Computational Continuum Physics

(TIF330/FYM330), 2023

Problem set 2

Deadline: 23:59 on 2023-05-08

For submission requirements see guidance to written reports on the course page.

Problem 1. Galerkin method (5 points)

Apply Galerkin method to obtain function $f(x)$ in $0 \leq x \leq 1$ that satisfies the equation

$$\frac{\partial^2}{\partial x^2} f(x) = x + 1,$$

and the boundary conditions $f(0) = f(1) = 0$, using the basis functions

$$\chi_j(x) = x(1-x)^j.$$

Perform analytical computations and demonstrate that for $N = 2$ basis functions the resultant approximate solution converges to the exact solution.

Comment: Use scalar product in the form:

$$(v, u) = \int_0^1 v(x)u(x)dx.$$

Problem 2. Split-step Fourier solvers for TDSE (10 points)

Suppose we need to simulate how an intense laser pulse causes ionization of the outer electron of an atom and what kind of secondary radiation causes the induced dynamics of the wave function $\psi(x, y, z, t)$ of the electron. We will assume that the dynamics of the outer electron is described by the Time-Dependent Schrödinger Equation (TDSE) that includes an effective potential $U_i(x, y, z) = -d(x^2 + y^2 + z^2 + w^2)^{-1/2}$ of the ion (averaged effect of the nucleus and the inner electrons, which are assumed unperturbed) and an effective potential $U_l(x, y, z, t) = a(t)x$ that describes the external electric field imposed by the laser pulse in the dipole approximation (the wavelength of the laser is assumed to be much larger than spatial scales of the problem):

$$i\frac{\partial}{\partial t}\psi + \nabla^2\psi - (U_i + U_l)\psi = 0.$$

Hereafter dimensionless units are used. We assume that initially the electron is in the ground state ψ_0 that is known. The real constants d and w characterize the depth and the width of the effective ion potential. The function $a(t) = a_{\max}\exp(-(t-3D)^2/D^2)\sin\omega t$ describes temporal evolution of the electric field strength experienced by the electron; D is the duration of the pulse, ω is the laser frequency. Our goal is to compute the evolution of ψ over $t \in [0, 6D]$. The straightforward implementation of the Fourier-based split-step approach implies splitting the step into the propagators related to ∇^2 and $(U_i + U_l)$ that can be carried out in momentum and coordinate representations, respectively. However, in certain cases the computational routine can be optimized so that the amount of computations can be reduced (assuming the same accuracy level).

Find a way to optimize the solver in the following cases:

(a) The external field is much stronger than the atomic field ($d \ll a_{\max}w^2$) but the frequency ω is too high to cause a prominent detachment of the electron (i.e. of its entire wave packet).

(b) The external field is much stronger than the atomic field ($d \ll a_{\max}w^2$) while the frequency ω is low enough to cause a prominent detachment of the electron (i.e. of its entire wave packet) and its motion far beyond the influence of U_i. At the same time, due to shortness of the pulse (small value of D) there is no overwhelming spread of the initial wave packet ψ_0 (i.e. the electron remains its localization around certain point that moves) over the entire course of the laser pulse action $t \in [0, 6D]$.

In both cases you are supposed to derive and present the explicit form of the propagator and to explain the benefit.

Hint: Consider the effects of the operators $exp(i\alpha(t)x)$ and $exp\left(\alpha(t)\frac{\partial}{\partial x}\right)$.

Extra hint: Observe that requiring the propagator of $(U_i + U_l)$ to be close to unity imposes a strong restriction on time step due to U_l (under the specified conditions). A way to bypass this restriction is to transform the equation into some useful equivalent form. The effect of the first operator specified in the previous hint (consider its substitution to the equation) may lead you to the insight.

Clarification for the extra hint: The substitution of an operator into the given TDSE implies the context: the operator acts on a function and returns another function that is to be substituted to TDSE, i.e. we substitute $\psi(x,y,z,t) = e^{i\alpha(t)x}\varphi(x,y,z,t)$. *One can notice that multiplying by* $e^{-i\alpha(t)x}$ *(from left, to not misinterpret the subject of* ∇^2*) leads to another form of TDSE for* φ *and by setting* $-\dot{\alpha} = a(t)$ *we can cancel the term that caused the unwanted restriction on time step. From the physics point of view, you can now recognize that the effect of external electric field is now to be accounted by the modification of the momentum operator (the shift of* k_x*). This should lead you to the idea that in case (b) we can also transform the equation in a beneficial way (the other suggested operator can help you to change the reference frame).*

Problem 3. Spectral split-step solver for 2D Schrödinger equation (15 points)

Develop a C++ implementation of 2D split-step spectral solver for the time-dependent Schrödinger equation in the following form:

$$i\frac{\partial}{\partial t}\psi(x,y,t) = \left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x,y)\right)\psi(x,y,t),$$

where the coordinates belong to the region $-10 \le x, y \le 10$ with periodic boundary conditions, and $V(x,y)$ is the potential that does not change in time.

Consider the case

$$V(x,y) = -5\left(1 + \left(\frac{x}{5}\right)^2 + \left(\frac{y}{4}\right)^2\right)^{-4}$$

and perform a simulation of the wave function evolution to see the spectrum of this two-dimensional potential: simulate the evolution of the wave function ψ during the time interval $t \in [0, 100]$, starting from the state

$$\psi(t=0) = \frac{1}{\sqrt{\pi}} e^{-\left((x-1)^2 + (y-1)^2\right)},$$

and plot the temporal spectrum of $\psi(0.1, 0)$. What do the peaks in this spectrum correspond to? Determine and specify the location of the first (the lowest frequency) peak.

Comment: For performing FFT consider the use of fftw library (http://www.fftw.org/). You may find useful notes on linking the fftw library via modification of "json" file in VSC under Windows (see pdfs under Module 2); similar modifications should be relevant to other IDEs and OS.