1 Some aspects of the finite size scaling : first-order transition

Let us consider discontinuous (or first-order) phase transitions. One can show that, in the vicinity of the transition, the partition function of a finite size system of linear size L, with periodic boundary conditions is given by

$$Z = \sum_{i=1}^{k} \exp(-\beta f_i(\beta) L^d) \tag{1}$$

where k is the number of coexisting phases (often $k = 2$, but it is not necessary), $f_i(\beta_c)$ is the free energy per site of the $i$the phase in the thermodynamic limit. At the transition temperature, the free energies of each phase are equal. For the sake of simplicity, one assumes only two coexisting phases. The first-order expansion of the free energy densities is given

$$\beta f_i(\beta) = \beta_c f_i(\beta_c) - \beta_c e_i t + O(t^2) \tag{2}$$

where e_i is the free energy per site of the phase i and $t = 1 - T_c/T$.

1. Express the partition function by keeping first-order terms in t. Infer that the two phases coexist only if $tL^d << 1$.

Solution: Expanding to first-order in t gives

$$Z \simeq \exp(-\beta_c f(\beta_c)) \sum_{i=1}^{2} \exp(\beta_c e_i t L^d) \tag{3}$$

by using that $\beta_c f(\beta_c) = \beta_c f_1(\beta_c) = \beta_c f_2(\beta_c)$ In order to have a phase coexistence, the two exponentials must contribute significantly to the partition function, where implies that $tL^d << 1$

One can show that the probability of finding an energy E per site is given for large L as

$$P(E) = \frac{K\delta(E - e_1) + \delta(E - e_2)}{1 + K} \tag{4}$$

where K is a scaling function $K = K(tL^d)$, with the properties $K(x) \to \infty$ when $x \to -\infty$ and $K(x) \to 0$ when $x \to +\infty$.

Knowing that the specific heat per site $C(L, T)$ for a lattice of size L is given by

$$C(L, T)L^{-d} = \beta(< E^2 > - < E >^2) \tag{5}$$

2. Show that $C(L, T)$ goes to zero for temperature much larger and much smaller than the temperature of the transition.

Solution: When T is small $P(X) \simeq \delta(E - e_1)$ and conversely when T is large $P(X) \simeq \delta(E - e_2)$. In both cases $< E^2 > \simeq < E >^2$

3. Determine the value of K where $C(L, T)$ is maximal.

Solution: One calculates

$$< E >= \frac{Ke_1 + e_2}{1 + K}$$

and

$$< E^2 >= \frac{Ke_1^2 + e_2^2}{1 + K}$$

$$C(L, T)L^{-d} = \beta K \frac{(e_1 - e_2)^2}{(1 + K)^2} \tag{6}$$

4. Show that there exists a maximum of $C(L, T)$.

Solution:

$$\frac{\partial C_v}{\partial K} \propto \frac{K - 1}{(1 + K)^3} \tag{7}$$

which gives $K = 1$

5. Determine the corresponding value of $C(L, T)$, expressed as a function of e_1 e_2, β_c.

Solution:

$$C(L, T) = L^d \beta \frac{(e_1 - e_2)^2}{4}$$

6. For characterizing a first-order transition, one can consider the Binder parameter

$$V_4(L, T) = 1 - \frac{< E^4 >}{3 < E^2 >^2}. \tag{8}$$

Express V_4 as a function of e_1, e_2, and K.

Solution: One has

$$< E^4 >= \frac{Ke_1^4 + e_4^2}{1 + K}$$

which gives

$$V_4(L, T) = 1 - \frac{(Ke_1^4 + e_2^4)(1 + K)}{3(Ke_1^2 + e_2^2)^2} \tag{9}$$

7. Determine the value of K where V_4 is minimum. Calculate the corresponding value of V_4.

Solution: Taking the derivative V versus K one obtains that

$$K_m = \left(\frac{e_2}{e_1}\right)^2$$

which gives

$$V_4 = \frac{2}{3} - \frac{1}{12}\frac{(e_1 - e_2)^2(e_1 + e_2)^2}{e_1^2 e_2^2}$$

At large and small K V_4 is close $2/3$.

8. What can one say about the specific heat and V_4 when e_1 is close to e_2 ?

Solution: When e_1 is close to e_2, the amplitude of C_v goes to zero et the minimum of V_4 is close to $2/3$

2 Finite size scaling for continuous phase transitions : logarithm corrections

The goal of this problem is to recover the results of the finite size analysis with a simple method.

1. Give the scaling laws for a infinite system, of the specific heat $C(t)$, of the correlation length $\xi(t)$ and of the susceptibility $\chi(t)$ as a function of usual critical exponents α, ν, γ and of $t = \frac{T-T_c}{T_c}$, the dimensionless temperature, where T_c is the critical temperature.

Solution: Close a phase transition, one has

$$C(t) \propto t^{-\alpha}$$
$$\xi(t) \propto t^{-\nu}$$
$$\chi(t) \propto t^{-\gamma}$$

2. In a simulation, explain why there are no divergences of quantities previously defined.

Solution: The system is finite, there is no true phase transition and the thermodynamic quantities are analytical.

Under an assumption of finite size analysis, one has the relation

$$\frac{C_L(0)}{C(t)} = \mathcal{F}_C\left(\frac{\xi_L(0)}{\xi(t)}\right) \tag{10}$$

where $\mathcal{F}_C$ is a scaling function, $C_L(0)$ the maximum value of the specific heat obtained in a simulation of a finite system with a linear dimension L.

3. By assuming that $\xi_L(0) = L$ and that the ratio $\left(\frac{\xi_L(0)}{\xi(t)}\right)$ is finite and independent of L, infer that $t \sim L^x$ where x is an exponent to be determined.

Solution: If $\left(\frac{\xi_L(0)}{\xi(t)}\right)$ is finite and independent of L, on has $t^{-nu} \propto L$ which gives

$$t \propto L^{-1/\nu}$$

and $x = -1/\nu$

4. By using the above result and Eq. (10), show that

$$C_L(0) \sim L^y \tag{11}$$

Solution: $C_L(0) \propto t^{-1/\nu}$ with $t \propto L^{-1/\nu}$ which gives

$$C_L(0) \propto L^{\frac{\alpha}{\nu}}$$

and one recovers that $y = \frac{\alpha}{\nu}$

where y is an exponent to calculate.

5. By assuming that

$$\frac{\chi_L(0)}{\chi(t)} = \mathcal{F}_\chi\left(\frac{\xi_L(0)}{\xi(t)}\right) \tag{12}$$

show that

$$\chi_L(0) \sim L^z \tag{13}$$

where z is an exponent to be determined.

Solution: Using similar reasoning one obtains that

$$\chi_L(0) \sim L^{\frac{\gamma}{\nu}} \tag{14}$$

Various physical situations occur where scaling laws must be modified to account for logarithmic corrections. The rest of the problem consists of obtaining relations between exponents associated with these corrections. We now assume that for an infinite system

$$\xi(t) \sim |t|^{-\nu}|\ln|t||^{\hat{\nu}} \tag{15}$$

$$C(t) \sim |t|^{-\alpha}|\ln|t||^{\hat{\alpha}} \tag{16}$$

$$\chi(t) \sim |t|^{-\gamma}|\ln|t||^{\hat{\gamma}} \tag{17}$$

6. By assuming that $\xi_L(0) \sim L(\ln(L))^{\hat{q}}$ and the finite size analysis is valid for the specific heat, Eq.(10), show that

$$C_L(0) \sim L^x(\ln(L))^{\hat{y}} \tag{18}$$

where $\hat{y}$ is expressed as a function of α, $\hat{\alpha}$, ν, $\hat{\nu}$ and of $\hat{q}$.
Hint : Consider the equation $y\ln(y)^c = x^{-a}|\ln(x)|^b$; for $y > 0$ and going to infinity, the asymptotic solution is given by

$$x \sim y^{-1/a}\ln(y)^{(b-c)/a} \tag{19}$$

Solution: One has

$$C_L(0) \propto |t|^{-\alpha}\ln(|t|)^{\hat{\alpha}}$$

with

$$t^{-\nu}\ln(|t|)^{\hat{\nu}} = L(\ln(L)^{\hat{q}})$$

Inverting the second equation, one has

$$t \propto L^{-1/\nu}\ln(L)^{(\hat{\nu}-\hat{q})/\nu}$$

Inserting this relation in the first equation and taking the leading order

$$C_L(0) \propto L^{\frac{\alpha}{\nu}}\ln(|t|)^{\hat{\alpha}-\alpha(\hat{\nu}-\hat{q})/\nu}$$

which give $x = \frac{\alpha}{\nu}$ and

$$y = \hat{\alpha} - \alpha(\hat{\nu} - \hat{q})/\nu$$

A finite size analysis of the partition function (details are beyond of the scope of this problem) shows that if $\alpha \neq 0$ the specific heat of a finite size system behaves as

$$C_L(0) \sim L^{-d+\frac{2}{\nu}}(\ln(L))^{-2\frac{\hat{\nu}-\hat{q}}{\nu}} \tag{20}$$

7. By using the results of question 6 show that one recovers the hyperscaling relation and an additional relation between $\hat{\alpha}$, $\hat{q}$, $\hat{\nu}$, ν and α.

Solution: Equating the exponents of the variable L one obtains

$$\frac{\alpha}{\nu} = -d + \frac{2}{\nu}$$

Multiplying this equation by ν, one obtais $\nu d = (2-\alpha) = 1$ which is the hyperscaling relation.
Equating the exponents of the variable $\ln(L)$ one obtains

$$\hat{\alpha} = (\alpha - 2)(\hat{\nu} - \hat{q})/\nu$$

8. By using the hyperscaling relation, show that the new relation can be expressed as a function of $\hat{\alpha}$, $\hat{q}$, $\hat{\nu}$, and d.

Solution: By using that $2 - \alpha = \nu d$ one obtains

$$\hat{\alpha} = d(\hat{q} - \hat{\nu})$$

.

When $\alpha = 0$, the specific heat of a finite size system behaves as

$$C_L(0) \sim (\ln(L))^{1-2\frac{\hat{\nu}-\hat{q}}{\nu}} \tag{21}$$

9. What is the relation between $\hat{\alpha}$, $\hat{q}$, $\hat{\nu}$ and d?

Solution: Using similar arguments, one obtains

$$\hat{\alpha} = 1 + d(\hat{q} - \hat{\nu})$$

Let us consider now the logarithmic corrections of the correlation function

$$g(r,t) = \frac{(\ln(r))^{\hat{\eta}}}{r^{d-2+\eta}} D\left(\frac{r}{\xi(t)}\right) \tag{22}$$

10. By calculating the susceptibility $\chi(t)$ from the correlation function, recover Fisher's law as well as a new relation between the exponents $\hat{\eta}$, $\hat{\gamma}$, $\hat{\nu}$ and η.

Solution: Integrating the correlation function over the volume one obtains the susceptibility. Equating the exponents of the variable L one recovers

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

and the additional relation for the logarithmic terms

$$\hat{\eta} = \hat{\gamma} - \hat{\nu}(2 - \eta)$$

Références

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