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Computational many-body quantum dynamics using Hagedorn wavepackets

We consider the approximation of multi-particle quantum dynamics in the semiclassical regime by Hagedorn wavepackets, which are products of complex Gaussians with polynomials that form an orthonormal L^2 basis and preserve their type under propagation in Schrödinger equations with quadratic potentials. We build a time-reversible, fully explicit time-stepping algorithm to approximate the solution of the Hagedorn wavepacket dynamics. The algorithm is based on a splitting between the kinetic and potential part of the Hamiltonian operator, as well as on a splitting of the potential into its local quadratic approximation and the remainder. The algorithm reduces to the Strang splitting of the Schrödinger equation in the limit of the full basis set, and it is robust in the semiclassical limit.

This is joint work with C. Lubich and V. Gradinaru (Tübingen).