



New Version Announcement

Program for quantum wave-packet dynamics with time-dependent potentials (new version announcement) [☆]

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ABSTRACT

WAVEPACKET is a program to simulate the dynamics of a wave packet interacting with a time-dependent potential, with the time-dependent Schrödinger equation being solved on a one-, two-, or three-dimensional spatial grid using the split operator method. This new version fixes bugs present in the original program.

New version program summary

Program Title: wavepacket

CPC Library link to program files: <https://doi.org/10.17632/gnxmkygxrw.1>

Licensing provisions: GPLv3

Programming language: C (iso C99)

Journal reference of previous version: Comput. Phys. Commun. 185 (2014) 407–414.

Does the new version supersede the previous version?: Yes

Reasons for the new version: Bug fixes.

Summary of revisions: This new version fixes bugs in the program WAVEPACKET [1]. In the original version, the function `print_wf_bin`, used (optionally) to write out the wave function as a binary file, contained a bug that would result in only part of the full wave function being written out when the program was run in parallel.

Additionally, negative values of the parameters `nt` and/or `nprint` could lead to the program being stuck in an infinite loop. Additional checks have been added to ensure that both these parameters are positive (or zero).

Nature of problem: Solves the time-dependent Schrödinger equation for a single particle interacting with a time-dependent potential.

Solution method: The wave function is described by its value on a spatial grid and the evolution operator is approximated using the split-operator method [2,3], with the kinetic energy operator calculated using a Fast Fourier Transform.

Additional comments including restrictions and unusual features: Simulation can be in one, two, or three dimensions. The FFTW [4] implementation of the fast Fourier transform is used, so the corresponding library must be installed. Serial and parallel versions are compiled from the same source files. The parallel version is based on the Message-Passing Interface (MPI) [5].

References

- [1] C.M. Dion, A. Hashemloo, G. Rahali, Comput. Phys. Commun. 185 (2014) 407–414.
- [2] M.D. Feit, J.A. Fleck, Jr., A. Steiger, Solution of the Schrödinger equation by a spectral method, J. Comput. Phys. 47 (1982) 412–433.
- [3] M.D. Feit, J.A. Fleck, Jr., Solution of the Schrödinger equation by a spectral method II: Vibrational energy levels of triatomic molecules, J. Chem. Phys. 78 (1) (1983) 301–308.
- [4] <http://www.fftw.org>
- [5] <http://www.mpi-forum.org>

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[☆] The review of this paper was arranged by Prof. J. Ballantyne.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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