Simulations in Statistical Physics

Course for MSc physics students

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Information

- Coordinates:
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    - F III building, first floor 6 (after the first stairs to the right, at the end of the corridor), Department of Theoretical Physics
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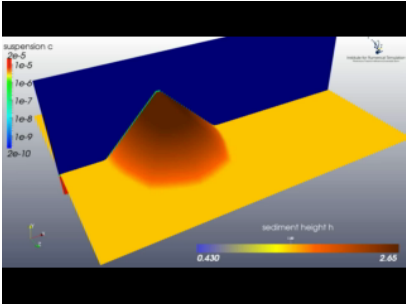
    - Upon demand (Email)
- Webpage: http://www.phy.bme.hu/~torok
- Homework: http://newton.phy.bme.hu/moodle

Required knowledge

- Knowledge of basic statistical physics
- C, or C++ language (only basic things)
- English



Examination requirements

- Signature
  - Mid November: home work
  - A problem to be solved by simulation
  - Code written in C or C++, which compiles easily
  - Documented working code (no extra libaries except for `gsl`)
  - Using fancy visualization techniques does not impove the mark which is given for the algorithm, the efficiency of the code and the solution of the problem
  - A pdf documentation of the results and explanation (3-5 pages)
  - Language: English, Hungarian
- Exam: mark
  - 3/5: From the code and documentations
  - 2/5: Lecture material
    - Both must be at least 2 to have a final note larger than 1
  - Presentation random part of the code
  - Language: English, Hungarian, German, French

Literature

- D.W. Heermann: Computer simulation methods in theoretical physics, Springer, 1995
- D. Landau and K. Binder: A guide to Monte Carlo simulations in statistical physics (Cambridge UP, 2000)
- D. Rapaport: The art of molecular dynamics programming (Cambridge UP, 2004)
- J. Kertész and I. Kondor (eds): Advances in computer simulation (Springer, 1998)
- W.G. Hoover: Molecular Dynamics (Springer, 1986)

Overview of statistical physics

Aim

- Microscopic explanation of thermo dynamics
- Calculate macroscopic properties from microscopic principles
- Explain phenomena (phase transitions, pattern formation, etc.)

Major parts

- Equilibrium
- Non-equilibrium
  - Perturbation of an equilibrium system
  - Far-from equilibrium system

Definitions in statistical physics

- Isolated system: No interactions with the world
- Closed system: Only energy transfer with the world
- Reservoir: Part of an isolated or closed system which is much larger than the rest and any change in the rest leaves this part unaffected
- Microstate: a point in the phase space, snapshot of the system with all required quantities (e.g. position, speed, etc.)
- Macrostate: thermodynamic or hydrodynamic state.
- Equilibrium: Not flow of energy in the system
- Detailed balance: in thermodynamic equilibrium

$$\pi_i P_{ij} = \pi_j P_{ji}$$

π_i: probability of state i, P_{ij}: transition probability $i \to j$

Averages

- Time average:

$$\overline{A} = \lim_{T \to \infty} \frac{1}{T} \int_0^T A(q(t), p(t)) dt$$

- Ensemble average:

$$\langle A \rangle = \frac{1}{h^{3N}(N!)} \int A(q,p) P^{eq}(q,p) dqdp$$

E.g. $P^{eq}(q,p) = \exp(-betaH)$.

- Equivalence: Ergodicity, Thermodynamic limit $N \to \infty$
- Problems:
  - Order of limits (glasses)
  - Non-equilibrium: $T \to \infty$

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Fluctuation-dissipation theorem

- Dynamical system $H_0(x)$ subject to thermal fluctuations
- Observable $x(t)$ fluctuates around $\langle x \rangle_0$.
- Power spectrum of fluctuations of x: $S_x(\omega) = \hat{x}(\omega)\hat{x}^*(\omega)$
- Linear perturbation of the Hamiltonian: $H(x) = H_0(x) + fx$
- Susceptibility (linear response):

$$\langle x(t) \rangle = \langle x \rangle_0 + \int_{-\infty}^{t} f(\tau)\chi(t-\tau)d\tau$$

- The Fluctuation-dissipation theorem relates the above as

$$S_x(\omega) = \frac{2k_\mathrm{B}T}{\omega}\mathrm{Im}\hat{\chi}(\omega)$$

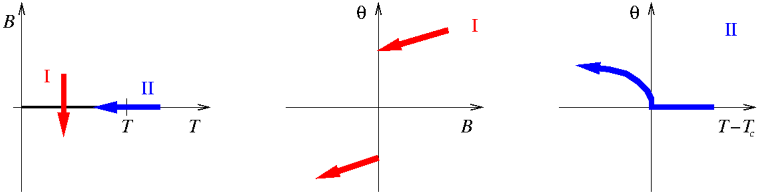
- Can be used to define temperature

Phase transitions

Equilibrium	order parameter	Non-equilibrium	order parameter
liquid-gas	density	traffic jam	flux
ferromagnetic	magnetization	flocking	average speed
		jamming	$\phi_c - \phi$
		glass	replicas

- Order of phase transition: which derivative of Gibbs free energy becomes discontinuous
- Better classification:
  - First order: discontinuous transition (latent heat)
  - Second order: continuous transition, order parameter is continuous but susceptibility is divergent

Phase transitions



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Correlation function

- e.g. Magnetic systems

$$G(r) = \langle s(R)s(R+r)\rangle - \langle s\rangle^2$$

- Close to the critical point:

$$G(r) = r^{-(d-2+\eta)}\exp(-r/\xi),$$

where

$$\xi \propto |T - T_c|^{-\nu}$$

is the correlation length. The correlation length, i.e., the characteristic size of the regions, where the fluctuations are correlated diverges at the critical point.

- ν and η are critical exponents.

Correlation function

- Near to the critical point G is a generalized homogeneous function of its variables:

$$G(r,t,h) \propto b^{-2\beta/\nu} G(r/b, b^{y_t} t, b^{y_h} h),$$

where $t = (T - T_c)/T_c$ and $t \to 0$, $h \to 0$.

- The susceptibility

$$\chi = \beta V \int G(\mathbf{r}) dr^3 = \beta \langle (s - \langle s \rangle)^2 \rangle$$

- Magnetization (OP), susceptibility, specific heat

$$\chi = \frac{\partial M}{\partial h}, \qquad M = \frac{\partial F}{\partial h}, \qquad C = \frac{\partial F}{\partial T}$$

Scaling relations

- $C(h=0) \propto |t|^{-\alpha}$
- $M(h=0) \propto (-t)-\beta,\ t<0$
- $\chi(h=0) \propto |t|^{-\gamma}$
- $M(t=0) \propto h^{1/\delta}$
- 8 exponents: $\alpha, \beta, \gamma, \delta, \eta, \nu, y_t, y_h$
- Scaling relations (d dimension):
  - $y_t = 1/\nu,\ y_h = d - \beta/\nu$
  - $\alpha + 2\beta + \gamma = 2$
  - $\delta = 1 + \gamma/\beta$
  - $d\nu = 2 - \alpha$
  - $\nu = \gamma/(2-\eta)$
- Two independent exponents left $\rightarrow$ universality classes