COMPUTATIONAL PHYSICS
Second assignment WS 2022/2023

Deadline: 20th of November 2022
Final date for the mini-exam: 21st/22nd of November

The aim of this assignment is to get familiar with the numerical solution of linear differential equations and the Gauss-Seidel method.

Note: The assignments contain questions and tasks, labeled (a), (b), etc. For some of these tasks, you are supposed to create and hand in one of the following:

- 🖥 a script or a part of a script written in the computer language of your choice;

- 📈 a figure with legends and axis titles.

Other questions primarily serve to guide you through the exercises; you do not need to submit the answers in writing. However, you may be asked these or similar questions during the assessment discussions.

Note: Many tasks in the exercises can be performed using an existing library or toolbox. In line with the aim of the course, however, programming your own analysis tools is encouraged. If libraries or toolboxes are used, you are expected to be able to explain in detail how these algorithms work.

Note: When collaborating in groups of up to 3 students, you are allowed to hand in identical code. Please list all collaborators, for example in the header.

Note: The scripts in the programming exercises should be considered to be intended for general use, and a corresponding coding style will be appreciated. For example, using input parameters as variables, clear presentation of input and output, naming of variables and/or comprehensive comments in the script are among the grading criteria.

1 Solving a system of linear equations

We intend to solve the equation $A\boldsymbol{x} = \boldsymbol{b}$ without inverting the matrix A. Writing the equation element-wise, the set of equations has the following form:

$$\sum_{j=1}^{n} a_{ij}x_j = b_i \qquad \text{for } i = 1, \dots, n \tag{1}$$

with a_{ij} and b_i being the real-valued coefficients of the square matrix A and the vector $\boldsymbol{b}$. To solve this system for $\boldsymbol{x}$ we extract the value x_i from the sum and rewrite it in the following form

$$x_i = -\frac{1}{a_{ii}} \left(\sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij}x_j - b_i \right) = x_i - \left[x_i + \frac{1}{a_{ii}} \left(\sum_{j=1}^{i-1} a_{ij}x_j + \sum_{j=i+1}^{n} a_{ij}x_j - b_i \right) \right]. \tag{2}$$

This leads us to the Gauss-Seidel and Jacobi algorithm. [1]

> ## The Gauss-Seidel method
>
> The Gauss-Seidel method is an iterative method to approximate the solution of a system of linear equations. It uses the already calculated values of the solution vector $x_k^{(p+1)}$ in the calculation of the next values $x_i^{(p+1)}$ for $i > k$, where p is the iteration index. At every iteration, the value of x_i is calculated from
> $$x_i^{(p+1)} = x_i^{(p)} - \Delta x_i^{(p)}. \tag{3}$$
> The corresponding equation for $\Delta x_i^{(p)}$ is:
>
> $$\Delta x_i^{(p)} = x_i^{(p)} + \frac{1}{a_{ii}} \left(\sum_{j=1}^{i-1} a_{ij}x_j^{(p+1)} + \sum_{j=i+1}^{n} a_{ij}x_j^{(p)} - b_i \right), \tag{4}$$
>
> for $a_{ii} \neq 0$.

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[1]More information on the Gauss-Seidel and Jacobi algorithm, may be found in last years lecture notes p.89-92 (link in the teachcenter)

(a) 🖥 Implement the Gauss-Seidel method and Jacobi method for solving a set of n linear equations. Make sure that the input consists of A, $\boldsymbol{b}$ and optionally the convergence and abortion criteria. The output should consist of the vector $\boldsymbol{x}$ and optionally a status parameter.

(b) 📈 Create now a random matrix of reasonably large dimensions (e.g. 100×100 or 1000×1000) and a vector $\boldsymbol{b}$ and solve $\boldsymbol{b} = A\boldsymbol{x}$. Use your Gauss-Seidel and Jacobi method to solve for $\boldsymbol{x}^{(p)}$ and get back your vector $\boldsymbol{b}^{(p)} = A\boldsymbol{x}^{(p)}$. Plot the difference of the initial vector $\boldsymbol{b}$ and the vector $\boldsymbol{b}^{(p)}$ your methods return over the number of iterations p (use the sum over the absolute value of the difference).

2   Electron transmission through a molecular transport system

We consider the system shown in Fig. 1, consisting of a hydrocarbon molecule with 6 atomic sites, two of which are connected to gold electrodes. We are interested in the transmission probability of an electron from one electrode to the other, which determines the electric conductance of the molecular system.
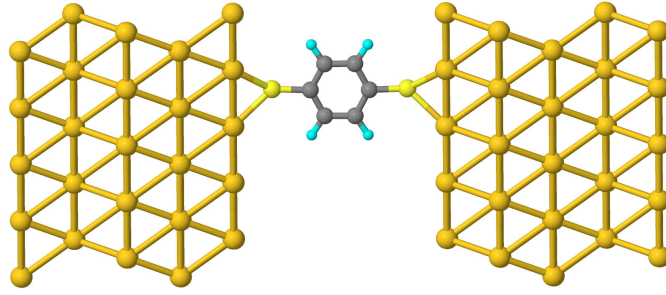
Figure 1: Example of a quantum transport system. *Color code*: Au (gold), S (yellow), C (gray), H (cyan)

The Schrödinger equation

The time-dependent Schrödinger equation reads

$$i\hbar\partial_t\big|\Psi(t)\big\rangle = \hat{H}\big|\Psi(t)\big\rangle.$$

When we limit ourselves to steady-states (i.e. no *explicit* time dependence) the time-dependent Schrödinger equation turns into an eigenvalue equation

$$\hat{H}\big|\Psi\big\rangle = E\big|\Psi\big\rangle,$$

with E being the energy. Solving for the wavefunction $\big|\Psi\big\rangle$ is cumbersome at times. Therefore we choose a complete orthonormal basis set $\big|\Phi_i\big\rangle$ and expand $\big|\Psi\big\rangle$ as

$$\big|\Psi\big\rangle = \sum_i c_i\big|\Phi_i\big\rangle.$$

Our problem has now simplified to finding the coefficients c_i, for which we can write the equation

$$H\boldsymbol{c} = E\boldsymbol{c},$$

where H is a matrix and $\boldsymbol{c}$ contains the coefficients of the basis functions.

Instead of solving the Schrödinger equation directly, we will take advantage of the Green's function $G(E)$, which is defined by the equation

$$(H - E\mathcal{I})\, G(E) = \mathcal{I},$$

where $\mathcal{I}$ is the identity matrix. Furthermore, since the Hamiltonian of the complete system has too many degrees of freedom, we partition the system into a region of interest (the central ring) and the environment (the electrodes), and write

$$\left(H_R - E\mathcal{I} + i\Delta(E)\right) G_R(E) = \mathcal{I}, \tag{6}$$

where H_R, $G_R(E)$ are the parts of H and $G(E)$ describing the ring and the matrix $\Delta(E)$ describes the influence of the electrodes on the ring. Entering and leaving the ring is taken into account through the matrix $\Delta(E)$, which quantifies a 'broadening' of the energy levels of the ring by the contact with the electrodes. To calculate the transmission between sites α and β, we set $\Delta_{\alpha\alpha}(E) = \Delta_{\beta\beta}(E) = \delta$, independent of E. Through Heisenberg's uncertainty, the energy broadening δ is related to the time τ it takes an electron to escape to the electrode by $\delta\tau = \hbar/2$.[2] After solving Eq. (6), the transmission properties of the system can be calculated directly from $G_R(E)$, which has the same dimensions as the Hamilton matrix H_R.

(a) Verify that Eq. (6) can be solved for each column of $G_R(E)$ individually, reducing every calculation to the form $A\boldsymbol{x} = \boldsymbol{b}$.

To write down the Hamiltonian of the ring we use *second quantization*.[3] For simplicity we limit ourselves to non-interacting particles, which can only move between the sites α and β of the N-site ring,

$$\hat{H}_R = \sum_{\alpha,\beta=1}^{N} t_{\alpha\beta}\hat{a}_\alpha^\dagger \hat{a}_\beta,$$

where $\hat{a}_\alpha^\dagger$ is an operator creating an electron in state α, while $\hat{a}_\beta$ is an operator destroying it in state β. The coefficients $t_{\alpha\beta}$ quantify the probability for an electron to move from state β to state α.[4]

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[2]The lifetime of a particle (or its state) is related to the width of an energy level, so the bigger $\Delta(E)$, the wider the peak and the smaller the lifetime. Describing an isolated system of non-interacting particles we expect infinite lifetimes due to the particles neither having the possibility to leave the system nor to transfer energy to other particles. Coupled to the environment, our system has the possibility to pick up electrons from the enviroment and return them later on, so we expect to observe peaks of finite width. For the present exercise, it is not necessary to be able to reproduce the physics behind this broadening mechanism in detail.

[3]For details on second quantization we refer to any standard quantum mechanics textbook.

[4]If the indices α and β of the creation and annihilation operators are taken to describe the location of the electrons (e.g. lattice site, orbital index, etc.), $\hat{H}_R$ can be expressed as a sum of terms describing hopping processes, so that the matrix representation of $\hat{a}_\alpha^\dagger \hat{a}_\beta$ is a matrix equal to 1 at index $\alpha\beta$ and zero elsewhere.

(b) 🖥 Write a function `ring(N, t, E, delta, alpha, beta)` returning the complex matrix $(H_R - E\mathcal{I} + i\Delta)$ describing a system containing N sites. The electrons are able to hop onto their closest neighbouring sites only (consider $t_{\alpha\beta} = t$ for $\alpha = \beta \pm 1$ and zero otherwise). Make sure to take the ring shape of the molecule into account: electrons are allowed to hop between sites 1 and N. The parameter `delta` is the value of the energy broadening (inverse time scale) of entering and leaving the system through the contacts `alpha` and `beta`.

(c) 🖥 Use the function `ring` to generate the terms of Eq. (6) for two systems: one with electrodes connected to $\alpha = 1$ and $\beta = 3$ and one with $\alpha = 1$ and $\beta = 4$. Use $N = 6$, $t = -2.6$ and $\delta = 0.5$. Use your implementation of the Gauss-Seidel method to calculate $G_{R,\alpha\alpha}$, $G_{R,\beta\beta}$, $G_{R,\alpha\beta}$ and $G_{R,\beta\alpha}$ for the energy interval $E = [-6, 6]$.

Hint: One has the freedom to choose the reference energy of these calculations. This can be done by shifting all elements on the main diagonal of H_R by the same amount.

The transmission probability between contacts α and β is given by the absolute value of the elements of the Green's function,

$$T_{\alpha\beta}(E) = |G_{R,\alpha\beta}(E)|^2. \tag{7}$$

(d) 📈 Plot the transmission for both systems used in (c) as a function of the energy. Additionally calculate the eigenvalues of the Hamiltonian H_R of the ring and compare them to the peaks of your plot. In this exercise it is fine to use a build-in eigenvalue solver. What do you observe and how do you explain it?

3   Poisson equation in more than one dimension

In electrostatics the Poisson equation is a 2nd order linear differential equation which relates the potential $\phi(\boldsymbol{r})$ to the charge density $\rho(\boldsymbol{r})$. (The Heaviside Lorentz system of units is used)

$$\Delta\phi(\boldsymbol{r}) = -\rho(\boldsymbol{r}),$$

where Δ is the Laplace-operator, which in two dimensions reads

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

On a one-dimensional grid with equal spacing h between adjacent grid points x_{n_1} this operator can be discretized as

$$\frac{\partial^2}{\partial x^2} f(x_{n_1}) \approx \frac{f(x_{n_1+1}) - 2f(x_{n_1}) + f(x_{n_1-1})}{h^2} \tag{8}$$

For the two-dimensional Poisson equation on a grid with equal spacing in both x and y direction this implies:

$$\phi(x_{n_1+1}, y_{n_2}) + \phi(x_{n_1-1}, y_{n_2}) + \phi(x_{n_1}, y_{n_2+1}) + \phi(x_{n_1}, y_{n_2-1}) \approx 4\phi(x_{n_1}, y_{n_2}) - h^2 \rho(x_{n_1}, y_{n_2}). \quad (9)$$

In general, the $N_1 \times N_2 \times ... \times N_d$ points of a d dimensional grid are characterized by the vectors $(n_1, n_2, ... n_d)$, with the indices $n_i = 0, 1, ... N_i - 1$ for $i \in \{1, 2, ... d\}$. To transform a d-dimensional problem to the form $A\boldsymbol{x} = \boldsymbol{b}$, the grid points may be adressed by one single index k ("rolled-up index") using

$$k = n_1 + n_2 N_1 + n_3 N_1 N_2 + ... + n_d N_1 N_2 ... N_{d-1}, \quad (10)$$

where $k \in \{0, 1, ... N_1 \times N_2 \times ... \times N_d - 1\}$. Every point(except on the boundary) is surrounded by $2d$ neighbouring points. With the help of the single index, the discretized Poisson equation in two dimensions may be written as:

$$\phi_{k+1} + \phi_{k-1} + \phi_{k+N_1} + \phi_{k-N_1} - 4\phi_k = -h^2 \rho_k. \quad (11)$$

where $\phi_k = \phi(x_{n_1}, y_{n_2})$ with $k = n_1 + n_2 N_1$. Eq. (11) can then be written as

$$-4\phi_k + \sum_{i=nb(k)} \phi_i = -h^2 \rho_k, \quad (12)$$

where $nb(k)$ contains the indices of all neighbours of k.

(a) ⌨ Write a function $\texttt{nb(k, mu)}$ or $\texttt{nb(k, d)}$ which either gives the adress (single index) of a specific neighbour of the point k, indexed by μ, or a list of all neighbours in d dimensions. In the first case, μ runs e.g. from 1 to $2d$ and $\texttt{nb(k, mu)}$ should return the addresses of neighbors in positive direction for $\mu = 1, 2, ... d$ whereas $\texttt{nb(k, d + mu)}$ returns the adresses in negative μ-direction for $\mu = 1, 2, ... d$.

If we interpret ϕ_k and ρ_k as vector elements, Eq. (12) is an equation in vector matrix form:

$$\sum_j A_{ij} \phi_j = -h^2 \rho_i. \quad (13)$$

For the boundary conditions, we either use Dirichlet boundaries (fixed $\phi(x, y)$ at the boundary) or periodic boundary conditions, which for a rectangular grid in two dimensions are given by

$$\phi(0, y) = \phi(L_x, y) \quad (14)$$
$$\phi(x, 0) = \phi(x, L_y). \quad (15)$$

where L_x and L_y are the corresponding sizes of the domain.

(b) 🖥 Implement a program which creates the discretized Laplace operator A for a two dimensional grid with periodic boundary conditions. As grid size you may e.g. use $N_1 \times N_2 = 50 \times 50$ or 100×100.

(c) 🖥 Use the matrix A together with your Gauss-Seidl algorithm to solve Eq. (12) for the electrostatic potential of a dipole configuration.

(d) How does the computational time scale with the size (N_1, N_2) of the domain?

In general A will be a very sparse matrix, this means most off-diagonal values are zero. This sparsity can be used to speed up the calculation by using Gauss-Seidl only on the non-zero elements.

(e) 🖥 Modify your script to keep a list of non-zero elements when constructing the matrix A and use this list to speed up the Gauss-Seidl algorithm. Alternative implementations, for example based on the function $\mathtt{nb(k, mu)}$, are also possible. Check whether the new calculation is indeed faster.

(f) 🖥 Repeat step (b) and (c) for a Faraday cage. Proceed in the following way: Choose a square inside your grid (e.g. 25×25) where the potential is not allowed to change $\phi(square) = 0$ (these are the grounded rods of your cage). On the upper and the lower bound apply a voltage of $\phi(x, 0) = U$ and $\phi(x, L_y) = -U$, $U = 1$. The charge density ρ is zero everywhere and you should use periodic boundary conditions for the remaining boundaries of your grid: $\phi(0, y) = \phi(L_x, y)$. You may use either the standard Gauss-Seidl or the modified script for sparse matrices from (e).

(g) 📈 Make a 3D-surface plot or a 2D-contour plot of $\phi(x, y)$ for both the dipole and the Faraday cage. Additionally you should make a comparison of your results with the corresponding analytical solution for the dipole configuration.

4 Transport system (Bonus-Task)

The coupling to the left (L) and right (R) electrodes are often not identical. In the general case, the transmission $T(E)$ can be calculated by the formula

$$T(E) = \text{Tr}\big(G_R^\dagger(E)\Gamma^R(E)G_R(E)\Gamma^L(E)\big), \tag{16}$$

with $\Gamma^L(E) = \big(\Delta_L(E) - \Delta_L^\dagger(E)\big)$ and $\Gamma^R(E) = \big(\Delta_R(E) - \Delta_R^\dagger(E)\big)$ with $\dagger$ standing for "complex conjugate".

(a) Assume that all matrix elements of $\Gamma^L(E)$ and $\Gamma^R(E)$ are zero except for $\Gamma_{\alpha\alpha}^L(E) = \Gamma_{\beta\beta}^R(E) = 1$. Show that for this case Eq. (16) simplifies to the transmission of Eq. (7).

(b) 🖥 Generalize the function `ring` in at least one of the following ways:

- Include further hopping processes in your Hamiltonian.[5]

- Allow for more freedom of how the system couples to its enviroment (e.g.: different coupling for both electrodes, `deltaL` and `deltaR` or coupling to sites other than α and β).[6]

- Redo your calculations for a variety of values `deltaL` and `deltaR`. How do your results change for the different values?

- Redo your calculations for a linear hydrocarbon molecule of N sites connecting the two electrodes.

  Hint: A generalized $\Delta(E)$ might require the use of eq. (16). Therefore `ring` should create $\Delta_L(E)$ and $\Delta_R(E)$ seperately, where $\Delta_L(E)$ describes the coupling to the left electrode and $\Delta_R(E)$ the coupling to the right electrode[7] and return both matrices in addition to the Hamiltonian.

(c) 📈 Redo the calculations from before including the generalizations and plot your results.

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[5]Think about a physically reasonable choice of the $t_{\alpha\beta}$ for the new hopping processes.

[6]Here should also be taken care of choosing reasonable values for the new elements of $\Delta(E)$.

[7]For eq. (6) we just have to use $\Delta(E) = \Delta_L(E) + \Delta_R(E)$