Numerical Analysis and Scientific Computing Seminar

Numerical simulations for quantum many-body systems

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Abstract: The rapidly evolving quantum science calls for profound understanding and predictive control of entangled quantum many-body systems, such as quantum materials, synthetic qubits, and correlated molecules. I will use this talk to give an introduction to the application of numerical linear algebra theory and techniques in quantum applications. I will start with an introduction to quantum many-body systems and their mathematical descriptions. A second-quantized quantum system can be mapped to variational and algebraic problems, whose popular solvers include exact diagonalization, matrix-product state, and a few other variational techniques. These techniques have been tightly embedded into high-performance computing hardware nowadays. Then, I will use three examples to show a few aspects of exotic phenomena in quantum many-body systems and their solutions through large-scale linear algebra. The first example is the entangled spin polaron states discovered in a material-relevant model called the Hubbard model; the second example is the unconventional spectral features in quantum materials, where I will also introduce typical methods for excited-state spectral simulations; the last example is the nonequilibrium dynamics and time-resolved x-ray theory for entanglement probe and control, where I will also introduce typical methods for time evolution simulations. This talk won't cover all aspects where large-scale numerical linear algebra challenges existing intuitions and constructs new frameworks for quantum science, but is expected to stimulate discussions about possible collaborations.

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