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On variational approximations in quantum molecular dynamics

The Dirac-Frenkel-McLachlan variational principle is the basic tool for obtaining computationally accessible approximations in quantum molecular dynamics. It determines equations of motion for an approximate time-dependent wave function on an approximation manifold of reduced dimension. This talk gives a near-optimality result for variational approximations. It bounds the error in terms of the distance of the exact wave function to the approximation manifold and identifies the parameters that control the deviation of the variational approximation from the best-approximation on the manifold.