





Einladung

zum Vortrag im Rahmen des SFB Colloquiums (Standort Linz), mit dem Titel

Lattice point sets and exponential operator splitting for time-dependent Schrödinger equations

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Abstract: We propose a numerical method to approximate solutions for time-dependent Schrdinger equations (TDSEs). Our method consists of two steps: (i) we first discretize the physical domain using a lattice point set and its Pontryagin dual, which can be seen as a Fourier pseudo-spectral method on a lattice point set. In other words, by using the Pontryagin dual of a lattice point set (i.e., no oversampling), we can obtain desirable properties for pseudo-spectral methods; (ii) then we discretize time by exponential operator splitting which will give us the higher order convergence. We analyze the combination of a lattice point set and exponential operator splitting, and derive the smoothness conditions which assure higher order convergence in temporal discretization. The proposed method has two distinctive features from a numerical perspective: (i) numerical results show the error convergence of temporal discretization is consistent even for higher-dimensional problems; (ii) by using a rank-1 lattice point set, the solution can be efficiently computed (and further time stepped) using only 1-dimensional Fast Fourier Transforms.

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