|VI WECIQ>

VI Workshop Escola de Computação e Informação Quântica

Subspace-Search Variational Quantum Eigensolver (SSVQE) as a tool in materials science, a benchmark

Raphael César de Souza Pimenta[1], **Anibal Tiago Bezerra**[2]

[1]Universidade Federal de Santa Catarina, SC, Brasil

[2] Universidade Federal de Alfenas, MG, Brasil

anibal.bezerra@unifal-mg.edu.br[2]

Abstract

We present an analysis on quantum simulations of k·p Hamiltonians applying the SSVQE hybrid algorithm. Using the PennyLane framework we estimate the ground and excited states for different materials of interest. Also, we make a benchmark of the viability of NISQ computers to perform band structure calculations. Our results showed the time and number of cycles needed to run the algorithm with NISQ technology are not competitive with classical simulations. Nevertheless, the k·p approximation allows for the use of shallow circuits, with limited number of qubits, which is beneficial to deal with nowadays quantum computers.

Keywords Quantum Computing, Semiconductor Band Structure, k·p method

Introduction

- Materials science is benefited by simulations, shortening devices' development time;
- Increasing the system size is a challenging for classical algorithms. Simulation time grows exponentially with number of constituents;
- Quantum computers can potentially reduce simulation times, with polynomial growth;
- Nowadays quantum technology - NISQ (Noise Intermediate Quantum) - is a reality, and can be tested, but are limited to be employed with shallow algorithms;
- Mapping the system with k·p can be a solution to represent periodic systems.

Objectives

We aimed to benchmark the viability of the use of NISQ computers to evaluate band structure of semiconductor periodic structures using k·p Hamiltonians.

Subspace Search Variational Quantum Eigensolver (SSVQE)

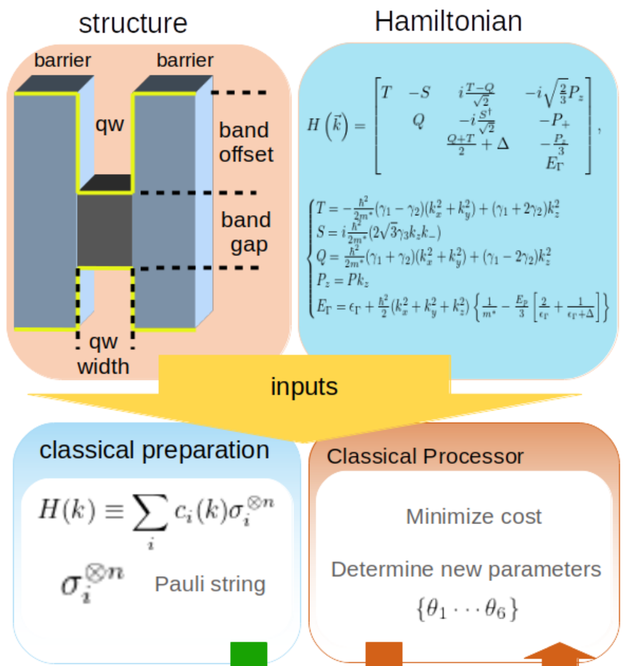

Figura 1: SSVQE framework

- Variational Quantum Eigensolver (VQE) methods form a class of hybrid quantum-classical algorithm showed to obtain the ground states using NISQ computers (1);
- Excited states require a specialized VQE, namely the SSVQE method (2);
- **p**-copies of the quantum circuit are initialized with p-orthogonal states $|\psi_p\rangle = |\psi\rangle^{\otimes n}$. **p** is the desired number of excited states;
- A weighted cost function is minimized iteratively using both the quantum and classical processor, returning a set of optimized parameters;
- Once the minimization attains to a minimum, the ansatz becomes unitary mapping the states $|\psi_p\rangle$ to the orthonormal eigenstates of the Hamiltonian.

Results

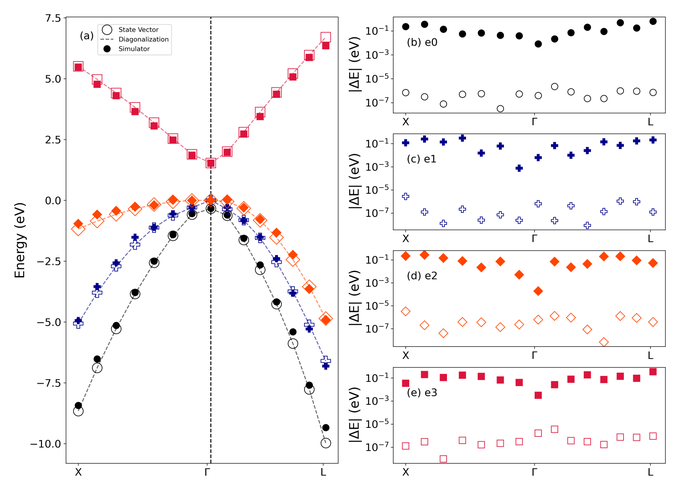

Figura 2: (a) GaAs band structure for the conduction band (red squares), and heavy hole (blue pluses), light hole (orange diamonds) and split-off (black circles) states, evaluated using the state vector solver (open symbols), the probabilistic simulator (full symbols), and numerical diagonalization (dashed lines). Error for the state vector solver (open symbols), and the probabilistic simulator (full symbols) for (b) split-off band, (c) heavy hole band, (d) light hole, and (e) conduction band.

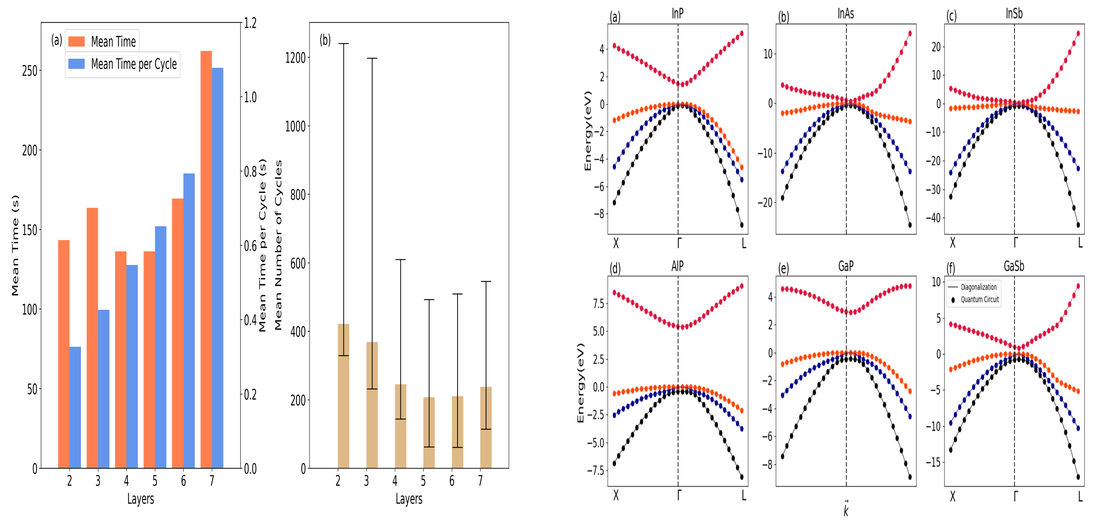

Figura 3: [Left](a) In orange, mean time in seconds for convergence of each point in the k-path and in blue the mean time to complete each cycle of convergence attempt. (b) Filled bars is the mean number of cycles to complete the convergence, thin black bars represent the maximum and minimum number of cycle for a point. [Right] Simulation for 6 other band structures

Conclusions

We presented an evaluation of feasibility and benchmark of the use of quantum computers in favor of materials problems, in special the calculation of band structures of periodic semiconductors compounds. We employed the exact state vector solver and the real device simulator. In comparison to direct diagonalization of the Hamiltonian both machines were able to return the band structure of a couple of semiconductor structures. The simulation time is directly dependent on the ansatz depth and the diagonalization method. The results showed the possibility of simulating semiconductor band structures, however the time used in the simulations is still not competitive with the classical solution. Notwithstanding, the use of k·p method allows for shallow circuits, which is mandatory with NISQ computers.

Referências

[1] Peruzzo, A., McClean, J., Shadbolt, P., Yung, M.-H., Zhou, X.-Q., Love, P. J., Aspuru-Guzik, A., and O'brien, J. L. *A variational eigenvalue solver on a photonic quantum processor*. Nature communications 5, 1 (2014), 1–7

[2] Nakanishi, Ken M and Mitarai, Kosuke and Fujii, Keisuke. *Subspace-search variational quantum eigensolver for excited states*. Physical Review Research, 1 (2019)

Acknowledgments

We acknowledge the use of IBM Quantum services for this work. The views expressed are those of the authors, and do not reflect the official policy or position of IBM or the IBM Quantum team. Our special thanks to the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and to the Fundação de Amparo à Pesquisa e Inovação do Estado de Santa Catarina (FAPESC) for providing resources to this research.