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Explore 2D groundstates by iPEPS optimization with VUMPS

We present a general computational framework for studying ground-state properties of quantum spin models on infinite two-dimensional lattices. Our approach combines automatic differentiation (AD)-based gradient optimization of infinite projected entangled-pair states (iPEPS) with variational uniform matrix product states (VUMPS) to efficiently contract infinite tensor networks with unit cell structures.

We demonstrate the effectiveness of this framework by applying it to the Kitaev-type model, which features complex interactions and competing ground states. Benchmarking against exact solutions, our method achieves higher accuracy in computing various observables compared to previous tensor network approaches, such as imaginary-time projection or corner transfer matrix renormalization group (CTMRG). By employing dominant eigensolver techniques and GPU acceleration, we can handle large unit cells (e.g., 2×6) with bond dimensions up to 10.

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