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"Krylov subspace spectral methods for the time-dependent Schrödinger equation with non-smooth potentials"

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Review

In this paper some modifications of Krylov subspace spectral (KSS) methods for discretizing the time-dependent Schrödinger equation with periodic boundary conditions are suggested. Specifically, problems for which the initial data and/or the potential functions are non-smooth are targeted. A thorough introductory discussion on KSS methods in general and their applications to the Schrödinger equation in particular is also offered.

KSS methods construct approximations to time-dependent solutions in the spectral domain. Evolving the Fourier components is then tantamount to computing the matrix exponential applied to the basis vectors. In turn, as suggested earlier by Golub and others, this can be done accurately and efficiently using Gaussian quadratures obtained from the Lanczos iteration.

In the paper, the one-dimensional *one-node* case is analyzed and results for consistency, stability, energy conservation and convergence are established. Generalizations to the multi-node (high order) case are also briefly discussed and it is clear that higher demands are put on the smoothness of the data and on the time step in order to also observe high order convergence. Given the multistep nature of the scheme, this behaviour is rather the expected one.

It is demonstrated by simple examples that these problems can be mitigated by employing a symmetric scaled perturbation which improves the stability of the Lanczos iteration. The paper concludes by commenting on implementation issues and presenting results from numerical experiments in one and two spatial dimensions. Several considerations for future research are also mentioned.

Lacking in the paper are comparisions with more standard methods which would be of some interest given that the orders reported here are attainable in other ways too. The paper is probably of interest to anyone who wishes to be informed about this ongoing area of research.

MSC 2010 classification: 65M12 (primary); 65M70 (secondary).