Density matrix renormalization group:

time-dependent formalism, light-emitting, carrier transport, and singlet fission

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Electron correlation and electron-phonon coupling are the competing factors in organic/polymeric functional materials. DMRG has been proposed by White to treat correlated system which has been successfully extended to quantum chemistry, for example for studying the low-lying excited state orderings problem in conjugated polymers [1]. We present here some of our recent progresses on developing the DMRG time-dependent formalism as applied to the optical spectra for molecular aggregates[2], carrier transport for organic semiconductors [3], and singlet fission phenomena in donor-acceptor conjugated polymers [4]. An inner space perturbation algorithm is also introduced to replace the expensive matrix diagonalization procedures [5].

References

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