

Karlsruher PDE-Seminar

Computing quantum dynamics in the semiclassical regime using Hagedorn wavepackets

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(joint work with Erwan Faou and Vasile Gradinaru)

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 is robust in the classical limit. It reduces to the Strang splitting of the Schrödinger equation in the limit of the full basis set, and it advances positions and momenta by the Störmer–Verlet method for the classical equations of motion. The algorithm allows for the efficient treatment of multi-particle problems by thinning out the basis according to a hyperbolic cross approximation and a rapid algorithm for computing the action of the potential matrix with a coefficient vector.

Termin: Donnerstag, 16.12.2010, 16:00 Uhr
Ort: Raum 1C-04, Allianz Building 5.20
Gastgeber: Die Dozenten des Schwerpunktes Partielle Differentialgleichungen