

Lectures IV & V: Examples from the Physical Sciences and Sociology

Morten Hjorth-Jensen

¹Department of Physics and Center of Mathematics for Applications
University of Oslo, N-0316 Oslo, Norway

²Department of Physics and Astronomy, Michigan State University
East Lansing, Michigan, USA

January 28 - February 2

Outline

- 1 Repetition
- 2 Variational and Diffusion Monte Carlo
- 3 Modelling Phase Transition in Statistical Physics
- 4 Peer Pressure and Electoral Behavior

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'lacta Alea est', the die is cast!

Plan for the lectures

- 1 January 28: Introduction to Monte Carlo methods, probability distributions and Monte Carlo Integration.
- 2 January 29: Random numbers, Markov chains, diffusion and the Metropolis algorithm.
- 3 January 30: Applications in sociology, simulations of phase transitions in physics and quantum physics.
- 4 All material taken from my text on Computational Physics, see <http://www.uio.no/studier/emner/matnat/fys/FYS3150/h06/undervisningsmateriale/LectureNotes/>.

Reminder: What is Monte Carlo?

- 1 **Monte Carlo** methods are nowadays widely used, from the integration of multi-dimensional integrals to solving ab initio problems in chemistry, physics, medicine, biology, or even Dow-Jones forecasting. Computational finance is one of the novel fields where Monte Carlo methods have found a new field of applications, with financial engineering as an emerging field.
- 2 **Numerical methods** that are known as Monte Carlo methods can be loosely described as statistical simulation methods, where statistical simulation is defined in quite general terms to be any method that utilizes sequences of random numbers to perform the simulation.

Reminder: Monte Carlo Keywords

Consider it is a numerical experiment

- Be able to generate random variables following a given probability distribution function (PDF). The starting point for any calculation is the derivation of random numbers based on the uniform distribution.
- Sampling rule for accepting a move, important algo Metropolis-Hastings
- Compute standard deviation and other expectation values
- Techniques for improving errors

Metropolis-Hastings Algorithm

The equation for detailed balance with the acceptance probability A is

$$\frac{A(\mu \rightarrow \nu)}{A(\nu \rightarrow \mu)} = \exp(-\beta(E_\nu - E_\mu))$$

is general and we could replace the Boltzmann distribution with other distributions as well. It specifies the ratio of pairs of acceptance probabilities, which leaves us with quite some room to manouvre.

- We give the largest of the two acceptance ratios the value 1 and adjust the other to satisfy the constraint.
- If $E_\mu < E_\nu$ then the larger of the two acceptance ratios is $A(\nu \rightarrow \mu)$ and we set to 1.
- Then we must have

$$A(\mu \rightarrow \nu) = \exp(-\beta(E_\nu - E_\mu))$$

if $E_\nu - E_\mu > 0$ and 1 otherwise. And that is the **Metropolis-Hastings** algorithm.

More general Definition

A Markov chain Monte Carlo method for the simulation of a distribution p is any method producing an ergodic Markov chain of events x whose stationary distribution is p .

- Generate an initial value $x^{(i)}$.
- Generate a trial value y_t with probability $f(y_t|x^{(i)})$.
- Take a new value

$$x^{(i+1)} = \begin{cases} y_t & \text{with probability} = \rho(x^{(i)}, y_t) \\ x^{(i)} & \text{with probability} = 1 - \rho(x^{(i)}, y_t) \end{cases}$$

- We have defined

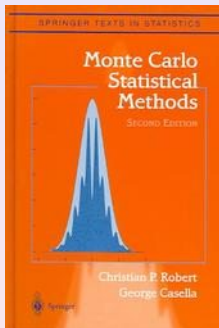
$$\rho(x, y) = \min \left\{ \frac{p(y)f(x|y)}{p(x)f(y|x)}, 1 \right\}.$$

The distribution f is often called the instrumental (we will relate it to the jumping of a walker) or proposal distribution while ρ is the Metropolis-Hastings acceptance probability.

Implementation

- Establish an initial state with some selected features to test.
- Do a random change of this initial state.
- Compute the Metropolis-Hastings acceptance probability ρ
- Compare ρ with a random number r . If $r \leq \rho$ accept, else keep the old configuration.
- Compute the terms needed to obtain expectations values.
- Repeat the above steps in order to have as good statistics as possible.
- For a given number of MC cycles, compute then the final expectation values.

A good introductory Text



Casella and Roberts

- C. R. Robert and G. Casella, *Monte Carlo Statistical Methods*, Springer, 2nd edition 2004.
- Chapters 1-7 cover to a large extent my lectures, with proofs and many more examples.

Quantum Monte Carlo

Most quantum mechanical problems of interest in e.g., atomic, molecular, nuclear and solid state physics consist of a large number of interacting electrons and ions or nucleons. The total number of particles N is usually sufficiently large that an exact solution cannot be found. Typically, the expectation value for a chosen hamiltonian for a system of N particles is

$$\langle H \rangle = \frac{\int d\mathbf{R}_1 d\mathbf{R}_2 \dots d\mathbf{R}_N \Psi^*(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N) H(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N) \Psi(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N)}{\int d\mathbf{R}_1 d\mathbf{R}_2 \dots d\mathbf{R}_N \Psi^*(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N) \Psi(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N)},$$

an in general intractable problem.

Quantum Monte Carlo

As an example from the nuclear many-body problem, we have Schrödinger's equation as a differential equation

$$\hat{H}\Psi(\mathbf{r}_1, \dots, \mathbf{r}_A, \alpha_1, \dots, \alpha_A) = E\Psi(\mathbf{r}_1, \dots, \mathbf{r}_A, \alpha_1, \dots, \alpha_A)$$

where

$$\mathbf{r}_1, \dots, \mathbf{r}_A,$$

are the coordinates and

$$\alpha_1, \dots, \alpha_A,$$

are sets of relevant quantum numbers such as spin and isospin for a system of A nucleons ($A = N + Z$, N being the number of neutrons and Z the number of protons).

Quantum Monte Carlo

There are

$$2^A \times \binom{A}{Z}$$

coupled second-order differential equations in $3A$ dimensions.

For a nucleus like ^{10}Be this number is **215040**. This is a truly challenging many-body problem.

Methods like partial differential equations can at most be used for 2-3 particles.

Quantum Many-particle(body) Methods

- 1 Monte-Carlo methods
- 2 Renormalization group (RG) methods, in particular density matrix RG
- 3 Large-scale diagonalization (Iterative methods, Lanczo's method, dimensionalities 10^{10} states)
- 4 Coupled cluster theory, favoured method in quantum chemistry, molecular and atomic physics. Applications to ab initio calculations in nuclear physics as well for large nuclei.
- 5 Perturbative many-body methods
- 6 Green's function methods
- 7 Density functional theory/Mean-field theory.....

The physics of the system hints at which many-body methods to use. For systems with strong correlations among the constituents, item 5 and 7 are ruled out.

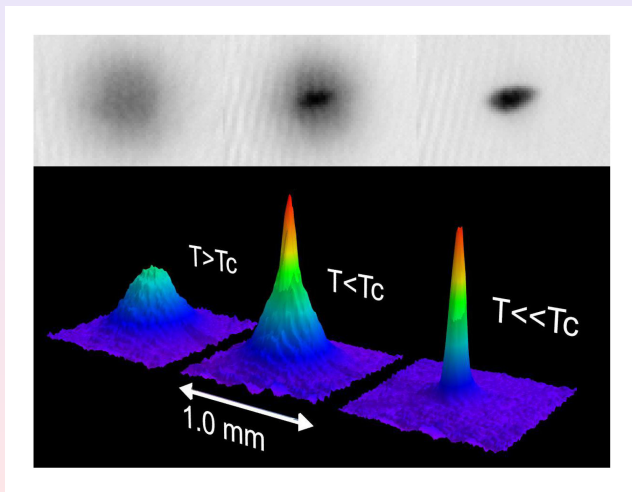
Pros and Cons of Monte Carlo

- Is physically intuitive.
- Allows one to study systems with many degrees of freedom. Diffusion Monte Carlo (DMC) and Green's function Monte Carlo (GFMC) yield in principle the exact solution to Schrödinger's equation.
- Variational Monte Carlo (VMC) is easy to implement but needs a reliable trial wave function, can be difficult to obtain.
- DMC/GFMC for fermions (spin with half-integer values, electrons, baryons, neutrinos, quarks) has a sign problem. Nature prefers an anti-symmetric wave function. PDF in this case given distribution of random walkers ($p \geq 0$).
- The solution has a statistical error, which can be large. Hard to compete with light systems in quantum chemistry (less than 100 electrons).
- There is a limit for how large systems one can study, DMC needs a huge number of random walkers in order to achieve stable results.
- Obtain only the lowest-lying states with a given symmetry. Difficult to get excited states.

Where and why do we use Monte Carlo Methods in Quantum Physics

- Quantum systems with many particles at finite temperature: Path Integral Monte Carlo with applications to dense matter and quantum liquids (phase transitions from normal fluid to superfluid). Strong correlations.
- Bose-Einstein condensation of dilute gases, method transition from non-linear PDE to Diffusion Monte Carlo as density increases.
- Light atoms, molecules and nuclei. In quantum chemistry, atomic and molecular physics however precision not good enough. Applications in nuclear physics for systems with less than 12 nucleons.
- Lattice Quantum-Chromo Dynamics. Impossible to solve without MC calculations.
- Simulations of systems in solid state physics, from semiconductors to spin systems. Many electrons active and possibly strong correlations.

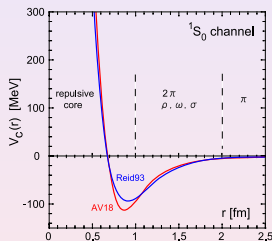
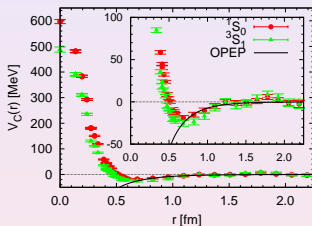
Bose-Einstein Condensation of atoms, thousands of Atoms in one State



Lattice QCD

Brief Description

Analytic or perturbative solutions in QCD are hard or impossible due to the highly nonlinear nature of the strong force. The formulation of QCD on a discrete rather than continuous space-time naturally introduces a momentum cut off at the order $1/a$, which regularizes the theory. As a result lattice QCD is mathematically well-defined. Most importantly, lattice QCD provides the framework for investigation of non-perturbative phenomena such as confinement and quark-gluon plasma formation, which are intractable by means of analytic field theories.

Lattice QCD, Ishii *et al*, nucl-th/0611096

The nucleon-nucleon interaction, Phenomenology vs Lattice calculations.

Quantum Monte Carlo and Schrödinger's equation

For one-body problems (one dimension)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x,t) + V(x,t)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t},$$

Quantum mechanical probability distribution function (PDF)

$$P(x,t) = \Psi(x,t)^*\Psi(x,t)$$

$$P(x,t)dx = \Psi(x,t)^*\Psi(x,t)dx$$

Interpretation: probability of finding the system in a region between x and $x + dx$.
Always real

$$\Psi(x,t) = R(x,t) + iI(x,t)$$

yielding

$$\Psi(x,t)^*\Psi(x,t) = (R - iI)(R + iI) = R^2 + I^2$$

Variational Monte Carlo uses only $P(x,t)$!!

Quantum Monte Carlo and Schrödinger's equation

Petit digression

Choose $\tau = it/\hbar$.

The time-dependent (1-dim) Schrödinger equation becomes then

$$\frac{\partial \Psi(x, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, \tau)}{\partial x^2} - V(x, \tau) \Psi(x, \tau).$$

With $V = 0$ we have a diffusion equation in complex time with diffusion constant

$$D = \frac{\hbar^2}{2m}.$$

Used in diffusion Monte Carlo calculations. The wave function is given by the distribution of random walkers. Leads to problems if the wave function is anti-symmetric.

Quantum Monte Carlo and Schrödinger's equation

Conditions which Ψ has to satisfy:

- 1 Normalization

$$\int_{-\infty}^{\infty} P(x, t) dx = \int_{-\infty}^{\infty} \Psi(x, t)^* \Psi(x, t) dx = 1$$

meaning that

$$\int_{-\infty}^{\infty} \Psi(x, t)^* \Psi(x, t) dx < \infty$$

- 2 $\Psi(x, t)$ and $\partial\Psi(x, t)/\partial x$ must be finite
- 3 $\Psi(x, t)$ and $\partial\Psi(x, t)/\partial x$ must be continuous.
- 4 $\Psi(x, t)$ and $\partial\Psi(x, t)/\partial x$ must be single valued

Square integrable functions.

First Postulate

Any physical quantity $A(\vec{r}, \vec{p})$ which depends on position \vec{r} and momentum \vec{p} has a corresponding quantum mechanical operator by replacing $\vec{p} \rightarrow -i\hbar\vec{\nabla}$, yielding the quantum mechanical operator

$$\hat{A} = A(\vec{r}, -i\hbar\vec{\nabla}).$$

Quantity	Classical definition	QM operator
Position	\vec{r}	$\hat{\vec{r}} = \vec{r}$
Momentum	\vec{p}	$\hat{\vec{p}} = -i\hbar\vec{\nabla}$
Orbital momentum	$\vec{L} = \vec{r} \times \vec{p}$	$\hat{\vec{L}} = \vec{r} \times (-i\hbar\vec{\nabla})$
Kinetic energy	$T = (\vec{p})^2/2m$	$\hat{T} = -(\hbar^2/2m)(\vec{\nabla})^2$
Total energy	$H = (p^2/2m) + V(\vec{r})$	$\hat{H} = -(\hbar^2/2m)(\vec{\nabla})^2 + V(\vec{r})$

Second Postulate

The only possible outcome of an ideal measurement of the physical quantity A are the eigenvalues of the corresponding quantum mechanical operator $\hat{\mathbf{A}}$.

$$\hat{\mathbf{A}}\psi_\nu = a_\nu\psi_\nu,$$

resulting in the eigenvalues a_1, a_2, a_3, \dots as the only outcomes of a measurement.

The corresponding eigenstates $\psi_1, \psi_2, \psi_3 \dots$ contain all relevant information about the system.

Third Postulate

Assume Φ is a linear combination of the eigenfunctions ψ_ν for $\hat{\mathbf{A}}$,

$$\Phi = c_1\psi_1 + c_2\psi_2 + \dots = \sum_{\nu} c_{\nu}\psi_{\nu}.$$

The eigenfunctions are orthogonal and we get

$$c_{\nu} = \int (\Phi)^* \psi_{\nu} d\tau.$$

From this we can formulate the third postulate:

When the eigenfunction is Φ , the probability of obtaining the value a_{ν} as the outcome of a measurement of the physical quantity A is given by $|c_{\nu}|^2$ and ψ_{ν} is an eigenfunction of $\hat{\mathbf{A}}$ with eigenvalue a_{ν} .

Third Postulate

As a consequence one can show that:

when a quantal system is in the state Φ , the mean value or expectation value of a physical quantity $A(\vec{r}, \vec{p})$ is given by

$$\langle A \rangle = \int (\Phi)^* \hat{\mathbf{A}}(\vec{r}, -i\hbar\vec{\nabla}) \Phi d\tau.$$

We have assumed that Φ has been normalized, viz., $\int (\Phi)^* \Phi d\tau = 1$. Else

$$\langle A \rangle = \frac{\int (\Phi)^* \hat{\mathbf{A}} \Phi d\tau}{\int (\Phi)^* \Phi d\tau}.$$

Fourth Postulate

The time development of of a quantal system is given by

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{\mathbf{H}}\Psi,$$

with $\hat{\mathbf{H}}$ the quantal Hamiltonian operator for the system.

Quantum Monte Carlo

Given a hamiltonian H and a trial wave function Ψ_T , the variational principle states that the expectation value of $\langle H \rangle$, defined through

$$E[H] = \langle H \rangle = \frac{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) H(\mathbf{R}) \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})},$$

is an upper bound to the ground state energy E_0 of the hamiltonian H , that is

$$E_0 \leq \langle H \rangle.$$

In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. Traditional integration methods such as the Gauss-Legendre will not be adequate for say the computation of the energy of a many-body system.

Quantum Monte Carlo

The trial wave function can be expanded in the eigenstates of the hamiltonian since they form a complete set, viz.,

$$\Psi_T(\mathbf{R}) = \sum_i a_i \Psi_i(\mathbf{R}),$$

and assuming the set of eigenfunctions to be normalized one obtains

$$\frac{\sum_{nm} a_m^* a_n \int d\mathbf{R} \Psi_m^*(\mathbf{R}) H(\mathbf{R}) \Psi_n(\mathbf{R})}{\sum_{nm} a_m^* a_n \int d\mathbf{R} \Psi_m^*(\mathbf{R}) \Psi_n(\mathbf{R})} = \frac{\sum_n a_n^2 E_n}{\sum_n a_n^2} \geq E_0,$$

where we used that $H(\mathbf{R})\Psi_n(\mathbf{R}) = E_n\Psi_n(\mathbf{R})$. In general, the integrals involved in the calculation of various expectation values are multi-dimensional ones. The variational principle yields the lowest state of a given symmetry.

Quantum Monte Carlo

In most cases, a wave function has only small values in large parts of configuration space, and a straightforward procedure which uses homogeneously distributed random points in configuration space will most likely lead to poor results. This may suggest that some kind of importance sampling combined with e.g., the Metropolis algorithm may be a more efficient way of obtaining the ground state energy. The hope is then that those regions of configurations space where the wave function assumes appreciable values are sampled more efficiently.

The tedious part in a VMC calculation is the search for the variational minimum. A good knowledge of the system is required in order to carry out reasonable VMC calculations. This is not always the case, and often VMC calculations serve rather as the starting point for so-called diffusion Monte Carlo calculations (DMC). DMC is a way of solving exactly the many-body Schrödinger equation by means of a stochastic procedure. A good guess on the binding energy and its wave function is however necessary. A carefully performed VMC calculation can aid in this context.

Quantum Monte Carlo

- Construct first a trial wave function $\psi_T^\alpha(\mathbf{R})$, for a many-body system consisting of N particles located at positions $\mathbf{R} = (\mathbf{R}_1, \dots, \mathbf{R}_N)$. The trial wave function depends on α variational parameters $\alpha = (\alpha_1, \dots, \alpha_N)$.
- Then we evaluate the expectation value of the hamiltonian H

$$E[H] = \langle H \rangle = \frac{\int d\mathbf{R} \Psi_{T_\alpha}^*(\mathbf{R}) H(\mathbf{R}) \Psi_{T_\alpha}(\mathbf{R})}{\int d\mathbf{R} \Psi_{T_\alpha}^*(\mathbf{R}) \Psi_{T_\alpha}(\mathbf{R})}.$$

- Thereafter we vary α according to some minimization algorithm and return to the first step.

Quantum Monte Carlo

Choose a trial wave function $\psi_T(\mathbf{R})$.

$$P(\mathbf{R}) = \frac{|\psi_T(\mathbf{R})|^2}{\int |\psi_T(\mathbf{R})|^2 d\mathbf{R}}.$$

This is our new probability distribution function (PDF). The approximation to the expectation value of the Hamiltonian is now

$$E[H] \approx \frac{\int d\mathbf{R} \psi_T^*(\mathbf{R}) H(\mathbf{R}) \psi_T(\mathbf{R})}{\int d\mathbf{R} \psi_T^*(\mathbf{R}) \psi_T(\mathbf{R})}.$$

Define a new quantity

$$E_L(\mathbf{R}) = \frac{1}{\psi_T(\mathbf{R})} H \psi_T(\mathbf{R}),$$

called the local energy, which, together with our trial PDF yields

$$E[H] = \langle H \rangle \approx \int P(\mathbf{R}) E_L(\mathbf{R}) d\mathbf{R} \approx \frac{1}{N} \sum_{i=1}^N P(\mathbf{R}_i) E_L(\mathbf{R}_i)$$

with N being the number of Monte Carlo samples.

Quantum Monte Carlo

Algo:

- Initialisation: Fix the number of Monte Carlo steps. Choose an initial \mathbf{R} and variational parameters α and calculate $|\psi_T^\alpha(\mathbf{R})|^2$.
- Initialise the energy and the variance and start the Monte Carlo calculation (thermalize)
 - 1 Calculate a trial position $\mathbf{R}_p = \mathbf{R} + r * \text{step}$ where r is a random variable $r \in [0, 1]$.
 - 2 Metropolis algorithm to accept or reject this move

$$w = P(\mathbf{R}_p)/P(\mathbf{R}).$$

- 3 If the step is accepted, then we set $\mathbf{R} = \mathbf{R}_p$. Update averages
- Finish and compute final averages.

Observe that the jumping in space is governed by the variable *step*. Called brute-force sampling. Need importance sampling.

Importance Sampling

We need to replace the brute force Metropolis algorithm with a walk in coordinate space biased by the trial wave function. This approach is based on the Fokker-Planck equation and the Langevin equation for generating a trajectory in coordinate space. For a diffusion process characterized by a time-dependent probability density $P(x, t)$ in one dimension the Fokker-Planck equation reads (for one particle/walker)

$$\frac{\partial P}{\partial t} = D \frac{\partial P}{\partial x} \left(\frac{\partial P}{\partial x} - F \right) P(x, t),$$

where F is a drift term and D is the diffusion coefficient. The drift term is

$$F = 2 \frac{1}{\Psi_T} \nabla \Psi_T$$

where Ψ_T is our trial wave function. The new positions in coordinate space are given as the solutions of the Langevin equation using Euler's method, namely, we go from the Langevin equation

$$\frac{\partial x(t)}{\partial t} = DF(x(t)) + \eta,$$

with η a random variable, yielding a new position

$$y = x + DF(x)\Delta t + \xi,$$

where ξ is gaussian random variable and Δt is a chosen time step.

Importance Sampling

The Fokker-Planck equation yields a transition probability given by the Green's function

$$G(y, x, \Delta t) = \frac{1}{(4\pi D\Delta t)^{3N/2}} \exp\left(-\frac{(y - x - D\Delta t F(x))^2}{4D\Delta t}\right)$$

which in turn means that our brute force Metropolis algorithm

$$A(y, x) = \min(1, q(y, x)),$$

with $q(y, x) = |\Psi_T(y)|^2 / |\Psi_T(x)|^2$ is now replaced by

$$q(y, x) = \frac{G(x, y, \Delta t) |\Psi_T(y)|^2}{G(y, x, \Delta t) |\Psi_T(x)|^2}$$

Quantum Monte Carlo

The radial Schrödinger equation for the hydrogen atom can be written as

$$-\frac{\hbar^2}{2m} \frac{\partial^2 u(r)}{\partial r^2} - \left(\frac{ke^2}{r} - \frac{\hbar^2 l(l+1)}{2mr^2} \right) u(r) = Eu(r),$$

or with dimensionless variables

$$-\frac{1}{2} \frac{\partial^2 u(\rho)}{\partial \rho^2} - \frac{u(\rho)}{\rho} + \frac{l(l+1)}{2\rho^2} u(\rho) - \lambda u(\rho) = 0,$$

with the hamiltonian

$$H = -\frac{1}{2} \frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} + \frac{l(l+1)}{2\rho^2}.$$

Use variational parameter α in the trial wave function

$$u_7^\alpha(\rho) = \alpha \rho e^{-\alpha \rho}.$$

Quantum Monte Carlo

Inserting this wave function into the expression for the local energy E_L gives

$$E_L(\rho) = -\frac{1}{\rho} - \frac{\alpha}{2} \left(\alpha - \frac{2}{\rho} \right).$$

α	$\langle H \rangle$	σ^2	σ/\sqrt{N}
7.00000E-01	-4.57759E-01	4.51201E-02	6.71715E-04
8.00000E-01	-4.81461E-01	3.05736E-02	5.52934E-04
9.00000E-01	-4.95899E-01	8.20497E-03	2.86443E-04
1.00000E+00	-5.00000E-01	0.00000E+00	0.00000E+00
1.10000E+00	-4.93738E-01	1.16989E-02	3.42036E-04
1.20000E+00	-4.75563E-01	8.85899E-02	9.41222E-04
1.30000E+00	-4.54341E-01	1.45171E-01	1.20487E-03

Quantum Monte Carlo

We note that at $\alpha = 1$ we obtain the exact result, and the variance is zero, as it should. The reason is that we then have the exact wave function, and the action of the hamiltonian on the wave function

$$H\psi = \text{constant} \times \psi,$$

yields just a constant. The integral which defines various expectation values involving moments of the hamiltonian becomes then

$$\langle H^n \rangle = \frac{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) H^n(\mathbf{R}) \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})} = \text{constant} \times \frac{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})}{\int d\mathbf{R} \Psi_T^*(\mathbf{R}) \Psi_T(\mathbf{R})} = \text{constant}.$$

This gives an important information: the exact wave function leads to zero variance! Variation is then performed by minimizing both the energy and the variance.

Quantum Monte Carlo

The helium atom consists of two electrons and a nucleus with charge $Z = 2$. The contribution to the potential energy due to the attraction from the nucleus is

$$-\frac{2ke^2}{r_1} - \frac{2ke^2}{r_2},$$

and if we add the repulsion arising from the two interacting electrons, we obtain the potential energy

$$V(r_1, r_2) = -\frac{2ke^2}{r_1} - \frac{2ke^2}{r_2} + \frac{ke^2}{r_{12}},$$

with the electrons separated at a distance $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$.

Quantum Monte Carlo

The hamiltonian becomes then

$$\hat{H} = -\frac{\hbar^2 \nabla_1^2}{2m} - \frac{\hbar^2 \nabla_2^2}{2m} - \frac{2ke^2}{r_1} - \frac{2ke^2}{r_2} + \frac{ke^2}{r_{12}},$$

and Schrödinger's equation reads

$$\hat{H}\psi = E\psi.$$

All observables are evaluated with respect to the probability distribution

$$P(\mathbf{R}) = \frac{|\psi_T(\mathbf{R})|^2}{\int |\psi_T(\mathbf{R})|^2 d\mathbf{R}}.$$

generated by the trial wave function. The trial wave function must approximate an exact eigenstate in order that accurate results are to be obtained. Improved trial wave functions also improve the importance sampling, reducing the cost of obtaining a certain statistical accuracy.

Quantum Monte Carlo

Choice of trial wave function for Helium: Assume $r_1 \rightarrow 0$.

$$E_L(\mathbf{R}) = \frac{1}{\psi_T(\mathbf{R})} H \psi_T(\mathbf{R}) = \frac{1}{\psi_T(\mathbf{R})} \left(-\frac{1}{2} \nabla_1^2 - \frac{Z}{r_1} \right) \psi_T(\mathbf{R}) + \text{finite terms.}$$

$$E_L(R) = \frac{1}{\mathcal{R}_T(r_1)} \left(-\frac{1}{2} \frac{d^2}{dr_1^2} - \frac{1}{r_1} \frac{d}{dr_1} - \frac{Z}{r_1} \right) \mathcal{R}_T(r_1) + \text{finite terms}$$

For small values of r_1 , the terms which dominate are

$$\lim_{r_1 \rightarrow 0} E_L(R) = \frac{1}{\mathcal{R}_T(r_1)} \left(-\frac{1}{r_1} \frac{d}{dr_1} - \frac{Z}{r_1} \right) \mathcal{R}_T(r_1),$$

since the second derivative does not diverge due to the finiteness of Ψ at the origin.

Quantum Monte Carlo

This results in

$$\frac{1}{\mathcal{R}_T(r_1)} \frac{d\mathcal{R}_T(r_1)}{dr_1} = -Z,$$

and

$$\mathcal{R}_T(r_1) \propto e^{-Zr_1}.$$

A similar condition applies to electron 2 as well. For orbital momenta $l > 0$ we have

$$\frac{1}{\mathcal{R}_T(r)} \frac{d\mathcal{R}_T(r)}{dr} = -\frac{Z}{l+1}.$$

Similarly, studying the case $r_{12} \rightarrow 0$ we can write a possible trial wave function as

$$\psi_T(\mathbf{R}) = e^{-\alpha(r_1+r_2)} e^{r_{12}/2}.$$

The last equation can be generalized to

$$\psi_T(\mathbf{R}) = \phi(\mathbf{r}_1)\phi(\mathbf{r}_2)\dots\phi(\mathbf{r}_N) \prod_{i<j} f(r_{ij}),$$

for a system with N electrons or particles.

Diffusion Monte Carlo

Choose $\tau = it/\hbar$. The time-dependent Schrödinger equation becomes then

$$\frac{\partial \Psi(x, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, \tau)}{\partial x^2}$$

Diffusion constant

$$D = \frac{\hbar^2}{2m}$$

Can solve this equation with a random walk algorithm for the above diffusion equation. What happens with an interaction term?

$$\frac{\partial \Psi(x, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, \tau)}{\partial x^2} - V(x)\Psi(x, \tau)$$

Diffusion Monte Carlo

Without the kinetic energy term we have

$$\frac{\partial \Psi(x, \tau)}{\partial \tau} = -V(x)\Psi(x, \tau)$$

which is the same as a decay or growth process (depending on the sign of V). We can obtain the solution to this first-order differential equation by replacing it by a random decay or growth process. We can thus interpret the full SE as a combination of diffusion and branching processes. For the latter, the number of random walkers at a point x depends on the sign of $V(x)$.

Diffusion Monte Carlo

A crucial aspect (which leads to the Monte Carlo sign problem for Fermions, particles with half-integer angular momentum) is that the probability distribution is no longer

$$P(x, \tau) = \Psi^*(x, \tau)\Psi(x, \tau)dx$$

but

$$P(x, \tau) = \Psi(x, \tau)dx$$

Ψ must be nonnegative! It is related to distribution of walkers.
The general solution to SE

$$\Psi(x, \tau) = \sum_n c_n \phi_n(x) e^{-E_n \tau}$$

For sufficiently large τ the dominant term becomes the eigenvalue with lowest energy

$$\Psi(x, \tau \rightarrow \infty) = c_0 \phi_0(x) e^{-E_0 \tau}$$

Diffusion Monte Carlo

Note

- Spatial dependence of $\Psi(x, \tau \rightarrow \infty)$ proportional to ϕ_0
- The population of walkers will however decay to zero unless $E_0 = 0$!
- Can avoid this problem by introducing an arbitrary reference energy V_{ref} , which is adjusted so that an approximate steady state distribution of random walkers is obtained.

We obtain then

$$\frac{\partial \Psi(x, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, \tau)}{\partial x^2} - [V(x) - V_{\text{ref}}] \Psi(x, \tau),$$

and

$$\Psi(x, \tau) \approx c_0 \phi_0(x) e^{-(E_0 - V_{\text{ref}})\tau}$$

Diffusion Monte Carlo

The DMC method is based on rewriting the SE in imaginary time, by defining $\tau = it$. The imaginary time SE is then

$$\frac{\partial \psi}{\partial \tau} = -\hat{\mathbf{H}}\psi.$$

The wave function ψ is again expanded in eigenstates of the Hamiltonian

$$\psi = \sum_i^{\infty} c_i \phi_i,$$

where

$$\hat{\mathbf{H}}\phi_j = \epsilon_j \phi_j,$$

ϵ_j being an eigenstate of $\hat{\mathbf{H}}$. A formal solution of the imaginary time Schrödinger equation is

$$\psi(\tau_1 + \delta\tau) = e^{-\hat{\mathbf{H}}\delta\tau} \psi(\tau_1).$$

Diffusion Monte Carlo

The DMC equation reads

$$-\frac{\partial\psi(\mathbf{R},\tau)}{\partial\tau} = \left[\sum_i^N -\frac{1}{2}\nabla_i^2\psi(\mathbf{R},\tau) \right] + (V(\mathbf{R}) - E_T)\psi(\mathbf{R}).$$

This equation is a diffusion equation where the wave function ψ may be interpreted as the density of diffusing particles (or “walkers”), and the term $V(\mathbf{R}) - E_T$ is a rate term describing a potential-dependent increase or decrease in the particle density. The above equation may be transformed into a form suitable for Monte Carlo methods, but this leads to a very inefficient algorithm. The potential $V(\mathbf{R})$ is unbounded in e.g., atomic systems and hence the rate term $V(\mathbf{R}) - E_T$ can diverge. Large fluctuations in the particle density then result and give impractically large statistical errors.

Diffusion Monte Carlo

These fluctuations may be substantially reduced by the incorporation of importance sampling in the algorithm. Importance sampling is essential for DMC methods, if the simulation is to be efficient. A trial or guiding wave function $\psi_T(\mathbf{R})$, which closely approximates the ground state wave function is introduced. For the trial wave function and energy, one typically uses the results from a as best as possible VMC calculation. A new distribution is defined as

$$f(\mathbf{R}, \tau) = \psi_T(\mathbf{R})\psi(\mathbf{R}, \tau),$$

which is also a solution of the SE when $\psi(\mathbf{R}, \tau)$ is a solution. Modified to

$$\frac{\partial f(\mathbf{R}, \tau)}{\partial \tau} = \frac{1}{2} \nabla [\nabla - F(\mathbf{R})] f(\mathbf{R}, \tau) + (E_L(\mathbf{R}) - E_T) f(\mathbf{R}, \tau).$$

Diffusion Monte Carlo

In this equation we have introduced the so-called force-term F , given by

$$F(\mathbf{R}) = \frac{2\nabla\psi_T(\mathbf{R})}{\psi_T(\mathbf{R})},$$

and is commonly referred to as the “quantum force”. The local energy E_L is defined as previously

$$E_L(\mathbf{R}) = -\frac{1}{\psi_T(\mathbf{R})} \frac{\nabla^2\psi_T(\mathbf{R})}{2} + V(\mathbf{R}),$$

and is computed, as in the VMC method, with respect to the trial wave function.

Diffusion Monte Carlo

We can give the following interpretation. The right hand side of the importance sampled DMC equation consists, from left to right, of diffusion, drift and rate terms. The problematic potential dependent rate term of the non-importance sampled method is replaced by a term dependent on the difference between the local energy of the guiding wave function and the trial energy. The trial energy is initially chosen to be the VMC energy of the trial wave function, and is updated as the simulation progresses. Use of an optimised trial function minimises the difference between the local and trial energies, and hence minimises fluctuations in the distribution f .

DMC

Our previous Green's function, (the diffusion part only)

$$G_{\text{Diff}}(y, x, \Delta t) = \frac{1}{(4\pi D\Delta t)^{3N/2}} \exp\left(-\frac{(y - x - D\Delta t F(x))^2}{4D\Delta t}\right)$$

is replaced by a diffusion piece and a branching part

$$G_{\text{B}}(y, x, \Delta t) = \exp\left(-\left[\frac{1}{2}(E_L(y) + E_L(x)) - E_T\right] \Delta t\right)$$

yielding

$$G_{\text{DMC}}(y, x, \Delta t) \approx G_{\text{Diff}}(y, x, \Delta t) G_{\text{B}}(y, x, \Delta t)$$

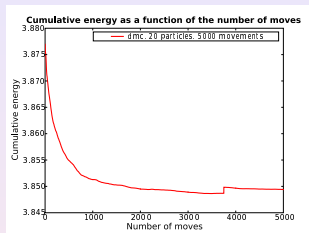
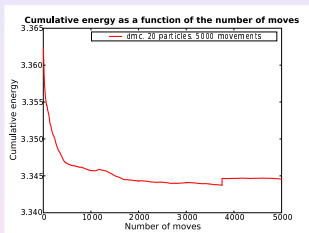
with E_L being the local energy and E_T our trial energy. The Metropolis algorithm is still

$$A(y, x) = \min(1, q(y, x)),$$

with

$$q(y, x) = \frac{G_{\text{DMC}}(x, y, \Delta t) |\Psi_T(y)|^2}{G_{\text{DMC}}(y, x, \Delta t) |\Psi_T(x)|^2}$$

Applications: Bose-Einstein Condensation



Energy evolution of the ground state and an excited vortex state. See Jon Nilsen's article at <http://xxx.lanl.gov/abs/physics/0609191>. A very interesting usage of Python in parallelizing Diffusion Monte Carlo codes.

Statistical Physics

	Microcanonical	Canonical	Grand canonical	Pressure canon
Exchange of heat with the environment	no	yes	yes	yes
Exchange of particles with the environment	no	no	yes	no
Thermodynamical parameters	$V, \mathcal{M}, \mathcal{D}$ E N	$V, \mathcal{M}, \mathcal{D}$ T N	$V, \mathcal{M}, \mathcal{D}$ T μ	$P, \mathcal{H}, \mathcal{E}$ T N
Potential	Entropy	Helmholtz	PV	Gibbs
Energy	Internal	Internal	Internal	Enthalpy

Canonical Ensemble

Helmholtz Free Energy

$$F = -k_B T \ln Z = \langle E \rangle - TS$$

What is the free energy?

$$dF = -SdT - pdV + \mu dN$$

Entropy

$$S = k_B \ln Z + k_B T \left(\frac{\partial \ln Z}{\partial T} \right)_{N,V}$$

Pressure

$$p = k_B T \left(\frac{\partial \ln Z}{\partial V} \right)_{N,T}$$

Chemical Potential

$$\mu = -k_B T \left(\frac{\partial \ln Z}{\partial N} \right)_{V,T}$$

Energy (internal only)

$$E = k_B T^2 \left(\frac{\partial \ln Z}{\partial T} \right)_{V,N}$$

Expectation Values

At a given temperature we have the probability distribution

$$P_i(\beta) = \frac{e^{-\beta E_i}}{Z}$$

with $\beta = 1/kT$ being the inverse temperature, k the Boltzmann constant, E_i is the energy of a state i while Z is the partition function for the canonical ensemble defined as

$$Z = \sum_{i=1}^M e^{-\beta E_i},$$

where the sum extends over all states M . P_i expresses the probability of finding the system in a given configuration i .

Expectation Values

For a system described by the canonical ensemble, the energy is an expectation value since we allow energy to be exchanged with the surroundings (a heat bath with temperature T). This expectation value, the mean energy, can be calculated using the probability distribution P_i as

$$\langle E \rangle = \sum_{i=1}^M E_i P_i(\beta) = \frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i},$$

with a corresponding variance defined as

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \sum_{i=1}^M E_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^M E_i e^{-\beta E_i} \right)^2.$$

If we divide the latter quantity with kT^2 we obtain the specific heat at constant volume

$$C_V = \frac{1}{kT^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right).$$

Expectation Values

We can also write

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta}.$$

The specific heat is

$$C_V = \frac{1}{kT^2} \frac{\partial^2 \ln Z}{\partial \beta^2}$$

These expressions link a physical quantity (in thermodynamics) with the microphysics given by the partition function. Statistical physics is the field where one relates microscopic quantities to observables at finite temperature.

Expectation Values

$$\langle \mathcal{M} \rangle = \sum_i^M \mathcal{M}_i P_i(\beta) = \frac{1}{Z} \sum_i^M \mathcal{M}_i e^{-\beta E_i},$$

and the corresponding variance

$$\sigma_{\mathcal{M}}^2 = \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 = \frac{1}{Z} \sum_{i=1}^M \mathcal{M}_i^2 e^{-\beta E_i} - \left(\frac{1}{Z} \sum_{i=1}^M \mathcal{M}_i e^{-\beta E_i} \right)^2.$$

This quantity defines also the susceptibility χ

$$\chi = \frac{1}{kT} \left(\langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \right).$$

Phase Transitions

NOTE: Helmholtz free energy and canonical ensemble

$$F = \langle E \rangle - TS = -kT \ln Z$$

meaning $\ln Z = -F/kT = -F\beta$ and

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} = \frac{\partial(\beta F)}{\partial \beta}.$$

and

$$C_V = -\frac{1}{kT^2} \frac{\partial^2(\beta F)}{\partial \beta^2}.$$

We can relate observables to various derivatives of the partition function and the free energy. When a given derivative of the free energy or the partition function is discontinuous or diverges (logarithmic divergence for the heat capacity from the Ising model) we talk of a phase transition of order of the derivative.

Phase Transitions

- An important quantity is the correlation length (ξ , to be discussed during friday's lecture). The correlation length defines the length scale at which the overall properties of a material start to differ from its bulk properties. It is the distance over which the fluctuations of the microscopic degrees of freedom (for example the position of atoms) are significantly correlated with each other. Usually it is of the order of few interatomic spacings for a solid.
- The correlation length ξ depends however on external conditions such as pressure and temperature.
- A phase transition is marked by abrupt macroscopic changes as external parameters are changed, such as an increase of temperature.
- The point where a phase transition takes place is called a critical point.

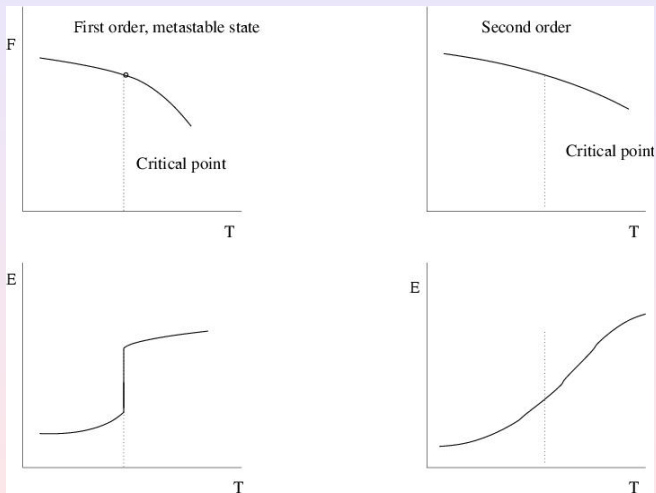
Two Scenarios for Phase Transitions

- 1 First order/discontinuous phase transitions: Two or more states on either side of the critical point also coexist exactly at the critical point. As we pass through the critical point we observe a discontinuous behavior of thermodynamical functions, see figure in forthcoming slides. The correlation length is normally finite at the critical point. Phenomena such as hysteresis occur, viz. there is a continuation of state below the critical point into one above the critical point. This continuation is metastable so that the system may take a macroscopically long time to readjust. Classical example, melting of ice.
- 2 Second order or continuous transitions: The correlation length diverges at the critical point, fluctuations are correlated over all distance scales, which forces the system to be in a unique critical phase. The two phases on either side of the critical point become identical. Smooth behavior of first derivatives of the partition function, while second derivatives diverge. Strong correlations make a perturbative treatment impossible. Renormalization group theory.

Examples of Phase Transitions

System	Transition	Order Parameter
Liquid-gas Binary liquid Quantum liquid Liquid-solid Magnetic solid Dielectric solid	Condensation/evaporation mixture/Unmixing Normal fluid/superfluid Melting/crystallisation Ferromagnetic Antiferromagnetic Ferroelectric Antiferroelectric	Density difference $\Delta\rho = \rho_{liquid} - \rho_{gas}$ Composition difference $\langle \phi \rangle$, $\psi = \text{wavefunction}$ Reciprocal lattice vector Spontaneous magnetisation M Sublattice magnetisation M Polarization P Sublattice polarisation P

Examples of Phase Transitions



Ising and Potts Model

The model we will employ in our studies of phase transitions at finite temperature for magnetic systems is the so-called Ising model. In its simplest form the energy is expressed as

$$E = -J \sum_{\langle kl \rangle}^N s_k s_l - B \sum_k^N s_k,$$

with $s_k = \pm 1$, N is the total number of spins, J is a coupling constant expressing the strength of the interaction between neighboring spins and B is an external magnetic field interacting with the magnetic moment set up by the spins. The symbol $\langle kl \rangle$ indicates that we sum over nearest neighbors only.

Ising Model

Notice that for $J > 0$ it is energetically favorable for neighboring spins to be aligned. This feature leads to, at low enough temperatures, to a cooperative phenomenon called spontaneous magnetization. That is, through interactions between nearest neighbors, a given magnetic moment can influence the alignment of spins that are separated from the given spin by a macroscopic distance. These long range correlations between spins are associated with a long-range order in which the lattice has a net magnetization in the absence of a magnetic field. This phase is normally called the ferromagnetic phase. With $J < 0$, we have a so-called antiferromagnetic case. At a critical temperature we have a phase transition to a disordered phase, a so-called paramagnetic phase.

Potts Model

Another popular set of models are the so-called Potts models. The energy is given by

$$E = -J \sum_{\langle kl \rangle}^N \delta_{s_l, s_k},$$

where the spin s_k at lattice position k can take the values $1, 2, \dots, q$. N is the total number of spins. For $q = 2$ the Potts model corresponds to the Ising model, we can rewrite the last equation as

$$E = -\frac{J}{2} \sum_{\langle kl \rangle}^N 2(\delta_{s_l, s_k} - \frac{1}{2}) - \sum_{\langle kl \rangle}^N \frac{J}{2}.$$

Now, $2(\delta_{s_l, s_k} - \frac{1}{2})$ is $+1$ when $s_l = s_k$ and -1 when they are different. Equivalent except the last term which is a constant and that $J \rightarrow J/2$.

Analytic Results: two-dimensional Ising model

The analytic expression for the Ising model in two dimensions was obtained in 1944 by the Norwegian chemist Lars Onsager (Nobel prize in chemistry). He obtained analytic results for the partition function and various expectations values.

The specific heat is given by

$$C_V = \frac{4k_B}{\pi} (\beta J \operatorname{coth}(2\beta J))^2$$

$$\left\{ K_1(q) - K_2(q) - (1 - \tanh^2(2\beta J)) \left[\frac{\pi}{2} + (2 \tanh^2(2\beta J) - 1) K_1(q) \right] \right\},$$

with

$$K_2(q) = \int_0^{\pi/2} d\phi \sqrt{1 - q^2 \sin^2 \phi}.$$

is the complete elliptic integral of the second kind. Near the critical temperature T_C the specific heat behaves as

$$C_V \approx -\frac{2}{k_B \pi} \left(\frac{J}{T_C} \right)^2 \ln \left| 1 - \frac{T}{T_C} \right| + \text{const.}$$

Analytic Results: two-dimensional Ising model

In theories of critical phenomena one has that

$$C_V \sim \left| 1 - \frac{T}{T_C} \right|^{-\alpha},$$

and Onsager's result is a special case of this power law behavior. The limiting form of the function

$$\lim_{\alpha \rightarrow 0} \frac{1}{\alpha} (Y^{-\alpha} - 1) = -\ln Y,$$

meaning that the analytic result is a special case of the power law singularity with $\alpha = 0$.

Analytic Results: two-dimensional Ising model

One can also show that the mean magnetization per spin is

$$\left[1 - \frac{(1 - \tanh^2(\beta J))^4}{16 \tanh^4(\beta J)} \right]^{1/8}$$

for $T < T_C$ and 0 for $T > T_C$. The behavior is thus as $T \rightarrow T_C$ from below

$$M(T) \sim (T_C - T)^{1/8}$$

The susceptibility behaves as

$$\chi(T) \sim |T_C - T|^{-7/4}$$

Correlation Length

Another quantity (given by the covariance) is the correlation function (defined in friday's lecture)

$$G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle.$$

and the correlation length

$$\xi^{-1} = - \lim_{r \rightarrow \infty} \frac{\partial}{\partial r} \ln G(r),$$

with $r = |i - j|$.

Scaling Results

Near T_C we can characterize the behavior of many physical quantities by a power law behavior. As an example, the mean magnetization is given by

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^\beta,$$

where β is a so-called critical exponent. A similar relation applies to the heat capacity

$$C_V(T) \sim |T_C - T|^{-\alpha},$$

the susceptibility

$$\chi(T) \sim |T_C - T|^\gamma.$$

and the correlation length

$$\xi(T) \sim |T_C - T|^{-\nu}.$$

$\alpha = 0$, $\beta = 1/8$, $\gamma = 7/4$ and $\nu = 1$. Later we will derive these coefficients from finite size scaling theories.

Scaling Results

Through finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) \sim aL^{-1/\nu},$$

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^\beta \rightarrow L^{-\beta/\nu},$$

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\gamma/\nu},$$

and

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\alpha/\nu}.$$

We can compute the slope of the curves for M , C_V and χ as function of lattice sites and extract the exponent ν .

Modelling the Ising Model

The code uses periodic boundary conditions with energy

$$E_i = -J \sum_{j=1}^N s_j s_{j+1},$$

In our case we have as the Monte Carlo sampling function the probability for finding the system in a state s given by

$$P_s = \frac{e^{-(\beta E_s)}}{Z},$$

with energy E_s , $\beta = 1/kT$ and Z is a normalization constant which defines the partition function in the canonical ensemble

$$Z(\beta) = \sum_s e^{-(\beta E_s)}$$

This is difficult to compute since we need all states. In a calculation of the Ising model in two dimensions, the number of configurations is given by 2^N with $N = L \times L$ the number of spins for a lattice of length L . Fortunately, the Metropolis algorithm considers only ratios between probabilities and we do not need to compute the partition function at all.

Metropolis Algorithm

- 1 Establish an initial state with energy E_b by positioning yourself at a random position in the lattice
- 2 Change the initial configuration by flipping e.g., one spin only. Compute the energy of this trial state E_t .
- 3 Calculate $\Delta E = E_t - E_b$. The number of values ΔE is limited to five for the Ising model in two dimensions, see the discussion below.
- 4 If $\Delta E \leq 0$ we accept the new configuration, meaning that the energy is lowered and we are hopefully moving towards the energy minimum at a given temperature. Go to step 7.
- 5 If $\Delta E > 0$, calculate $w = e^{-(\beta\Delta E)}$.
- 6 Compare w with a random number r . If

$$r \leq w,$$

then accept the new configuration, else we keep the old configuration and its values.

- 7 The next step is to update various expectations values.
- 8 The steps (2)-(7) are then repeated in order to obtain a sufficiently good representation of states.

Modelling the Ising Model

In the calculation of the energy difference from one spin configuration to the other, we will limit the change to the flipping of one spin only. For the Ising model in two dimensions it means that there will only be a limited set of values for ΔE . Actually, there are only five possible values. To see this, select first a random spin position x, y and assume that this spin and its nearest neighbors are all pointing up. The energy for this configuration is $E = -4J$. Now we flip this spin as shown below. The energy of the new configuration is $E = 4J$, yielding $\Delta E = 8J$.

$$E = -4J \quad \begin{array}{c} \uparrow \\ \uparrow \uparrow \uparrow \\ \uparrow \end{array} \quad \Longrightarrow \quad E = 4J \quad \begin{array}{c} \uparrow \\ \uparrow \downarrow \uparrow \\ \uparrow \end{array}$$

Modelling the Ising Model

The four other possibilities are as follows

$$E = -2J \quad \downarrow \begin{array}{c} \uparrow \\ \uparrow \\ \uparrow \end{array} \uparrow \quad \Longrightarrow \quad E = 2J \quad \downarrow \begin{array}{c} \uparrow \\ \downarrow \\ \uparrow \end{array} \uparrow$$

with $\Delta E = 4J$,

$$E = 0 \quad \downarrow \begin{array}{c} \uparrow \\ \uparrow \\ \downarrow \end{array} \uparrow \quad \Longrightarrow \quad E = 0 \quad \downarrow \begin{array}{c} \uparrow \\ \downarrow \\ \downarrow \end{array} \uparrow$$

with $\Delta E = 0$

Modelling the Ising Model

$$E = 2J \quad \downarrow \uparrow \uparrow \quad \Rightarrow \quad E = -2J \quad \downarrow \downarrow \uparrow$$

\downarrow \downarrow \downarrow \downarrow

with $\Delta E = -4J$ and finally

$$E = 4J \quad \downarrow \uparrow \downarrow \quad \Rightarrow \quad E = -4J \quad \downarrow \downarrow \downarrow$$

\downarrow \downarrow \downarrow \downarrow

with $\Delta E = -8J$. This means in turn that we could construct an array which contains all values of $e^{\beta\Delta E}$ before doing the Metropolis sampling. Else, we would have to evaluate the exponential at each Monte Carlo sampling.

The loop over T in main

```

for ( double temp = initial_temp; temp <= final_temp; temp+=temp_ste
//   initialise energy and magnetization
E = M = 0.;
// setup array for possible energy changes
for( int de =-8; de <= 8; de++) w[de] = 0;
for(int de =-8; de <= 8; de+=4) w[de+8] = exp(-de/temp);
// initialise array for expectation values
for( int i = 0; i < 5; i++) average[i] = 0.;
initialize(n_spins, temp, spin_matrix, E, M);
// start Monte Carlo computation
for (int cycles = 1; cycles <= mcs; cycles++){
    Metropolis(n_spins, idum, spin_matrix, E, M, w);
    // update expectation values
    average[0] += E;    average[1] += E*E;
    average[2] += M;    average[3] += M*M; average[4] += fabs(M);
}
// print results
output(n_spins, mcs, temp, average);
}

```








The Metropolis function

```

// loop over all spins
for(int y =0; y < n_spins; y++) {
  for (int x= 0; x < n_spins; x++){
    int ix = (int) (ran1(&idum)*(double)n_spins); // RANDOM SPIN
    int iy = (int) (ran1(&idum)*(double)n_spins); // RANDOM SPIN
    int deltaE = 2*spin_matrix[iy][ix]*
(spin_matrix[iy][periodic(ix,n_spins,-1)]+
spin_matrix[periodic(iy,n_spins,-1)][ix] +
spin_matrix[iy][periodic(ix,n_spins,1)] +
spin_matrix[periodic(iy,n_spins,1)][ix]);
    if ( ran1(&idum) <= w[deltaE+8] ) {
spin_matrix[iy][ix] *= -1; // flip one spin and accept new confi
      M += (double) 2*spin_matrix[iy][ix];
      E += (double) deltaE;
    }
  }
}
}

```

Computational Sociophysics

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Monte Carlo Simulations of Opinion Dynamics

Statistical physics teaches us that, even when it is impossible to foresee what a single particle will do, one can often predict how a sufficiently large number of particles will behave, in spite of the eventually large differences between the variables describing the state of the individual particles.

This principle holds, to some extent, for human societies too. It is nearly impossible to predict when one person will die, as death depends on many factors, most of which are hard to control: nevertheless statistics of the mortality rates of large populations are stable for long times and have been studied for over three centuries.

Crucial question:

Can one describe social behaviour through statistical physics?

Monte Carlo Simulations of Opinion Dynamics

Early mathematical models of opinion dynamics date back to the 50's, but the starting point for quantitative investigations in this direction is marked by the theory of social impact proposed by Bibb Latané. The impact is a measure of the influence exerted on a single individual by those agents which interact with him/her (social neighbours). Models based on social impact[3] were among the first microscopic models of opinion dynamics. They are basically cellular automata, where one starts by assigning, usually at random, a set of numbers to any of the N agents of a community. One of these numbers is the opinion, the others describe specific features of the agents, like persuasiveness, supportiveness, tolerance, etc. Society is modelled as a graph, and each agent interacts with its geometric neighbours, which represent friends or close relatives.

Monte Carlo Simulations of Opinion Dynamics

The procedure is iterative: at each iteration one takes a set of interacting agents and updates their opinions (or just the opinion of a single agent), according to a simple dynamical rule. After many iterations, the system usually reaches a state of static or dynamic equilibrium, where the distribution of the opinions among the agents does not change shape, even if the agents themselves still change their mind. The dynamics usually favours the agreement of groups of agents about the same opinion, so that one ends up with just a few opinions in the final state. In particular it is possible that all agents share the same opinion (consensus), or that they split in two or more factions.

The Sznajd Model (SM)

The SM is probably the most studied consensus model of the last years. The reasons of its success are the intuitive “convincing rule” and the deep relationship with spin models like Ising. One starts with a simple remark: an individual is more easily convinced to change its mind if more than just a single person try to persuade him/her. So, if two or more of our friends share the same view about some issue, it is likely that they will convince us to accept that view, sooner or later.

The Sznajd Model

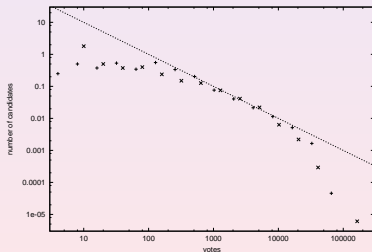
In the most common implementation of the model, a group of neighbouring agents which happen to share the same opinion imposes this opinion to all their neighbours. The “convincing” pool of friends can be a pair of nearest-neighbours on a graph, or groups of three or more neighbours like triads on networks or plaquettes on a lattice. One usually starts from a random distribution of opinions among the agents, with a fraction p of agents sharing the opinion $+1$ (the rest of the agents having opinion -1). In the absence of perturbing factors like noise, the state of the system always converges towards consensus and a phase transition is observed as a function of the initial concentration p : for $p < 1/2$ ($> 1/2$) all agents end up with opinion -1 ($+1$).

The Sznajd Model

Since the original formulation of the model of the Sznajds, for a one-dimensional chain of agents, countless refinements have been made, which concern the type of graph, the updating rule, the introduction of external factors like a social temperature, advertising and ageing, etc. (for more details see the reference list).

The Sznajd dynamics has been used to devise simple election models which reproduce the bulk behaviour of votes distributions of real elections, see the example on the next slide.

Brazilian Election



The Sznajd Model

Histogram of the fraction of candidates receiving a given number of votes for 1998 election in the state of Minas Gerais (Brazil). A simple election model based on Sznajd opinion dynamics reproduces well the central pattern of the data. The data points are indicated by \times , the results of the election model by $+$.