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Finite temperature properties of strongly correlated systems via variational Monte Carlo[1] JAHAN CLAES, BRYAN CLARK, University of Illinois at Urbana Champaign — Variational methods are a common approach for computing properties of ground states but have not yet found analogous success in finite temperature calculations. In this talk I present a new variational finite temperature algorithm (VAFT) which combines ideas from maximally entangled thermal states (METTS), variational Monte Carlo optimization (VMC) and path integral Monte Carlo (PIMC) to define an implicit variational finite-temperature density matrix. The algorithm allows us to calculate temperature-averaged observables without ever explicitly representing the full density matrix. On the 2D bipartite Heisenberg lattice, VAFT agrees with exact results at low and intermediate temperatures, and qualitatively reproduces exact results at high temperatures. VAFT is sign-free and works in arbitrary dimensions.

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