Analyse Numérique / Computational Physics (M1) - T. Roscilde, F. Caleca

General rule for the TD sessions: the TD sessions are fully *hands-on* – namely, in every TD session you are supposed to *write computer codes* to learn about the phenomenology and efficiency of important algorithms, or, more ambitiously, to learn the physics of simple, yet fundamental models. You should choose a programming platform (Python, Matlab, Mathematica, C, Fortran, etc.), and you should be able to plot your results in the form of two-dimensional functions $y = f(x)$ (using matplotlib in Python, the plotting utilities of Matlab and Mathematica, Gnuplot, etc.), or occasionally in a more complicated form. We assume that you have some familiarity with at least one programming platform; if this is not the case, you should be able to familiarize yourself rapidly *e.g.* by attending online tutorials.

TD1: Exact diagonalization

In this exercise sheet, we shall use exact diagonalization to learn about the physics of particles in a periodic or quasi-periodic potential; and we will explore the use of the Lanczos algorithm in a simplified form

1 Periodic potential for a quantum particle in a tight-binding chain

In this programming exercise, we will learn about the quantum physics of a particle moving in one dimension in the presence of a periodic potential. This problem will flesh out many fundamental aspects of the physics of solids (cfr. the Condensed Matter lectures in M1). We will focus our attention on the following *tight-binding Hamiltonian*, describing a quantum particle which hops between N discrete positions in one dimension (with periodic boundary conditions), and which is immersed in a periodic potential:

$$\hat{\mathcal{H}}(q,V) = -\sum_{i=1}^{N-1} (|i\rangle\langle i+1| + |i+1\rangle\langle i|) - (|1\rangle\langle N| + |N\rangle\langle 1|) + V\sum_{i=1}^{N} \cos(qi)\ |i\rangle\langle i| \qquad (1)$$

The first two terms describe the kinetic energy of the particle ($|i+1\rangle\langle i|$ is the operator making the particle hop from the state $|i\rangle$ to the state $|i+1\rangle$); and the last term describes the periodic potential (in the form of a cosine) with

$$q = \frac{2\pi}{N}\ p \qquad\qquad p \in \mathbb{N}, \quad 0 \le p \le N/2\ .$$

In particular m is chosen so that $N/p = m \in \mathbb{N}$ – this is the case of a so-called commensurate potential, which describes an integer number m of periods over the periodic chain of length N.

1.1

Write the matrix $H_{i,j} = \langle i|\hat{\mathcal{H}}|j\rangle$ in your computer code, for a length N and a value m and V of your choice.

1.2

Diagonalize the matrix using a library of your choice (standard diagonalization libraries under numpy in Python, in Matlab or Mathematica; LAPACK library in C or Fortran; etc.), namely solving the problem

$$H\boldsymbol{\psi}_k = \lambda_k \boldsymbol{\psi}^{(k)} \qquad k = 1, ..., N \ .$$

Plot the spectrum of eigenvalues for $V = 0$ and $V \neq 0$ (e.g. for $m = N/2$): can you see the appearance of "holes" (so called "band gaps") in the spectrum when $V > 0$?

1.3

How does the number of gaps depend on m?

1.4

How does the width of the gaps depend on V? Make a plot for a given gap and a fixed m.

1.5

Visualize some selected eigenvectors – namely plot the Hamiltonian eigenfunctions $\psi_i^{(k)} = \langle i|\psi^{(k)}\rangle$ as a function of $i = 1, ..., N$. What is the main difference between the ground state and the most excited state? And can you see a defining feature for the eigenvectors corresponding to the two eigenvalues bounding an energy gap from below and from above?

2 Quantum particle in a quasi-periodic potential and Aubry-André transition

In this programming exercise we shall consider the same model as in the previous exercise, but this time the potential will be taken to be incommensurate, namely $q = 2\pi\alpha$ where α is an irrational number. For definiteness, you can take α as the inverse of the golden ratio

$$\alpha = \frac{2}{\sqrt{5}+1}$$

but other values would give you the same physics (you can check this!). In this case the potential never exactly repeat itself on the chain – it is called then "quasi-periodic".
You can use the same construction of the Hamiltonian matrix as in the previous exercise, and just change the parameter q.

2.1

Diagonalize the Hamiltonian matrix for $V = 0.5, 1, 1.5, 2, 2.5, 3$. Plotting the spatial structure of any eigenstate (e.g. the ground state $\psi_i^{(0)}$, and more simply its square modulus $|\psi_i^{(0)}|^2$) you should observe a radical change of behavior around a particular value of V. Which one?

2.2

You can capture this transition (the so-called Aubry-André transition for a quantum particle in a quasi-periodic potential) by studying a spatial property of the ground-state wavefunction, called the participation ratio

$$P^{(0)}(V) = \frac{1}{N} \frac{1}{\sum_i \left|\psi_i^{(0)}\right|^4}$$

where $\psi_i^{(0)}$ is the ground state of $\hat{\mathcal{H}}(q,V)$ and we assume that the ground state is normalized. The participation ratio P expresses the fraction of the chain which is effectively covered by the wavefunction (e.g. $P=1$ for a constant normalized wavefunction $\psi_i^{(0)}=1/\sqrt{N}$, as you can easily verify). Plot $P^{(0)}(V)$ vs. V to visualize the Aubry-André transition in the ground state.
Extra question. Repeat the same study using the k-the eigenstate with arbitrary k. What do you observe for the behavior of $P^{(k)}(V)$?

3 Modified Lanczos algorithm

In this programming exercise, we will try to find the lowest-energy eigenvalue and eigenstate of the previous problem (particle in an incommensurate potential) by using a simplified version of the Lanczos algorithm – the so-called modified Lanczos approach.

3.1

Use same matrix as in the previous exercises, for instance the $H(q,V)$ with $V=2$ and $q=4\pi/(1+\sqrt{5})$.

3.2

Generate a random vector $\boldsymbol{u}_0$ of length N, and normalize it. If you do not know how to generate random numbers, just take a uniform vector with $1/\sqrt{N}$ on all entries.

3.3

Build the second Lanczos vector

$$\beta_1 \boldsymbol{u}_1 = H\boldsymbol{u}_0 - \left(\boldsymbol{u}_0^T H \boldsymbol{u}_0\right)\boldsymbol{u}_0 \tag{2}$$

where β_1 is the normalization factor.

3.4

Build the 2x2 matrix

$$H^{(1)} = \begin{pmatrix} \boldsymbol{u}_0^T H \boldsymbol{u}_0 & \boldsymbol{u}_0^T H \boldsymbol{u}_1 \\ \boldsymbol{u}_1^T H \boldsymbol{u}_0 & \boldsymbol{u}_1^T H \boldsymbol{u}_1 \end{pmatrix} \tag{3}$$

which you can then diagonalize (even analytically!! It is possible for a 2x2 matrix) in order to find the lowest-energy state

$$\boldsymbol{\psi}_0^{(1)} = a\ \boldsymbol{u}_0 + b\ \boldsymbol{u}_1 \qquad (a^2+b^2=1) \tag{4}$$

with corresponding eigenvalue $E_0^{(1)}$.

3.5

Use $\boldsymbol{\psi}_0^{(1)}$ as the new initial trial vector for the Lanczos approach, namely consider the reduced 2-dimensional subspace spanned by $\boldsymbol{\psi}_0^{(1)}$ and $\boldsymbol{\psi}_1^{(1)}$ defined as

$$\gamma_1 \boldsymbol{\psi}_1^{(1)} = H\boldsymbol{\psi}_0^{(1)} - \left[(\boldsymbol{\psi}_0^{(1)})^T H \boldsymbol{\psi}_0^{(1)}\right]\boldsymbol{\psi}_0^{(1)} \tag{5}$$

where γ_1 is the normalization factor. Then build the new matrix

$$H^{(2)} = \begin{pmatrix} (\boldsymbol{\psi}_0^{(1)})^T H \boldsymbol{\psi}_0^{(1)} & (\boldsymbol{\psi}_0^{(1)})^T H \boldsymbol{\psi}_1^{(1)} \\ (\boldsymbol{\psi}_1^{(1)})^T H \boldsymbol{\psi}_0^{(1)} & (\boldsymbol{\psi}_1^{(1)})^T H \boldsymbol{\psi}_1^{(1)} \end{pmatrix} \tag{6}$$

which you can again diagonalize to find its ground state $\boldsymbol{\psi}_0^{(2)}$ and corresponding eigen-energy $E_0^{(2)}$.

3.6

Reiterating the above procedure you will obtain new estimates $E_0^{(3)}$, $E_0^{(4)}$, ... for the ground-state energy. Monitor the convergence of the sequence $E_0^{(k)}$ to the exact value of E_0 (which you could determine in the previous exercise).