Neural-network wave functions for quantum many-body problems

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While the race for breakthroughs in quantum computing continues, classical techniques are simultaneously expanding their capabilities to tackle more difficult challenges. The rapid development of machine learning has led to neural networks establishing themselves as efficient ground state ansätze for quantum many-body systems [1]. In this talk, we will explore how the use of such neural quantum states, particularly those generated with the game-changing transformer architectures [2], in conjunction with variational quantum Monte Carlo techniques, allow us to reproduce the phase diagrams of Ising-type models with long-range interactions [3,4], to elucidate the nature of the phase transition (first or second order), or to tackle frustrated models such as the elusive spin liquids [5] – a challenge even for established techniques like matrix product states (MPS), dynamical mean field theory (DMFT), or tensor networks. The inherent flexibility in constructing different types of neural networks enables us to circumvent issues like the sign problem characteristic of frustrated systems—an Achilles' heel of other quantum Monte Carlo methods—or to reproduce correlation lengths that exceed those achievable with DMFT. Those techniques can also be useful in connection with experiment, assisting for instance in the characterization of real materials believed to exhibit physics consistent with spin liquids, like 2D heterometallic oxalate complexes [6].

References

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