Efficient approaches to multidimensional quantum dynamics:
Dynamical pruning in phase, position and configuration space

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Widespread practical use of quantum dynamics is strongly hampered by exponential scaling with dimensionality. In part, this unfavourable scaling is due to employing many basis functions that are rarely or never used in the actual dynamics. Hence, by dynamically pruning (DP) the basis down to the actually used functions at each time step, substantial savings in computing time and memory are obtained [1, 2]. This idea has been combined with different types of basis functions [1, 3–6] in conventional quantum dynamics, resulting in speed-ups of up to 25 for nonadiabatic dynamics of six-dimensional pyrazine, without jeopardizing accuracy.

Recently, DP has been combined with the multiconfiguration time-dependent Hartree method (MCTDH) [7, 8], and extended to both the primitive basis in which the single-particle functions (SPFs) are represented and the SPF configurations themselves [2]. As we illustrate for nonadiabatic 24-dimensional pyrazine, pruning the primitive basis allows for the propagation of higher-dimensional SPFs and partially lifts the sum-of-product-form requirement onto the structure of the Hamiltonian. Dynamical pruning the set of configurations (DP-MCTDH) yields significant speed-up factors between 5 and 50, making it competitive with the multilayer MCTDH method.
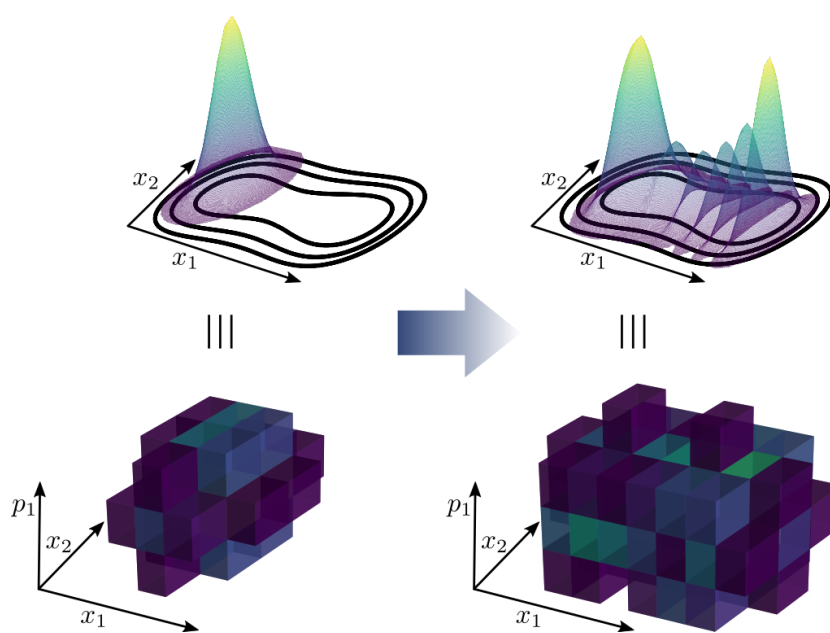
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