Exact diagonalization (ED), Monte Carlo (MC) projects and Molecular Dynamics (MD) - Numerical Methods II, 2019/2020

18 marzo 2020

1 Rules of the game

Each student selects 2 or 3 projects they're interested in by March 20th. The projects can be chosen from the MD, ED or MC part. You should choose at least one project from the MD part, and one from the MC/ED part.

Hand-in your project 5 days before the exam - both the codes, documentation, and the plots shall be sent to the correspondent examiner by March 29th.

The oral exam will consist of an oral presentation about the code and the problem it takes (10 minutes), followed by questions. The exam will take place on Zoom. The oral exam is scheduled for the 1st of April 2020 beginning at 2pm. Note that the oral exam will include questions not only about your project but also material learnt throughout the course.

1.1 General Tips for All Projects

Important 1! A good code becomes immediately bad if there is no documentation. You should write a short documentation for your code, explaining in brief its structure (functions, input variables, outputs) and its mathematical methodology. Typically, a pair of pages are more than enough. Please, write this in Latex and send that as a pdf file.

Important 2! When writing MC or MD programs, do never forget how to deal with statistical errors! A good code should always return values with their corresponding error bars well in sight.

Important 3! Plots should always be clear: fonts sufficiently large, points visible, axis properly labelled. A good simulation which is not well presented is not of much use.

2 Project list

The list of projects for 2019/2020 includes:

1. **Exact diagonalization of the quantum Ising model in a ladder geometry: from antiferromagnet to decoupled chain**;
2. **Numerical study of disordered systems: the Heisenberg model with exact diagonalization**;
3. **Spectral statistics of the quantum Ising model: from integrable to non-integrable regimes**;
4. **Critical point of the 2D Ising model: correlation functions**;
5. **Finite-temperature phase transition in the 4D Ising model**
6. **Quantum Monte Carlo simulations of the 1D quantum Ising model**
7. **Molecular Dynamics of Liquid Argon**
8. **Structure and Dynamics of Water Clusters**
9. **Transport Properties: Diffusion from Molecular Dynamics**
10. **Exploring Verlet Algorithms in Molecular Dynamics with Lennard-Jones Liquid: Standard Verlet, Leap-Frog Verlet vs Velocity Verlet**

The project has to be discussed at the exam (please send all files in advance - see below). There is no preference for the language used to code: python is recommended for simplicity, C/C++ is also acceptable. For the Molecular Dynamics exercises, Fortran is recommended. Please, check that the code is working on the machines in the lab well in advance.

Below is a detailed description of the projects and the corresponding to-do-lists. Each to-do-list contains mandatory and optional points. A good mark requires solely the mandatory points to be carried out correctly. The best mark can be achieved with all mandatory points and one optional one carried out correctly.

3 Projects

3.1 Exact diagonalization of the quantum Ising model in a ladder geometry: from antiferromagnet to decoupled chain

Preamble.– Here, we are interested in the ground state phase diagram of the quantum Ising model in a two-leg ladder geometry. We denote as a, b the two legs of the ladder, and as $S^{\alpha}_{a,j}$ the spin operator α at the site j of the chain a. The model Hamiltonian is:

$$H = -\sum_{i=1}^{L}(S^{x}_{a,i}S^{x}_{a,i+1} + S^{x}_{b,i}S^{x}_{b,i+1}) + h\sum_{i=1}^{L} S^{z}_{i} + J_{\perp}\sum_{i=1}^{L} S^{x}_{a,i}S^{x}_{b,i} \qquad (1)$$

where we have considered periodic boundary conditions, e.g., $S^{\alpha}_{L+1} = S^{\alpha}_{1}$.

Goals of this project. – The goals of this project are:

- write a code for the exact diagonalization of the model in Eq. (1); use sparse matrices. Use periodic boundary conditions. Compare, for $L = 10$, the computational time required to solve the problem using full or Lanczos diagonalization for a single point in parameter space;
- investigate the $J_{\perp} = 0$ line: the transition point is approximately signalled by a minimum of the gap between the ground state and the first excited state, $\Delta(L)$, at given system size;
- perform the same gap analysis for $h = 0.25$ as a function of $J_{\perp}$: is there a minimum? in case, where?
- perform a finite-size scaling analysis of $\Delta(L)$ at the point where the gap is minimal: plot it as a function of $1/L$ and show if, within numerical accuracy, the gap vanishes.

3.2 Numerical study of disordered systems: the Heisenberg model with exact diagonalization

Preamble. – The one-dimensional Heisenberg model with disorder in the magnetic field term is defined as:

$$H = -J\sum_{i=1}^{L}(S^{x}_{i}S^{x}_{i+1} + S^{y}_{i}S^{y}_{i+1} + S^{z}_{i}S^{z}_{i+1}) + \sum_{i=1}^{L} h_{i}S^{z}_{i} \qquad (2)$$

where h_i are uniformly distributed variables in the interval $[-h_m+h_0, h_0+h_m]$, that is, centered around h_0.

Goals of this project. – The goals of this project are:

- write a code for the exact diagonalization of the model in Eq. (2); use sparse matrices. Use periodic boundary conditions. Compare, for $L = 10$, the computational time required to solve the problem using full or Lanczos diagonalization for a single point in parameter space;
- investigate the $h_m = 0$ point (no disorder): this is a transition point, and is approximately signalled by a minimum of the gap between the ground state and the first excited state, $\Delta(L)$, at given system size; evaluate this gap and discuss its scaling with L;
- *optional*: perform a full, exact diagonalization of the entire spectrum, and compute the energy level statistics: is it Poisson or Wigner-Dyson type? [ask help if needed] Compare the $h_m = 0$ and $h_m = J$ cases.

3.3 Spectral statistics of the quantum Ising model: from integrable to non-integrable regimes

Preamble. – We consider the following spin chain:

$$H = -J \sum_{i=1}^{L} (S_i^x S_{i+1}^x) + J_2 S_i^z S_{i+2}^z + h \sum_{i=1}^{L} S_i^z; \tag{3}$$

For $J_2 = 0$, this spin chain corresponds to the Ising model, which is analytically soluble, while for $J_2 \neq 0$ the model is not integrable.

Goals of this project. – The goals of this project are:

- write a code for the exact diagonalization of the model in Eq. (3); use sparse matrices. Use periodic boundary conditions.
- compute the full spectrum of the model $\{\epsilon_n\}$ for $L = 4, 6, 8, 10$. How does the CPU time required for this operation scale with L?
- the difference between the integrable regime $J_2 = 0$ and the non-integrable one can be diagnosed by studying the level statistics of the model. Carry on the following analysis:

1. calculate the distribution of energy level differences $\delta_n = \epsilon_{n+1} - \epsilon_n$ for $L = 8$ and for values of $J_2 = 0, 0.45$. Do you notice any difference?
2. compute the average level spacing ratio, defined as:

$$r = \frac{1}{2^N} \sum_n r_n \tag{4}$$

where $r_n = \min(\delta_n, \delta_{n+1})/\delta_n$. In the two regimes, is this value different?

3.4 Critical properties of the 2D Ising model on the square and cubic lattices using single spin updates

Preamble.– The starting point is the 2D classical Ising model:

$$H_{Is} = J \sum_{<i,j>} \sigma_i \sigma_j + h \sum_j \sigma_j \tag{5}$$

with $\sigma = \{-1, +1\}$, and the sum in the first term running over nearest-neighbors. We are interested here in the two-point correlation function, defined as:

$$g(r) = \langle \sigma_j \sigma_{j+r} \rangle - \langle \sigma_j \rangle \langle \sigma_{j+r} \rangle \tag{6}$$

where $\langle ... \rangle$ corresponds to a thermal average.

On the square lattice, the Ising model is known to have a second order phase transition for $h = 0$ around $T_c \simeq 2.27$. At the transition point, $g(r)$ is 'critical' - i.e., it decays as a power -, while away from it, it decays as $g(r) \propto \exp[-r/\xi]$, with ξ being the correlation length, which depends on temperature. For a pedagogical review on the Ising model, see Ref.[1].

Goal of this project. – The goals of this project are:

- write a code for the 2D Ising model on the square lattice. Use periodic boundary conditions and single spin updates.
- implement a routine to measure $g(r)$; check analytically if Eq. (6) can be further simplified before coding it.
- evaluate the correlation length ξ for several system sizes $L = [8, 10, 12, 14]$ and temperatures $T = [1, 2, 2.27, 3, 4]$. **Plot** ξ vs T at fixed sizes: can one predict the position of the transition point based on this data?

3.5 Finite-temperature phase transition in the 4D Ising model

Preamble.– The starting point is the 4D classical Ising model:

$$H_{Is} = J \sum_{<i,j>} \sigma_i \sigma_j + h \sum_j \sigma_j \tag{7}$$

with $\sigma = \{-1, +1\}$, and the sum in the first term running over nearest-neighbors. We are interested here in the value of the average magnetization, defined as:

$$M = \sum_j |\sigma_j|/N \tag{8}$$

where N is the number of spins in the system. For convenience, we shall choose an hypercubic lattice wuth dimensions L, so that $N = L^4$

Goal of this project. – The goals of this project are:

- write a code for the 4D Ising model on the hypercubic lattice. Use periodic boundary conditions and single spin updates.
- implement a routine to measure the expectation value of the magnetization, and check that the low-temperature regime returns expectation from analytical calculations;
- study the magnetization as a function of temperature, and try to locate the transition point between ferromagnet and paramagnet.

3.6 Quantum Monte Carlo simulations of the 1D quantum Ising model

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For this project, we refer to the additional notes on the Quantum Ising model from Adriano, available on request.

Goal of this project. – The goals of this project are:

- write a code for the one-dimensional Ising model using the path integral MC method. Using periodic boundary conditions in real space.
- evaluate and **plot** the mean energy value for various temperatures $T = [0.1, 1.0, 10.0]$ and values of the transverse field $h = [0.1, 0.5, 1.0, 2.0]$ at fixed system size L (take L as large as you manage to run in few minutes).

- *optional:* discuss how truncation in imaginary time works. Provide examples of cases where the truncation is affecting the result, and discuss how to performing simulations at smaller imaginary time steps improve the results.

- *optional:* show that the transition is of second order by proving the absence of bi-stability in the energy histogram.

3.7 Molecular Dynamics of Liquid Argon

Preamble.– The goal of this project is to get experience with the numerical algorithms associated with molecular dynamics. The idea will be to write your own molecular dynamics code to simulate liquid Argon. Your goal will be to study a publication by Rahman et al.: Correlations in the Motion of Atoms in Liquid Argon, Phys. Rev. 136, A405 and then write a code (in Fortran preferably).

Goal of this project. – The goals of this project are:

- Study the paper by Rahman.

- Write a molecular dynamics code to simulate 864 Lennard-Jones particles with the potential defined in the paper by Rahman.

- within your molecular dynamics code implement a poor-mans thermostat - scale the velocities of all the particles so that they correspond to a Maxwell-Boltzmann distribution at 94.4K.

- write a code to compute the g(r) between the particles and the running coordination number.

- comment/think about how long it takes to converge a property like the g(r).

3.8 Structure and Dynamics of Water Clusters

Preamble.– The starting point is the hexamer water cluster that we studied in class. You already have the potential for this system given by the sum of electrostatic and Lennard-Jones interactions. In this project you will use the DLPOLY to conduct various types of simulations and then write your own codes to analyze your trajectories. Preference for language in which to write the code is Fortran.

Goal of this project. – The goals of this project are:

- Run the DLPOLY code for the water cluster at 4 temperatures: 50K, 100K, 150K and 200K using the Nose-Hoover thermostat.
- write a code to compute the O-O and O-H g(r): how does temperature affect the g(r)
- sitting yourself on an oxygen atom, write a code to compute the running coordination number around it (the oxygen atom). what does this plot tell you about the physical properties of the cluster as a function of temperature?
- how long does it take to converge the g(r)?
- optional: can you devise a way to determine the melting temperature of the water cluster?

3.9 Transport Properties: Diffusion from Molecular Dynamics

Preamble.– The starting point will be a trajectory of 32 water molecules which I am happy to share with you. If you want, you can also generate it yourself in DLPOLY. You have to use the trajectory to extract the diffusion constant of water molecules. This can be done using either the mean square displacement or the Green Kubo relationship that relates the diffusion constant to the velocity-velocity auto-correlation function.

Goal of this project. – The goals of this project are:

- Run a simulation of bulk water at 300K using DLPOLY. If you have trouble with this, I can share the trajectory with you.
- Compute the mean-square displacement (MSD) of the water molecules as a function of time.
- Try to extract the diffusion constant of the water molecules from the MSD.
- optional: extract the diffusion constant from the velocity-velocity autocorrelation function.

3.10 Exploring Verlet Algorithms in Molecular Dynamics with Lennard-Jones Liquid: Standard Verlet, Leap-Frog Verlet vs Velocity Verlet

Preamble.– The idea will be to write your own molecular dynamics code to simulate liquid Argon. Your goal will be to study a publication by Rahman et al.: Correlations in the Motion of Atoms in Liquid Argon, Phys. Rev. 136, A405 and then write a code (in Fortran preferably). Then your goal is to implement different numerical integrators and compare the quality of the simulations. In particular, you should compare the Verlet, Leap-Frog Verlet and Velocity Verlet integrators.

Goal of this project. – The goals of this project are:

- Study the paper by Rahman.
- Write a molecular dynamics code to simulate 864 Lennard-Jones particles with the potential defined in the paper by Rahman.
- Make a plot of the conserved quantity in the system as a function of time.
- Compare how the quality of your simulations change when you use the standard Verlet, Leap-Frog Verlet and finally the Velocity-Verlet.

Riferimenti bibliografici

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[4] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).

[5] *Introduction to Frustrated Magnetism: Materials, Experiments, Theory*, edited by C. Lacroix, P. Mendels, and F. Mila (Springer, Heidelberg, 2011).