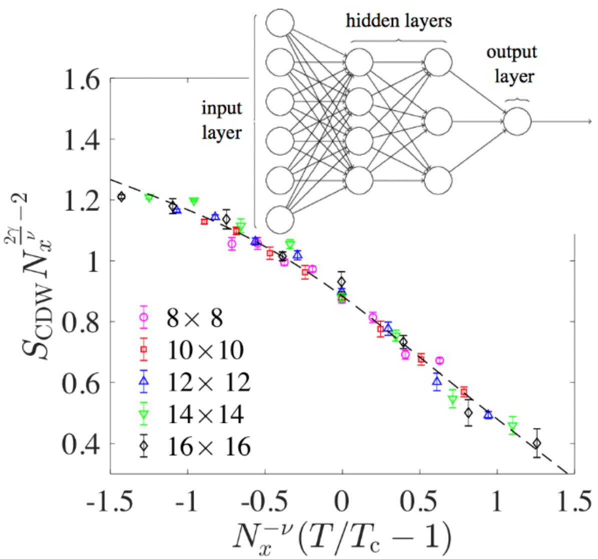
AI accelerates lattice quantum Monte Carlo simulations



A thermodynamic scaling analysis of the charge density wave structure factor of the half-filled two-dimensional Holstein model in proximity to the metal-to-CDW insulator transition T_c, which demonstrates that the transition belongs to the Ising universality class. Data were obtained using an ANN sampling algorithm. The ANNs for this simulation were taught *both* an underlying effective physics model and its parameters using training examples generated by the conventional determinantal QMC algorithm on smaller inexpensive 6×6 lattices before being scaled to larger lattices.

Reference: S. Li, P. M. Dee, E. Khatami, and S. Johnston, “Accelerating lattice quantum Monte Carlo simulations using artificial neural networks: Application to the Holstein model,” *Physical Review B* **100,** 020302(R) (2019).

Scientific Achievement

Researchers have designed artificial neural networks (ANNs) that predict with near-perfect accuracy state change probabilities in quantum Monte Carlo (QMC) simulations of many-body Hamiltonians and obtain an order of magnitude reduction in the run time.

Significance and Impact

Demonstration that machines can learn to perform efficient QMC simulations—without an underlying physics model and given only limited information about the configuration space—means the method can be easily generalized even to other challenging models, such as the Fermi-Hubbard model.

Research Details

- ANNs were designed to predict *local* and *global* state changes in determinantal QMC simulations of the Holstein model.
- This development in artificial intelligence (AI) granted access to large systems at low-temperatures, overcame long autocorrelation times for the model, and facilitated a thermodynamic scaling analysis.

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