Implementation of Quantum Machine Learning for Electronic Structure Calculations of Periodic Systems on Quantum Computing Devices

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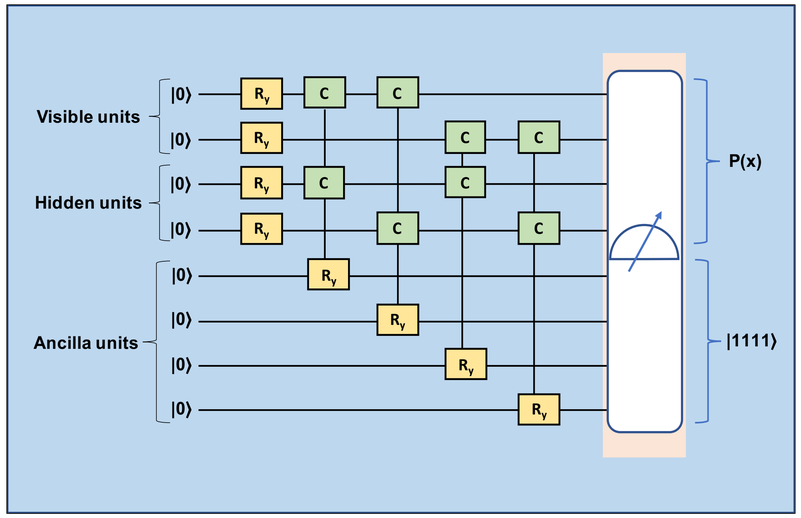
Abstract

- Quantum Machine Learning (QML): The interplay of machine learning techniques with quantum computation.
- QML provides tantalizing prospects to solve quantum many-body problems by reducing the large complexity of the wavefunction.
- Solving the quantum many-body problem accurately is an important task for the advancement of material science and chemistry.
- Electronic structure calculations has been considered as one among the first real applications of a quantum computer.
- Thus, solving for the electronic structure of materials using machine learning on a quantum computer paves the way for further advancement of the domain of quantum chemistry.
- Here, we implement the benchmark test of a hybrid quantum machine learning algorithm on the IBM-Q quantum computer to calculate the electronic structure of typical 2-dimensional crystal structures: hexagonal-Boron Nitride (h-BN) and graphene.

Gibbs Sampling

- The quantum circuit to sample Gibbs distribution is shown in the figure.
- The quantum circuit consists of a single qubit rotation (R_y) and a controlled-controlled rotation operations ($C-C-R_y$).
- The angle by which the R_y operation rotates is determined by the visible and hidden bias parameters a_i and b_j. The angle by which the $C-C-R_y$ operation rotates, is determined by the weights connecting the visible and hidden layers w_{ij}.
- The target qubits for the controlled-controlled Rotations are the ancilla qubits. Once all the rotations are completed, the ancilla qubits are measured. If the ancilla qubits are in $|1\rangle$, then the sampling is deemed successful. Then, the final states corresponding to the visible and hidden units provide the distribution *P(x)*.
- With *P(x)* computed through the QML algorithm and *s(x)* computed classically, the wavefunction $|\Psi\rangle$ is computed and through this the energy expectation value is obtained. This value of the energy expectation value is optimized through gradient descent until the eigenvalue of the Hamiltonian is obtained.

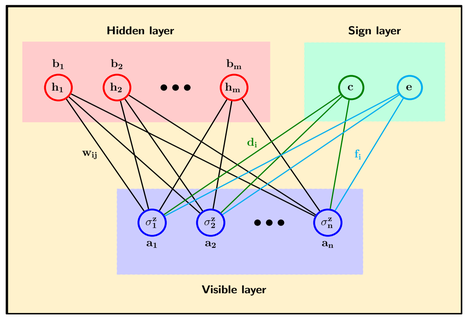


Conclusion

- The primary goal of this study was to examine the performance of an RBM on Noisy Intermediate-Scale Quantum (NISQ) devices in order to calculate the electronic structure of materials.
- By using an RBM and a quantum circuit to sample Gibbs distribution, the electronic structures for h-BN and graphene were obtained.
- For this algorithm, the number of qubits required scales as *O(mn)* and the complexity of the gates turns out to be *O(mn)* for one sampling.
- With the field of quantum computing developing rapidly, the curiosity of combining machine learning and quantum computing has led to very interesting researches.
- The development of quantum computers and their capability scaling very fast, quantum machine learning can prove to be useful in not only electronic structure methods, but also as a significant tool in developing new materials and understanding complex phenomena.

Methodology

- Here, a three-layered Restricted Boltzmann Machine (RBM) is used.



- In contrast with the conventional RBMs, which contain just visible and hidden layers, the three-layered RBM contains a visible, a hidden and a sign layer.
- The sign layer is added in order to consider the real and imaginary values of the wavefunction of a quantum state.
- The wavefunction can be expressed as:

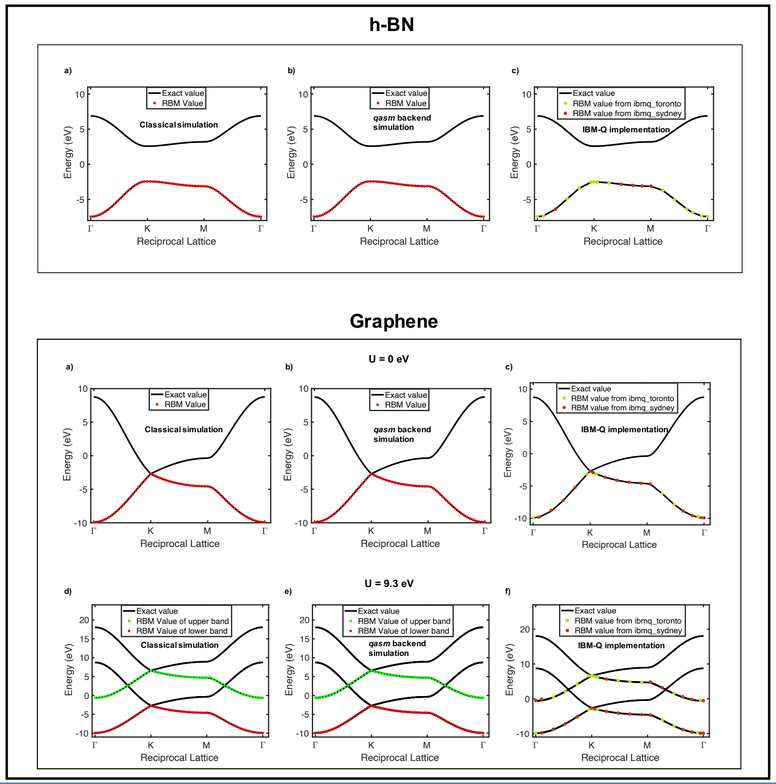
$$|\Psi\rangle = \sum_x \sqrt{P(x)}\, s(x)|x\rangle$$

$$P(\mathbf{x}) = \frac{\sum_{\{h\}} e^{\sum_i a_i \sigma_i^z + \sum_j b_j h_j + \sum_{ij} w_{ij} \sigma_i^z h_j}}{\sum_{x'} \sum_{\{h\}} e^{\sum_i a_i \sigma_i^z + \sum_j b_j h_j + \sum_{ij} w_{ij} \sigma_i^z h_j}}$$

$$s(x) = tanh\left(\left(c + \sum_i d_i \boldsymbol{\sigma}_i\right) + i\left(e + \sum_i f_i \boldsymbol{\sigma}_i\right)\right)$$

Results

- The electronic structures of h-BN and graphene are shown in the figure.
- The implementation was done in three parts:
- Firstly, the QML algorithm was implemented classically. (Classical simulation implies that the gates were simulated on a classical computer).
- Then, the implementation is carried out using Qiskit, which is IBM's Quantum Information Software Kit. Specifically, the algorithm was implemented on the *qasm* backend, which is a high-performance quantum circuit simulator.
- Finally, the implementation of this procedure is demonstrated on the actual IBM-Q quantum computers('*ibmq_toronto*' and '*ibmq sydney*', both of which are 27 qubit devices).
- For the case of h-BN, the tight binding Hamiltonian is considered.
- For graphene, the Hubbard model is taken as the Hamiltonian.
- Initially, the electronic structure is computed for the case when the Hubbard on-site interaction U = 0 eV.
- Then, the band splitting in graphene is shown when U = 9.3 eV.
- The number of qubits required:
  - 2 qubits for visible units (n)
  - 2 qubits for hidden units (m)
  - 4 ancilla qubits (n+m)
- The number of gates:
  - 4 single-qubit rotations (n+m)
  - 4 Controlled-Controlled rotations (n×m)
  - 24 X(bit-flip) gates (6 × n×m)



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