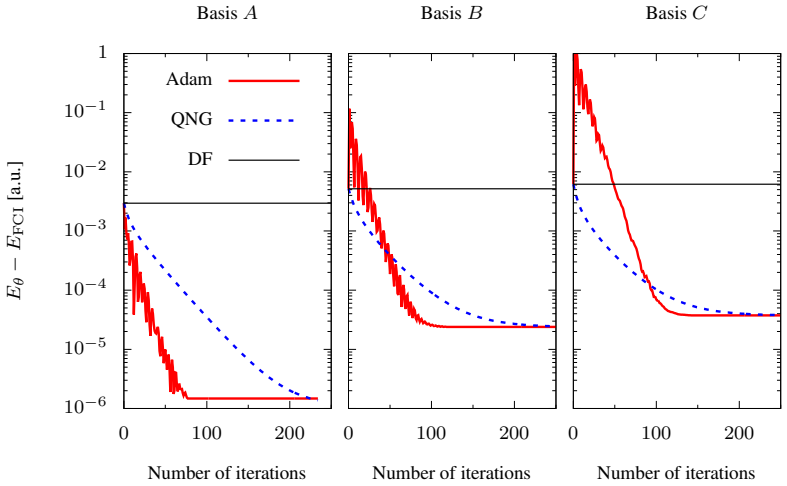
Algorithm for the direct calculation of the ionization energy



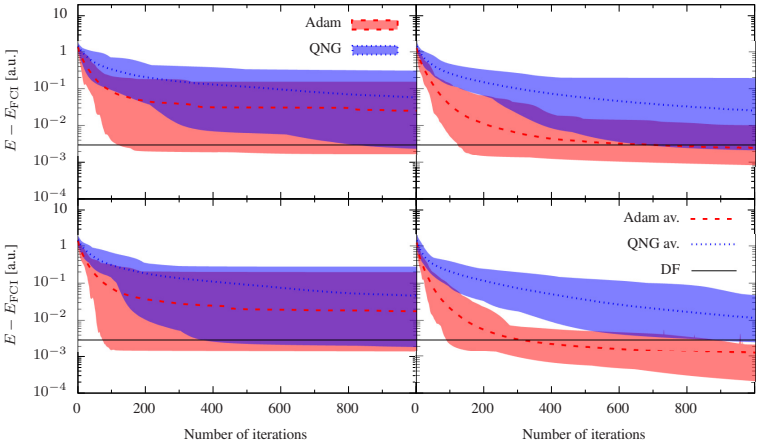
Radial orbitals

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

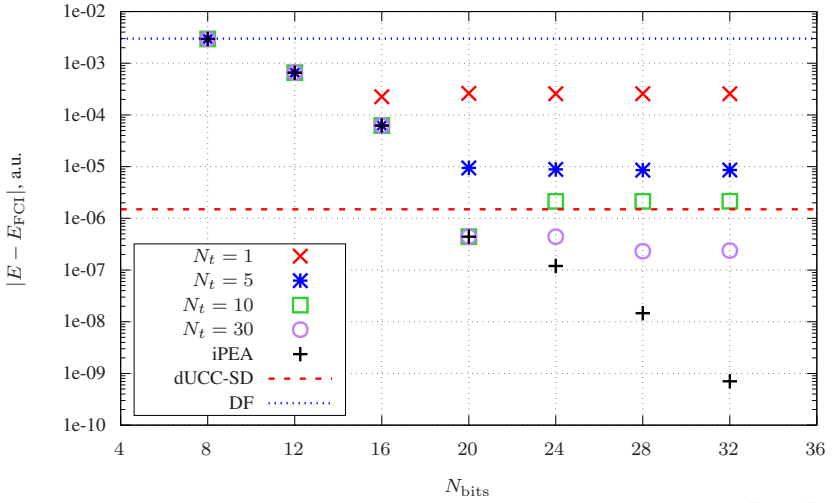
The difference between the expectation value of the VQE obtained with the use of the dUCC-SD ansatz and E_{FCI}



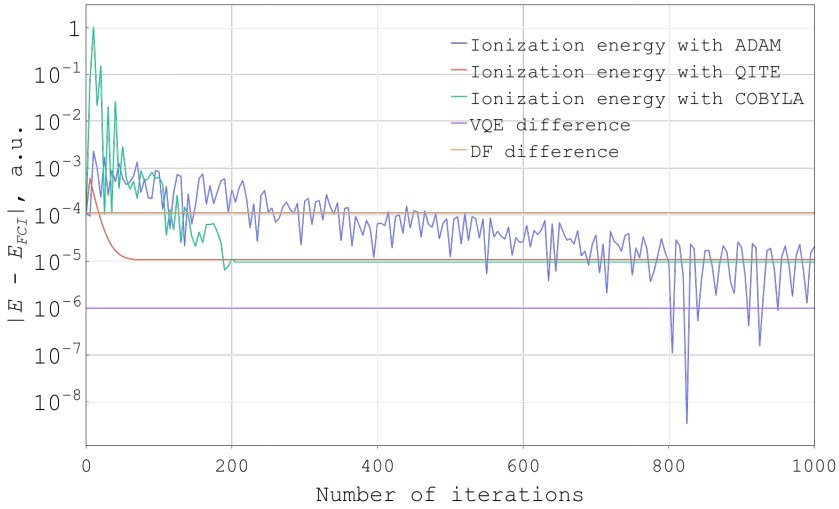
The difference between the expectation value of the VQE obtained with the use of the HE ansatz and E_{FCI}



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.