Thermal Schrodinger equation:
Modeling of exciton-vibrational dynamics with many degrees of freedom at finite temperature and simulation of nonlinear spectroscopic signals

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I will give a brief overview of the recently developed wave-function-based method for the simulation of quantum dynamics of systems with many degrees of freedom at finite temperature. The method is inspired by the ideas of Thermo Field Dynamics (TFD). As TFD, the method is based on the doubling of the system's degrees of freedom and thermal Bogoliubov transformation. As distinct from TFD, the method implements the doubling of thermalized degrees of freedom only, and relies upon the explicitly constructed generalized thermal Bogoliubov transformation, which is not restricted to fermionic and bosonic degrees of freedom. The solution of TFD dynamic equations is based on the Tensor Trains (Matrix Product States) propagation technique. The methodology is illustrated by the simulation of the exciton dynamics as well as time- and frequency-resolved fluorescence spectra of the Fenna-Mathews-Olsen complex using a realistic structured spectral density for modeling the electron-phonon interaction. The results of the simulations highlight the effect of specific vibrational modes on the exciton dynamics and energy transfer process, as well as call for careful modeling of electron-phonon couplings in natural and artificial light-harvesting systems.