Renormalization group study of first-order phase transitions: scaling properties and finite-size effects

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Outline of the talk

1. Review of RG fixed point properties
2. An example: first-order transition in low-temperature Ising model
3. Coexisting phases and RG exponents
4. Finite-size effects

Critical exponents and local RG flow

The fundamental insight the RG provides is the connection between critical exponents and the local behavior of the RG flow in the vicinity of a given RG fixed point (FP). Let b be the parameter ruling the renormalization group (for example, the decimation parameter in the Kadanoff scheme). Local structure of the RG flow in the vicinity of a FP can be analyzed by linearizing the RG transformation $\mathcal{R}(b, \mathbf{g})$, as

$$T_{\alpha\beta}(b, \mathbf{g}) = \frac{\partial \mathcal{R}_\alpha(b, \mathbf{g})}{\partial g_\beta},$$

where $\mathbf{g}$ is the coupling vector, that, at the FP, satisfy the property

$$\mathbf{g}^* = \mathcal{R}(b, \mathbf{g}^*)$$

Supposing the matrix to be in diagonal form, the couplings are then classified depending on the eigenvalues of the matrix. Due to semigroup property, the eigenvalues are appearing in the exponential form b^{y_α}, and the couplings are:

- Relevant, if $y_\alpha > 0$

- Irrelevant, if $y_\alpha < 0$
- Marginal, if $y_\alpha = 0$, so we need to go to the next order beyond linearization.

The FP can be classified on the basis of their couplings being in the above classes. An important property of the FP is that, by construction, the correlation length ξ can be only 0 or $+\infty$. This can be proven by the scaling relation of the correlation length

$$\xi(\mathcal{R}(b, \mathbf{g})) = b^{-1}\xi(\mathbf{g})$$

when applied to the FP. By iteratively applying the RG transformation, and approaching the FP, one sees that it is impossible to have a finite correlation length. By converse, if $\xi = +\infty$ at FP, all the values in the basin of attraction must have $\xi = +\infty$, and will be called **critical**, corresponding to **second-order transitions**.

Instead, for a FP related to first-order transition, or to a bulk phase, $\xi = 0$.

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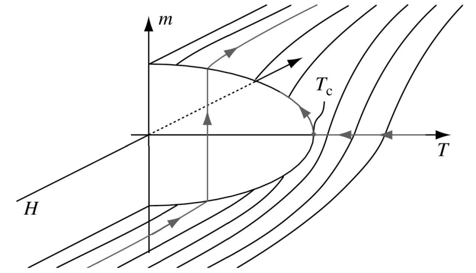
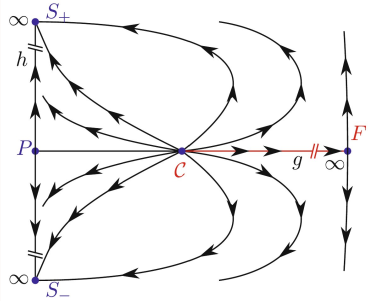
Let H be the external field, T the temperature and $g = T^{-1}$. It is possible to coarse-grain the model, by using approximate arguments as the Migdal-Kadanoff one, to obtain the RG flow.



(a) Phase diagram of the Ising coupling plane [A. Altland and B. Simons, *Condensed Matter Field Theory*, Cambridge University Press (2010)]



(b) RG flow in the Ising coupling plane [P. Kopietz, L. Bartosch and F. Schütz, *Introduction to the Functional Renormalization Group*, Springer (2010)]

Ising model at $T < T_C$

The RG flow establishes some FPs:

- $F = (T = 0, H = 0)$ is related to the whole line of first-order phase transition below the critical temperature. This is called a **discontinuity FP**.
- $\mathcal{C}$ is the critical FP.
- $S_{\pm}$ are the one related to bulk phases.
- P is an infinite temperature FP, noncritical.

We now consider a simple proof of the following property

Theorem

In the discontinuity FP $(T = 0, H = 0)$, whose basin of attraction is the line of first-order phase transition, it holds $y_h = d$, where d is the dimensionality of the system.

Ising model at $T < T_C$

Informal proof.

Consider the fundamental scaling of the free energy per degree of freedom, considering a coarse-graining of step b

$$f(h,t) = b^{-d} f(h',t'),$$

where

$$h' = b^{y_h} h \quad \text{and} \quad t' = b^{y_t} t.$$

In order to have a first-order phase transition,

$$M_\pm(t) = \frac{\partial f(h,t)}{\partial h}\bigg|_{h=0^\pm},$$

so we can use the scaling relation to have

$$M_\pm(t) = b^{-d+y_h} \frac{\partial f(h',t')}{\partial h'}\bigg|_{h'=0^\pm},$$

Ising model at $T < T_C$

Informal proof.

and this relation can be expressed using the magnetization in another point of the transition line:

$$M_{\pm}(t) = b^{-d+y_h} M_{\pm}(t').$$

Let us consider to reach, asymptotically, the FP. Then, for $t = 0$ we can express the magnetization jump as

$$\Delta M(0) = M_{+}(0) - M_{-}(0) = b^{-d+y_h} \Delta M(0),$$

and since $\Delta M(0) \neq 0$ we conclude $y_h = d$. □

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RG transformation for thermodynamic densities

From the definition of the thermodynamic densities in a size N system,

$$M_\alpha = \frac{1}{N}\frac{\partial}{\partial g_\alpha}\ln Z_N\,,$$

it is possible to relate the densities to the linearized RG matrix

$$M_\alpha = \frac{1}{b^d N'}\left(\frac{\partial \ln Z_N}{\partial g'_\beta}\right)\left(\frac{\partial g'_\beta}{\partial g_\alpha}\right) = b^{-d} M'_\beta T_{\beta\alpha}\,,$$

finally obtaining, at the FP,

$$M^*_\alpha = b^{-d} M^*_\beta T_{\beta\alpha}\,.$$

The couplings in the Hamiltonian must satisfy the inherent symmetry requirements even after the RG transformation. This implies

$$g_{\text{even}} \implies +g_{\text{even}}\ ,\ g_{\text{odd}} \implies -g_{\text{odd}}\ .$$

RG transformation for thermodynamic densities

The general structure of the linearized matrix of the RG transformation at a FP in which the odd coupling are zero is

$$T_{\beta\alpha} = \left[\begin{array}{c|c|c} b^d & \text{even} & 0 \\ \hline 0 & \text{even} & \text{odd} \\ \hline 0 & 0 & \text{odd} \end{array}\right].$$

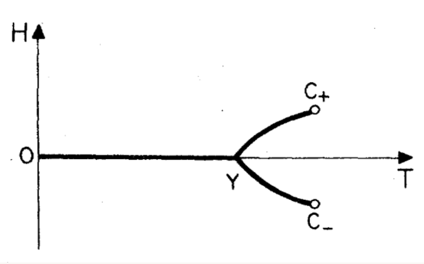
Notice that the eigenvalue b^d is always present for the insertion into the Hamiltonian of the parameter Ng_0 related to the chemical potential. By applying the previous argument, we deduce that the presence of a first-order transition fixes another exponent to the value of d.

One can also conclude similarly, by stating that coexisting phases are described by **independent thermodynamic** densities, in the sense that an additional density is introduced for specifying the state of the system. An example is the order parameter $(n_L - n_G)$, difference between the liquid and gas densities in the liquid-gas transition (see for example [K. Huang, *Statistical Mechanics*, John Wiley and Sons (2008)]).

From this we conclude that the number of eigenvalue exponents equal to d are equal to the **number of coexisting phases**.

Special case of discontinuity at the Curie point

In some cases, it turns out that a discontinuous transition is found at the **crossing of the critical temperature**, by following a constant $H = 0$ line. This can be explained by the presence of a **triple** point Y, in which three phases are together. We expect to have three eigenvalue exponent equal to d.



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Special case of discontinuity at the Curie point

One expects a critical-point variation, as $t \to 0^-$

$$M(t) \approx B|t|^{\beta},$$

with $\beta > 0$.

If M has to vanish discontinuously, we need to have $\beta = 0$. We use now the scaling relation $2 - \alpha = \beta(1 + \delta)$, where $\alpha \leq 1$, and δ enters the equation

$$M(h) \approx \pm D|h|^{1/\delta}.$$

The scaling relation implies $\delta = +\infty$, and from this requirement one can deduce the the corresponding eigenvalue exponent at the fixed point, that has to be $y_h = d$. So by scaling relations we have been able to obtain an additional eigenvalue exponent equal to d. We also remark that, instead of the normally expected critical behavior of the internal energy

$$U(t) - U_c \approx \pm A_{\pm}|t|^{1-\alpha},$$

with U_c the average value before and after the transition, we could have in this case a nonzero latent heat, i.e. a discontinuity in the internal energy.

Outline of the talk

Scaling for finite-size system

We want to describe the effects of having a system of finite-size, namely **rounding** of the diverging quantities, and **shifting** of the transition couplings. Let us focus on the transition of the Ising model for $t < 0$ and h crossing $h = 0$. This can be accomplished by using the following scaling hypotesis for the singular free energy per mode.

$$f(h; L) \approx L^{-\zeta} Z(L/\xi),$$

where we have the correlation length $\xi(h; L) \sim a|h|^{-\nu}$. Equivalently, one can use a function Y such that:

$$f(h; L) \approx L^{-\zeta} Y(hL^{\frac{1}{\nu}}),$$

to have the magnetization jump

$$\Delta M \approx L^{\frac{1}{\nu}-\zeta} Y'(hL^{\frac{1}{\nu}}).$$

In the thermodynamic limit, we know $\Delta M \to \pm M_{\pm}$ for $h \to 0^{\pm}$. This implies $Y'(y) \to \pm M_{\pm}$ as $y \to \pm\infty$ and $\zeta = \frac{1}{\nu}$, from which the susceptibility reads

$$\chi(h; L) \approx L^{\frac{1}{\nu}} Y''(hL^{\frac{1}{\nu}}).$$

Scaling for finite-size system

Moreover, by using the definition of the susceptibility, one gets a maximum value

$$\chi_{\max}(L) < cN \propto L^d,$$

implying $\frac{1}{\nu} \le d$. If one assumes that the correlator $\langle s_{\mathbf{r}} s_{\mathbf{r}'} \rangle \to M_0^2$ when $|\mathbf{r} - \mathbf{r}'| \to \infty$, then $\chi_{\max}(L) \approx M_0^2 N$, so $\zeta = d = \frac{1}{\nu}$. Rounding should become relevant for $\xi \approx L$, so by looking at the h dependence of ξ, we expect a **rounding field** amounting to

$$h_\times \approx L^{-d}.$$

Consider a discrete spin model at $T = 0$, with boundary spins pointed in the positive H $(+)$ way. The ground-state energies of the uniform configurations are

$$E_+ = -\frac{1}{2} zNJ - NH,$$
$$E_- = -\frac{1}{2} zNJ + NH + c_s L^{d-1} J_s,$$

Scaling for finite-size system

where z is the valence number in the bulk, c_s a surface geometry factor, and J_s the coupling to the boundary. The two energies cross at a **nonzero** field, so the transition experiences a **shift**

$$H_s = \frac{1}{2} c_s J_s L^{d-1}/N,$$

that scales as $H_s \sim L^{-1}$. From this argument, we see that the shift is typically larger than the rounding, in opposition to second-order phase transitions.

Conclusions

- A first-order phase transition can be analyzed by RG transformation, in terms of the eigenvalue exponents related to the **discontinuity FP**.
- The number of **coexisting phases** in the transition corresponds to the number of eigenvalue exponents that are exactly equal to the dimension of the system d.
- In the case of a system with finite-size, it is possible to obtain the **rounding** and the **shifting** of the diverging properties in the phase transition. In a different way to second-order transitions, the shift is bigger than the rounding.

Thanks for the attention!

Relevant references

[1] A. Altland and B. D. Simons. *Condensed matter field theory*. Cambridge university press, 2010.

[2] M. E. Fisher and A. N. Berker. “Scaling for first-order phase transitions in thermodynamic and finite systems”. In: *Physical Review B* 26.5 (1982), p. 2507.

[3] K. Huang. *Statistical mechanics*. John Wiley & Sons, 2008.

[4] P. Kopietz, L. Bartosch, and F. Schütz. *Introduction to the functional renormalization group*. Vol. 798. Springer Science & Business Media, 2010.

[5] B. Nienhuis and M. Nauenberg. “First-order phase transitions in renormalization-group theory”. In: *Physical Review Letters* 35.8 (1975), p. 477.