Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.

- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.

- Include the source code of your program. Comment your program properly.

- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.

- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.

- Try to evaluate the reliabilty and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.

- Try to give an interpretation of you results in your answers to the problems.

- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.

- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.

Format for electronic delivery of report and programs

The preferred format for the report is a PDF file. You can also use DOC or postscript formats. As programming language we prefer that you choose between C/C++, Fortran or Python. The following prescription should be followed when preparing the report:

- Use Fronter to hand in your projects, log in at blyant.uio.no and choose 'fellesrom fys3150'. Thereafter you will see an icon to the left with 'hand in' or 'innlevering'. Click on that icon and go to the given project. There you can load up the files within the deadline.

- Upload **only** the report file and the source code file(s) you have developed. The report file should include all of your discussions and a list of the codes you have developed. Do not include library files which are available at the course homepage, unless you have made specific changes to them.

- Comments from us on your projects, approval or not, corrections to be made etc can be found under your Fronter domain and are only visible to you and the teachers of the course.

Finally, we do prefer that you work two and two together. Optimal working groups consist of 2-3 students. You can then hand in a common report.

Project 5, The time-dependent Schrödinger equation, deadline November 30 12am (midnight)

This project deals with the solution of the time-dependent Schrödinger method. We need here the results from project 2 and you should not do this project if you did not solve the optional part of project 2. You will namely need the eigenvectors you generated in order to solve the time-dependent Schrödinger equation.

This project can lead, with extensions, to an eventual publication. However, in its present form it is meant to be finished by the deadline. The project is however demanding.

We give first a general background to the problem.

Given a complete set of of orthonormal basis vectors $|\phi_k\rangle$, we expand the state vector $|\Psi\rangle$ in this basis, and truncate after the first N basis vectors

$$|\Psi\rangle = \sum_{k=1}^{N} c_k |\phi_k\rangle, \quad c_k = \langle \phi_k | \Psi \rangle. \tag{1}$$

The above coefficients c_k are those which where computed in project 2. Conversely, any coefficient vector $\mathbf{c}$ defines a unique wave function on this truncated basis. In the case where the basis vectors are labelled by several quantum numbers, we will have to define some mapping of these onto the single index k. The action of operators can now be viewed as matrix multiplication on the coefficient vector. That is, the action of an operator A on the state vector corresponds to $\mathbf{Ac}$, where the matrix elements of A in the basis of vectors $|\phi_k\rangle$ are given by

$$(\mathbf{A})_{jk} = \langle \phi_j | A | \phi_k \rangle. \tag{2}$$

In this basis the time-dependent Schrödinger equation may be written

$$i\frac{\partial}{\partial t}\mathbf{c}\left(\mathbf{t}\right) = \mathbf{Hc}\left(\mathbf{t}\right). \tag{3}$$

This is the general case of the semi-discrete Schrödinger equation. If we use the eigenvectors $|\psi_k\rangle$ of the Hamiltonian as a basis, the problem becomes trivial when H is time-independent. In this basis H is diagonal, with the diagonal elements being the eigenvalues of H. Equation (3) decouples

$$i\frac{\partial}{\partial t}\mathbf{c}\left(\mathbf{t}\right) = \mathbf{D}\mathbf{c}\left(\mathbf{t}\right), \qquad \mathbf{D} = \mathrm{diag}\left(\mathrm{E}_1, \mathrm{E}_2, \ldots, \mathrm{E}_\mathrm{N}\right), \tag{4}$$

which is what was done in project 2.

The time development is given simply as $c_k\left(t\right) = \exp\left[-i(t-t_0)E_k\right]c_k\left(t_0\right)$. We now look at the case where H has a time-dependent perturbation $H_1\left(t\right)$

$$H\left(t\right) = H_0 + H_1\left(t\right). \tag{5}$$

Here, H_0 is the stationary part of the Hamiltonian of an, as of yet, unspecified number of particles. Here we will consider H_0 to be the full Hamiltonian of the two-electron problem, including the two-particle Coulomb terms, as it was solved in project 2. We will use the eigenvectors $|\psi_k\rangle$ of H_0 as a basis to approximate the total Hamiltonian H. To find the eigenvectors of the many-body Hamiltonian, an approximation method that gives the ground state and the excited states up to some specified cut-off value must be used. The full diagonalization from project 2 is one possible approach. Using the N vectors, obtained in project 2, $|\psi_k\rangle$ of the many-body basis, the matrix version of the Hamiltonian becomes

$$\mathbf{H} = \mathbf{H_0} + \mathbf{H_1}\left(\mathbf{t}\right), \tag{6}$$

where

$$\mathbf{H_0} = \mathrm{diag}\left(\mathrm{E}_1, \mathrm{E}_2, \ldots, \mathrm{E}_\mathrm{N}\right), \qquad \left[\mathbf{H_1}\left(\mathbf{t}\right)\right]_{\mathrm{jk}} = \langle\psi_\mathrm{j}|\mathrm{H}_1|\psi_\mathrm{k}\rangle. \tag{7}$$

There is one potential difficulty however: To use the eigenfunctions $|\psi_k\rangle$ of the stationary part of the Hamiltonian, we have to be able to calculate the matrix elements $\langle\psi_j|H_1\left(t\right)|\psi_k\rangle$. In the case of the many-particle Hamiltonian this can be prohibitively expensive. In most cases, this certainly rules out calculating these matrix elements for each time step. In many cases, however, the time-dependent perturbation $H_1\left(t\right)$ can be written as a product of a function depending only on time, and a function of spatial coordinates. The form of perturbation of interest in this project is that of a system which is influenced by an electric field. Here we will simply limit this perturbation to be time-dependent only for the two particles

$$H_1\left(\vec{x}, t\right) = E_0\sin\left(\omega t\right). \tag{8}$$

To solve the time-dependent Schrödinger equation we will use a so-called multi-step method developed by Blanes and Moan (Physics Letters A, Vol. 265, pages 35 - 42, (2005)).

We start with our solution to the time-independent Schrödinger equation from project 2, rewritten as

$$H_0\psi_j\left(\mathbf{r}_1, \mathbf{r}_2\right) = E_j\psi_j\left(\mathbf{r}_1, \mathbf{r}_2\right). \tag{9}$$

We have limited ourselves to the spatial part of the wave function. Our problem in project 2 does also not have an angular dependence. Here, H_0 is the time-independent part of the Hamiltonian.

The fourth-order time stepping scheme of Blanes and Moan is given for a time step $n + 1$ as

$$\mathbf{\Psi^{n+1}} \approx [\exp -(\mathbf{M_2}) \exp \mathbf{M_1} \exp \mathbf{M_2}] \mathbf{\Psi^n}, \tag{10}$$

where $\mathbf{M_1}$ and $\mathbf{M_2}$ are defined below and consist of terms proportional to integrals of the form $\int \mathbf{H}(\mathbf{s}) \, d\mathbf{s}$ and $\int s\mathbf{H}(\mathbf{s}) \, d\mathbf{s}$. The error goes like $O(\Delta t^5)$. The variable n represents the number of time steps that have been performed.

When applying a time-dependent perturbation, which in our case is given by Eq. 8, the Hamiltonian matrix $\mathbf{H}$ is in the eigenvector basis given by

$$\mathbf{H} = \mathbf{H_0} + \mathbf{H_1}(\mathbf{t}), \tag{11}$$

where $\mathbf{H_0}$ is a diagonal matrix of the energy-eigenvalues, $\mathbf{H_0} = \text{diag}(E_1, E_2, \ldots, E_N)$, and $\mathbf{H_1}(\mathbf{t})$ is given by, in our case,

$$[\mathbf{H_1}(\mathbf{t})]_{jk} = E(t) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi_j^*(\mathbf{r_1}, \mathbf{r_2}) \psi_k(\mathbf{r_1}, \mathbf{r_2}) \, d\mathbf{r_1} d\mathbf{r_2}. \tag{12}$$

The two terms M_1 and M_2 are given as

$$M_1 = -i \int_{t_n}^{t_n + \Delta t} H(s) \, ds, \tag{13}$$

and

$$M_2 = \frac{i}{\Delta t} \int_{t_n}^{t_n + \Delta t} \left(s - \left(\frac{\Delta t}{2} - t_n \right) \right) H(s) \, ds = \frac{i}{\Delta t} \left[\int_{t_n}^{t_n + \Delta t} sH(s) \, ds \right] + \left(\frac{\Delta t}{2} - t_n \right) M_1. \tag{14}$$

Since our perturbation depends on time only, it is easy to calculate the above integrals. In case we need to compute a more involved expectation value (including for example a spatial dependence), then the exponential functions would be matrices and one would need to evaluate the exponential of a matrix.

a) Set up a program which solves Eq. (10) for the ground state and the first excited state from project 2. Allow for different values of the strength in front of the Coulomb interaction from project 2. Test your program for the ground state of the non-interacting two-particle case with a frequency of the electric field given by the energy difference between the ground state and the first excited state. Set $E_0 = 1$ and choose a time interval with

$$t_{\text{final}} = 600 \quad \Delta t = 0.05$$

A good test of your code is to test the one-particle case with no time-dependent perturbation. In this case it is possible to find a simple closed form expression. Study the ground state and compare with your numerical results.

b) It is often difficult to see the physics of a two-variable complex function (three, counting time). It is helpful to introduce the *single-particle density* $\rho_i(\mathbf{r}_i, t)$ defined by integrating the two-particle density, $|\psi(\mathbf{r}_1, \mathbf{r}_2, t)|$, over one of the particles, say particle one

$$\rho_1(\mathbf{r}_1, t) = \int_{-\infty}^{\infty} |\psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 \, d\mathbf{r}_2. \tag{15}$$

In our case we have no angular dependence of the wave function. Furthermore, we will only focus on the density of the relative motion. The center of mass motion is not of interest since the both the time-dependent part and the interacting part do not depend affect the center of mass motion. The density of interest is therefore

$$\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2. \tag{16}$$

Since there is no angular dependence (we have chosen $l = 0$) the radius $\mathbf{r}$ reduces simply to r. The angular dependence has been integrated out.

Compute the above density for both the non-interacting and the interacting systems. Study the time-development of the density function for the ground state and the first excited state using the same strength parameters in front of the Coulomb interaction as in project 2. Use now the spacing between the ground state and the first excited state of the interacting system to define the frequency ω. Comment your results.

There are several tests which have been to be done in addition to those listed above. For example one needs to check that unitarity is observed and that the norm is conserved. However, these topics are beyond the aim of this project. Furthermore, a realistic perturbation has a spatial dependence as well. In this case one needs to develop a function which computes the exponential of a matrix. With these ingredients in place, this method can be extended to consider realistic quantum mechanical cases and could form the background for a possible scientific article. One very hot topic is to study the temporal evolution of electrons in so-called quantum dots.