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Ab-initio study of interacting fermions at finite temperature with neural canonical transformation

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Summary for general readers:
Accurate prediction of thermal properties of quantum matter has been a challenging task in physics. At finite temperatures, Nature tries to balance the energy and entropy to bring physical systems into a minimal free energy state. Ironically, it was rather difficult to turn such a free energy minimization principle into a practical algorithm to simulate quantum matters, especially those consisting of fermionic particles. Such a difficulty is mainly due to the prohibitive cost associated with entropy calculation in the free energy, also known as the "intractable" partition functions problem. The present work makes such a variational calculation possible by capitalizing on the latest advances in generative machine learning.

Generative machine learning aims at modeling, learning, and sampling from high-dimensional probability distributions. To achieve these goals, the machine learning community has developed a variety of expressive neural network models with tractable partition functions. By jointly optimizing two generative models, one for the classical Boltzmann distribution and one for the quantum wavefunction, the authors successfully solved a system of a few electrons in a quantum dot. Further applications of the approach to prototypical quantum matters such as the uniform electron gas and dense hydrogen have offered new insights into these problems. In addition, this paper is also an example of how physical principles should be integrated with machine learning techniques.

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