TDStool

Time Dependent Schrödinger equation simulation tool

Notes on Numerical Methods

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June 17, 2009
Version 0.2
TDStool Version 0.2

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Preface

The software TDStool is a numerical solver for the Time Dependent (linear) Schrödinger equation and (nonlinear) Gross-Pitaevskii equation. This document provides the theoretical basis for TDStool. It describes the discretization methods and the main numerical algorithms used in the code. It aims to be a technical reference guide and a means to reach an in-depth understanding of the source code. In fact, it should be the starting point for whoever is willing to modify the code (released as an open-source project) and hopefully contribute to the project. Since the discussion in this note has been kept at a tutorial level, it can represent a nimble introduction to some of the numerical techniques used in the code. However, we urge newcomers to read the references suggested in the text.

Disclaimer

We make no warranty to users of TDStool and accept no responsibility for its use and for any conclusion drawn from its results. Although we endeavour to provide an easy-to-use software with an intuitive interface, TDStool is primarily intended for use by those competent in the field of quantum mechanics and numerical analysis.

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Acknowledgements

TDStool has been developed within the *TDStool* INFM Seed project 2008. We are pleased to thank Guido Goldoni (Università di Modena e Reggio Emilia) and Massimo Rudan (Università di Bologna) for most helpful discussions and suggestions.

Contents

1 Introduction

The single-particle dynamics of a nonrelativistic quantum system follows the so-called time-dependent Schrödinger equation (TDSE) that relates the time derivative of the system state with the system Hamiltonian $\mathcal{H}$ and the state itself [1]. In the real-space representation, for a spinless particle the TDSE is the partial differential equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \mathcal{H}\psi(\mathbf{r},t), \tag{1}$$

where $\mathbf{r}$ is the position, t the time coordinate, $\psi(\mathbf{r},t)$ a complex-valued function representing the quantum state, with $|\psi(\mathbf{r},t)|^2$ the probability density in $\mathbf{r}$ and t. The Hamiltonian $\mathcal{H}$ in the above equation is a differential operator written in the real-space representation.

The aim of TDStool is to solve numerically Eq. (1) once the initial condition $\psi(\mathbf{r}, t = 0)$ and a proper boundary condition on the computational domain are given.

We will first deal with a single particle moving in a static scalar (e.g. electric) potential, then we will generalize the discussion to include time-dependent fields. The effect of a time-dependent uniform magnetic field will be added in a future version of these notes.

For the sake of brevity, we will only consider 2D systems and domains, i.e. with $\mathbf{r} = (x, y)$. Formulas for different dimensionality will be explicitly reported only if the generalization is not straightforward. Where manifest, the spatial or time coordinates of the wave function and operators will be implied.

2 Schrödinger equation with a scalar potential

We consider a single particle subject to a potential $U(x, y, t)$, eventually dependent on the time t. We want to solve the TDSE Eq. (1) on a rectangular domain

$$D = (x, y) \mid x \in [0, X], y \in [0, Y] \tag{2}$$

with given X and Y. We assume Dirichlet conditions on the domain boundaries

$$\partial(D) = (0, y) \cup (X, y) \cup (x, 0) \cup (x, Y) \mid x \in [0, X], y \in [0, Y] \tag{3}$$

i.e. the values of the wave function $\psi(x, y, t)$ in the points $(x, y) \in \partial(D)$ are given.

The Hamiltonian of the system reads $\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(x, y, t)$, where m is the mass of the particle. Equation (1) becomes the standard real-space TDSE for a single particle in a scalar potential:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(x, y, t) + U(x, y, t)\psi(x, y, t). \tag{4}$$

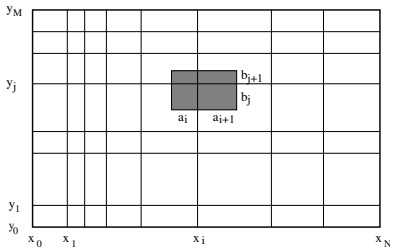

Figure 1: Discretization grid on the 2D domain D. The box C_{ij} of area $s_{ij} = \frac{a_i+a_{i+1}}{2}\frac{b_i+b_{i+1}}{2}$ is shaded.

3 Box Integration Method

In order to discretize the spatial coordinates of the TDSE we employ the Box Integration Method, also known as Finite Volume Method [2]. We start by semidiscretizing the Schrödinger equation in the space. We work on the above special case where the domain D is a box and we take an orthogonal and separable discretization grid. We are going to consider a 2D grid, but the discretization can easily be extended to a higher dimensional domain. Furthermore, for brevity we rewrite Eq. (4) as

$$\frac{\partial \psi}{\partial t} = -\beta \nabla G + v\,\psi\,, \tag{5}$$

where we have used the definitions

$$\beta = i\frac{\hbar}{2m}, \tag{6}$$

$$v = \frac{1}{i\hbar}U, \tag{7}$$

$$G = \nabla\psi\,. \tag{8}$$

Let $x_0 < x_1 < \cdots < x_{N+1}$ and $y_0 < y_1 < \cdots < y_{M+1}$ be the coordinates of an orthogonal grid, with $x_0 = 0$, $x_{N+1} = X$, $y_0 = 0$, $y_{M+1} = Y$. The domain D will be given by

$$D = [x_0, x_{N+1}] \times [y_0, y_{M+1}]\,. \tag{9}$$

Note that we take a non-uniform but x-y separable discretization grid, as shown in Fig. 1.

We will have $N \times M$ internal nodes in which the function ψ is unknown. The function $\psi(x, y, t)$ in the points where $x = x_0$ or $x = x_{N+1}$ or $y = y_0$ or $y = y_{M+1}$ is known thanks to the Dirichlet boundary conditions.

In order to solve the TDSE we use here a vertex-centred Box Integration Method. First, we consider the internal grid points and partially cover the domain D with $N \times M$ boxes

$$C_{ij} = [\frac{x_i - x_{i-1}}{2}, \frac{y_j - y_{j-1}}{2}] \times [\frac{x_{i+1} - x_i}{2}, \frac{y_{j+1} - y_j}{2}], \tag{10}$$

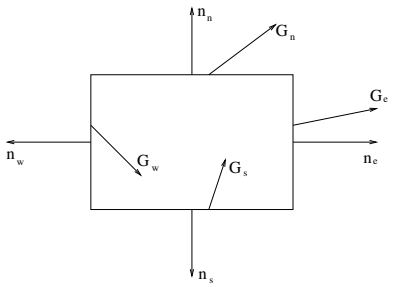

Figure 2: Single box scheme

where $i = 1, \cdots, N$ and $j = 1, \cdots, M$.

If we call $a_i = x_i - x_{i-1}$ and $b_j = y_j - y_{j-1}$, the area of the box C_{ij} is $s_{ij} = \frac{a_i + a_{i+1}}{2} \frac{b_i + b_{i+1}}{2}$. Following the Box Integration Method we integrate Eq. (5) on each box C_{ij}:

$$\int_{C_{ij}} \frac{\partial \psi}{\partial t}\, ds = \beta \int_{C_{ij}} \nabla G\, ds + \int_{C_{ij}} v\, \psi\, ds\,. \tag{11}$$

The three integrals can be approximated as follow:

$$\int_{C_{ij}} \frac{\partial \psi}{\partial t}\, ds \;\approx\; s_{ij} \frac{d\psi}{dt}(x_i, y_j, t)\,, \tag{12}$$

$$\int_{C_{ij}} v\, \psi\, ds \;\approx\; s_{ij} (v\psi)(x_i, y_j, t)\,, \tag{13}$$

$$\int_{C_{ij}} \nabla G\, ds = \oint_{\partial C_{ij}} G \bar{\boldsymbol{n}}\, dl \;\approx\; (G_e \bar{\boldsymbol{n}}_e + G_n \bar{\boldsymbol{n}}_n + G_w \bar{\boldsymbol{n}}_w + G_s \bar{\boldsymbol{n}}_s)\,, \tag{14}$$

where the Green's theorem has been used in the latter expression. $\bar{\boldsymbol{n}}_e$, $\bar{\boldsymbol{n}}_n$, $\bar{\boldsymbol{n}}_w$ and $\bar{\boldsymbol{n}}_s$ are the vectors normal to the four edges of the box C_{ij}, and whose modulus is equal to the length of the edge (area of the surface in the 3D case); G_e, G_n, G_w and G_s are the values of G, namely the gradient of ψ, in the mid point of each edge, as shown in Fig 2.

Let define the space-discretized wave function $\psi_{i,j}(t) = \psi(x_i, y_i, t)$. For ease of notation, here we use a two-index representation for ψ_{ij} although this quantity is represented in the code as a 1D array. Specifically, $\psi_{i,j}$ means that we are referring to the element $iM + j$. Using a centred difference formula, the gradient values G can be approximated from the $\psi_{i,j}$ values on the nodes:

$$\begin{aligned}
G_e \bar{\boldsymbol{n}}_e &\approx \frac{\psi_{i,j} - \psi_{i-1,j}}{a_i} \frac{b_j + b_{j+1}}{2}\,, \\
G_n \bar{\boldsymbol{n}}_n &\approx \frac{\psi_{i,j} - \psi_{i+1,j}}{a_{i+1}} \frac{b_j + b_{j+1}}{2}\,, \\
G_w \bar{\boldsymbol{n}}_w &\approx \frac{\psi_{i,j} - \psi_{i,j-1}}{b_j} \frac{a_i + a_{i+1}}{2}\,,
\end{aligned} \tag{15}$$

$$G_s \bar{\boldsymbol{n}}_s \approx \frac{\psi_{i,j} - \psi_{i,j+1}}{b_{j+1}} \frac{a_i + a_{i+1}}{2} .$$

Let us now define

$$\begin{aligned} k_1 &= \frac{b_j + b_{j+1}}{2a_i}, \qquad k_2 = \frac{b_j + b_{j+1}}{2a_{i+1}} , \\ k_3 &= \frac{a_i + a_{i+1}}{2b_j}, \qquad k_4 = \frac{a_i + a_{i+1}}{2b_{j+1}} . \end{aligned} \tag{16}$$

The approximation of the integral in Eq. (14) becomes

$$\begin{aligned} &\int_{C_{ij}} \nabla G \, ds \approx \\ &\approx \quad (k_1 + k_2 + k_3 + k_4)\, \psi_{i,j} + k_1\, \psi_{i-1,j} + k_2\, \psi_{i+1,j} + k_3\, \psi_{i,j-1} + k_4\, \psi_{i,j+1} . \end{aligned} \tag{17}$$

If a box is adjacent to the boundary of the domain, some of the $\psi_{i,j}$ terms of the summation are defined by the boundary conditions rather than being unknown. In this case we can group all these terms in one constant term. For example, if $(i, j) = (1, 1)$, then $\psi_{i-1,j}$ and $\psi_{i,j-1}$ are on the boundaries and the above expression becomes

$$\begin{aligned} &\int_{C_{11}} \nabla G \, ds \approx \\ &\approx \quad (k_1 + k_2 + k_3 + k_4)\, \psi_{1,1} + k_2\, \psi_{2,1} + k_4\, \psi_{1,2} + d_{11} . \end{aligned} \tag{18}$$

where $d_{11} = k_1\, \psi_{0,1} + k_3\, \psi_{1,0}$ is the constant term that includes the known values of ψ at the boundaries.

In vector form, for each given box C_{ij} these summations can be represented as a scalar product:

$$\boldsymbol{m}_{ij} \boldsymbol{\psi} + d_{ij} = \sum_{(k,l)=(1,1)}^{(N,M)} m_{ij}^{k,l}\, \psi_{k,l} + d_{ij} \tag{19}$$

with $\boldsymbol{\psi}$ representing the column vector of the wave function and with $\boldsymbol{m}_{ij} \in R^{N \times M}$ defined by

$$\begin{aligned} &\boldsymbol{m}_{ij} = (m_{ij}^{1,1}, m_{ij}^{1,2}, \cdots, m_{ij}^{N,M}) = \\ &= \quad (0, \cdots, 0,\, k_1, 0, \cdots, 0,\, k_3, k_1 + k_2 + k_3 + k_4, k_4\, , 0, \cdots, 0,\, k_2, 0, \cdots, 0) . \end{aligned} \tag{20}$$

Thus, the Schrödinger equation can be approximately integrated on the box C_{ij} with

$$s_{ij} \frac{d\psi_{i,j}}{dt}(t) = \beta \boldsymbol{m}_{ij} \boldsymbol{\psi}(t) + s_{ij}\, v_{ij}\, \psi_{i,j}(t) + \beta d_{ij} , \tag{21}$$

where $v_{ij} = v(x_i, x_j)$.

By defining the diagonal matrices $S = \mathrm{diag}(s_{ij})$ and $V = \mathrm{diag}(v_{ij})$, and the matrix whose columns are the vectors $\boldsymbol{m}_{ij}$: $M = \beta[\boldsymbol{m}_{ij}]$, the equation can be written in matrix form:

$$S\frac{d\boldsymbol{\psi}}{dt}(t) = M\boldsymbol{\psi}(t) + SV\boldsymbol{\psi} + \beta\boldsymbol{d}\,, \tag{22}$$

where the vector symbol $\boldsymbol{d}$ represents the column vector $\boldsymbol{d} = (d_{11}, d_{12}, \cdots, d_{NM})$, as usual.

For the *time discretization* we use a Cranck-Nicholson scheme (also known as trapezoidal rule). By considering a time step Δ_t, Eq. (22) becomes:

$$S\boldsymbol{\psi}(t+\Delta_t) = S\boldsymbol{\psi}(t) + \frac{(M+SV)\Delta_t}{2}\left(\boldsymbol{\psi}(t) + \boldsymbol{\psi}(t+\Delta_t)\right) + \beta\Delta_t\boldsymbol{d} \tag{23}$$

or equivalently

$$\left(S - \frac{(M+SV)\Delta_t}{2}\right)\boldsymbol{\psi}(t+\Delta_t) = \left(S + \frac{(M+SV)\Delta_t}{2}\right)\boldsymbol{\psi}(t) + \beta\Delta_t\boldsymbol{d} \tag{24}$$

Note that in case the potential v is dependent on the time, the two matrices V on the left and right sides of Eq. (24) must be computed at the later and earlier time step, respectively. By making explicit the above equation for $\psi(t+\Delta_t)$ one gets

$$\boldsymbol{\psi}(t+\Delta_t) = \frac{2\beta\Delta_t\boldsymbol{d} \;+\; \left(2S + \left(M + S\,V(t)\right)\Delta_t\right)\boldsymbol{\psi}(t)}{2S - \left(M + S\,V(t+\Delta_t)\right)\Delta_t} \tag{25}$$

4 Gross-Pitaevskii equation

The time-dependent Gross-Pitaevskii equation describes the collective coherent dynamics of an ensemble of quantum particles, interacting through a Hartree pseudopotential. This approximation results in an additional potential-like term in the time-dependent Scrödinger equation, proportional to the local particle density $|\psi(\mathbf{r})|^2$. In fact, the Gross-Pitaevskii model leads to the following nonlinear form of the Schrödinger equation [3]

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi(x,y,t) + \left(U(x,y,t) + \frac{4\pi\hbar^2 a_s}{m}|\psi(x,y,t)|^2\right)\psi(x,y,t)\,, \tag{26}$$

where U is an external potential, as in the linear case, and a_s is the particle-particle scattering length.

In this case, we suppose periodic boundary conditions on the domain D. We rewrite Eq. (26) highlighting the linear part and the nonlinear part of the operator, $\mathcal{L}$ and $\mathcal{N}$, respectively:

$$\frac{\partial}{\partial t}\psi = \mathcal{L}\psi + \mathcal{N}\psi \tag{27}$$

with

$$\mathcal{L} = \frac{i\hbar}{2m}\nabla^2 \qquad \text{and} \qquad \mathcal{N} = -i\left(\frac{1}{\hbar}U + \frac{4\pi\hbar a_s}{m}|\psi|^2\right). \tag{28}$$

The evolution of the wave function can be obtained through the evolution operator $\mathcal{U}$

$$\psi(t+dt) = \mathcal{U}(t, t+dt)\,\psi(t) = \mathcal{T}\exp\left(\int_t^{t+dt}(\mathcal{L}+\mathcal{N}(t'))\,dt'\right)\psi(t)\,, \tag{29}$$

where $\mathcal{T}$ is the time-ordering operator and the time dependence of $\mathcal{N}$ has been explicitated.

Note that, if the operator $\mathcal{N}$ did not depend on the time, the evolution operator would be $\mathcal{U}(t, t+dt) = e^{(\mathcal{L}+\mathcal{N})dt}$. However, in the following we do not impose such a condition.

5 Split-step Fourier Method

In order to compute numerically the evolution of the wave function, we use a second-order approximation formula to decompose the evolution operator $\mathcal{U}$.

In fact, we suppose that the operator $\mathcal{N}$, containing the time-dependent potential and the particle density, varies slowly with the time. Thus, a suitable n-th order decomposition formula for the time-ordered exponential can be used[**?**, 5], with a negligible error of the order $O(dt^{n+1})$

The first-order approximate decomposition of $\mathcal{U}$ reads:

$$\mathcal{U}(t, t+dt) \approx e^{\mathcal{L}dt}e^{\mathcal{N}(t+\frac{dt}{2})dt} + O(dt^2)\,, \tag{30}$$

while the second-order decomposition reads:

$$\mathcal{U}(t, t+dt) \approx e^{\frac{1}{2}\mathcal{N}(t+\frac{dt}{2})dt}e^{\mathcal{L}dt}e^{\frac{1}{2}\mathcal{N}(t+\frac{dt}{2})dt} + O(dt^3)\,, \tag{31}$$

It is easy to see that the wave function evolution obtained with the above first-order approximation, $\psi(t+dt) = e^{\mathcal{L}dt}e^{\mathcal{N}(t+\frac{dt}{2})dt}\psi(t)$ is equivalent to perform two subsequent dt steps through the equations

$$\frac{\partial}{\partial t}\psi = \mathcal{N}\left(t+\frac{dt}{2}\right)\psi \qquad \text{and} \qquad \frac{\partial}{\partial t}\psi = \mathcal{L}\psi\,. \tag{32}$$

Similarly, the second-order evolution is equivalent to first perform a step of $\frac{dt}{2}$ with the nonlinear operator $\mathcal{N}$ at time $t+\frac{dt}{2}$, then a dt step with $\mathcal{L}$, finally another $\frac{dt}{2}$ step with $\mathcal{N}(t+\frac{dt}{2})$. Now, the problem comes down to compute the separate evolutions generated by $\mathcal{N}$ and $\mathcal{L}$.

From Eq. (28), it is clear that the operator $\mathcal{N}$ is diagonal in the real-space representation. Thus, its effect is local on each point of the wave function:

$$\mathcal{N}\left(t+\frac{dt}{2}\right)\psi(x,y,t) = e^{-i\left(\frac{1}{\hbar}V(x,y)+\frac{4\pi\hbar a_s}{m}|\psi(x,y,t)|^2\right)dt}\,\psi(x,y,t) \tag{33}$$

On the other hand, the eigenvectors of the operator $i\hbar\mathcal{L}$ are known analytically since they are the set of plane waves $e^{i\mathbf{k}\cdot\mathbf{r}}$. The linear evolution of ψ can be obtained easily on the reciprocal k space. In order to do so, the wave function must be Fourier transformed. Then, the linear evolution can be applied directly since its effect is local in k space.

Starting from $\psi(x, y, t)$, the steps are the following:

$$\bar{\psi}(k_x, k_y, t) = \mathsf{FFT}[\psi(x, y, t)] \tag{34}$$

$$\bar{\psi}(k_x, k_y, t + dt) = \bar{\psi}(k_x, k_y, t) e^{\frac{i\hbar}{2m}(k_x^2 + k_y^2)dt} \tag{35}$$

$$\psi(x, y, t + dt) = \mathsf{IFFT}[\bar{\psi}(k_x, k_y, t + dt)], \tag{36}$$

where FFT and IFFT indicate the Fourier transform and inverse Fourier transform, respectively. A Fast Fourier Transform algorithm is used to compute the above transformations.

Let $x_0 < x_1 < \cdots < x_{N+1}$ and $y_0 < y_1 < \cdots < y_{M+1}$ be the coordinates of a *uniform* orthogonal grid, with $x_0 = 0$, $x_{N+1} = X$, $y_0 = 0$, $y_{M+1} = Y$. It is important to properly define the frequency components on the corresponding k grid. In fact, if a wave function is defined on $[0, X] \times [0, Y]$ and the x axis is discrtized on $N + 2$ points, the $(k_x)_i$ are defined as:

$$(k_x)_i = \begin{cases} \frac{2\pi(i-1)}{X} & i = 1, \ldots, \frac{N+2}{2} \\ - \frac{2\pi(N+3-i)}{X} & i = \frac{N+2}{2} + 1, \ldots, (N+2) \end{cases} . \tag{37}$$

Appendices

A Notation

The following notation will be used for the spatial derivatives of a complex functional $f : (x_1, \cdots, x_n) \mapsto C$:

$$\nabla f = \text{grad}(f) = \left(\frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_n} \right) \tag{38}$$

$$\nabla \cdot f = div(f) = \frac{\partial f}{\partial x_1} + \cdots + \frac{\partial f}{\partial x_n} \tag{39}$$

$$\nabla^2 f = \nabla \cdot \nabla f = \frac{\partial^2 f}{\partial x_1^2} + \cdots + \frac{\partial^2 f}{\partial x_n^2} \tag{40}$$

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See also

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