



## QUANTUM OPTICS SEMINAR

**Title:** Numerical Solution of the Time-Dependent Schrödinger Equation using the FEDVR/RSP2 Method

**Speaker:** Dr Barry I. Schneider, Physics Division, National Science Foundation, Arlington, VA

**Time:** Tuesday, October 4, 2005 at 14:15

**Place:** 520-616

**Abstract:**

A solution of the time-dependent Schrödinger equation (TDSE) is required in a variety of problems in physics and chemistry. These include atoms and molecules in time dependent electromagnetic fields, time-dependent approaches to atomic collision problems and in describing the behavior of materials subjected to internal and external forces. We present a new approach in which the Finite Element Discrete Variable Representation (FEDVR) is combined with the Real-Space Product (RSP) algorithm to generate an efficient and highly accurate method for the solution of the time-dependent linear/nonlinear Schrödinger equation. The FEDVR provides a highly-accurate spatial representation (FEDVR) using a minimum number of grid points ( $N$ ) while the RSP algorithm propagates the wavefunction in  $O(N)$  operations per time step. Parallelization of the method is transparent and is implemented by distributing one spatial dimension across the available processors, within the Message-Passing-Interface (MPI) scheme. The complete formalism and a number of three-dimensional (3D) examples will be given to demonstrate its high accuracy and efficacy.

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