Molecular simulation with neutral atoms

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Abstract

We compute the ground state energy of small molecules on neutral-atom quantum computing platforms, comparing the digital and analog paradigms. The smart arrangement of the register makes the analog drive competitive with digital quantum computing.

In the near term, Rydberg atom devices are one of the most promising platforms to carry out useful quantum simulations and computations. Their programmable arrays of up to several hundreds atoms, the efficient control of interactions through the Rydberg blockade mechanisms and the precise control of single atom positioning allow the implementation of high-fidelity quantum gates, as well as the native evolution of the system as analog quantum simulators[1].

We investigate the behavior of variational quantum eigensolvers using both digital (gate-based) and analog approaches, extending the results obtained in[2], with the computation of ground-state energy of small molecules as target problem and benchmark. Both treatements are implmeneted at low (single pulse) level, using Pasqal's Pulser library[3].

In particular, in the digital case, instead of the usual UCC-like ansatzes, we implement some hardware-efficient ansatzes, using single-qubit rotations and native CZ entangling gates, exploiting the connectivity of the atomic register.

On the other hand, in the analog case, we realize a QAOA-like ansatz using alternating global pulses, corresponding to two non-commuting driving Hamiltonians $H_m = \frac{\hbar}{2}\sum_i \left(\Omega\hat{X}_i - \delta\hat{Z}_i\right)$ and $H_p = \frac{\hbar}{2}\sum_i \left(\Omega\hat{X}_i - \delta\hat{Z}_i\right)$, that are applied subsequently in different layers to construct the variational state $|\vec{\beta},\vec{\gamma}\rangle = \prod_{l=1}^{L} e^{-i\beta_l \hat{H}_M} e^{-i\gamma_l \hat{H}_P} |\psi_0\rangle$. Moreover, we strategically optimize the arrangement of atomic registers, tuning the Ising-like Rydberg-interaction term $H_{Ising} = \sum_{i<j} \frac{C_6}{r_{ij}^6}\hat{n}_i\hat{n}_j$ to specific features of the molecular Hamiltonian and problem constraints.

We further make use of the classical shadow estimation technique[4]. Our results demonstrate that energy estimates can be achieved with minimal error, typically within a few percentage points.

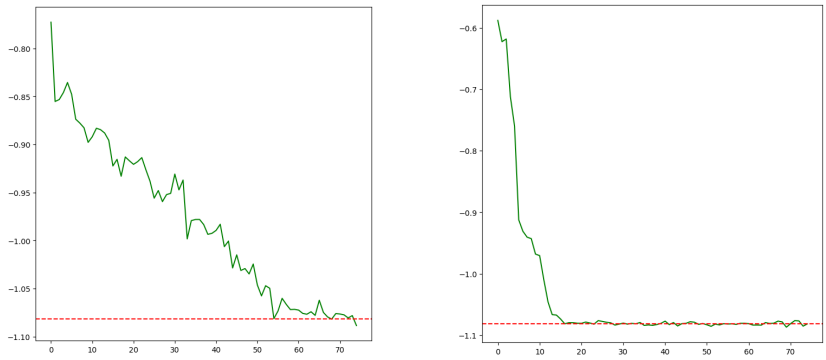

Figure 1: Estimated ground-state energy of the LiH molecule during the optimization process, in the analog case (right) and digital case (left).

References

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