Abstract Submitted
for the APR07 Meeting of
The American Physical Society

Accurate numerical solutions of the time-dependent Schrödinger equation[1] W. VAN DIJK, Redeemer University College and McMaster University, F.M. TOYAMA, Kyoto Sangyo University — We present a generalization of the often-used Crank-Nicolson (CN) method of obtaining numerical solutions of the time-dependent Schrödinger equation. The generalization yields numerical solutions accurate to order $(\Delta x)^{2r-1}$ in space and $(\Delta t)^{2M}$ in time for any positive integers r and M, while CN employ $r = M = 1$. We note dramatic improvement in the attainable precision (circa 10 or greater orders of magnitude) along with several orders of magnitude reduction of computational time. We show that the cumulative error and the CPU time of the numerical calculations scale as functions of r and M. The method can be generalized further to obtain solutions of nonhomogeneous Schrödinger-type equations such as those arising when perturbation theory is applied to coupled-channel systems. The improved method is shown to lead to feasible studies of coherent-state oscillations with additional short-range interactions, wavepacket scattering, and long-time studies of decaying systems. Examples of solutions of nonhomogeneous equations will also be presented.

[1]This research is supported by the Natural Sciences and Engineering Research Council of Canada

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Date submitted: 11 Jan 2007 Electronic form version 1.4