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MCQM PhD Lecture: Dominik Sulz

Wednesday, 25 March 2026 11:30 (1 hour)

Title: Numerical methods for quantum dynamics using Gaussian wave packets

Abstract: This talk aims to provide an introduction to numerical methods for quantum dynamics using Gaussian wave packets. Solving the time-dependent Schrödinger equation in high dimensions remains one of the most significant challenges in quantum dynamics due to the so-called 'curse of dimensionality'. Gaussian wave packets provide a mesh-free ansatz to approximate the wave function and therefore are a powerful tool for high-dimensional numerical simulations.
We will discuss the underlying geometry of the Gaussian manifold and apply the Dirac-Frenkel time-dependent variational principle to derive efficient equations of motion. A particular focus will be placed on the semiclassical regime: we discuss how Gaussian methods handle the occurring high oscillations of the wave function—a fundamental numerical difficulty.