Frequency Domain Density Matrix Renormalization Group Algorithms for Dynamical Correlation Function of Molecular Aggregates at both Zero and Finite Temperature

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Recent work of our group [1] presented the time dependent density matrix renormalization group (TD-DMRG) approach at both zero and finite temperature for vibronic model to calculate the linear spectrum of molecular aggregates. Here we focus on the frequency domain DMRG approaches within the same matrix product states/operators (MPS/MPO) framework: the correction vector approach is extended to finite temperature; the Chebyshev expansion approach is implemented to access the dynamical property of molecular vibronic model. The absorption spectrum of a real molecular aggregate Perylene bisimide at both zero and finite temperature is calculated to show the effectiveness of frequency domain approaches. CV-DMRG and Cheb-DMRG exhibit similar accuracy compared to that of TD-DMRG. Furthermore, CV-DMRG is favorable for pleasingly parallel computation, and Cheb-DMRG could capitalize the fact that the spectral band of vibronic model is much smaller than the full many-body band to greatly reduce the number of expansion terms. The frequency domain treatment provides an efficient and reliable way for the calculation of the dynamical correlation function of molecular aggregates at zero and finite temperature.

References

1. J. Ren, Z. Shuai, G Kin-Lic Chan, *J. Chem. Theory Comput.* **14** (2018), 5027-5039.
2. T. Jiang, J. Ren, Z. Shuai, *in preparation.*