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Strategies for solving the Anderson model via Quantum Computer

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Summary. — We apply the Variational Quantum Eigensolver to the study of the periodic Anderson model in the atomic limit. After presenting the steps necessary for the implementation of the algorithm, such as the fermionic mapping of the Hamiltonian and the construction of the variational ansatz, we will discuss the results obtained by simulations carried out using resources provided by IBM, as well as the performance of the chosen ansatz for the considered system, in ideal and noisy environment. Finally, we apply a simple mitigation scheme to the noisy scenario to improve the algorithm's accuracy.

1. – Introduction

The Variational Quantum Eigensolver (VQE) [1] is a quantum-classical algorithm used to estimate the ground state energy of physical systems. In particular, its hybrid structure is believed to be useful for problems whose complexity scales exponentially with the system size. Several applications of this algorithm to relevant physical systems, such as Heisenberg [2] and Hubbard [3] models, have been presented in the past years. Here, we apply the VQE to the Anderson impurity model, which describes a rich physics linked to several relevant phenomena ranging from magnetism to unconventional superconductivity to topological properties [4, 5]. The paper is organized as follows: in sect. **2** we introduce the Anderosn model together with a brief description of the algorithm employed to solve the above mentioned model, as well as the principal steps required for an efficient implementation, such as the fermionic mapping and the construction of the variational ansatz. In sect. **3** we discuss the result obtained from simulations with and without quantum noise while the conclusions are summarized in sect. **4**.

2. – Model and methods

We will apply the VQE algorithm to the study of the Anderson Model [6] in its *atomic limit*, which in the case of a single impurity is described by the following Hamiltonian:

$$\begin{aligned}\hat{H} =& \hat{H}_c + \hat{H}_f + \hat{H}_{Coul} + \hat{H}_{hyb} \\ =& \varepsilon_c \sum_\sigma \hat{c}^\dagger_\sigma \hat{c}_\sigma + \varepsilon_f \sum_\sigma \hat{f}^\dagger_\sigma \hat{f}_\sigma + U \hat{n}_{f\uparrow} \hat{n}_{f\downarrow} + V \sum_\sigma \left(\hat{c}^\dagger_\sigma \hat{f}_\sigma + \hat{f}^\dagger_\sigma \hat{c}_\sigma \right),\end{aligned} \tag{1}$$

where $\hat{c}_\sigma$ and $\hat{f}_\sigma$ are fermionic operators for conduction and localized electrons respectively, with σ representing the electron's spin. To efficiently apply the VQE we first recast the second quantized Hamiltonian (1) in terms of Pauli spin operators. This can be achieved using Jordan-Wigner mapping [7] after a suitable choice of the ordering for generic state vector for the system; we specifically choose the following ordering: $|c_\uparrow f_\uparrow f_\downarrow c_\downarrow\rangle$. The construction of the variational ansatz represents a crucial choice for the implementation of VQE: here, we used the Hamiltonian Variational Ansatz (HVA) [8]. We propose the following form for the HVA circuit [9, 10]:

$$|\psi(\boldsymbol{\theta})\rangle = \prod_{l=1}^{L}\prod_{\alpha=1}^{4} \exp\left[i\theta_{\alpha,l}\hat{H}_\alpha\right]|\psi_0\rangle, \tag{2}$$

where the $\{\hat{H}_\alpha\}$ are the terms in Hamiltonian (1), $l = 1, \ldots, L$ is the number of circuit layers and $\{\theta_{\alpha,l}\}$ is the set of variational parameters. The initial state $|\psi_0\rangle$ is chosen as the ground state of the $\hat{H}_{hyb}$ term since it has the same quantum numbers as the ground state of the complete model, thus allowing to search for the energy minimum in a restricted subspace of the whole system's Hilbert space. On real quantum devices, computation is always affected by the presence of quantum noise. It is possible to mitigate these effects using internal symmetries of the system: indeed, if one finds a unitary operator $\hat{S}$ such that $[\hat{H}, \hat{S}] = 0$, then it is possible to define a *symmetry-verified* state $\hat{\rho}_s$ by projecting the noisy state $\hat{\rho}$ onto a subspace $\mathcal{S}$ of $\hat{S}$ [11]. For the Anderson Hamiltonian we applied this mitigation scheme choosing the fermion parity as unitary symmetry, described by the operators $\hat{S}_\sigma = (-1)^{\sum_i \hat{n}_{i,\sigma}}, \sigma \in \{\uparrow, \downarrow\}$.

3. – Experimental setup and results

Simulations were performed using the following values for the microscopic parameters of the model: $\varepsilon_c = 0, \varepsilon_f = -1, U \in \{1, 3, 5\}, V \in (0, 1]$. To be specific, in what follows we present results referring to the case with $U = 3$ and V ranging from $V_{min} = 0.1$ to $V_{max} = 1$ with steps $\Delta V = 0.1$. Computation has been carried out using the IBM-Qiskit Python library to simulate the behavior of both ideal and noisy quantum devices. Moreover, we employed Bayesian optimization [12] as the minimization routine. The analysis focuses on the convergence of the algorithm's estimation of the ground state energy as well as on the relative error achieved. Furthermore, we studied the capacity of the algorithm to extract the correct ground state by evaluating its fidelity $\mathcal{F} = \mathrm{Tr}(\sqrt{\sqrt{\hat{\rho}}\hat{\sigma}\sqrt{\hat{\rho}}})^2$, where $\hat{\sigma} = |\psi_{exact}\rangle\langle\psi_{exact}|$ is the exact ground state. For values of $\mathcal{F} \geq 0.99$, we can conclude that the algorithm has successfully found the exact ground state.

3˙1. *Ideal simulations.* – In ideal environment we neglect the effects of quantum noise on the computation and we only consider the errors coming from a limited number of measurements on the output state of the quantum computer at each iteration of the algorithm. The proposed ansatz for the model is then capable of obtaining a good accuracy of the energy estimation, with a relative error of $E_r \lessapprox 2\%$ on average using only one layer, as shown in fig. 1(a). Raising the number of layers to $L = 2, 3$ gives a similar result and a similar relative error but in these cases, convergence is reached in a slightly higher number of iterations due to the increase of variational parameters to be optimized. Focusing on the output state of the algorithm, we can see in fig. 1(b) how the fidelity varies throughout the optimization process. We can see that for every layer

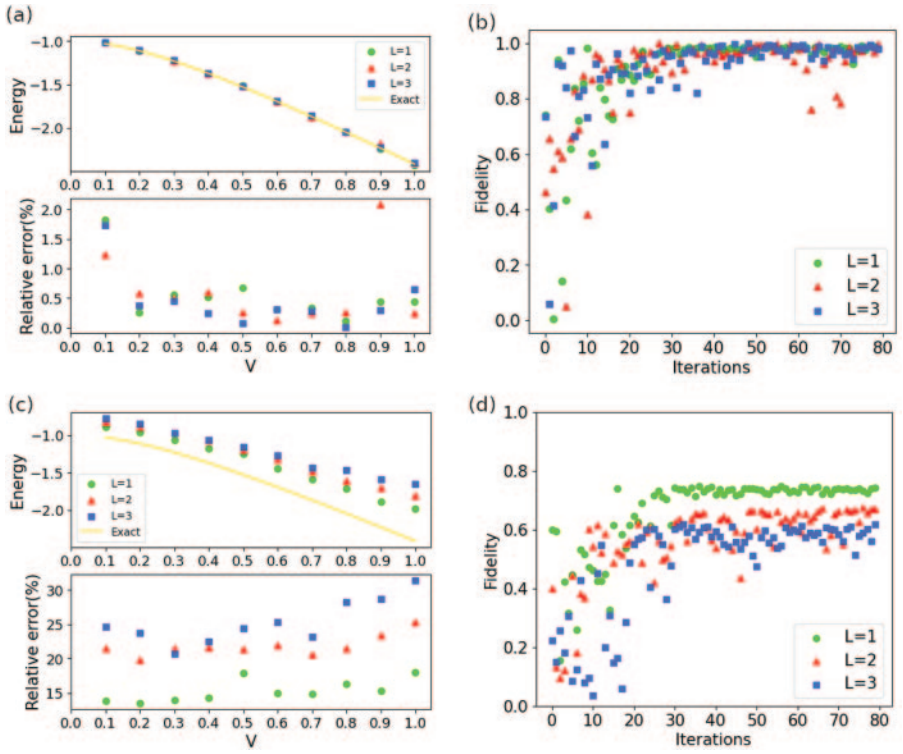

Fig. 1. – Results of the algorithm for the Anderson model: ground state energy and relative error in (a) ideal environment and (c) noisy environment. For $V = 0.5$: evolution of ground state fidelity during the optimization process in (b) ideal environment and in (d) noisy environment.

the estimated optimal state reaches a fidelity of $\mathcal{F} \geq 0.99$, thus we can conclude that the algorithm can find the exact ground state for the chosen model and the chosen set of microscopic parameters.

3˙2. *Noisy simulations*. – Noisy simulations have been performed using a noise model generated from the calibration data of the quantum computer "Osaka" of IBM. Due to the noise, mostly coming from the entangling CNOT gates, the ansatz is now unable to search for the energy minimum in the selected subspace of the total system's Hilbert space. As a consequence, the fidelity of the output state reaches its maximum at $\mathcal{F} \approx 0.74$ for $L = 1$, with decreasing values for higher layers number, see fig. 1(d). The relative error achieved on the energy estimation is shown in fig. 1(c). We can see that for $L = 1$ the relative error is already $E_r \approx 15\%$ and the scenario worsens in the $L = 2, 3$ cases due to the higher number of CNOT gates required. We reduced the effect of noise using the symmetry verification scheme, which allowed us to improve the accuracy of the result obtaining a final relative error on the energy of $E_r^{mit} \lessapprox 10\%$ in almost all cases, as can be seen in fig. 2(a). The same improvement trend can be seen in the fidelity of the output state, depicted in fig. 2(b), which now reaches its maximum at $\mathcal{F} \approx 0.91$.

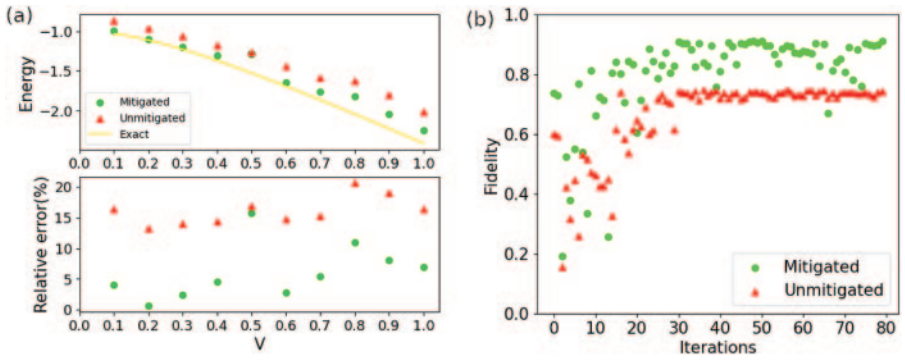

Fig. 2. – Comparison between the noisy cases for $L = 1$: (a) ground state energy and relative error; (b) evolution of ground state fidelity during the optimization process for $V = 0.5$.

4. – Conclusions

We have shown how to apply the Variational Quantum Eigensolver to the study of the Anderson model using the Hamiltonian Variational Ansatz. We have seen that the HVA, in ideal environment, can find the ground state energy of the model with high accuracy. Moreover, it is also possible to achieve a high fidelity on the corresponding ground state. The quality of the results drastically changes in noisy simulations; however, using a mitigation scheme, we were able to improve both energy estimation and fidelity for the ground state and its energy. Considering the results obtained, we plan to investigate the behavior of the algorithm under the effect of quantum noise varying the ansatz circuit and classical optimization routine. Furthermore, we plan to extend the analysis to lattices with different geometries as well as to the calculation of the excited states.

REFERENCES

[1] Peruzzo A. *et al.*, *Nat. Commun.*, **5** (2014) 4213.
[2] Villani L. *et al.*, *Testing the variational quantum eigensolver on the four-site Heisenberg model*, in *2023 IEEE Nanotechnology Materials and Device Conference (NMDC)* (IEEE) 2023, pp. 740–745.
[3] Stanisic S. *et al.*, *Nat. Commun.*, **13** (2022) 5743.
[4] Skolimowski J. *et al.*, *Phys. Rev. B*, **109** (2024) 075147.
[5] Dzero M. *et al.*, *Annu. Rev. Condens. Matter Phys.*, **7** (2016) 249.
[6] Noce C., *Phys. Rep.*, **431** (2006) 173.
[7] Jordan P. and Wigner E., *Z. Phys.*, **47** (1928) 631.
[8] Wecker D. *et al.*, *Phys. Rev. A*, **92** (2015) 042303.
[9] De Riso G. *et al.*, *New J. Phys.*, **26** (2024) 063041.
[10] De Riso G. *et al.*, *Simulating Kondo quantum dots on NISQ devices*, in *2023 IEEE Nanotechnology Materials and Devices Conference (NMDC)* (IEEE) 2023, pp. 735–739.
[11] Bonet-Monroig X. *et al.*, *Phys. Rev. A*, **98** (2018) 062339.
[12] Frazier P.I., *A Tutorial on Bayesian Optimization*, arXiv:1807.02811v1 (2018).