



Program for quantum wave-packet dynamics with time-dependent potentials[☆]



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ABSTRACT

We present a program to simulate the dynamics of a wave packet interacting with a time-dependent potential. The time-dependent Schrödinger equation is solved on a one-, two-, or three-dimensional spatial grid using the split operator method. The program can be compiled for execution either on a single processor or on a distributed-memory parallel computer.

Program summary

Program title: wavepacket

Catalogue identifier: AEQW_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEQW_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, <http://cpc.cs.qub.ac.uk/licence/licence.html>

No. of lines in distributed program, including test data, etc.: 7231

No. of bytes in distributed program, including test data, etc.: 232209

Distribution format: tar.gz

Programming language: C (iso C99).

Computer: Any computer with an iso C99 compiler (e.g. gcc [1]).

Operating system: Any.

Has the code been vectorized or parallelized?: Yes, parallelized using MPI. Number of processors: from 1 to the number of grid points along one dimension.

RAM: Strongly dependent on problem size. See text for memory estimates.

Classification: 2.7.

External routines: fftw [2], mpi (optional) [3]

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 [4, 5], with the kinetic energy operator calculated using a Fast Fourier Transform.

Unusual features:

Simulation can be in one, two, or three dimensions. Serial and parallel versions are compiled from the same source files.

[☆] This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

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Running time:

Strongly dependent on problem size. The example provided takes only a few minutes to run.

References:

- [1] <http://gcc.gnu.org>
- [2] <http://www.fftw.org>
- [3] <http://www.mpi-forum.org>
- [4] 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.
- [5] 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.

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1. Introduction

Quantum wave-packet dynamics, that is, the evolution of the spatial distribution of a quantum particle, is an important part of the simulation of many quantum systems. It can be used for studying problems as diverse as scattering, surface adsorption, and laser control, just to name a few.

We propose here a general-purpose program to solve the spatial part of the time-dependent Schrödinger equation (TDSE), aimed particularly at a quantum particle interacting with a time-dependent potential. Our interest mainly concerns such applications as laser control of quantum systems [1,2], but the program can be used with any user-supplied potential function.

The program is based on the split-operator method [3–6], which has successfully been used to solve the time-dependent Schrödinger equation in many different settings, from the calculation of vibrational bound states (see, e.g., [5]) and the simulation of high-power laser–matter interactions (see, e.g., [7]), to the laser control of chemical reactions (see, e.g., [8]). The method can also be applied to Schrödinger-like equations, such as the Gross-Pitaevskii [9] and Dirac [10] equations.

2. Numerical approach

2.1. Split-operator method

In this section, we present a detailed description of the split-operator method to solve the time-dependent Schrödinger equation. While everything presented here can be found in the original works developing the method [3–6], we think it useful to review all the elements necessary to understand the inner workings of the program.

We consider the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \psi(t) = \hat{H} \psi(t), \quad (1)$$

with \hat{H} the Hamiltonian for the motion of a particle interacting with an external time-dependent potential $V(t)$, i.e.,

$$\hat{H} = \hat{K} + \hat{V} = \frac{\hat{P}^2}{2m} + V(t), \quad (2)$$

where \hat{K} and \hat{V} are the kinetic and potential energy operators, respectively, \hat{P} is the momentum operator, and m the mass of the particle. (The same Hamiltonian is obtained for a vibrating diatomic molecule, where the spatial coordinate is replaced by the internuclear distance, and the potential $V(t)$ is the sum of the internal potential energy and an external, time-dependent potential, as will be shown in Section 4.1.)

The formal solution to Eq. (1) is given by the time evolution operator \hat{U} , itself a solution of the time-dependent Schrödinger equation [11],

$$i\hbar \frac{\partial}{\partial t} \hat{U} = \hat{H} \hat{U}, \quad (3)$$

such that, given an initial wave function at time t_0 , $\psi(t_0)$, the solution at any time t is obtained from

$$\psi(t) = \hat{U}(t, t_0) \psi(t_0). \quad (4)$$

As the Hamiltonian is time dependent, we have that [12]

$$\begin{aligned} \hat{U}(t, t_0) &= \hat{T} \exp \left[-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(t') dt' \right] \\ &= \hat{T} \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t [\hat{K} + \hat{V}(t')] dt' \right\}. \end{aligned} \quad (5)$$

In Eq. (5), the time-ordering operator \hat{T} ensures that the Hamiltonian is applied to the wave function in order of increasing time, as in general the Hamiltonian does not commute with itself at a different time, i.e., $[\hat{H}(t), \hat{H}(t')] \neq 0$ iff $t \neq t'$ [11,13]. By considering a small time increment Δt , we can do without the time-ordering operator by considering the approximate short-time evolution operator [13],

$$\hat{U}(t + \Delta t, t) = \exp \left\{ -\frac{i}{\hbar} \int_t^{t+\Delta t} [\hat{K} + \hat{V}(t')] dt' \right\}. \quad (6)$$

We are concerned here with time-dependent potentials that also have a spatial dependence, $\hat{V} \equiv V(\mathbf{x}, t)$, such as those produced by ion traps or focused laser pulses, such that $\hat{V} \equiv V(\mathbf{x}, t)$, in which case \hat{K} and \hat{V} do not commute. For two non-commuting operators \hat{A} and \hat{B} , $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}}e^{\hat{B}}$, but the split-operator method [4,5] allows the approximation of the evolution operator with minimal error,

$$\begin{aligned} \hat{U}(t + \Delta t, t) &= \exp \left[-\frac{i\Delta t}{2\hbar} \hat{K} \right] \exp \left[-\frac{i}{\hbar} \int_t^{t+\Delta t} \hat{V}(t') dt' \right] \\ &\quad \times \exp \left[-\frac{i\Delta t}{2\hbar} \hat{K} \right] + O(\Delta t^3). \end{aligned} \quad (7)$$

Using the midpoint formula [14] for the integral of the potential,

$$\int_t^{t+\Delta t} f(t') dt' = f(t + \Delta t/2) \Delta t + O(\Delta t^3), \quad (8)$$

we get

$$\begin{aligned} \hat{U}(t + \Delta t, t) \\ \approx \exp \left[-\frac{i\Delta t}{2\hbar} \hat{K} \right] \exp \left[-\frac{i\Delta t}{\hbar} V \left(t + \frac{\Delta t}{2} \right) \right] \exp \left[-\frac{i\Delta t}{2\hbar} \hat{K} \right], \end{aligned} \quad (9)$$

where the global error is $O(\Delta t^3)$. The choice of the order of the operators \hat{K} and \hat{V} in the above equations is arbitrary, but the choice

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