Fast Iterative Eigenvalue Solver for Heisenberg Spin ½ Models

Scientific Achievement

Developed an iterative eigensolver capable of computing interior eigenvalues of Heisenberg spin ½ models with more than 28 spins. (The previous record was 26 spins)

Significance and Impact

Such a solver will enable EFRC researchers to study localization and thermalization properties of quantum materials that depend on the interplay between many-body interaction and disorder.

Research Details

- Use LOBPCG to compute the largest eigenvalues of $(H-\sigma_i I)^2$
- Precondition by solving $(H-\sigma_i I)^2 x = b$ with PCG
- Diagonal preconditioner used in PCG
- Multiple linear systems solved simultaneously
- HX can be performed without forming the entire Hamiltonian due to the tensor structure of H
- Achieve multiple levels of concurrency

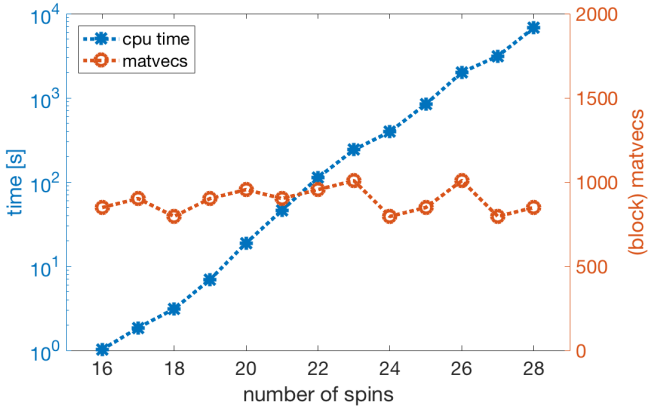
Spin Model:

$$H = \sum_{i=1}^{L-1} \vec{S}_i \cdot \vec{S}_{i+1} - h_i S_i^Z$$

Tensor Eigenvalue Problem $H\psi = E\psi$,

$H = \left[\sum_{i=1}^{L-1} I \otimes \cdots \otimes A_i \otimes I \cdots\right] + D$

dim: $\binom{L}{L/2}$, e.g. L=34 yields 2.3×10^9



MATVEC count and wallclock time required to compute 50 interior eigenvalues of models with different # of spins

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