Boosting quantum many-body simulations via deep neural networks

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Abstract: We employ neural networks to boost many-body simulations based on Monte Carlo and on density functional theory, allowing simulating the spin-glass quantum phase transition. We explore how this transition could be observed with Rydberg atoms.

Quantum simulators based on Rydberg atoms in optical tweezers or on ion traps present us with new challenging quantum many-body problems. Here, we discuss how deep learning techniques can be used to boost the efficiency of computational techniques such as quantum Monte Carlo algorithms and density functional theory. This strategy allows us simulating the ground state or the dynamical properties of quantum spin models with frustrated interactions, which can be implemented in quantum-simulation platforms.

In a first example, we show that generative neural networks allow boosting projection quantum Monte Carlo algorithms, so that the spin-glass quantum phase transition can be efficiently simulated. We study the critical properties of the two-dimensional Edwards-Anderson model [1] (see Fig. 1), and we explore the possible occurrence of spin-glass phases with positional disorder realizable in Rydberg-atom platforms.

In the second example, we show that deep neural networks can learn universal energy-density functionals [2,3]. Thanks to an appropriately designed scalable network architecture, the learned functional allows one to simulate larger spin models than those used for training. Furthermore, dynamical simulations can be performed by deep-learning the van Leeuwen map. This allows us simulating the long-time dynamics of quantum spin models at an affordable computational cost.

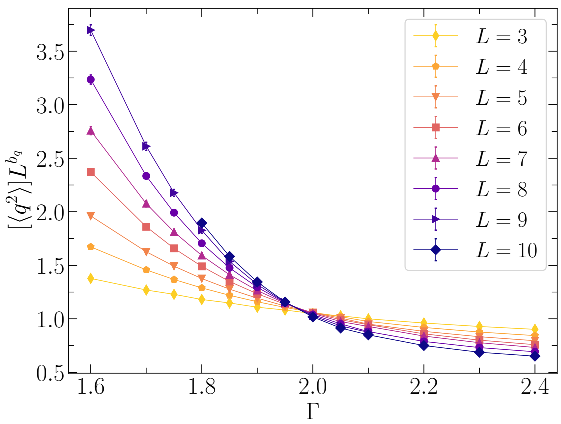

Fig. 1 Finite-size scaling of the spin-glass quantum phase transition in the two-dimensional Edwards-Anderson model. The rescaled (realization-averaged) mean-squared replica spin-overlap $[\langle q^2 \rangle]$ is plotted as a function of the transverse field Γ, for different system sizes L. For the critical exponents, we find $b_q = 1.68(8)$, $1/\nu = 1.11(22)$, and for the critical point $\Gamma_c = 1.98(7)$.

References

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