Absolute Irreversibility in Classical Phase Transitions: Ising Model

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March 24, 2015 (v2.6 since January 13, 2015)

Prepared for discussions with Gentaro, Prasana and Seungju about the absolute irrevisibility in classical phase transitions. In this note, we are focused on the Ising model.

- ▷ See Murashita et al. (2014).

- ▷ New in v2.6: In Section 5.4, a third method to get $\rho(\hat{S})$ is discussed, which reveals exactly how the discrepancy between Gentaro and Seunju's and my method occurs.
- ▷ New in v2.5: Gentaro's Questions 5.1 and 5.3 are discussed. Additional my own Question 5.4 is discussed as well.
- ▷ New in v2.4: Section 5.1 has been split into two, Sections 5.1 and 5.2.
- ▷ New in v2.3: Several typos in Section 5 fixed.
- ▷ New in v2.2: New section 5, where I obtain a rigorous distribution function $\rho(S)$ in the mean-field approximation and which shows that the width of the distribution function $\rho(S)$ should depend on the coupling strength.
- ▷ New in v2.1: Section 4 is new.
- ▷ New in v2.0: Ising model exclusively. Revisions are managed separately for each section.

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1 Model and Notations

- March 23, 2015 (v1.2)
- New in v1.2: Notations slightly changed, see (1.2).

■ The model is described by the Hamiltonian

$$H = -J\sum_{ij} S_i S_j - B\sum_j S_j\,, \quad S_j = \pm 1 \tag{1.1}$$

Recall that finite-temperature phase transition occurs only in 2D or higher dimensions. We will be interested in the order parameter $S \equiv \langle \hat{S} \rangle$, where

$$\hat{S} \equiv \frac{1}{N}\sum_j S_j\,. \tag{1.2}$$

■ The quenching process changes the *reduced temperature*

$$\epsilon(t) = \frac{T(t) - T_c(t)}{T_c(t)} \tag{1.3}$$

in general. We are particularly interested in the case where T is kept constant and J is varied:

$$\epsilon(t) = \frac{J_c(T) - J(t)}{J_c(T)} \tag{1.4}$$

We will assume a linear queching *from the ordered to disordered phase* in the form

$$\epsilon(t) = \frac{t}{\tau_Q}\,, \quad \epsilon(0) = 0\,, \quad (-\infty \le t \le \infty) \tag{1.5}$$

where τ_Q is the quenching time.[1.1]

(1.1) Physically, $J(t) \ge 0$ and hence $-\infty < \epsilon(t) \le 1$ $(-\infty < t \le \tau_Q)$ However, as we are mostly concerned about the critical phenomena near $\epsilon \sim 0$, extending time to ∞ would not affect the final results much.

2 Symmetry Considertation

- March 23, 2015 (v1.1)
- Here I argue that in principle, $\langle e^{-\sigma}\rangle = 1/2$ for any quenching rate. The conclusion is quite boring. Then I will argue that the result may be different if we allow for some tolerance in the initial distribution. This may be interesting if it exhibits some scaling behavior peculiar to second-order phase transitions.

Let's denote a spin configuration by $\boldsymbol{S}$:

$$\boldsymbol{S} = (S_1, S_2, \cdots, S_N). \tag{2.1}$$

Let

$$\mathcal{H} \equiv \mathcal{H}_+ \cup \mathcal{H}_- \cup \mathcal{H}_0\,, \quad \mathcal{H}_\pm \equiv \{\, \boldsymbol{S} \mid \textstyle\sum_j S_j \gtrless 0\,\}\,, \quad \mathcal{H}_0 \equiv \{\, \boldsymbol{S} \mid \textstyle\sum_j S_j = 0\,\}\,. \tag{2.2}$$

Of course, $\mathcal{H}_0$ is empty for odd N. Even for even N, the contribution of $\mathcal{H}_0$ is relatively negligible (probability measure is zero) in the thermodynamic limit. Nevertheless, I keep it because it helps to make the argument clearer.

■ Let us first consider N even. Let ρ_i (ρ_f) be the initial equilibrium state for the forward (backward) process starting from the symmetry-breaking (disordered) phase

$$\rho_i = \frac{1}{Z_i}\sum_{\boldsymbol{S}\in\mathcal{H}_+} e^{-\beta H(t_i)}\,, \quad \rho_f = \frac{1}{Z_f}\sum_{\boldsymbol{S}\in\mathcal{H}} e^{-\beta H(t_f)} \tag{2.3}$$

The reason why $\rho_i(\mathcal{H}_0) = 0$ can be argued by the standard recipe for symmetry breaking

$$\langle S_i\rangle = \lim_{B\to 0}\lim_{N\to\infty}\sum_{\boldsymbol{S}} S_i e^{-\beta H}/Z \tag{2.4}$$

For infinitely fast quenching, the initial spin configuration for any forward path is completely frozen. Of course, the initial spin configuration belongs to $\mathcal{H}_+$. Therefore, any reverse path starting from $\boldsymbol{S} \in \mathcal{H}_- \cup \mathcal{H}_0$ has no corresponding forward path. Note that

$$\rho_f(\mathcal{H}_+) + \rho_f(\mathcal{H}_-) + \rho_f(\mathcal{H}_0) = 2\rho_f(\mathcal{H}_-) + \rho_f(\mathcal{H}_0) = 1 \tag{2.5}$$

Therefore, we conclude that

$$\lambda_S = \rho_f(\mathcal{H}_-) + \rho_f(\mathcal{H}_0) = \frac{1}{2} + \frac{1}{2}\rho_f(\mathcal{H}_0) > \frac{1}{2}\,, \quad \langle e^{-\sigma}\rangle < \frac{1}{2}\,. \tag{2.6}$$

As mentioned above, in the thermodynamic limit

$$\rho_f(\mathcal{H}_0) \to 0\,, \quad \langle e^{-\sigma}\rangle \to \frac{1}{2}\,. \tag{2.7}$$

But the point related to later arguments is that the existence of a third set other than $\mathcal{H}_\pm$ leads to $\langle e^{-\sigma}\rangle < 1/2$.

■ Now I argue that $\langle e^{-\sigma}\rangle = 1/2$ for any quenching rate (I now ignore $\mathcal{H}_0$). See Fig. 2.1, where I define sets $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$ and their relations to $\mathcal{H}_\pm$. $\mathcal{A}$ is the subset of $\mathcal{H}$ that cannot be reached by any path from $\mathcal{H}_+$. $\mathcal{C} = \{\, -\boldsymbol{S} \mid \boldsymbol{S} \in \mathcal{A}\,\}$ is the symmetric counterpart of $\mathcal{A}$. $\mathcal{B}$ is the rest of $\mathcal{H}$; it is the set of spin configurations that can be reached from $\mathcal{H}_\pm$.

Note that

$$P[\Gamma(\mathcal{A}\to\mathcal{H}_-)] + P[\Gamma(\mathcal{C}\to\mathcal{H}_+)] + P[\Gamma(\mathcal{B}\to\mathcal{H}_-)] + P[\Gamma(\mathcal{B}\to\mathcal{H}_+)] = 1\,, \tag{2.8}$$

$$P[\Gamma(\mathcal{A}\to\mathcal{H}_-)] = P[\Gamma(\mathcal{C}\to\mathcal{H}_+)]\,, \tag{2.9}$$

$$P[\Gamma(\mathcal{B}\to\mathcal{H}_-)] = P[\Gamma(\mathcal{B}\to\mathcal{H}_+)]\,. \tag{2.10}$$

I conclude that

$$\lambda_S = P[\Gamma(\mathcal{A} \to \mathcal{H}_-)] + P[\Gamma(\mathcal{B} \to \mathcal{H}_+)] = \frac{1}{2}. \tag{2.11}$$

The conclusion is rather boring!

■ So far, the argument was given as a matter of principle. In practice, especially when the process starts from a deep symmetry-breaking phase, the initial distribution should be strongly dominated by the configurations close to $\boldsymbol{S}_0 = (1, 1, \cdots, 1)$. The tails of the distribution might be ignorable. Then this ignored portion plays the same role as the set $\mathcal{H}_0$ above, leading to $\langle e^{-\sigma} \rangle < 1/2$.

In this sense, we may have to introduce some tolerance in the initial distribution function. The deviation, of course, will depend on the tolerance we introduce. But the deviation may exhibits some scaling behavior inherited from that of second-order phase transitions. The results in Section A.1 may reflect this fact (note that the KZM is also an approximation in the first place and it may have effectively introduced a tolerance.)

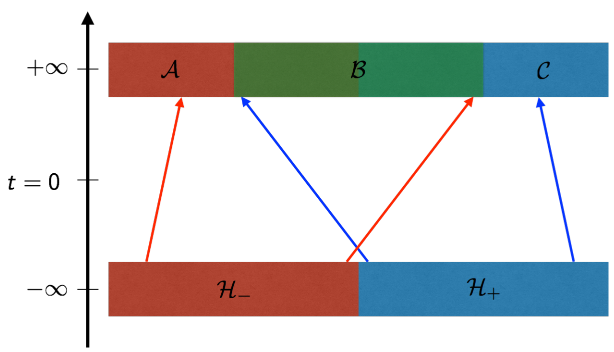

Figure 2.1: Possible forward paths and images of them.

3 Kibble-Zurek Mechanism

- March 9, 2015 (v1.2)

3.1 Overview

Within the spirit of the KZM, we find the *adiabatic-impulse crossover points* $\pm t_*$ ($t_* > 0$), determined by the condition

$$\tau(t_*) = \left|\frac{\epsilon(t)}{\partial_t \epsilon}\right|_{t=t_*} = |t_*| \,. \tag{3.1}$$

For later use, we define

$$\epsilon_* \equiv \epsilon(t_*) \tag{3.2}$$

Usually t_* and ϵ_* are smaller for slower quenching; for example, see

At the crossover times, the coupling stength is given by

$$K(\mp t_*) = (1 \pm \epsilon_*) K_c \gtrless K_c \tag{3.3}$$

and hence the order parameter by

$$S_* \equiv S(-t_*) = \langle \hat{S} \rangle_{t=-t_*} \neq 0 \,, \quad S(t_*) = 0 \tag{3.4}$$

■ For $t \in (-\tau_\infty, -t_*)$, the relaxation rate $1/\tau(t)$ of the system is fast enough to follow the external change of $\epsilon(t)$. The process in this period is thus regarded as *quasi-static*. Namely, at each moment the system is in *local* equilibrium with broken symmetry. Therefore, there is no entropy change and the amount of work done during this period is entirely given by the free energy change:

$$\beta W(-t_*, -\tau_\infty) = \Delta F(t_*, -t_*) \tag{3.5}$$

S.2

■ For $t \in (-t_*, t_*)$, the relaxation rate $1/\tau(t)$ is too slow to follow the external variation of $\epsilon(t)$. The system is assumed to remain in its state where it was at $t = -t_*$. Then one has

$$\langle e^{-\beta W} \rangle\Big|_{-t_*}^{t_*} = \langle e^{-\beta \Delta H(t_*, -t_*)} \rangle_{t=-t_*} \tag{3.6}$$

It is stressed that the average $\langle \cdots \rangle_{t=-t_*}$ is over the equilibrium distribution at time $t = -t_*$. Putting the Ising model (1.1) into (3.6) leads to

$$\begin{aligned} \langle e^{-\beta \Delta H(t_*, -t_*)} \rangle_{t=-t_*} &= \sum_{\boldsymbol{S} \in \mathcal{H}_+} e^{-\beta[H(t_*) - H(-t_*)]} \frac{e^{-\beta H(-t_*)}}{Z(-t_*)} \\ &= \frac{1}{Z(-t_*)} \sum_{\boldsymbol{S} \in \mathcal{H}_+} e^{-\beta H(t_*)} = \frac{1}{Z(-t_*)} \frac{1}{2} \sum_{\boldsymbol{S} \in \mathcal{H}} e^{-\beta H(t_*)} = \frac{1}{2} \frac{Z(t_*)}{Z(-t_*)} \end{aligned} \tag{3.7}$$

Notice the factor $1/2$ which is required for $Z(t_*)$ as the equilibrium state corresponding to $H(t_*)$ is disordered. We have just shown that

$$\langle e^{-\sigma} \rangle\Big|_{-t_*}^{t_*} = \frac{1}{2} \tag{3.8}$$

Remark Equation (3.8) is exact (as a matter of principle). Considering the argument leading to it, it should hold for any infinitely fast quenching (not limited to the KZM).

- For $t \in (t_*, \tau_\infty)$, the process becomes quasi-static again. Therefore, the work is given by

$$\beta W(\tau_\infty, t_*) = \Delta F(\tau_\infty, t_*) \tag{3.9}$$

In this period, there is no order ($\langle S \rangle = 0$), and one expects that no work is done on the system.(3.1)

- Summing up, the total work done on the system is given by

$$\begin{aligned} \beta W(\tau_\infty, -\tau_\infty) &= \overbrace{\Delta F(\tau_\infty, t_*)}^{\text{adiabatic}} + \overbrace{\beta W(t_*, -t_*)}^{\text{impulse}} + \overbrace{\Delta F(-t_*, -\tau_\infty)}^{\text{adiabatic}} \\ &= \Delta F(\tau_\infty, -\tau_\infty) + \underbrace{\beta W(t_*, -t_*) - \Delta F(t_*, -t_*)}_{\sigma(t_*, -t_*)} \end{aligned} \tag{3.10}$$

Therefore, within the Kibble-Zurek mechanism, the entropy production occurs soley from the impulse interval of the whole process:

$$\sigma \equiv \sigma(\tau_\infty, -\tau_\infty) = \sigma(t_*, -t_*)\,. \tag{3.11}$$

In Sections A.1–A.3 below, we will work out $W(t_*, -t_*)$ and $\Delta F(t_*, -t_*)$ more closely.

Remark 3.1 If Eqs. (3.10) and (3.11) are correct, then it follows from (3.8) that $\langle e^{-\sigma} \rangle = \frac{1}{2}$ regardless of the quenching speed and the system size.

Question 3.1 Two questions are:

(a) The classification in (3.11) is under the assumption that the average in $\langle e^{-\sigma} \rangle(\infty, -\infty)$ can be done separately in the three sections.

$$\langle e^{-\sigma} \rangle|_{-\infty}^{\infty} = \langle e^{-\sigma} \rangle|_{t_*}^{\infty} \times \langle e^{-\sigma} \rangle|_{-t_*}^{t_*} \times \langle e^{-\sigma} \rangle|_{-\infty}^{-t_*}? \tag{3.12}$$

Is it true, when σ is not a state function? As Gentaro mentioned in his note, during the quasi-static process, the work is usually supposed to be deterministic $W = \langle W \rangle$. How serious should we take this when the quasi-static process is combined with a highly irreversible process? I'm getting now confused about everything.

(b) The fast relaxation to equilibrium right after the impulse regime ($t = t_*$). We've ignored it so far. Would it affect the result? As we briefly discussed over Skype before, I tend to think that this effect is ignorable. In the case of the quenching from the disordered to ordered phase, created are topological defects, which surve for asymptotically long time (see, e.g., Laguna and Zurek 1997; Laguna and Zurek 1998). However, in the opposite direction, at the end of the impulse period, there is no free-energy barrier against the non-equilibrium spin configurations to relax to equlibrium ones.

(3.1) Indeed, using the mean-field result demonstrate this,

$$\beta W(\tau_\infty, t_*) \approx -N \log \frac{\cosh[zK(\tau_\infty)S(\tau_\infty)]}{\cosh[zK(t_*)S(t_*)]} = 0$$

.

3.2 Introducing the Tolerance

We focus on the impulse regime, $-t_* < t < t_*$. Introducting a tolerance ε in the spin distribution function[(3.2)] [to be comapred with (3.7)]

$$\langle e^{-\beta W}\rangle\big|_{-t_*}^{t_*} = \langle e^{-\beta\Delta H(t_*,-t_*)}\rangle_{t=-t_*} = \sum_{\boldsymbol{S}\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta[H(t_*)-H(-t_*)]}\frac{e^{-\beta H(-t_*)}}{Z(-t_*)}$$
$$= \frac{1}{Z(-t_*)}\sum_{\boldsymbol{S}\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta H(t_*)} \quad (3.13)$$

where $\mathcal{H}_\varepsilon(-t_*)$ is the Hilbert space allowed for the given tolerance ε. Note that

$$Z(-t_*) = \sum_{\boldsymbol{S}\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta H(-t_*)} \quad (3.14)$$

Therefore, we have [to be compared with (3.8)]

$$\langle e^{-\sigma}\rangle\big|_{-t_*}^{t_*} = \frac{1}{Z(t_*)}\sum_{\boldsymbol{S}\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta H(t_*)} = \frac{\sum_{\boldsymbol{S}\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta H(t_*)}}{\sum_{\boldsymbol{S}\in\mathcal{H}_\varepsilon(+t_*)} e^{-\beta H(t_*)}} \quad (3.15)$$

Namely, the effect of the tolerance depends how much the *initially* allowed Hilbert space $\mathcal{H}_\varepsilon(-t_*)$ contribute the *final* Boltzmann weight $e^{-\beta H(t_*)}$. For $\varepsilon = 0$, we have $\mathcal{H}_0(-t_*) = \mathcal{H}_+$ and recover the result (3.8).

Question 3.2 For the process from ordered to disorder phase, $\mathcal{H}_\varepsilon(-t_*)$ is centered around $S(-t_*) = S_*$ while $e^{-\beta H(t_*)}$ is maximum around $S(t_*) = 0$. In the opposite direction, $\mathcal{H}_\varepsilon(-t_*)$ is centered around $S(-t_*) = 0$ while $e^{-\beta H(t_*)}$ is maximum around $S(t_*) = S_*$. The relative relations between $\mathcal{H}_\varepsilon(-t_*)$ and $e^{-\beta H(t_*)}$ thus seem quite symmetric for both directions (except for the factor of $1/2$). Therefore, at least in the MFA, it seems that $\langle e^{-\sigma}\rangle$ is the same for both directions. What do you think, Gentaro?

(3.2) Here I introduce the tolerance to the spin distribution rather than to the work distribution function.

4 Ginzbug-Landau Description

- March 23, 2015 (v1.1)
- See Goldenfeld (1992) and Binney et al. (1992).

S.2

In the neighborhood of a critical point all macroscopic processes are slowing down. Microscopic kinetics, scattering of particles, exchange of momentum and energy, and so on, are not affected by the slowing of the macroscopic behavior of the system. This leads to the situation where all other degrees of freedom can be considered as being in a *local equilibrium state* characterized by some slowly changing value of the order parameter $\psi(t, \boldsymbol{r})$. Therefore, the Ginzburg-Landau (GL) theory is a natural way to describe the system in this regime.

Here we want evaluate Eq. (3.15) within the GL theory. In terms of the order paramter, it reads as

$$\langle e^{-\sigma}\rangle|_{-t_*}^{t_*} = \frac{\sum_{\psi\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta H(t_*)}}{\sum_{\psi\in\mathcal{H}_\varepsilon(+t_*)} e^{-\beta H(t_*)}} \tag{4.1}$$

where βH has the form

$$\beta H[\psi] = \int d^d\boldsymbol{x}\, \left[(\boldsymbol{\nabla}\psi)^2 + \alpha(t)\psi^2 + \frac{1}{2}g\psi^4\right] \tag{4.2}$$

4.1 Relevant Configuration Space: Ordered Phase

In the ordered phase,

$$\psi(t, \boldsymbol{x}) = \psi_0 + \phi(t, \boldsymbol{x}) \tag{4.3}$$

$$\beta H[\psi] \approx \beta H(\psi_0) + \int d^d\boldsymbol{x}\, \left[(\boldsymbol{\nabla}\phi)^2 + m^2(-t_*)\phi^2\right]\,, \quad m^2 \equiv 1/\xi^2 \tag{4.4}$$

Equation (4.4) is *not* a simple Gaussian approximation, which is equivalent to the mean-field approximation, because $m^2 = 1/\xi^2$ is the true correlation length.(Q4.1)

$$\phi(\boldsymbol{x}) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\phi_{\boldsymbol{k}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\frac{(\varphi_{\boldsymbol{k}} + i\varphi'_{\boldsymbol{k}})}{\sqrt{2}}\,, \quad \varphi_{\boldsymbol{k}}, \varphi'_{\boldsymbol{k}} \in \mathbb{R} \tag{4.5}$$

$$\phi_{\boldsymbol{k}} = \phi^*_{-\boldsymbol{k}}\,, \quad \varphi_{\boldsymbol{k}} = \varphi_{-\boldsymbol{k}}\,, \quad \varphi'_{\boldsymbol{k}} = -\varphi'_{-\boldsymbol{k}}\,. \tag{4.6}$$

$$\rho[\psi]\mathscr{D}[\psi] = \frac{1}{Z}e^{-\beta H[\psi]}\mathscr{D}[\psi] \sim \prod_{\boldsymbol{x}} d\phi(\boldsymbol{x})\exp\left\{-\int d^d\boldsymbol{x}\, \left[(\boldsymbol{\nabla}\phi)^2 + m^2\phi^2\right]\right\} \tag{4.7}$$

(Q4.1) 2015-03-23: Unfortunately, this method does not seem to incorporate properly the *anomalous dimension* η.

$$
\begin{aligned}
\rho[\psi]\mathscr{D}[\psi] &= \frac{1}{Z(-t_*)}\prod_{\boldsymbol{k}\in\mathcal{B}} d\phi_{\boldsymbol{k}} \exp\left\{-|\phi_{\boldsymbol{k}}|^2(\boldsymbol{k}^2+m^2)\right\} \\
&= \frac{1}{Z(-t_*)} d\phi_0 \prod_{\boldsymbol{k}\in\mathcal{B}/2} d\phi^*_{\boldsymbol{k}} d\phi_{\boldsymbol{k}} \exp\left\{-|\phi_{\boldsymbol{k}}|^2(\boldsymbol{k}^2+m^2)\right\} \\
&= \frac{1}{Z(-t_*)} d\varphi_0 e^{-\varphi_0^2 m^2} \prod_{\boldsymbol{k}\in\mathcal{B}/2} d\varphi_{\boldsymbol{k}} d\varphi'_{\boldsymbol{k}} \exp\left\{-\frac{1}{2}(\varphi^2_{\boldsymbol{k}}+\varphi'^2_{\boldsymbol{k}})(\boldsymbol{k}^2+m^2)\right\} \\
&= \frac{1}{Z(-t_*)} \underbrace{\left[\frac{1}{\sqrt{2m^2}}\prod_{\boldsymbol{k}\in\mathcal{B}/2}\frac{1}{\boldsymbol{k}^2+m^2}\right]}_{\text{to be canceled by } Z} d\eta_0 e^{-\frac{1}{2}\eta_0^2} \prod_{\boldsymbol{k}\in\mathcal{B}/2} d\eta_{\boldsymbol{k}} d\eta'_{\boldsymbol{k}} \exp\left\{-\frac{1}{2}(\eta^2_{\boldsymbol{k}}+\eta'^2_{\boldsymbol{k}})\right\}
\end{aligned}
$$

The probability distribution of the rescaled field η is given by

$$
\rho[\psi]\mathscr{D}[\psi] = \rho[\eta]\mathscr{D}[\eta] = \frac{1}{Z_\eta(-t_*)} d\eta_0 e^{-\frac{1}{2}\eta_0^2} \prod_{\boldsymbol{k}\in\mathcal{B}/2} d\eta_{\boldsymbol{k}} d\eta'_{\boldsymbol{k}} \exp\left\{-\frac{1}{2}(\eta^2_{\boldsymbol{k}}+\eta'^2_{\boldsymbol{k}})\right\} \tag{4.8}
$$

where

$$
Z_\eta(-t_*) = \int d\eta_0 e^{-\frac{1}{2}\eta_0^2} \prod_{\boldsymbol{k}\in\mathcal{B}/2} \int d\eta_{\boldsymbol{k}} d\eta'_{\boldsymbol{k}} \exp\left\{-\frac{1}{2}(\eta^2_{\boldsymbol{k}}+\eta'^2_{\boldsymbol{k}})\right\} = (2\pi)^{N/2} \tag{4.9}
$$

Here N is the number of *coarse-grained* sites (not the original sites), and yet it scales like the number of original sites. We conclude that

$$
\mathcal{H}_\varepsilon(-t_*) = \left\{ \eta_{\boldsymbol{k}} \;\middle|\; \eta_0^2 + \sum_{\boldsymbol{k}\in\mathcal{B}/2} (\eta^2_{\boldsymbol{k}}+\eta'^2_{\boldsymbol{k}}) \le R^2_\varepsilon \right\}, \tag{4.10}
$$

where R_ε is defined by the relation

$$
\int_{|\boldsymbol{\eta}|<R_\varepsilon} \frac{d^N\boldsymbol{\eta}}{(2\pi)^{N/2}}\, e^{-\boldsymbol{\eta}^2/2} = 1 - \frac{\Gamma(N/2, R^2_\varepsilon/2)}{\Gamma(n/2)} \equiv 1-\varepsilon \tag{4.11}
$$

and $\Gamma(z,\zeta)$ is the incomplete Gamma function

$$
\Gamma(z,\zeta) \equiv \int_\zeta^\infty dt\, t^{z-1}e^{-t}\,, \quad \Gamma(z,0)=\Gamma(z)\,. \tag{4.12}
$$

Note that

$$
R_\varepsilon \sim \sqrt{N} \quad (N\gg 1\,, \quad \varepsilon \ll 1) \tag{4.13}
$$

4.2 Relevant Configuration Space: Disordered Phase

The order parameter is chosen similarly as in the ordered phase, but setting $\phi_0 = 0$:

$$
\psi(t,\boldsymbol{x}) = \phi(t,\boldsymbol{x}) \tag{4.14}
$$

and

$$
\beta H[\psi] \approx \int d^d\boldsymbol{x}\, \left[(\boldsymbol{\nabla}\phi)^2 + m^2(t_*)\phi^2\right]\,, \quad m^2 \equiv 1/\xi^2 \tag{4.15}
$$

We thus have

$$\mathcal{H}_\varepsilon(t_*) = \left\{ \eta_{\boldsymbol{k}} \;\middle|\; \eta_0^2 + \sum_{\boldsymbol{k}\in\mathcal{B}/2} (\eta_{\boldsymbol{k}}^2 + \eta_{\boldsymbol{k}}'^2) \le R_\varepsilon^2 \right\} \tag{4.16}$$

For the moment, we assume that $m(-t_*) = m(t_*)$ and hence that R_ε deines the relevant area in both phases.

4.3 Jarzynski Equality

Let us now examine the Jaryzinski equality using the identity (4.1).

- The denominator of (4.1) is given by

$$\sum_{\psi\in\mathcal{H}_\varepsilon(+t_*)} e^{-\beta H(t_*)} = \frac{Z_\eta(t_*)}{Z(t_*)} \int_{|\boldsymbol{\eta}|<R_\varepsilon} \frac{d^N\boldsymbol{\eta}}{(2\pi)^{N/2}}\, e^{-\boldsymbol{\eta}^2/2} = \frac{Z_\eta(t_*)}{Z(t_*)}\,[1-\varepsilon] \tag{4.17}$$

- The numerator of (4.1) is the hard part.

$$\sum_{\psi\in\mathcal{H}_\varepsilon(-t_*)} e^{-\beta H(t_*)} = \frac{Z_\eta(-t_*)}{Z(-t_*)} \int_{|\boldsymbol{\eta}|<R_\varepsilon} \frac{d^N\boldsymbol{\eta}}{(2\pi)^{N/2}}\, e^{-(\boldsymbol{\eta}-\boldsymbol{a})^2/2} \tag{4.18}$$

where

$$a = \psi_0 \frac{\sqrt{N}}{\xi} \sim L^{(d/2-1)-\beta/\nu} \frac{\Phi_S(\epsilon(-t_*)L^{1/\nu})}{\Phi_\xi(\epsilon(-t_*)L^{1/\nu})} \tag{4.19}$$

$$a \sim N^{(1/2-1/d)-\beta/d\nu} \tag{4.20}$$

- 2D Ising: $\beta = 1/8$, $\nu = 1$, $a \sim N^{-1/16}$.
- 3D Ising: $\beta = 0.326$, $\nu = 0.63$, $a \sim N^{-0.006}$.
- 4D Ising: $\beta = 1/2$, $\nu = 1/2$, $a \sim 1$.
- Ising in larger dimensions: $a \sim N^{\text{positive power}}$.

Therefore, a is mostly small.

- For $a \ll 1$,

$$\int_{|\boldsymbol{\eta}|<R_\varepsilon} \frac{d^N\boldsymbol{\eta}}{(2\pi)^{N/2}}\, e^{-(\boldsymbol{\eta}-\boldsymbol{a})^2/2} \approx [1-\varepsilon] - \underbrace{\left[\frac{\Gamma(N/2+1, R_\varepsilon^2/2)}{\Gamma(N/2+1)} - \frac{\Gamma(N/2, R_\varepsilon^2/2)}{\Gamma(N/2)}\right]}_{\text{very rapidly descreasing with } N} \frac{a^2}{2} + \mathscr{O}(a^4) \tag{4.21}$$

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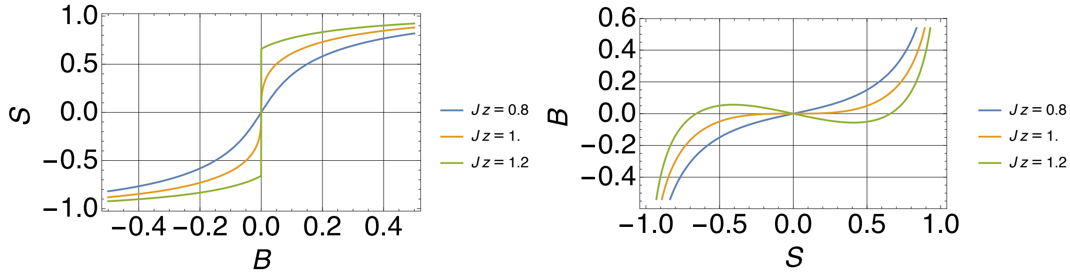

Figure 5.1: Two different forms of the (self-consistent) equation of state within the mean-field approximation.

5 Mean-Field Approximation

- March 24, 2015 (v1.8 since March 16, 2015)
- New in v1.8: In Section 5.4, a third method to get $\rho(\hat{S})$ is discussed, which reveals exactly how the discrepancy between Gentaro and Seunju's and my method occurs.
- New in v1.7: Gentaro's Questions 5.1 and 5.3 are discussed. Additional my own Question 5.4 is discussed as well.
- New in v1.6: Section 5.1 has been split into two, Sections 5.1 and 5.2.
- New in v1.5: Several typos (mostly concerning β and N) corrected.

Recently Gentaro and Seunju worked on the test of Jarzynski equality allowing for a finite value of tolerance within the mean-field (MF) approximation. One key difference from the GL approach in Section 4 is that the width of the distribution does not depend on the initial and final values of (dimensionless) coupling constant $J(-t_*)$ and $J(t_*)$; it was simply given by $\sim 1/\sqrt{N}$ regardless of J. I find this weird because even in the MF approximation, the susceptibility $\chi(J)$, which gives the width of the distribution, diverges near the critical point ($J \to J_c$). Here I demonstrate that the width of the distribution should depend on J and does diverge as $J \to J_c$.

5.1 The Distribution Function $\rho(\hat{S})$ of $\hat{S}$

I write the Ising model in the form

$$\beta H = -J \sum_{<ij>} S_i S_j - B \sum_j S_j \tag{5.1}$$

where both the coupling J and the field B are dimensionless. The MF Hamiltonian is commonly written as [cf. (5.21)]

$$\beta H^0_{\rm MF} \stackrel{?}{=} -(zJS + B) \sum_j S_j\,, \quad S \equiv \langle \hat{S} \rangle\,, \quad \hat{S} \equiv \frac{1}{N} \sum_j S_j\,. \tag{5.2}$$

The self-consistent *equation of state* [see Fig. 5.1] is given by

$$S = \tanh(zJS + B) \tag{5.3}$$

We will see in Section 5.2 below that *this MF Hamiltonian is not self-consistent* – the MF Hamiltonian (5.2) and the equation of state (5.3) are not consistent with each other.

■ For the test of Jarzynski equality $\langle e^{-\sigma} \rangle = 1$, we want the distribution function $\rho(\hat{S})d\hat{S}$. I will use the following theorem.

Theorem 5.1 (Reif 1965, Chapter 8) Let $\mathcal{G}(J,S)$ be the Gibbs free energy *per spin*. In the thermodynamic limit and in the absence of spontaneous symmetry breaking,[(5.1)] the distribution function is given by (to be normalized)

$$\rho(J,B;\hat{S}) = e^{-NF(J,B;\hat{S})}\,, \quad F(J,B;S) \equiv \beta\mathcal{G}(J,S) - BS\,. \tag{5.4}$$

Two remarks are in order: First, $F(J,B;S)$ is *not* the Helmholtz free energy $\mathcal{F}(J,B)$ itself but related to it by

$$\beta\mathcal{F}(J,B) = \left[F(J,B;S)\right]_{S=S(B)}\,. \tag{5.5}$$

Second, the theorem is *exact*, and has nothing to do with the MF approximation.

I will get the MF approximation $\rho_{\rm MF}$ of the distribution function by putting into (5.4) the MF approximation $\mathcal{G}_{\rm MF}$ of the Gibbs free energy. As the Gibbs free energy gives the equation of state

$$B = \beta\frac{\partial\mathcal{G}}{\partial S} \tag{5.6}$$

one can get the MF approximation $\mathcal{G}_{\rm MF}$ of the Gibbs free energy by integrating the MF equation of state (5.3)

$$\begin{aligned}\beta\mathcal{G}_{\rm MF}(J,S) = \int_0^S dS'\,B(S') = \int_0^S dS'\,\left[\tanh^{-1}S' - zJS'\right]\\ = -\frac{1}{2}zJS^2 + S\tanh^{-1}(S) + \frac{1}{2}\log(1-S^2)\end{aligned} \tag{5.7}$$

Putting it into (5.4), I get the MF approximation $\rho_{\rm MF}(\hat{S})$ of the distribution function:

$$\rho_{\rm MF}(\hat{S}) = e^{-NF_{\rm MF}(\hat{S})}\,, \quad F_{\rm MF}(S) = -\frac{1}{2}zJS^2 + S\tanh^{-1}(S) + \frac{1}{2}\log(1-S^2) - BS\,. \tag{5.8}$$

Figure 5.2 shows $F_{\rm MF}(J,0;S)$ at $B=0$ as a function of S for various values of J.[(5.2)] For small S ($zJ \to 1$),

$$F_{\rm MF}(J,0;S) \approx -\log 2 + \frac{1}{2}(1-zJ)S^2 + \frac{1}{12}S^4 + \cdots \tag{5.9}$$

- **Summary**. The width $\sqrt{\chi_{\rm MF}}$ of the distribution function $\rho_{\rm MF}(\hat{S}) = e^{-NF_{\rm MF}(\hat{S})}$ is given by

$$\chi_{\rm MF} \equiv \langle\hat{S}^2\rangle_{\rm MF} - \langle\hat{S}^2\rangle_{\rm MF} \approx \frac{1}{N(1-zJ)} \tag{5.10}$$

This is consistent with the well-known result that the critical exponent $\gamma = 1$ in the MF approximation.

Question 5.1 Gentaro (March 20, 2015): I think the width of $\rho(\hat{S})$ as a function of $\hat{S}$ does *not* have to diverge even near the critical point.

(5.1) In the present of symmetry breaking ($J > J_c$), there is no simple way to get $\rho(\hat{S})$. For definiteness, I will thus focus on the disordered phase ($zJ_c < 1$) at the moment.
(5.2) Strictly speaking, $F_{\rm MF}(J,0;S)$ is valid only for $J < J_c$ because the identity (5.4) holds only for $J < J_c$. However, I think that it is valid even for $J > J_c$; see Eq. (5.48).

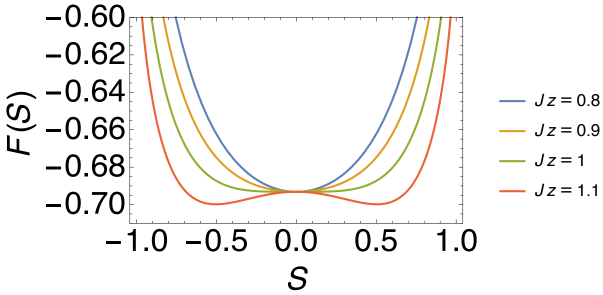

Figure 5.2: The exponent $F(S)$ of the probability distribution function $\rho(\hat{S}) = e^{-NF(\hat{S})}$ at $B = 0$.

(a) Suppose we have N spins. Then, there is only one configuration with $\hat{S} = 1$. On the other hand, the number of the configurations with $\hat{S} = 0$ is much larger, the "binomial distribution"[(5.3)] $B(N, N/2)$. If the width of $\rho(\hat{S})$ diverges so that ρ becomes a uniform function with respect to $\hat{S}$, we have extremely large enhancement of the probability to have the configuration $\hat{S} = 1$ compared to that of $\hat{S} = 0$. I think this cannot happen.

(b) I agree that the width of $\rho(\hat{S})$ increases by approaching the critical point (although it does not diverge). Actually, I have checked this point for $\rho(\hat{S})$ using the standard MF Hamiltonian numerically. The increase of the width near the critical point may be milder compared to $\rho(\hat{S})$ for the true Hamiltonian (that is why the approximate expression of Seungju and me, which assumes the coupling constant value around the critical point, does not depend on the coupling constant) but I think this would be the limitation of the mean-field theory.

Discussion I respond point by point to Gentaro's comments:

(a) I think this point is due to miscommunication. When I said that the "width" of the distribution of $\rho(\hat{S})$ "diverges," the Gaussian term in its exponent vanishes when expanded in small S; see Fig. 5.1 and Eq. (5.9). Namely, at the critial point ($zJ = 1$),

$$\rho_{\mathrm{MF}}(\hat{S}) \sim e^{-N\hat{S}^4/12} \tag{5.11}$$

and it becomes *flat* and

$$\chi_{\mathrm{MF}} \equiv \langle \hat{S}^2 \rangle_{\mathrm{MF}} - \langle \hat{S} \rangle_{\mathrm{MF}}^2 \to \infty\,. \tag{5.12}$$

In this sense, the (Gaussian) "width" is said to "diverges". On the other hand, for $zJ < 1$

$$\rho_{\mathrm{MF}}(\hat{S}) \sim e^{-N(1-zJ)\hat{S}^2/2 - N\hat{S}^4/12} \sim e^{-N(1-zJ)\hat{S}^2/2} \quad (|\hat{S}| \ll 1) \tag{5.13}$$

and

$$\chi_{\mathrm{MF}} \approx \frac{1}{N(1-zJ)}\,. \tag{5.14}$$

(b) Let us consider the probability distribution $\rho[\psi(\boldsymbol{r})]$ in the order-parameter space $\{\psi(\boldsymbol{r})\}$ within the Landau theory. As you agreed, the Gaussian approximation

$$\rho_G[\psi(\boldsymbol{r})] \sim \exp\left[-\int d^d\boldsymbol{r}\ \left\{(\boldsymbol{\nabla}\psi)^2 + \alpha(J)\psi^2\right\}\right]\,, \quad \alpha(J) \sim J_c - J \tag{5.15}$$

(5.3) Probably Gentaro means "binomial coefficient".

is equivalent to the MF approximation. Consider the uniform part

$$\psi_0 = \frac{1}{V}\int d^d\boldsymbol{r}\,\psi(\boldsymbol{r}) \tag{5.16}$$

of the order parameter $\psi(\boldsymbol{r})$. Near the critical point ($J \approx J_c$), we know that $\psi_0 = S$. Apparently, $\rho_G(\psi_0)$ has the same form of (5.9); following the same lines in Section 5.1, one can show more explicitly that the Gaussian model of the Ginzburg-Landau theory gives a distribution function of ψ_0 that has the same form as (5.9).

For these reasons, I believe that the "width" of the distribution should depend on the coupling J and "diverges" near the critical point *even in the mean-field picture*.

5.2 Self-Consistent Free Energies and MF Hamiltonian

I point out that Eqs. (5.2) and (5.3) are not consistent with each other. If one adopted the MF Hamiltonian (5.2), one would get the partition function

$$Z^0_{\mathrm{MF}} \stackrel{?}{=} [2\cosh(zJS+B)]^N \tag{5.17}$$

and the corresponding free energy (per spin)

$$\beta\mathcal{F}^0_{\mathrm{MF}}(J,B) \stackrel{?}{=} -\log[2\cosh(zJS+B)]_{S=S(B)}\,. \tag{5.18}$$

However, it leads to

$$S = -\beta\frac{\partial\mathcal{F}^0_{\mathrm{MF}}}{\partial B} = \tanh(zJS+B)\left[\frac{\partial S}{\partial B}+1\right] \neq \tanh(zJS+B)\,. \tag{5.19}$$

■ To get the *self-consistent* Helmholtz free energy, I make a Legendre transformation of the Gibbs free energy in (5.7) to get

$$\begin{aligned}\beta\mathcal{F}_{\mathrm{MF}}(J,B) &= \left[-\log[2\cosh(zJS+B)] + \frac{1}{2}zJS^2\right]_{S=S(B)} \\ &= -\log\left[2e^{-\frac{1}{2}zJS^2}\cosh(zJS+B)\right]_{S=S(B)}\,.\end{aligned} \tag{5.20}$$

This means that the self-consistent MF Hamiltonian should read as [cf. (5.2)]

$$\beta H_{\mathrm{MF}} = -(zJS+B)\sum_j S_j + \frac{1}{2}zJNS^2 \tag{5.21}$$

Question 5.2 Gentaro (March 19, 2015): My conclusion is that both the standard MF Hamiltonian (5.2) and the self-consistent equation of state (5.3) are correct. Hamiltonian with an extra term (5.21).

(a) An important point is that even though the magnetization S is given by

$$S = -\frac{\partial\mathcal{F}}{\partial B}, \tag{5.22}$$

where $\mathcal{F}$ is the Helmholtz free energy for the original Hamiltonian H without mean-field approximation, it is *incorrect* to write

$$S = -\frac{\partial\mathcal{F}^0_{MF}}{\partial B} \quad \text{wrong!} \tag{5.23}$$

for the free energy using the mean-field Hamiltonian.

To understand the above statement, we should return to think why S is given by $S = -\partial\mathcal{F}/\partial B$. The reason is the rhs of Eq. (5.22) is equivalent to

$$\sum_i \mathrm{Tr}[S_i e^{-\beta H}]/Z, \quad Z = \mathrm{Tr}\, e^{-\beta H} \tag{5.24}$$

Equation (5.22) is true only if there is no B-dependence in the Hamiltonian except for B itself; the mean-field Hamiltonian H^0_{MF} in (5.2) is not the case.

(b) Another point to raise is that we can directly calculate S for the mean-field Hamiltonian by

$$S = \sum_i \mathrm{Tr}\left[S_i e^{-\beta H^0_{\mathrm{MF}}}\right]/Z^0_{\mathrm{MF}}. \tag{5.25}$$

In the case of the standard MF Hamiltonian H^0_{MF} in (5.2), resulting value of S agrees with the value obtained by the self-consistent equation of state (5.3) for sufficiently large N (I have checked this fact). I think the Hamiltonian with an extra term (5.21) gives different value.

Discussion I respond point-by-point to Gentaro's comments:

(a) Note that the equation of state

$$S = -\beta\frac{\partial\mathcal{F}}{\partial B} \tag{5.26}$$

should hold even in thermodynamics, where the free energy is defined without any reference to partition function. It would be weird if one has to remember how the free energy was calculated assuming what (here that S was regarded as a fixed value) and to decide whether to apply it (or not) keeping in mind the assumption in detail. Namely, given the MF approximation $\mathcal{F}^0_{\mathrm{MF}}(J,B)$, one must remember that he cannot use the standard relation $S = -\beta\partial\mathcal{F}^0_{\mathrm{MF}}/\partial B$. To the contrary, with $\mathcal{F}_{\mathrm{MF}}(J,B)$ at hand, you are completely free to apply the standard method $S = -\beta\partial\mathcal{F}_{\mathrm{MF}}/\partial B$ to get the equation of state, without asking how the approximation was obtained. In this sense, I would prefer $\mathcal{F}_{\mathrm{MF}}$ to $\mathcal{F}^0_{\mathrm{MF}}$.

As long as you manage to be self-consistent, I think it's okay. The point is that my additional term does not affect the standard equation of state, and yet in addition helps us maintain self-consistency without extra caution or complexity.

(b) Both H^0_{MF} and H_{MF} lead to the same equation of state (5.3) when calculating in such a way. (This was confirmed by Gentaro.)

Question 5.3 Gentaro (March 20, 2015): The total energy given by the Hamiltonian (5.21) can significantly be different from that for the original Hamiltonian (5.1).

For clarity, please consider zero temperature case (ground state). We can see that the standard MF Hamiltonian (5.2) gives the same value of the energy as the original Hamiltonian at zero temperature. On the other hand, the energy given by the MF Hamiltonian with an additional term (5.21) differs by $zJS^2N/2$, which is not small compared to the other term. Since we are interested in the amount of work done on the system, this difference is crucial.

Discussion Actually, it's the other way around: It is H_{MF} in (5.21) [not H^0_{MF} in (5.2)] that gives a correct value of the ground-state energy. I think this issue can be seen in several different views:

(a) H^0_{MF} in (5.2) *double-counts* the self-energy and gives a wrong value of the ground-state energy. To the contrary, H_{MF} in (5.21) gives the correct value. In short, the three Hamiltonians give the ground-state energies as following:

$$\beta H/N = -\frac{1}{2}zJS^2 - BS \tag{5.27a}$$

$$\beta H^0_{\mathrm{MF}}/N = -zJS^2 - BS \quad \text{(wrong!)} \tag{5.27b}$$

$$\beta H_{\mathrm{MF}}/N = -\frac{1}{2}zJS^2 - BS \quad \text{(correct!)} \tag{5.27c}$$

Anyhow, this issue clarify the physical meaning of the additional term in (5.21): It corrects the double-counting in H^0_{MF} in (5.2). Thanks, Gentaro![5.4]

(b) One can also understand the 1/2-factor in the ground-state energy [either in (5.27a) or (5.27c)] within the self-consistency picture. Let us consider the amount of work that one has to do when S increases from $S = 0$ to a finite value S. First, due to the interaction with the external field, it is $-BS$. Second, due to the interaction with the self-consistent field $-zJS$ is given by $-zJSdS$ infinitismally, and hence for finite S, is given by

$$-zJ\int_0^S dS'S' = -\frac{1}{2}zJS^2 \tag{5.28}$$

Hence the ground-state energy is $\beta H/N = -\frac{1}{2}zJS^2$ at $B = 0$. This is reminiscent of the self-energy $Q^2/2C$ of the electric charge in a capacitor.

(c) I think that physically more significant is the energy *difference* not the absolute value of energy. Therefore let us consider some energy difference. As the free energy $\mathcal{F}_{\mathrm{MF}}$ in (5.20) gives the "required" equation of state (5.3) [via the standard prescription $S = -\beta\partial\mathcal{F}_{\mathrm{MF}}/\partial B$], one can safely assume that

$$\beta d\mathcal{F}_{\mathrm{MF}} = -SdB \quad (dH_{\mathrm{MF}} = -NSdB \quad \text{at} \quad T = 0), \tag{5.29}$$

and hence I think that any free energy change $\Delta\mathcal{F}_{\mathrm{MF}}$ (or ΔH_{MF} at $T = 0$) should be reasonably accurate as long as the mean-field picture itlsef is reasonable. Therefore it seems to me that the amount of work calculated from either (5.20) or (5.21) is reasonably accurate, again, up to the accuracy of the mean-field picture.

Neither $\mathcal{F}^0_{\mathrm{MF}}$ in (5.18) nor H^0_{MF} in (5.2) behaves in this way, and when using them one has to be careful to maintain the self-consistency.

Question 5.4 Then what's wrong (if any) with Gentaro and Seungju's approach?

Discussion As I understand, their approach is essentially as following

$$\rho^0_{\mathrm{MF}}(\hat{S}) \sim \sum_{\boldsymbol{S}}{}' e^{-\beta H^0_{\mathrm{MF}}(S,\hat{S})} = g(\hat{S})e^{-\beta H^0_{\mathrm{MF}}(S,\hat{S})} \tag{5.30}$$

where the restricted summation $\sum'_{\boldsymbol{S}}$ is over all spin configurations $\boldsymbol{S} = (S_1, \cdots, S_N)$ such that $\hat{S} = \frac{1}{N}\sum_j S_j$ and the *degeneracy factor* $g(\hat{S})$ is the number of such spin configurations.

(5.4) We would have arrived at an agreement far earlier if we had noticed it from the start. We could be cleverer. ;-)

The degeneracy factor $g(\hat{S})$ is related to the binonial coefficient and is approximated for large N by

$$g(\hat{S}) = \binom{N}{N\hat{S}} \approx \sqrt{\frac{2\pi}{N}} e^{-N\hat{S}^2/2} \tag{5.31}$$

Putting (5.31) into (5.30), they arrived at the conclusion (let us put $B = 0$)

$$\rho^0_{\mathrm{MF}}(J; S, \hat{S}) \sim \exp\left\{-N\left[\frac{1}{2}\hat{S}^2 - zJS\hat{S}\right]\right\} \tag{5.32}$$

Two noticeable features of this result are

(a) It depends on both S and $\hat{S}$. Gentaro argues that in the MF approximation, S should be regarded as a given parameter fixed by the MF equation of state (5.3). However, I am not sure if the distribution can be obtained independently of S. This is where I suspect that the self-consistency is lost (2015-03-24 this seems to be confirmed in Section 5.4). On the other hand, $\rho_{\mathrm{MF}}(\hat{S})$ in Eq. (5.8) is (if correct) given entirely as a function of $\hat{S}$ only and yet maintains the self-consistency.

(b) With S regarded as a fixed parameter, near the critical point without field ($J = J_c, B = 0, \hat{S} \sim S \sim 0$) $\rho^0_{\mathrm{MF}}(J; S, \hat{S})$ has the width

$$\sqrt{\chi^0_{\mathrm{MF}}} \approx \frac{1}{\sqrt{N}} \tag{5.33}$$

S.2 independent of J.

5.3 Physical Implication

In Section 5.1, I've shown that the width $\sqrt{\chi}$ of the distribution function depends on J and diverges as $J \to J_c$ ($zJ_c = 1$). What does it imply for the Jarzynski equality?

For $J > J_c$, the distribution $\rho_{\mathrm{MF}}(\hat{S})$ is centered around S and had width $\sqrt{\chi_{\mathrm{MF}}}$:

$$S_{\mathrm{MF}} \sim \epsilon^{\beta}\,, \quad \chi_{\mathrm{MF}} \sim \epsilon^{-\gamma}\,, \quad \epsilon \equiv \frac{J_c - J}{J_c} \tag{5.34}$$

with $\beta = 1/2$ and $\gamma = 1$ in the MF approximation.

For $J < J_c$, the distribution $\rho_{\mathrm{MF}}(\hat{S})$ is sentered around $\hat{S} = 0$ and had width $\sqrt{\chi_{\mathrm{MF}}}$:

$$\chi_{\mathrm{MF}} \sim \epsilon^{-\gamma} \tag{5.35}$$

with $\beta = 1/2$ and $\gamma = 1$ in the MF approximation.

Therefore, the centers of the two distributions below and above the critical point are still within the width. This means that even if we introduce the tolerance, $\langle e^{-\sigma}\rangle_{\mathrm{MF}}$ may still be finite. More detailed analyses are required, but at least, this seems to be (qualitatively) consistent with the results in the GL approach (Section 4).

5.4 A Third Method to Get $\rho(\hat{S})$

Here I try another method to get the distribution function $\rho(\hat{S})$ for the following two reasons.

- First, in Section 5.1 the distribution was obtained based on Theorem 5.1, which is guaranteed only in the absence of spontaneous symmetry breaking. I want to assure that the distribution function in (5.8) and (5.9) is valid even in the ordered phase.

- Second, I want to understand where Gentaro and Seungju's approach went (if ever) wrong. Their method seems intuitively appealing and I myself had suggested it to Seungju. There must be a reason for the discrepancy.

I start from

$$\rho(\hat{S})d\hat{S} = d\hat{S} \sum_{\boldsymbol{S}\in\mathcal{H}_{\hat{S}}} \frac{e^{-\beta H(\boldsymbol{S})}}{Z} = d\hat{S} \sum_{\boldsymbol{S}\in\mathcal{H}} \delta(N\hat{S} - \sum_j S_j) \frac{e^{-\beta H(\boldsymbol{S})}}{Z} \tag{5.36}$$

where

$$\mathcal{H}_{\hat{S}} = \{\, \boldsymbol{S} \mid \sum_j S_j = N\hat{S} \,\} \,. \tag{5.37}$$

Using the identity

$$2\pi\delta(x) = \int_{-i\infty}^{+i\infty} d\phi\, e^{-\phi x} \tag{5.38}$$

$$\rho(\hat{S}) = \frac{1}{Z} \int \frac{d\phi}{2\pi}\, e^{-N\phi\hat{S}} \sum_{\boldsymbol{S}} e^{-\beta H(J,B+\phi;\boldsymbol{S})}. \tag{5.39}$$

■ So far no approximation has been made and the expression (5.39) is exact. Now I make a MF approximation for the sum $\sum_{\boldsymbol{S}} e^{-\beta H(J,B+\phi;\boldsymbol{S})}$ by adopting the MF Hamiltonian

$$\beta H(J, B+\phi) \approx \beta H_{\mathrm{MF}}(J, B+\phi) = -(zJS + B + \phi) \sum_j S_j + \frac{1}{2} zJS^2 \tag{5.40a}$$

$$\sum_{\boldsymbol{S}} e^{-\beta H(J,B+\phi)} \approx \sum_{\boldsymbol{S}} e^{-\beta H_{\mathrm{MF}}(J,B+\phi)} = \left[2\cosh(zJS + B + \phi) e^{-zJS^2/2}\right]^N . \tag{5.40b}$$

Putting (5.40) into (5.39) leads to

$$\rho_{\mathrm{MF}}(\hat{S}) = \frac{1}{Z} \int \frac{d\phi}{2\pi}\, e^{-N\mathcal{A}}\,, \quad \mathcal{A} = \phi\hat{S} - \log\cosh(zJS + B + \phi) + \frac{1}{2} zJS^2 - \log 2 \tag{5.41}$$

Here it is stressed that $S = S(\phi)$ should be regarded as a function of ϕ determined *self-consistently* by[(5.5)]

$$S(\phi) = \tanh[zJS(\phi) + B + \phi]\,. \tag{5.42}$$

The exponent of the integrand in (5.41) has a large prefactor N, and the integral is dominated by the saddle point. The saddle point is determined by

$$\left.\frac{\partial\mathcal{A}}{\partial\phi}\right|_{\phi=\phi_0} = \hat{S} - \tanh[zJS(\phi_0) + B + \phi_0] = 0 \tag{5.43}$$

Near the saddle point,

$$\begin{aligned}\mathcal{A}(\phi) &\approx \mathcal{A}(\phi_0) + \frac{1}{2}\frac{\partial^2\mathcal{A}}{\partial\phi^2}(\phi-\phi_0)^2 + \mathscr{O}(\phi-\phi_0)^3 \\ &= \mathcal{A}(\phi_0) - \frac{1}{2}\chi(B+\phi_0)(\phi-\phi_0)^2 + \mathscr{O}(\phi-\phi_0)^3\,,\end{aligned} \tag{5.44}$$

(5.5) Later I will also consider the case where S is regarded as a fixed parameter; see Eq. (5.52).

where $\chi(B)$ is the susceptibility at field B. Then the saddle point approximation of the integral gives

$$\rho_{\text{MF}}(\hat{S}) \approx \frac{e^{-N\mathcal{A}(\phi_0)}}{Z} \int_{-i\infty}^{+i\infty} \frac{d\phi}{2\pi}\, e^{N\chi(B+\phi_0)(\phi-\phi_0)^2/2} \approx \frac{e^{-N\mathcal{A}(\phi_0)}}{Z\sqrt{2\pi\chi N}} \tag{5.45}$$

The denominator contains a week $\hat{S}$ dependence through χ, but the major $\hat{S}$-dependence comes from the exponent, and hence

$$\rho_{\text{MF}}(\hat{S}) \approx e^{-N\mathcal{A}(\phi_0)}\,. \tag{5.46}$$

It follows from (5.42) and (5.43), namely,

$$\tanh[zJS(\phi_0) + B + \phi_0] = S(\phi_0) = \hat{S}\,, \tag{5.47}$$

that

$$\begin{aligned}
\mathcal{A}(\phi_0) &= \hat{S}\phi_0 - \log\cosh(zJS(\phi_0) + B + \phi_0) + \frac{1}{2}zJS^2(\phi_0) \\
&= \hat{S}(\tanh^{-1}\hat{S} - zJ\hat{S} - B) + \frac{1}{2}\log(1-\hat{S}^2) + \frac{1}{2}zJS^2(\phi_0) \\
&= -\frac{1}{2}zJ\hat{S} + \hat{S}\tanh^{-1}\hat{S} + \frac{1}{2}\log(1-\hat{S}^2) - BS \\
&= F(J,B;\hat{S})
\end{aligned} \tag{5.48}$$

Therefore, we have reproduced $\rho_{\text{MF}}(\hat{S})$ in (5.8). The difference is that here the derivation is valid even in the ordered phase ($zJ > 1$).

- What if we regard S as a fixed parameter in (5.41). We would have

$$\rho^0_{\text{MF}}(\hat{S}) = \frac{1}{Z}\int \frac{d\phi}{2\pi}\, e^{-N\mathcal{A}^0(\hat{S},S,\phi)}\,, \quad \mathcal{A}^0(\hat{S},S,\phi) = \phi\hat{S} - \log\cosh(zJS + B + \phi) + \text{constant}. \tag{5.49}$$

In this case, the saddle point is determined by [cf. (5.43)]

$$\left.\frac{\partial\mathcal{A}^0}{\partial\phi}\right|_{\phi=\phi_0} = \hat{S} - \tanh(zJS + B + \phi_0) = 0 \tag{5.50}$$

The saddle-point approximation of the integral leads to

$$\rho^0_{\text{MF}}(\hat{S}) \approx e^{-N\mathcal{A}^0(\hat{S},S,\phi_0)} \tag{5.51}$$

with [cf. (5.48)]

$$\begin{aligned}
\mathcal{A}^0(\hat{S},S,\phi_0) &= \hat{S}[\tanh^{-1}\hat{S} - (zJS + B)] + \frac{1}{2}\log(1-\hat{S}^2) \\
&\approx \frac{1}{2}\hat{S}^2 - (zJS + B)\hat{S} + \mathscr{O}(\hat{S}^4)
\end{aligned} \tag{5.52}$$

This is the result of Gentaro and Seunju's. It has two distinguished properties:

(a) It depends on both S and $\hat{S}$.

(b) The (Gaussian) width of the distribution, $1/\sqrt{N}$, is independent of J.

Therefore, as I speculated in the dicussion concerning Question 5.4, it seems that these two properties are due to the loss of self-consistency.

A Test of the Jarzynski Equality: Obsolete

- March 23, 2015 (v1.12 since January 22, 2015)
- 2015-02-13: The results here are incorrect as Eq. (A.5) is actually $\beta\langle W\rangle$ and $\langle e^{\beta W}\rangle \neq e^{\beta\langle W\rangle}$; Eq. (A.16) is actually $\langle\sigma\rangle$ and $\langle e^{\sigma}\rangle \neq e^{\langle\sigma\rangle}$; Eq. (A.24) is actually $\langle\sigma\rangle$ and $\langle e^{\sigma}\rangle \neq e^{\langle\sigma\rangle}$.

A.1 Kibble-Zurek Mechanism: Mean-Field Scaling

- For comparison, the KZM is combined with the mean-field approximation rather than with the true critical scaling.

■ The mean-field Hamiltonian reads

$$\beta H_{MF} = -(zKS + C)\sum_j S_j\,, \quad K \equiv \beta J\,, \quad C \equiv \beta B\,, \tag{A.1}$$

where z is the coordination number and $\langle\cdots\rangle$-sign has been omitted from $\langle S\rangle$. Within the mean-field approximation, $zK_c = 1$. The self-consistent equation for S is given by

$$S = \tanh(zKS) \tag{A.2}$$

For later use, we also note that

$$S \approx \tanh(zK) \quad (K \to \infty) \tag{A.3a}$$

$$zK(1-S) \approx zK(1-\tanh(zK)) \to 0 \quad (K \to \infty) \tag{A.3b}$$

S.2

$$\beta W(-t_*, -\tau_\infty) \approx -N \log\frac{\cosh[(1+\epsilon_*)zK_cS_*]}{\cosh[zK(-\tau_\infty)S(-\tau_\infty)]} \tag{A.4}$$

■ Focusing on the impulse period ($-t_* < t < t_*$),

$$\beta W(t_*, -t_*) \approx -Nz\left[K(t_*) - K(-t_*)\right]S_*^2 = 2NzK_cS_*^2\epsilon_* \tag{A.5}$$

The free-energy difference is given by

$$F(t_*) = -N\log\cosh[zK(t_*)S(t_*)] = 0 \tag{A.6a}$$

$$F(-t_*) = -N\log\cosh[(1+\epsilon_*)zK_cS_*] + \log 2 \tag{A.6b}$$

$$\Delta F(t_*, -t_*) = N\log\cosh[(1+\epsilon_*)zK_cS_*] - \log 2 \tag{A.6c}$$

About the additional term $\log 2$, see Gentaro's note.

Summing up, we have

$$\sigma = -\log 2 - N\log\cosh[(1+\epsilon_*)zK_cS_*] + \log 2 + 2NzK_cS_*^2\epsilon_* \tag{A.7}$$

■ Let us first consider the slow-quenching limit ($\tau_Q \to \infty$). In this case, $t_* \approx \epsilon_* \approx 0$ and hence $K_* \approx K_c$ and $S_* \sim \sqrt{\epsilon_*}$. Therefore,

$$\sigma \approx \log 2 - N\log\left[1 + (zK_cS_*)^2/2\right] + \mathscr{O}(\epsilon_*^2) \tag{A.8}$$

$$\sigma = \beta(W - \Delta F) \approx \log 2 - N\log\left(1 + (zK_cS_*)^2/2\right) \tag{A.9}$$

$$\langle e^{-\sigma} \rangle \approx \frac{1}{2}\left[1+\frac{1}{2}(zK_cS_*)^2\right]^N \to \frac{1}{2} \tag{A.10}$$

Therefore, Eq. (A.10) reproduces Gentaro's result. Further, Eq. (A.10) implies that for slow but finite queching rate ($\tau_0 \ll \tau_Q < \infty$), $\langle e^{-\sigma} \rangle$ tends to *recover*[(QA.1)] the Jarzynski equality ($\langle e^{-\sigma} \rangle > 1/2$).

■ In the opposite limit ($\tau_Q \to 0$), we note that $t_* \sim \tau_Q$ and $\epsilon_* \sim 1$. This means that $S_* \sim 1$. From Eq. (A.7), it follows that

$$\sigma \approx \log 2 + N \log 2 + NzK_cS_*(1-\epsilon_*) \tag{A.11}$$

which leads to

$$\langle e^{-\sigma} \rangle \approx \frac{1}{2}\left(\frac{e^{-zK_cS_*(1-\epsilon_*)}}{2}\right)^N \to 0. \tag{A.12}$$

A.2 Kibble-Zurek Mechanism: Critical Scaling

• Warning: The arguments and results need a careful check.

Near the critical point ($K \approx K_c$, $t \approx 0$) of a second-order phase transition, the correlation length ξ and the relaxation time τ diverges like

$$\xi_\infty(t) \approx \frac{\xi_0}{|\epsilon(t)|^\nu} = \frac{\xi_0}{|t/\tau_Q|^\nu}\,, \quad \tau(t) \approx \xi_\infty^z(t) \tag{A.13}$$

where ν and z are critical exponents.

Except for very fast quenching, ϵ_* is small enought to be in the critical fluctuation regime, and it inherites the following scaling behavior from (A.13)

$$\epsilon_* \approx \left(\frac{\tau_0}{\tau_Q}\right)^{1/(1+\nu z)} \tag{A.14}$$

Accordingly $F(\pm t_*)$ and S_* also exhibit scaling behaviors:

$$F(\pm t_*) \approx L^d \epsilon_*^{d\nu} \Phi_F^\pm(0)\,, \quad S_* \approx \epsilon_*^\beta \Phi_S(0) \tag{A.15}$$

■ Let us first consider the slow-quenching limit ($\tau_Q \to \infty$). In this case, $t_* \approx \epsilon_* \approx 0$ and hence $K_* \approx K_c$ and $S_* \approx 0$. Considering the scaling behaviors (A.15),

$$\sigma \approx \log 2 - L^d \epsilon_*^{d\nu}\left[\Phi_F^+(0) - \Phi_F^-(0)\right] + 2L^d zK_c\epsilon_*^{2\beta+1}\Phi_S(0)\,. \tag{A.16}$$

Unlike the MF scaling, the true critical scaling behavior gives

$$2\beta + 1 < d\nu \tag{A.17}$$

For example, in $d = 2$, $\nu = 1$ and $\beta = 1/8$. Therefore,

$$\sigma \approx \log 2 + 2L^d zK_c\epsilon_*^{2\beta+1}\Phi_S(0)\,. \tag{A.18}$$

(QA.1) Physically, shouldn't it be the other way around?

$$\langle e^{-\sigma} \rangle \approx \frac{1}{2}\left[1 - 2zK_c\epsilon_*^{2\beta+1}\Phi_S(0)\right]^{L^d} \to \frac{1}{2} \tag{A.19}$$

Again this reproduces Gentaro's result. However, unlike the MF scaling [see Eq. (A.10)], (A.19) implies that for slow but finite queching rate ($\tau_0 \ll \tau_Q < \infty$), $\langle e^{-\sigma}\rangle$ tends to *violates further* the Jarzynski equality ($\langle e^{-\sigma}\rangle < 1/2$).

■ In the opposite limit, where $\epsilon_* \gg \epsilon_{GL}$. Here ϵ_{GL} is the Ginzburg-Landau criteria. In this case, the MF scaling should be enough.

A.3 Kibble-Zurek Mechanism: Finite-Size Scaling

- Warning (2015-02-04): Very primitive for the moment.

For finite L, the phase transition becomes a crossover. The scaling behaviors thus changes. For the free energy,

$$F(\pm t_*, L^{-1}) \sim L^d\,\epsilon_*^{d\nu}\Phi_F^{\pm}(\epsilon_*^{-\nu}/L) \equiv L^d\,\epsilon_*^{d\nu}\,(\epsilon_*^{-\nu}/L)^d\tilde{\Phi}_F^{\pm}(\epsilon_* L^{1/\nu}) \tag{A.20}$$

where the last equality defines the new scaling function $\tilde{\Phi}_F^{\pm}$.

$$\tilde{\Phi}_F^{\pm}(z) \sim \begin{cases} 1 \text{ or } 0 & (z \to 0) \\ z^{d\nu} & (z \to \infty) \end{cases} \tag{A.21}$$

Therefore, one has

$$F(\pm t_*, 0) \sim L^d\epsilon_*^{d\nu}\,, \quad F(\pm t_*, L^{-1}) \sim \tilde{\Phi}_F^{\pm}(\epsilon_* L^{1/\nu}) \tag{A.22}$$

In the same manner, the finite-size scaling of $S_*(L^{-1})$ is given by

$$S_*(0) \sim \epsilon_*^{\beta}\,, \quad S_*(L^{-1}) \sim L^{-\beta/\nu}\tilde{\Phi}_S(\epsilon_* L^{1/\nu}) \tag{A.23}$$

■ Let us now consider the slow-quenching limit ($\tau_Q \to \infty$).

$$\sigma \approx \log 2 - \left[\tilde{\Phi}_F^{+}(\epsilon_* L^{1/\nu}) - \tilde{\Phi}_F^{-}(\epsilon_* L^{1/\nu})\right] + 2zK_c L^{d-2\beta/\nu}\tilde{\Phi}_S^2(\epsilon_* L^{1/\nu})\epsilon_* \tag{A.24}$$

$$\langle e^{-\sigma}\rangle \approx \frac{1}{2}\left[\tilde{\Phi}_F^{+}(\epsilon_* L^{1/\nu}) - \tilde{\Phi}_F^{-}(\epsilon_* L^{1/\nu})\right]\left[1 + 2zK_c\tilde{\Phi}_S^2(\epsilon_* L^{1/\nu})\epsilon_*\right]^{L^{d-2\beta/\nu}} \neq \frac{1}{2} \tag{A.25}$$

B Issues

- March 9, 2015 (v1.1 since January 13, 2015)

- Transition rates for the first- and second-order phase transitions
- Discrete and continuous phase transitions
- Two-dimensional phase transition with continuous phase transitions
- To vary temperature or external parameter?
- Non-Markovian (if ever) dynamics of phase transitions

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