Time-adaptive scaling of the Hagedorn basis

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Abstract

We solve the time-dependent Schrödinger equation for molecular dynamics using a spectral method based on Hagedorn function expansion. The basis follows the classical trajectories and coincides with the Hermite basis in one dimension. The method is much similar to the time-dependent discrete variable representation of Billing and co-workers, but is more flexible in several dimensions. The approximation properties of the Hagedorn basis depend strongly on the scaling of the independent variable. Using results from control theory we develop a time-dependent scaling which adaptively matches the basis to the wave packet.

The method is demonstrated on a model for the photodissociation of IBr, using a Fourier basis in the bound state and Hagedorn bases in the dissociative states. For photodissociation problems, classical dynamics does not give an accurate approximation of the midpoint of the wave packet since the wave function is excited during a long period of time. The same approach which is used to control the width of the wave packet can be used to control the position. The end result is a Gauss-Hermite spectral method with an adaptive basis set, based on the classical equations of motion but insensitive to the Ehrenfest time barrier.