Advanced methods in Simulation: Part II

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Introduction

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Phase Transition

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- Scaling laws are present in observables and critical exponents define the universalitty class of the phase transiton..
- First-order phase transition is characterized by a finite discontinuity of the thermudynamic potential. In finite systems, the derivative of the thermodynamic potential displays a maximum which increases as the system size.
- The finite-size analysis allows us to obtain observables in the thermodynamic limit

Scaling laws

Ising model

$$\mathcal{H} = -J \sum_{<i,j>}^{N} S_i S_j - H \sum_{i=1}^{N} S_i \qquad (1)$$

where $< i, j >$ denotes a summation over nearest sites, J is the ferromagnetic interaction strength, and H a uniform external field.

Scaling laws

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Critical exponents

The magnetization per spin is defined by

$$m(t, h) = \frac{1}{N} \sum_{i=1}^{N} \langle S_i \rangle, \qquad (2)$$

where $t = (T - T_c)/T_c$ is the dimensionless temperature and $h = H/k_B T$ the dimensionless external field.

Scaling laws

Critical exponents

In the absence of an external field, the scaling law is

$$m(t, h = 0) = \begin{cases} 0 & t > 0 \\ A|t|^\beta & t < 0 \end{cases} \tag{3}$$

where the exponent β characterizes the spontaneous magnetization in the ferromagnetic phase.

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Along the critical isotherm, one has

$$m(t = 0, h) = \begin{cases} -B|h|^{1/\delta} & h < 0 \\ B|h|^{1/\delta} & h > 0 \end{cases}$$

where δ is the exponent of the magnetization in the presence of an external field.

Scaling laws

Critical exponents

The specific heat c_v is given by

$$c_v(t, h = 0) \begin{cases} C|t|^{-\alpha} & t < 0 \\ C'|t|^{-\alpha'} & t > 0 \end{cases}$$

where α and α' are the exponents associated with the specific heat. Experimentally, one always observes that $\alpha = \alpha'$. The amplitude ratio C/C' is also a universal quantity.

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Isothermal susceptibility in zero external field diverges at the critical point as

$$\chi_T(h = 0) \sim |t|^{-\gamma},$$

where γ is the susceptibility exponent.

Scaling laws

Critical exponents

The spatial correlation function, denoted by $g(r)$, behaves in the vicinity of the critical point as

$$g(r) \sim \frac{\exp(-r/\xi)}{r^{d-2+\eta}},$$

where ξ is the correlation length, which behaves as

$$\xi \sim |t|^{-\nu},$$

where ν is the exponent associated with the correlation length.

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At the critical point,

$$g(r) \sim \frac{1}{r^{d-2+\eta}}$$

where η is the exponent associated with the correlation function.

Scaling laws

Critical exponents: summary

These six exponents $(\alpha, \beta, \gamma, \delta, \nu, \eta)$ are not independent! Assuming that the free energy per volume unit and the pair correlation function obey a scaling function, it can be shown that only two exponents are independent.

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These six exponents $(\alpha, \beta, \gamma, \delta, \nu, \eta)$ are not independent! Assuming that the free energy per volume unit and the pair correlation function obey a scaling function, it can be shown that only two exponents are independent. Scaling function of the singular part of free energy density

$$f_s(t, h) = |t|^{2-\alpha} F_f^{\pm}\left(\frac{h}{|t|^{\Delta}}\right)$$

where $F_f^{\pm}$ are functions defined below and above the critical temperature and which approach a non zero value when $h \to 0$ and have an algebraic behavior when the scaling variable goes to infinity,

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$$F_f^{\pm}(x) \sim x^{\lambda+1}, \qquad x \to \infty.$$

Scaling laws

Critical exponents

$$m(h,t) = -\frac{1}{k_B T}\frac{\partial f_s}{\partial h} \sim |t|^{2-\alpha-\Delta} F_f^{\pm'}\left(\frac{h}{|t|^{\Delta}}\right). \quad (4)$$

For $h \to 0$, one identifies exponents of the algebraic dependence in temperature:

$$\beta = 2 - \alpha - \Delta. \quad (5)$$

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Taking the second derivative of the free energy density with respect to the field h, the isothermal susceptibility is given by

$$\chi_T(t,h) \sim \frac{\partial^2 f_s}{\partial h^2} \sim t^{2-\alpha-2\Delta} F_f^{\pm''}\left(\frac{h}{|t|^\Delta}\right). \tag{6}$$

For $h \to 0$, one identifies exponents of the algebraic dependence in temperature:

$$-\gamma = 2 - \alpha - 2\Delta. \tag{7}$$

Scaling laws

Critical exponents

$$\beta = 2 - \alpha - \Delta.$$

and

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$$\alpha + 2\beta + \gamma = 2. \tag{8}$$

Rushbrooke scaling law

Scaling laws

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$$\alpha + 2\beta + \gamma = 2. \tag{8}$$

Rushbrooke scaling law
This relation does not depend on the space dimension d. Moreover, one has

$$\Delta = \beta + \gamma. \tag{9}$$

Critical exponents

One then obtains for the magnetization, along the critical isotherm: (let us recall $F(x) \sim x^{\lambda+1}$)

$$m(t,h) \sim |t|^{\beta} \left(\frac{h}{|t|^{\Delta}}\right)^{\lambda} \tag{10}$$

$$\sim |t|^{\beta-\Delta\lambda} h^{\lambda}. \tag{11}$$

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Finally, by using $\Delta = \beta + \gamma$, one obtains

$$\beta\delta = \beta + \gamma.$$

Scaling laws

Critical exponents

The next two relations are inferred from the scaling form of the free energy density and of the spatial correlation relation $g(r)$.

$$\frac{f_s}{k_B T} \sim \xi^{-d}\left(A + B_1\left(\frac{l_1}{\xi}\right) + \dots\right) \tag{12}$$

where l_1 is a microscopic length scale. When $t \to 0$, subdominant corrections can be neglected and one has

$$\frac{f_s}{k_B T} \sim \xi^{-d} \sim |t|^{\nu d}. \tag{13}$$

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Taking the second derivative of this equation with respect to the temperature, one obtains for the specific heat

$$c_v = -T\frac{\partial^2 f_s}{\partial T^2} \sim |t|^{\nu d-2}. \tag{14}$$

Josephson relation (so called the hyper scaling relation), $2 - \alpha = d\nu$,

Scaling laws

Critical exponents

Knowing that the space integral of $g(r)$ is proportional to the susceptibility, one integrates $g(r)$ over a volume whose linear dimension is ξ,

$$\int_0^{\xi} d^d r g(r) = \int_0^{\xi} d^d r \frac{\exp(-r/\xi)}{r^{d-2+\eta}} \tag{15}$$

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$$\chi_T(h=0) \sim |t|^{-(2-\eta)\nu}, \tag{17}$$

Using that $\xi \sim t^{-\nu}$
one has

$$\gamma = (2-\eta)\nu$$

Scaling laws

Critical exponents

A universality class is defined by 2 independent critical exponents.
An significant feature of the critical phenomena theory is the existence of a upper and lower critical dimensions: At the upper critical dimension d_{sup} and above, the mean-field theory (up to some logarithmic subdominant corrections) describes the critical phase transition. Below lower critical dimension d_{inf}, no phase transition can occur. For the Ising model, $d_{inf} = 1$ and $d_{sup} = 4$.

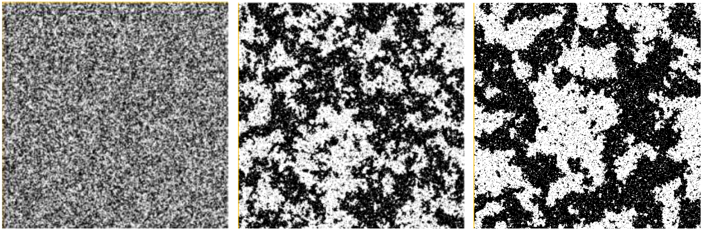
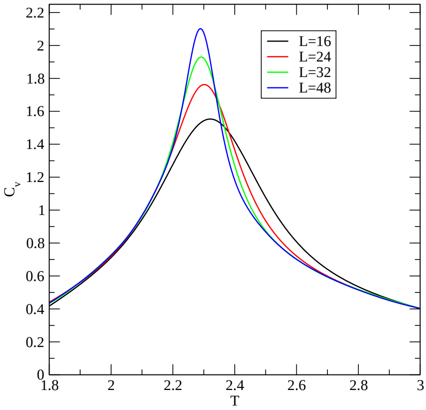


Figure: Spin configurations of the Ising model in 2 dimensions: From left to right, the temperature decreases.

Finite size scaling analysis

Specific heat for the Ising model in 2D



Free energy denity

Scaling functions

The thermodynamic quantities of a finite system of linear size L for a dimensionless temperature t, and a dimensionless field h,..., are the same of a system of size L/l for a dimensionless temperature tl^{y_t} and a dimensionless field hl^{y_h},..., which gives

$$f_s(t, h, \dots L^{-1}) = l^{-d} f_s(tl^{y_t}, hl^{y_h}, \dots, (l/L)^{-1}). \tag{18}$$

where y_t and y_h are the exponents associated with the fields.

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$$f_s(t, \ldots L^{-1}) = |t|^{2-\alpha} F_f^{\pm}(|t|^{-\nu}/L)$$

If the correlation length ξ is smaller than L, the system behaves like an infinite system. But, in simulation, the limit. Conversely, in the region where the correlation length is equal to size of the simulation cell, one observes a size-dependence of thermodynamic quantities.

Free energy denity

Specific heat for the Ising model in 2D

If we denote by F_c the scaling function associated with the specific heat, which depends on the scaling variable $|t|^{-\nu}/L$, one has

$$c_v(t, L^{-1}) = |t|^{-\alpha} F_c^{\pm}(|t|^{-\nu}/L). \tag{19}$$

Because $|t|^{-\alpha}$ goes to infinity when $t \to 0$, $F_c^{\pm}(x)$ must go to zero when x goes to zero. Reexpressing this function as

$$F_c^{\pm}(|t|^{-\nu}/L)) = (|t|^{-\nu}/L)^{-\kappa} D^{\pm}(Lt^{\nu}) \tag{20}$$

with $D^{\pm}(0)$ finite. Since the specific heat does not diverge when $|t|$ goes to zero, one requires that

Specific heat

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$$\kappa = \alpha/\nu \tag{21}$$

which gives for the specific heat

$$c_v(t, L^{-1}) = L^{\alpha/\nu} D(L|t|^{\nu}). \tag{22}$$

The function D goes to zero when the scaling variable is large and is always finite and positive. D is a continuous function, and displays a maximum for a finite value of the scaling variable, denoted x_0.

Specific heat

Specific heat for the Ising model in 2D

- The maximum of the specific heat occurs at a temperature $T_c(L)$ which is shifted with respect to that of the infinite system

$$T_c(L) - T_c \sim L^{-1/\nu}. \qquad (23)$$

- The maximum of the specific heat of a finite size system L is given by the scaling law

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Other quantities

$$\langle |m| \rangle = \frac{1}{N} \langle | \sum_{i=1}^{N} S_i | \rangle \tag{25}$$

and the isothermal susceptibility

$$k_B T \chi = N(\langle m^2 \rangle - \langle m \rangle^2). \tag{26}$$

FFS relations

Other quantities

It is possible to calculate a second susceptibility

$$k_B T\chi' = N(\langle m^2\rangle - \langle |m|\rangle^2) \tag{27}$$

χ increases as N when $T \to 0$, due to the existence of two peaks in the magnetization distribution and does not display a maximum at the transition temperature. Conversely, χ' goes to 0 when $T \to 0$ and has a maximum at the critical point. At high temperature, both susceptibilities are related in the thermodynamic limit by the relation $\chi = \chi'(1 - 2/\pi)$.

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Another quantity, useful in simulation, is the Binder parameter

$$U = 1 - \frac{\langle m^4\rangle}{3\langle m^2\rangle^2} \quad (28)$$

FFS relations

Other quantities

Scaling laws for finite size systems

$$\langle|m(t,0,L^{-1})|\rangle = L^{-\beta/\nu}F_m^{\pm}(tL^{1/\nu}) \quad (29)$$

$$k_B T\chi(t,0,L^{-1}) = L^{\gamma/\nu}F_\chi^{\pm}(tL^{1/\nu}) \quad (30)$$

$$k_B T\chi'(t,0,L^{-1}) = L^{\gamma/\nu}F_{\chi'}^{\pm}(tL^{1/\nu}) \quad (31)$$

$$U(t,0,L^{-1}) = F_U^{\pm}(tL^{1/\nu}) \quad (32)$$

where $F_m^{\pm}$, $F_\chi^{\pm}$, $F_{\chi'}^{\pm}$, and $F_U^{\pm}$ are 8 scaling functions (with different maxima).

Pratical rules

Overdetermination

- Practically, by plotting Binder's parameter as a function of temperature, all curves $U(t, 0, L^{-1})$ intersect at the same abscissa (within statistical errors), which determines the critical temperature of the system in the thermodynamic limit.
- Once the temperature of the transition obtained, one can compute β/ν from $\langle|m|\rangle$, then γ/ν from χ (or χ'). By considering the maximum of C_v or other quantities, one derives the value of the exponent $1/\nu$.
- Indeed, because of uncertainty and sub-dominant corrections to scaling laws, overdetermination allows us to determine more accurately critical exponents.