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Acceleration of Self Healing Diffusion Monte Carlo for nearly degenerate eigenstates[1] FERNANDO REBOREDO, Oak Ridge National Laboratory — The Self-Healing Diffusion-Monte-Carlo method (SHDMC) recurisvely applies an evolution operation for a finite imaginary time. SHDMC and finds the full configuration interaction coefficients of the many-body ground state by projecting out excited states. The convergence of the SHDMC, being a projection method, is dictated by the energy separation between the ground and excited states. In this talk we explore methods to accelerate the convergence of SHDMC for nearly degenerate states using the dynamical information of the excited states accumulated over the recursive iterations and to compute ground and excited states simultaneously.

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