Quantum Machine-Learning for Complex many-Body Systems on Quantum Devices

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Abstract :

In this talk, I will focus on quantum machine learning, particularly the Restricted Boltzmann Machine (RBM), as it emerged to be a promising alternative approach leveraging the power of quantum computers. Such algorithms have been developed to solve problems like electronic structure calculations of molecular systems and spin models in magnetic systems. Herein we demonstrate a quantum algorithm that can filter any energy eigenstate of the system based on either symmetry properties or a predefined choice of the user. The workhorse of our technique is a shallow neural network encoding the desired state of the system with the amplitude computed by sampling the Gibbs−Boltzmann distribution using a quantum circuit and the phase information obtained classically from the nonlinear activation of a separate set of neurons. We implement our algorithm not only on quantum simulators but also on actual IBM-Q quantum devices and show good agreement with the results procured from conventional electronic structure calculations. We thus expect our protocol to provide a new alternative in exploring the band structures and dynamics of exquisite quantum materials.

"Quantum Machine Learning for Electronic Structure Calculations"
Xia, Rongxin; Kais, Sabre, *Nature Comm*. 9, 4195 (2018)
"Implementation of Quantum Machine Learning for Electronic Structure Calculations of Periodic Systems on Quantum Computing Devices", Sureshbabu, Shree Hari; Sajjan, Manas; Oh, Sangchul; Kais, Sabre, *J. Chem. Inf.* 61, 2667 (2021).
"**Quantum Machine-Learning for Eigenstate Filtration in Two-Dimensional Materials",** Manas Sajjan, Shree Hari Sureshbabu, Sabre Kais, *JACS* 143, 44, 18426 (2021).

"Quantum Machine Learning for Chemistry and Physics"
Manas Sajjan, Junxu Li, Raja Selvarajan, Shree Hari Sureshbabu, Sumit Suresh Kale, Rishabh Gupta, Vinit Singh and Sabre Kais, *Chemical Society Reviews,* (in press 2022).

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