Neural Network and Its Applications to Emergent Quantum Phenomena

Tuesday, 26 August 2025 11:00 (1 hour)

I overview recent progress in explorations on efficient algorithms and their applications of neural network for strongly correlated electron systems. For correlated electron systems, restricted Boltzmann machines combined with the pair-product wavefunctions have shown a state-of-the-art accuracy among other quantum many-body solvers [1,2]. They have contributed to understanding of quantum spin-liquid phase in frustrated quantum spin models [2]. Not only to simplified theoretical models, the applications of the restricted Boltzmann machine to real materials with ab initio calculations have succeeded in reproducing detailed materials dependence as well as universality of physical properties observed in experiments for superconductivity in a number of high-Tc cuprate superconductors [3,4] and for quantum spin liquids in organic salts [5], which demonstrates that the AI has become NOT the level of the benchmark tests BUT a productive useful tool to uncover physics of challenging emergent quantum matter. It has also contributed to reveal the mechanisms of superconductivity and quantum spin liquids, which also enable to proceed to materials design by parameter search beyond ab initio calculations.

In the Boltzmann machine, the hidden variables are classical, in which the structure of the quantum entanglement is hidden and elusive as a black box. I also address recent attempts to quantize the hidden variable by using fermionic variables to make the entanglement structure more transparent and the solver more accurate, which has been made possible by enjoying the fractionalization of electrons discovered in the preceded Boltzmann machine simulations [6,7].

- [1] Y. Nomura. A. S. Darmawan, Y. Yamaji, M. Imada, Phys. Rev. B 96, 205152 (2017).
- [2] Y. Nomura, M. Imada, Phys. Rev. X, 11, 031034 (2021).
- [3] J.-B. Moree, M. Hirayama, M. T. Schmid, Y. Yamaji, M. Imada, Phys. Rev. B, 106, 235150 (2022).
- [4] M. T. Schmid, J.-B. Moree, R. Kaneko, Y. Yamaji, M. Imada, Phys. Rev. X, 13, 041036 (2023).
- [5] K. Ido, K.Yoshimi, T. Misawa, M. Imada npj Quantum Mater, 7, 48 (2022).
- [6] M. Imada, J. Phys. Soc. Jpn. 90, 111009 (2021).
- [7] M. Imada, J. Phys. Soc. Jpn. 93, 104002 (2024).

Primary author: Prof. IMADA, Masatoshi (Sofia University)

Presenter: Prof. IMADA, Masatoshi (Sofia University)

Session Classification: Invited talk

Track Classification: Invited talk