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On the Definition of Phase Transition

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It is shown that there exists a phase transition associated with a singularity of the free energy for a model such that for all temperatures the equilibrium state is unique and thus stable with respect to boundary perturbations. It is also shown on this model that there exist phase transitions without symmetry breakdown, which can be related to a phase transition with symmetry breakdown on an equivalent model.

KEY WORDS: Phase transition; unicity of equilibrium states.

Several definitions have been introduced in statistical mechanics to characterize a phase transition.[1] In particular, by analogy with thermodynamics, one can define a phase transition by the singularities of the free energy as a function of the thermodynamic variables; on the other hand, to prove the existence of a phase transition by means of Peierls' argument[1] or its natural generalization,[2] one defines a phase transition by means of the instability of the state with respect to boundary perturbation, i.e., nonuniqueness of the equilibrium state. It has been suspected[1] that these two definitions are closely related and the examples studied so far have confirmed this idea. In the following, we shall give an explicit example for which the two definitions are *not* equivalent. We shall show that it is possible to have a phase transition associated with a singularity of the free energy while the equilibrium state is unique at all temperatures.

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The model we consider is a spin-$\frac{1}{2}$ classical lattice system defined on a square lattice with an external field $H > 0$ and an alternating four-body force J_4, which is infinite. It is therefore defined by $\{\mathscr{L}, \mathscr{B}'\}$, where the lattice $\mathscr{L}$ is given by $\mathscr{L} = \mathbb{Z}^2$, and the family of bonds $\mathscr{B}'$ is given by $\mathscr{B}' = \mathscr{B} \cup \mathscr{B}_\infty$, with $\mathscr{B}$ the set of finite bonds defined by the one-point subset of $\mathscr{L}$ (external field) and $\mathscr{B}_\infty$ the set of infinite bonds defined by the four-point subsets of $\mathscr{L}$ represented by the hatched squares in Fig. 1.

The interactions are then given by the function J on $\mathscr{B}'$ defined by

$$J(x) = H \qquad \text{for all} \quad x \in \mathbb{Z}^2 = \mathscr{B}$$
$$J(B_\infty) = J_4 = +\infty \qquad \text{for all} \quad B_\infty \in \mathscr{B}_\infty$$

Introducing the function K on $\mathscr{B}'$ defined by

$$K(x) = (1/kT)J(x) = h, \qquad K(B_\infty) = (1/kT)J(B_\infty) = +\infty$$

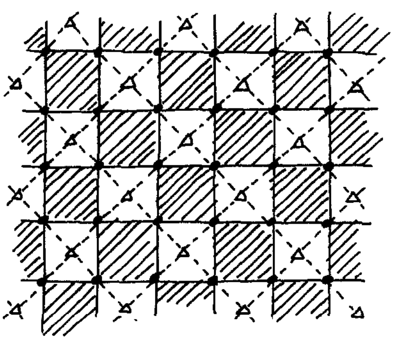
we find that the (reduced) partition function of the finite system $\{\Lambda, \mathscr{B}_\Lambda'\}$, $\Lambda \subset \mathbb{Z}^2, \mathscr{B}_\Lambda' = \mathscr{B}' \cap \mathscr{P}(\Lambda)$, is given by

$$Q'_{(\Lambda,h)} = \operatorname{Tr} \exp\left\{ \sum_{B \in \mathscr{B}_\Lambda'} K(B)[\sigma_B - 1] \right\} = \sum_{Y \subset \Lambda} C(Y) z^{|Y|}; \qquad z = e^{-2h}$$

where for any $X \subset \Lambda$ the function $\sigma_X = \prod_{x \in X} \sigma_x$ is the product of the spin variables belonging to the set X and $|X|$ denotes the cardinality of X; $C(Y)$ is the function which is one if Y is an admissible configuration, i.e., $\sigma_{B_\infty}(Y) = +1$ for all $B_\infty \in \mathscr{B}_{\infty,\Lambda}$ and is zero otherwise, $\mathscr{P}(\Lambda) = \{X; X \subset \Lambda\}$.

It has been shown[3] that this model is an HT–LT dual for the Ising model with two-body forces, which yields

$$f_H'(T) = f'^{(\text{Ising})}_{J_2 = H}(T) \tag{1}$$



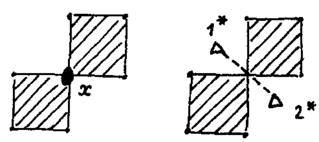


Fig. 1. The model (•) and its LT–LT dual (△). $h = \beta H > 0$, $K_4 = \beta J_4 = +\infty$. $d{:}\{x\} \mapsto B_x^* = \{1^*, 2^*\}$, $J_2^* = \text{H}$. $\mathscr{B}' = \{\{\bullet\}, \{\text{hatched square}\}\}$, $\mathscr{B}^* = \{\{\triangle - - - \triangle\}\}$.

where f' is the (reduced) free energy of the model and $f'^{(\text{Ising})}$ is the (reduced) free energy of the Ising model. We therefore conclude that there exists a phase transition at $T_c = T_c^{\text{Ising}}$ associated with a singularity of the free energy; moreover, the specific heat and susceptibility are proportional and both diverge at T_c with the indices of the Ising model; on the other hand, the magnetization is continuous.[4]

We shall now show that there exists a unique equilibrium state invariant under some subgroups τ of the translation group $\mathbb{Z}^2$ such that $\mathbb{Z}^2/\tau$ is finite. However, since there exist several definitions of the "equilibrium states of an infinite system," which have been shown to be equivalent only in the case where all interactions are finite[5] we shall show below that the equilibrium state is unique if one adopts any of the following definitions.

A state ω is an equilibrium state if:

D.1: It is a solution of the equation

$$\omega[\sigma_X] = \omega[\sigma_X \sigma_{B_\infty}]$$

$$\omega[\sigma_X] = \omega[\sigma_X \tanh(\textstyle\sum_{B \in \gamma(Z)} K(B)\sigma_B)]$$

for all $X \in \mathscr{P}_f(\mathscr{L})$, $B_\infty \in \mathscr{B}_\infty$, and for all $Z \in \mathscr{P}_f(\mathscr{L})$ such that Z is admissible, $|X \cap Z|$ is odd, and $\gamma(Z) = \{B \in \mathscr{B};\ \sigma_B(Z) = -1\}$; as usual $\mathscr{P}_f(\mathscr{L})$ denotes the family of finite subsets of $\mathscr{L}$.

D.2: It is a convex combination of thermodynamic limit of Gibbs states with specified boundary conditions.

D.3: It is a tangent plane to the graph of the free energy.

To establish this results, we consider an LT–LT duality transformation restricted to finite interactions,[6] which is defined in the following manner.

Let $\Gamma_f^{(a)}$ be the subgroup of $\mathscr{P}_f(\mathscr{B})$ defined by the element $\gamma(X) = \{B \in \mathscr{B};\ \sigma_B(X) = -1\}$ with X admissible and finite. The model $\{\mathscr{L}^*, \mathscr{B}^*\}$ with finite interactions only is called an LT–LT dual restricted to finite bonds for $\{\mathscr{L}, \mathscr{B}'\}$ if there exists a bijection d: $\mathscr{B} \to \mathscr{B}^*$ such that the induced mapping on subsets of $\mathscr{B}$ yields a bijection of $\Gamma_f^{(a)}$ onto $\Gamma_f{}^*$ with $K^*(B^*) = K(B)$. For our model, we shall take the transformation defined by the mapping $d{:}\,\mathscr{B} \to \mathscr{B}^*$, which associates to each point $x \in \mathbb{Z}^2$ [considered as bonds, i.e., elements of $\mathscr{P}_f(\mathbb{Z}^2)$] a pair of points $B_x{}^* = d\{x\}$ on the dual lattice $\mathbb{Z}^{2^*}$ defined by the center of the square for which $K_4 = 0$ (cf. Fig. 1).

For the model we consider, the group $\Gamma_f^{(a)}$ is generated by the four-point subsets of $\mathbb{Z}^2$ on white squares and those generators are mapped by the mapping d onto the four bonds containing the center of this square (see Fig. 2). We thus have a bijection between generators of $\Gamma_f^{(a)}$ and the generators of the group $\Gamma_f{}^*$ for the Ising model; it then follows that the Ising model with nearest neighbor interaction is an LT–LT dual restricted to finite bonds for our model.

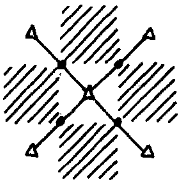


Fig. 2

1. If we adopt the definition of equilibrium states given by Eq. (1), we can use the result[6] that there exists a bijection between the equilibrium state ω invariant under the internal symmetry group $\mathscr{S}'$ and the equilibrium state ω^* invariant under $\mathscr{S}^*$ for the LT–LT dual; moreover, this bijection is given by

$$\omega\left[\prod_{B\in\beta}\sigma_B\right] = \omega^*\left[\prod_{B\in\beta}\sigma_{dB}\right] \qquad \text{for all} \quad \beta\in\mathscr{P}_f(\mathscr{B}) \tag{2}$$

With the LT–LT duality transformation considered, we then have that, for any equilibrium state ω, there exists a symmetric state $\omega^{*(\text{Ising})}$ of the Ising model, such that

$$\omega_{(H,T)}[\sigma_X] = \omega^{*(\text{Ising})}_{(J_2^*=H,T^*=T)}\left[\prod_{x\in X}\sigma_{dx}\right] \tag{3}$$

Since for all temperatures there exists a unique symmetric state of the two-dimensional Ising model invariant under translations,[7] we conclude that for all temperatures there exists a unique equilibrium state of our model invariant under some subgroup τ of the translation group such that $\mathbb{Z}^2/\tau$ is finite.

2. Let us then consider the definition given by the thermodynamic limit of a Gibbs state. The finite system Λ with boundary conditions Y such that $\sigma_B(Y) = +1$ for any B for which $K_4(B) = +\infty$ (compatibility of the boundary conditions with the constraints given by $K_4 = +\infty$) is defined by the interactions

$$\begin{aligned} h_x &= h && \forall_x\in\Lambda \\ h_x &= -\infty && \forall_x\in Y/[\Lambda\cap Y] \\ h_x &= +\infty && \forall_x\notin\Lambda\cup Y \end{aligned}$$

In this case, the LT–LT dual model is an Ising model with boundary conditions defined by $J_2^* = \pm\infty$ outside Λ^* where $\prod_{B^*\in\kappa^*} J^*_{B^*} > 0$ for any closed graph κ^*.

It then follows that there are exactly two boundary conditions on the LT–LT dual system, boundary conditions defined by Y^* and $\mathbb{Z}^{2*}/Y^*$; moreover, these boundary conditions are equivalent for the even point correlation functions.

We thus conclude that to any Gibbs state of the finite system Λ with boundary conditions Y there corresponds on the dual model a Gibbs state with boundary conditions Y^* such that

$$\langle \sigma_X \rangle_{(\Lambda, Y)} = \left\langle \prod_{x \in X} \sigma_{dx} \right\rangle_{(\Lambda^*, Y^*)} \qquad \text{for all} \quad X \subset \Lambda$$

Again the proof is concluded by means of the result of Ref. 7.

3. Finally we can use one of the proofs of Ref. 7 to conclude that for any perturbation defined by $R \in \mathscr{P}_f(\mathbb{Z}^2)$ and

$$Q'(\Lambda, h, \lambda) = \sum_{X \subset \Lambda} c(X) z^{|X|} \exp\left[-\lambda \sum_a (\tau_a \sigma_R)(X) \right]$$

the perturbed free energy $f'(h, \lambda)$ is differentiable at $\lambda = 0$. From this result one can then prove that there exists a unique equilibrium state whose symmetry group is the symmetry group of the interactions.

In conclusion, we have shown that although there exists a phase transition associated with a singularity of the free energy, the equilibrium state is unique at all temperatures and is given by Eq. (3). Moreover, this phase transition, which is not associated with a symmetry breakdown, can be related to a phase transition with a symmetry breakdown on an equivalent model.

We conclude with a few remarks concerning the state and the nature of the phase transition.

1. Using the LT–LT duality transformation, one can show that the state ω is not invariant under the translation group $\mathbb{Z}^2$ but only under the translation group of the interaction.

2. The phase transition can be characterized by the *long-range order parameter*[4]

$$\eta = \lim_{n \to \infty} \omega(\sigma_1 \cdots \sigma_n)$$

such that

$$\eta = 0, \qquad T \geqslant T_c$$
$$\eta > 0, \qquad T < T_c$$

In fact

$$\eta_H(T) = [m_{J_2 = h}^{\text{Ising}}(T)]^2$$

3. The phase transition can be characterized by a "*local*" *parameter* $\mu(T)$ which varies continuously and is such that $\mu(T) = 0$ for $T \leqslant T_c$ and $\mu(T) > 0$ for $T > T_c$. In fact,

$$\mu_H(T) = \lim_{K_4 \to +\infty} \langle e^{-2K_4(B)\sigma_B} \rangle_{(h, K_4)} \equiv m_{J_2 = h}^{\text{Ising}}(T^*) \tag{4}$$

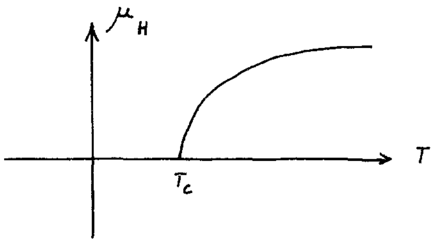


Fig. 3. Generator of $\Gamma_f^{(a)}$ and its image under the duality transformation.

where T^* is defined by $e^{(-2\beta^* J_2)} = \tanh \beta J_2$. (See Fig. 3.) It should be noticed that $\mu_H(T)$ is not a local order parameter in the usual sense, since (i)

$$\mu_H(T) = 0, \qquad T \leqslant T_c$$
$$\mu_H(T) > 0, \qquad T > T_c$$

and (ii)

$$\mu_H(T) \equiv \lim_{\lambda \stackrel{>}{\to} 0} (2\lambda)^{-1/2} \{\omega_{f,\lambda=0}(\mathfrak{S}_{B_4}) - \omega_{f,\lambda}(\mathfrak{S}_{B_4})\}$$

where $\omega_{f,\lambda}$ is the equilibrium state associated with the free boundary condition and $\tanh 2K_4 = 1 - \lambda$. On the other hand, for a standard order parameter such as the spontaneous magnetization, we have

$$-m_{J_2}(T) = \lim_{h \stackrel{>}{\to} 0} \{\omega_{f,h=0}(\sigma_x) - \omega_{f,h}(\sigma_x)\}$$

4. It can be easily seen that our model is equivalent to an eight-vertex model with weights $\omega_1 = \omega_2^{-1}$ and $\omega_3 = \cdots = \omega_8 = 1$ and the behavior of the local parameter $\mu_H = \mu_H(T)$ is analogous to the curve for the vertical polarization of the F model with respect to the vertical field.[8]

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