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Solution of the Schrödinger equation using exterior complex scaling and fast Fourier transform

V. V. Serov^a, and T. A. Sergeeva

Department of Theoretical Physics, Saratov State University, Astrakhanskaya 83, Saratov 410012, Russia

e-mail: ^a vladislav_serov@mail.ru

Abstract. The split-operator pseudo-spectral method based on the fast Fourier transform (SO-FFT) is a fast and accurate method for the numerical solution of the time-dependent Schrödinger-like equations (TDSE). As well as other grid-based approaches, SO-FFT encounters a problem of the unphysical reflection of the wave function from the grid boundaries. Exterior complex scaling (ECS) is an effective method widely applied for the suppression of the unphysical reflection. However, SO-FFT and ECS have not been used together heretofore because of the kinetic energy operator coordinate dependence that appears in ECS applying. We propose an approach for the combining the ECS with SO-FFT for the purpose of the solution of TDSE with outgoing-wave boundary conditions. Also, we propose an effective ECS-friendly FFT-based preconditioner for the solution of the stationary Schrödinger equation by means of the preconditioned conjugate gradients method.

Keywords: Schrödinger equation, exterior complex scaling, pseudo-spectral method, finite difference, fast Fourier transform

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