FYS-4096 Computational Physics: Project work 1

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Weeks 8-9, 2019

General remarks and instructions:

- You should have access to `miscellaneous_files` on teacher's repo.
- There you will find files that may be of help.
- **Everyone needs to do**
  - **The warm up problem** (2 points)
  - **and one of the problems 1-7!** (10 points)
- Deadline is March 8, 2019 before the exercise session at noon. Be prepared to demonstrate your solutions to others.
- In order to pass the project work a minimum of $1 + 2$ points are needed. That is, there has to be enough correctly done in both the warm up and the chosen problem.

Returning your Project work

1. Create a new git repo or make new folder to your existing Computational Physics repo.
2. Create a file problems_solved.txt at the root of your "Project_Work_1" git repo. Inside it, write for example "warm up and problem 3".
3. Make sure all your source files are under version control and push them to GitLab.
4. Tag your final solution (git commit) with "final" tag: `git tag final`
5. Push your commits and the final tag to GitLab before noon on Friday March 8, 2019: `git push --all && git push --tags`
6. Remember to share your GitLab project with the teacher and notify the teacher once you are ready (Teacher's GitLab account: kylanpaait, ilkka.kylanpaa@tuni.fi).

Warm up problem: 2D integration

- Calculate the below 2D integral with scipy's simpson rule over the area specified by the "lattice" vectors $\mathbf{a}_1 = (1.1, 0)$ and $\mathbf{a}_2 = (1/2, 1)$.

$$\int_\Omega (x+y) e^{-\frac{1}{2}\sqrt{x^2+y^2}} dxdy. \tag{1}$$

- Make a nice plot of the integrand and make the area Ω visible in the plot. Use for example contourf.

- The value of the integral should be close to 0.824887.

Problem 1: Induced magnetic field by current loops

- According to the law of Biot and Savart the magnetic field by a current element is given as

$$d\mathbf{B} = \frac{\mu_0}{4\pi} \frac{I d\mathbf{l} \times \hat{\mathbf{r}}}{r^2}, \tag{2}$$

  where $d\mathbf{l}$ is a vector of length dl in the direction of the current, and r is the distance of the segment dl from a position in space.

- For a single circular current loop in the yz-plane with radius a an analytical solution along the x-axis in the middle of the loop is

$$B_x = \frac{\mu_0 I a^2}{2(x^2+a^2)^{3/2}}. \tag{3}$$

- Write a code for calculating the magnetic field of a circular current loop in the yz-plane, and make a test function that compares your result with the above analytical result.

- Once the above code is working, consider the case where you have two parallel and identical circular current loops. These are placed a distance $4a$ apart from each other in a way that they share the axis going throught their mid-points (symmetry axis). The current is flowing in the same direction in both circuit.

- For the two loop system calculate the magnetic field in 3D and make a figure of the 3D vector field. Spend some time in tuning the figure (coloring, shape, labels, etc.).

Problem 2: Stationary state Schrödinger equation in 2D

- Using finite difference approach make a code that solves a single particle Schrödinger equation in 2D.

$$H\Psi(x,y) = E\Psi(x,y), \tag{4}$$

  where $H = -\frac{\hbar^2}{2m}\nabla^2 + V(x,y)$.

- Use harmonic potential as your test case, i.e., $V(x,y) = \frac{1}{2}m\omega^2(x^2+y^2)$. Choose for example $\hbar = m = \omega = 1$. Consider the accuracy of at least the two lowest eigenvalues and the ground state density ($|\Psi_{0,0}|^2$) in your testing. Notice that the energies are given as $E_{n_x,n_y} = \hbar\omega(n_x + n_y + 1)$, where $n_x = 0, 1, \ldots$ and $n_y = 0, 1, \ldots$, and the wave function as $\Psi_{n_x,n_y}(x,y) = \phi_{n_x}(x)\phi_{n_y}(y)$, where $\phi_n(\cdot)$ is the solution for the quantum harmonic oscillator in 1D:

$$\phi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \tag{5}$$

  where H_n are Hermite polynomials.

- Also use square domain with same spacing for both x and y directions.

- Remember that the kinetic term (T) in 2D can be represented as the kronecker sum: $T_x \oplus T_y = T_x \otimes I + I \otimes T_y$, where I is the identity matrix. In addition, the potential is diagonal.

- Once you are satisfied with the testing, include a gaussian perturbation into your harmonic potential. Choose such a perturbation that you can see the effect in both the ground state energy and the density.

- Make proper figures of the ground state electron density and comparison to the unperturbed case.

- Plot also some densities of the excited states.

Problem 3: Time-dependent two dimensional heat equation

- Make your own Python code that uses FTCS scheme for solving the Heat equation in 2D:

$$\frac{\partial u}{\partial t} = \alpha\nabla^2 u + f. \tag{6}$$

- Test your code with the "Test problem 1" that can be found at this link.

- In the test case compare the differences/accuracy between your numerical approach with the exact answer.

- After that solve the "Test problem 2" from the same location.

- That is, your code should be able to handle these two different cases.

- Make presentable figures of the temperature profiles.

Problem 4: Time-dependent Schrödinger equation in 1D

- Use the **Crank-Nicholson method** for solving the time propagation of a quantum particle in 1D.

$$i\hbar\frac{\partial\phi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x,t) + V(x,t)\phi(x,t). \tag{7}$$

- Use propagation of a Gaussian wave packet as your test case. That is, use for example the initial condition

$$\phi(x,t=0) = \frac{1}{\sqrt{\sigma_0\sqrt{\pi}}}e^{ik_0x}e^{-(x-x_0)^2/(2\sigma_0^2)}, \tag{8}$$

  where k_0 is the average wave number (or $\hbar k_0$ the average momentum), σ_0 the width of the packet and x_0 the position about which the packet is localized. When $V(x) = 0$ the probability density $P(x,t) = |\phi(x,t)|^2$ evolves as

$$P(x,t) = \frac{\sigma_0}{|\alpha|^2\sqrt{\pi}}\exp\left[-\frac{\sigma_0^4}{|\alpha|^4}\frac{(x - x_0 - \hbar k_0 t/m)^2}{\sigma_0^2}\right], \tag{9}$$

  where $\alpha^2 = \sigma_0^2 + i\hbar t/m$.

- Once your test case is working, consider a case where your wave packet is reflecting from a wall.

- Make proper figures of the electron density before and after reflection. Make also a figure of the electron density in the (x,t)-plane.

Problem 5: LU decomposition and thermal density matrix

- At this wikipedia link you will find a C code example of LU decomposition, how it can be used in solving linear matrix equations, inverting matrices, and calculating the determinant of a matrix.
- Transform these codes into working Python module with proper commenting.
- Make test functions that compare the results from your implementations against Python's own solvers.
- As your test matrix and equation use the 1D FEM Poisson case (Problem 2) of Exercise 6.
- Once your routines are working your task is to consider a system of three non-interacting identical Fermions. The thermal density matrix for such a system is given as the determinant below

$$\rho(R,R';\beta) = \begin{vmatrix} \rho^K(\mathbf{r}_1,\mathbf{r}'_1;\beta) & \rho^K(\mathbf{r}_1,\mathbf{r}'_2;\beta) & \rho^K(\mathbf{r}_1,\mathbf{r}'_3;\beta) \\ \rho^K(\mathbf{r}_2,\mathbf{r}'_1;\beta) & \rho^K(\mathbf{r}_2,\mathbf{r}'_2;\beta) & \rho^K(\mathbf{r}_2,\mathbf{r}'_3;\beta) \\ \rho^K(\mathbf{r}_3,\mathbf{r}'_1;\beta) & \rho^K(\mathbf{r}_3,\mathbf{r}'_2;\beta) & \rho^K(\mathbf{r}_3,\mathbf{r}'_3;\beta) \end{vmatrix} \tag{10}$$

  with

$$\rho^K(\mathbf{r},\mathbf{r}';\beta) = (4\pi\lambda\beta)^{-d/2} e^{-\frac{(\mathbf{r}-\mathbf{r}')^2}{4\lambda\beta}}, \tag{11}$$

  where $\beta = 1/(k_\mathrm{B}T)$, $\lambda = \hbar^2/(2m)$ and d is the dimensionality.
- Consider your three identical Fermions in 2D, that is, $d = 2$. Fix the initial configuration to $\mathbf{r}_1 = (1,0)$, $\mathbf{r}_2 = (-1,1)$, and $\mathbf{r}_3 = (0,0)$. For the primed coordinates keep $\mathbf{r}_1$ and $\mathbf{r}_2$ fixed at the same positions, but let $\mathbf{r}_3 = (x,y)$ have any values in the xy-plane, e.g., $x, y \in [-5,5]$. This way you are able to map out the so-called "nodal surface" for the third particle. This tells you, for example, if the density matrix would change its sign when particle 3 is moving from $\mathbf{r}_3$ to $\mathbf{r}'_3$.
- Use $\lambda = 1$ and at least $\beta = 10$, 1, and 0.1, and make proper plots of the xy-plane nodal surface, e.g, by using contourf and colormaps.
- Also, in the same plots make a circle around the initial position of $\mathbf{r}_3$ that has a radius of the thermal de Broglie wave length, i.e., $\sqrt{2\lambda\beta}$.

Problem 6: Classical scattering

- Consider scattering process of a particle with mass m in a central potential $V(r)$.
- Assume that the particle is coming from the left with an impact parameter b. This is given as the magnitude of $\mathbf{r} - \mathbf{r} \cdot \mathbf{v}/\|\mathbf{v}\|^2 \, \mathbf{v}$, where $\mathbf{r}$ is the initial position of the particle with respect to the scattering center, and $\mathbf{v}$ is the initial velocity vector.
- Differential cross section of the such a scattering is given by

$$\sigma(\theta) = \frac{b}{\sin(\theta)} \left| \frac{db}{d\theta} \right|, \tag{12}$$

  where $\theta \in [0, \pi/2]$ is the deflection angle.
- Due to the spherically symmetric potential the angular momentum and total energy of the system are conserved during the scattering process. Considering these it is possible to derive the following formulas for the minimum value of the distance (r_m) and the deflection angle (θ):

$$1 - \frac{b^2}{r_\mathrm{m}^2} - \frac{V(r_\mathrm{m})}{E} = 0, \tag{13}$$

$$\theta = 2b \left[\int_b^\infty \frac{dr}{r^2 \sqrt{1 - b^2/r^2}} - \int_{r_\mathrm{m}}^\infty \frac{dr}{r^2 \sqrt{1 - b^2/r^2 - V(r)/E}} \right], \tag{14}$$

  where E is the energy of the incident particle, i.e., $E = mv_0^2/2$.
- Code a program that calculates the differential cross section for arbitrary central potential.
- As your test case consider the Yukawa potential

$$V(r) = \frac{\kappa}{r} e^{-r/a}. \tag{15}$$

- In the limit as $a \longrightarrow \infty$, the Yukava potential approaches the Coulomb potential for which there is an analytical result (Rutherford formula):

$$\sigma(\theta) = \left(\frac{\kappa}{4E} \right)^2 \frac{1}{\sin^4(\theta/2)}. \tag{16}$$

- Plot $\ln(\sigma(\theta))$ as a function of θ for a few different values of parameter a, e.g., $a = 0.1, 1, 10, 100$, and compare your result to the Coulomb case with large a.
- Use, for example, $E = m = \kappa = 1$ in your calculations.

Problem 7: Planetary motion

- Make a code that describes the planetary motion, where Mercury, Venus, Earth, Mars, Jupiter, Saturn, Uranus, Neptune and Pluto are orbiting around the sun.
- Newton's law of gravitation states that the attractive force between two objects with masses m_i and m_j is

$$\mathbf{F}_{ij} = -\frac{Gm_i m_j}{r_{ij}^2}\hat{\mathbf{r}}_{ij}, \tag{17}$$

  where the gravitational constant $G \approx 6.67 \times 10^{-11} Nm^2 kg^{-2}$, $r_{ij} = \|\mathbf{r}_i - \mathbf{r}_j\|$ is the distance between the objects and $\hat{\mathbf{r}}_{ij}$ is the corresponding unit vector.
- Fix the sun at the origin.
- Calculate the trajectories of the planets and consider how the total energy of the system behaves. Notice that the potential energy between objects i and j is given as $U(r_{ij}) = -Gm_i m_j / r_{ij}$, and the kinetic energy of an object is $K = mv^2/2$.
- Regarding the trajectories store sufficiently many snapshots (or instances) of the coordinates as a function of time.
- What kind of initial conditions are satisfactory for relatively stable time evolution?
- Make an animation of the time evolution for example by using XCrySDen and the Fixed-cell animated XSF format. In this case, make a function that writes sufficiently many snapshots into the correct format, which you can straightforwardly convert into a good looking animation.
- Another type of animation is also acceptable as long as it will look better than one made with XCrySDen.