Computational Statistical Physics

Part I: Statistical Physics and Phase Transitions

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FS 2022

Dates and further information

- Lectures: Wednesday 9.45–11.45 in HCI J 7
- Exercises : Friday 9.45–11.45 in HPT C 103
- Tutors: Doruk Efe Gökmen and Pascal Engler
- Oral exams take place in Summer Exam Session 2022
- Moodle Course Page: https://moodle-app2.let.ethz.ch/course/view.php?id=17219

Dates and further information

- 80% of homeworks "meaningfully completed" and submitted $\rightarrow$ 0.25 bonus points. For details consult course catalogue and Exercise sheet 00 on the couse moodle page –> attempt before Friday, February 25
- Homework submission via gitlab: `https://gitlab.ethz.ch` [Detailed instructions in Exercise sheet 00] on moodle page under **Exercise Materials**.
- If not familiar with git, visit this week's exercises class
- Friday, 25.02., 9.45: git tutorial/setting up homework submission in HPT C 103 Please bring a laptop with you!

Course offered in (selection)

- Mathematics (Master)
- Physics (Master)
- Integrated Building Systems Master (Specialised Courses)
- Civil Engineering (Additional Courses)
- Biomedical Engineering (Master)
- Computational Science and Engineering (Bachelor and Master)
- Computer Science (Bachelor)
- Doctoral programs (qualifying exam: please get in touch before the end of the teaching term)

Phase transitions

- 23.02. Introduction to statistical physics and the Ising model
- 02.03. Monte Carlo methods
- 09.03. Finite size methods and cluster algorithms
- 16.03. Histogram methods
- 23.03. Renormalization group
- 30.03. Boltzmann machines
- 06.04. Non-equilibrium phase transitions

Molecular dynamics

- 13.04. Molecular Dynamics, Verlet scheme, Leapfrog scheme
- 20.04. ETH vacations
- 27.04. Optimization, Linked cell, Lagrange multipliers
- 04.05. Rigid bodies, quaternions
- 11.05. Nosé-Hoover thermostat, stochastic method, constant pressure ensemble

Event-driven dynamics

- 18.05. Event driven, inelastic collisions, friction
- 25.05. Contact dynamics
- 01.06. Advanced topics

Classical statistical mechanics

Classical statistical mechanics

Ringier reception in Zofingen, CH [Source:Wikipedia]

Phase space

Let us consider a classical physical system with N particles whose canonical coordinates and the corresponding conjugate momenta are given by $q_1, \ldots, q_{3N}$ and $p_1, \ldots, p_{3N}$, respectively. The $6N$-dimensional space Γ defined by the latter set of coordinates defines the *phase space*.

Ensemble average

The assumption that that all states in an ensemble are reached by the time evolution of the corresponding system is referred to as *ergodicity hypothesis*. We define the *ensemble average* of a quantity $Q(p, q)$ as

$$\langle Q \rangle = \frac{\int Q(p,q)\rho(p,q)\,\mathrm{d}p\mathrm{d}q}{\int \rho(p,q)\,\mathrm{d}p\mathrm{d}q}, \tag{1}$$

where ρ denotes the *phase space density* and $\mathrm{d}p\mathrm{d}q$ is a shorthand notation of $\mathrm{d}p^{3N}\mathrm{d}q^{3N}$.

Hamiltonian

The dynamics of the considered N particles is described by their *Hamiltonian* $\mathcal{H}(p, q)$, i.e., the equations of motions are

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} \quad \text{and} \quad \dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} \quad (i = 1, \ldots, 3N). \tag{2}$$

Moreover, we introduce the *phase space density* ρ and find for its temporal change in a volume V with boundary A

$$\frac{\partial}{\partial t} \int \rho \, \mathrm{d}V + \int_A \rho v \, \mathrm{d}A = 0, \tag{3}$$

where $v = (\dot{p}_1, \ldots, \dot{p}_{3N}, \dot{q}_1, \ldots, \dot{q}_{3N})$ is a generalized velocity vector.

Liouville Theorem

Applying the divergence theorem to Eq. (3), we find that ρ satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0, \tag{4}$$

where $\nabla = (\partial/\partial p_1, \ldots, \partial/\partial p_{3N}, \partial/\partial q_1, \ldots, \partial q_{3N})$.

Rewritting Eq. (4) using Poisson brackets

yields *Liouville's Theorem*

$$\frac{\partial \rho}{\partial t} = \{\mathcal{H}, \rho\} \tag{5}$$

which describes the time evolution of the phase space density ρ.

Thermal equilibrium

In *thermal equilibrium*, the system reaches a steady state in which the distribution of the configurations is constant and time-indepedent, i.e., $\partial\rho/\partial t = 0$. Liouville's theorem leads to the following condition

$$v \cdot \nabla\rho = \{\mathcal{H}, \rho\} = 0. \tag{6}$$

The latter equation is satisfied if ρ depends on quantities which are conserved during the time evolution of the system. We then use such a ρ to replace the *time average*

$$\langle Q \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T Q(p(t), q(t))\,\mathrm{d}t. \tag{7}$$

by its ensemble average as defined by Eq. (1).

Ensemble average

Considering a discrete and general configuration X, we define the ensemble average as

$$\langle Q \rangle = \frac{1}{\Omega} \sum_{X} Q(X)\rho(X), \tag{8}$$

where Ω is the normalizing volume such that $\Omega^{-1} \sum_X \rho(X) = 1$. With this definition, systems can be described by means of some macroscopic quantities, such as temperature, energy and pressure.

Ensembles

- Microcanonical ensemble: constant E, V, N
- Canonical ensemble: constant T, V, N
- Canonical pressure ensemble: constant T, p, N
- Grandcanonical ensemble: constant T, V, μ

Microcanonical ensemble

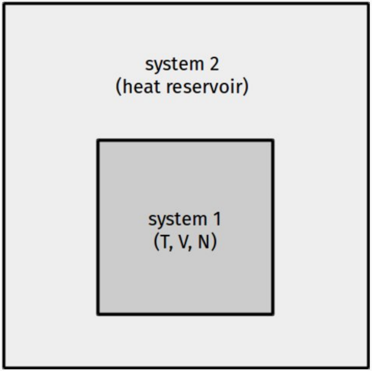
The *microcanonical ensemble* is defined by a constant number of particles, volume and energy. Thus, any configuration X of the system has the same energy $E(X) = \text{const.}$ Without proof, the phase space density is also constant and given by

$$\rho(X) = \frac{1}{Z_{\text{mc}}} \delta(\mathcal{H}(X) - E), \tag{9}$$

with Z_{mc} being the *partition function* of the microcanonical ensemble

$$Z_{\text{mc}} = \sum_X \delta(\mathcal{H}(X) - E).$$

Canonical ensemble



In a canonical ensemble setup, the system we study (system 1) is coupled to a heat reservoir (system 2) that guarantees a constant temperature. [Böttcher, Herrmann, Comp.Stat.Phys.,Cambridge University Press, 2021]

Canonical ensemble

At a given temperature T, the probability for a system to be in a certain configuration X with energy $E(X)$ is given by

$$\rho(X) = \frac{1}{Z_T}\exp\left[-\frac{E(X)}{k_B T}\right], \tag{10}$$

with

$$Z_T = \sum_X \exp\left[-\frac{E(X)}{k_B T}\right] \tag{11}$$

being the partition function of the canonical ensemble. According to the prior definition in Eq. (8), the ensemble average of a quantity Q is then given by

$$\langle Q\rangle = \frac{1}{Z_T}\sum_X Q(X)\, e^{-\frac{E(X)}{k_B T}}. \tag{12}$$

Ising model

Ising Model

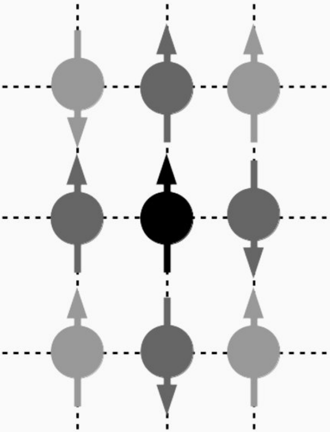


Figure 1: An illustration of the interaction of a magnetic dipole (black) with its nearest neighbors (dark grey) on a two-dimensional lattice. [Böttcher, Herrmann, Comp.Stat.Phys.,Cambridge University Press, 2021]

Ising Model

We consider a two-dimensional lattice with sites $\sigma_i \in \{1, -1\}$, which only interact with their nearest neighbors. Their interaction is given by the Hamiltonian

$$\mathcal{H}(\{\sigma\}) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - H \sum_{i=1}^{N} \sigma_i, \tag{13}$$

where the first term denotes the interaction between all nearest neighbors represented by a sum over $\langle i, j \rangle$, and the second one the interaction of each site with an external magnetic field H.

- Ferromagnetic case: $J > 0$ (parallel spins)
- Antiferromagnetic case: $J < 0$ (anti-parallel spins)
- No interaction: $J = 0$

Phase Transition in the Ferromagnetic Case

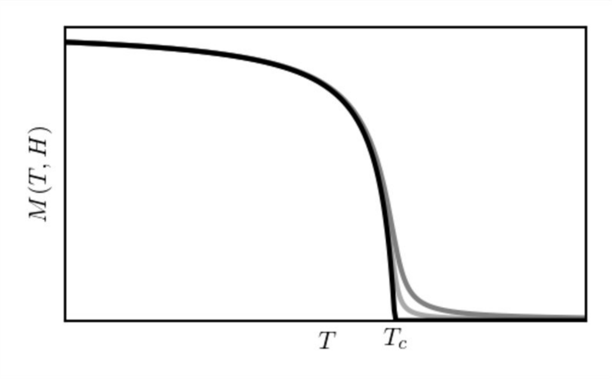


Figure 2: The magnetization $M(T, H)$ for different fields $H \geq 0$ as a function of T. For $T \leq T_c$, the system is characterized by a ferromagnetic phase. The black solid line represents the spontaneous magnetization $M_S(T)$ for $H = 0$ and should be interpreted in the sense that $\lim_{H \to 0^+} M(T, H)$. [Böttcher, Herrmann, Comp.Stat.Phys.,Cambridge University Press, 2021]

Phase Transition in the Ferromagnetic Case

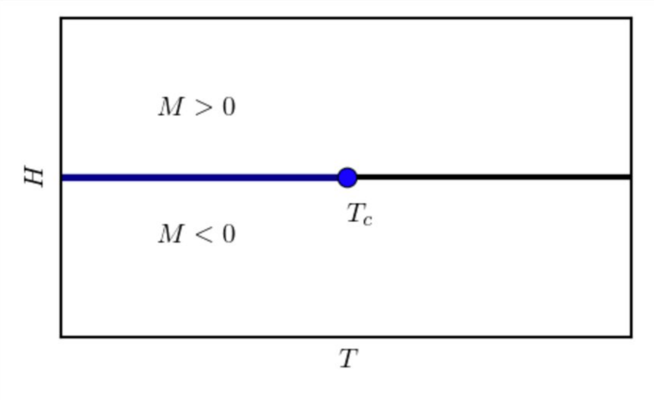


Figure 3: The first-order transition as a consquence of a sign change of the external field. [Böttcher, Herrmann, Comp.Stat.Phys.,Cambridge University Press, 2021]

Order parameter

The magnetization is defined as

$$M\left(T,H\right)=\left\langle \frac{1}{N}\sum_{i=1}^{N}\sigma_i\right\rangle, \tag{14}$$

and corresponds to the ensemble average of the mean value of all spins.

On average, $M\left(T\right)$ vanishes since for every configuration there exists one of opposite sign which neutralizes the other one. As a consequence, we define the *order parameter* of the Ising model as

$$M_{\mathsf{S}}\left(T\right)=\lim_{H\to 0^+}\left\langle \frac{1}{N}\sum_{i=1}^{N}\sigma_i\right\rangle \tag{15}$$

and refer to it as the *spontaneous magnetization*.

Magnetic Domains

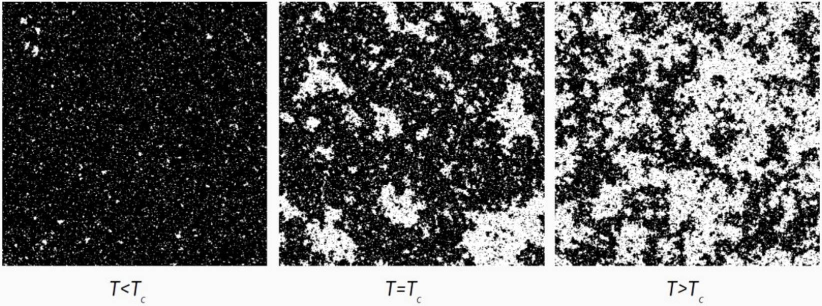


Figure 4: The formation of magnetic domains in the Ising model for temperatures $T < T_c$. For larger temperatures, the configurations are random due to thermal fluctuations. The simulations have been performed on a square lattice with 512×512 sites using `https://mattbierbaum.github.io/ising.js/`.

Critical Exponents I

In the vicinity of the critical temperature for $T < T_c$, the spontaneous magnetization scales as

$$M_{\mathsf{S}}(T) \propto (T_c - T)^{\beta} \,. \tag{16}$$

For $T = T_c$ and $H \to 0$, we find the following scaling

$$M(T = T_c, H) \propto H^{1/\delta}. \tag{17}$$

The exponents β and δ are so-called *critical exponents* and characterize together with other exponents the underlying phase transition.

- 2D: $\beta = 1/8$ and $\delta = 15$
- 3D: $\beta = 0.326$ and $\delta = 4.790$

Fluctuations

The magnetic sucsceptibility is defined as the change of the magnetization M in response to an applied magnetic field H, i.e.,

$$\chi(T) = \frac{\partial M(T,H)}{\partial H}. \tag{18}$$

We now use the definition of the spontaneous magnetization given by Eq. (15) and plug it into Eq. (18) leading to

$$\begin{aligned}
\chi(T) &= \lim_{H\to 0^+} \frac{\partial \langle M(T,H)\rangle}{\partial H} & (19)\\
&= \lim_{H\to 0^+} \frac{\partial}{\partial H} \frac{\sum_{\{\sigma\}} \sum_{i=1}^{N} \sigma_i \exp\left(\frac{E_0 + H\sum_{i=1}^{N}\sigma_i}{k_B T}\right)}{\underbrace{\sum_{\{\sigma\}} \exp\left(\frac{E_0 + H\sum_{i=1}^{N}\sigma_i}{k_B T}\right)}_{=Z_T(\mathcal{H})}}, & (20)
\end{aligned}$$

Fluctuations

Using the product rule yields

$$\begin{aligned}\chi(T) = & \lim_{H\to 0^+} \frac{1}{Nk_BT} \frac{\sum_{\{\sigma\}} \left(\sum_{i=1}^{N} \sigma_i\right)^2 \exp\left(\frac{E_0 + H\sum_{i=1}^{N}\sigma_i}{k_BT}\right)}{Z_T(\mathcal{H})} \\ & - \frac{1}{Nk_BT} \frac{\left[\sum_{\{\sigma\}} \sum_{i=1}^{N} \sigma_i \exp\left(\frac{E_0 + H\sum_{i=1}^{N}\sigma_i}{k_BT}\right)\right]^2}{\left[Z_T(\mathcal{H})\right]^2} \\ = & \frac{N}{k_BT}\left[\left\langle M_S(T)^2\right\rangle - \left\langle M_S(T)\right\rangle^2\right] \geq 0. \end{aligned} \tag{21}$$

The last equation defines fluctuation-dissipation theorem for the magnetic susceptibility. Analogously, the specific heat is connected to energy fluctuations as:

$$C(T) = \lim_{H\to 0^+} \frac{\partial \langle E\rangle}{\partial T} = \frac{1}{(k_BT)^2}\left[\left\langle E(T)^2\right\rangle - \left\langle E(T)\right\rangle^2\right]. \tag{22}$$

Critical Exponents II

Similarly to the power-law scaling of the spontaneous magnetization defined in Eq. (16), we find for the magnetic susceptibility in the vicinity of T_c

$$\chi(T) \propto |T_c - T|^{-\gamma} \tag{23}$$

$$C(T) \propto |T_c - T|^{-\alpha}, \tag{24}$$

- 2D: $\gamma = 7/4$ and $\alpha = 0$[1]
- 3D: $\gamma \approx 1.24$ and $\alpha \approx 0.11$

[1] An exponent of $\alpha = 0$ corresponds to a logarithmic decay since $\lim_{s\to 0} \frac{|x|^{-s}-1}{s} = -\ln|x|$.

Critical Exponents II

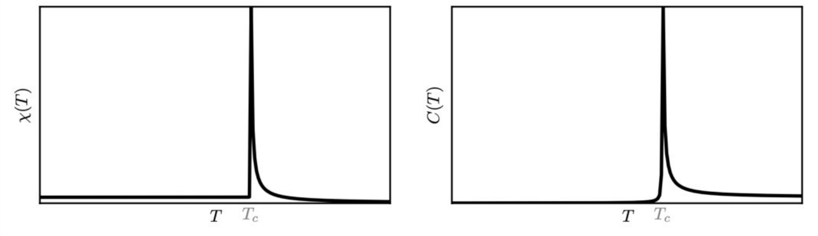


Figure 5: Susceptibility and specific heat as a function of temperature for the three dimensional Ising model. Both quantities diverge at the critical temperature T_c in the thermodynamic limit. [Böttcher, Herrmann, Comp.Stat.Phys.,Cambridge University Press, 2021]

Correlation length

The correlation function is defined by

$$G(r_1, r_2; T, H) = \langle \sigma_1 \sigma_2 \rangle - \langle \sigma_1 \rangle \langle \sigma_2 \rangle \,, \tag{25}$$

where the vectors r_1 and r_2 pointing in the direction of lattice sites 1 and 2. If the system is translational and rotational invariant, the correlation function only depends on $r = |r_1 - r_2|$. At the critical point, the correlation function decays as

$$G(r; T_c, 0) \sim r^{-d+2-\eta}, \tag{26}$$

where η is another critical exponent and d the dimension of the system.

- 2D: $\eta = 1/4$
- 3D: $\eta \approx 0.036$

Correlation length

For temperatures away from the critical temperature, the correlation function exhibits an exponential decay

$$G(r;T,0) \sim r^{-\vartheta} e^{-r/\xi}, \tag{27}$$

where ξ defines the *correlation length*. The exponent ϑ equals 2 above and $1/2$ below the transition point. In the vicinity of T_c, the correlation length ξ diverges since

$$\xi(T) \sim |T - T_c|^{-\nu} \tag{28}$$

- 2D: $\nu = 1$
- 3D: $\nu \approx 0.63$

Critical exponents and universality

The aforementioned six critical exponents are connected by four scaling laws

$$
\begin{aligned}
\alpha + 2\beta + \gamma &= 2 \quad \text{(Rushbrooke)}, &(29)\\
\gamma &= \beta(\delta - 1) \quad \text{(Widom)}, &(30)\\
\gamma &= (2 - \eta)\nu \quad \text{(Fisher)}, &(31)\\
2 - \alpha &= d\nu \quad \text{(Josephson)}, &(32)
\end{aligned}
$$

which have been derived in the context of the phenomenological scaling theory for ferromagnetic systems. Due to these relations, the number of independent exponents reduces to two.

Critical exponents and universality

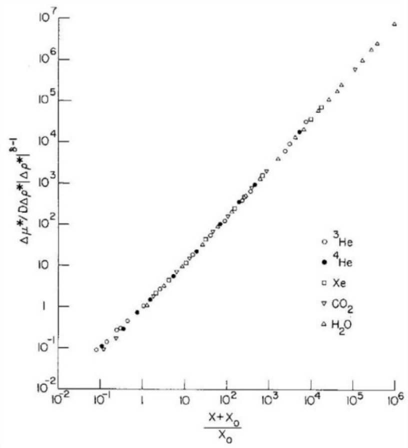


Figure 6: Universal scaling for five different gases. The scaling variable is define as $x = \Delta T\,|\Delta\rho|^{-1/\beta}$ and x_0 depends on the amplitude B of the power-law for the coexistence curve $\Delta\rho = B\Delta T^{\beta}$

[Sengers,Sengers,Croxton, Prog. in liquid physics, Wiley, 1978]

Critical exponents and universality

Table 1: The critical exponents of the Ising model in two and three dimensions [Pelissetto, Vicari, Phys. Rep. 368, 549–727 (2002)]

Exponent	$d = 2$	$d = 3$
α	0	$0.110(1)$
β	$1/8$	$0.3265(3)$
γ	$7/4$	$1.2372(5)$
δ	15	$4.789(2)$
η	$1/4$	$0.0364(5)$
ν	1	$0.6301(4)$