Rigorous Analysis of Singularities and Absence of Analytic Continuation at First Order Phase Transition Points in Lattice Spin Models *

Sacha Friedli
Institute of Theoretical Physics, EPFL, 1015 Lausanne, Switzerland

Charles-Édouard Pfister
Institute of Analysis and Scientific Computing, School of Mathematics, EPFL, 1015 Lausanne, Switzerland

We report about two new rigorous results on the non-analytic properties of thermodynamic potentials at first order phase transition. The first one is valid for lattice models ($d \geq 2$) with arbitrary finite state space, and finite-range interactions which have two ground states. Under the only assumption that the Peierls Condition is satisfied for the ground states and that the temperature is sufficiently low, we prove that the pressure has no analytic continuation at the first order phase transition point. The second result concerns Ising spins with Kac potentials $J_\gamma(x) = \gamma^d \varphi(\gamma x)$, where $0 < \gamma < 1$ is a small scaling parameter, and φ a fixed finite range potential. In this framework, we relate the non-analytic behaviour of the pressure at the transition point to the range of interaction, which equals γ^{-1}. Our analysis exhibits a crossover between the non-analytic behaviour of finite range models ($\gamma > 0$) and analyticity in the mean field limit ($\gamma \searrow 0$). In general, the basic mechanism responsible for the appearance of a singularity blocking the analytic continuation is that arbitrarily large droplets of the other phase become stable at the transition point.

Keywords: Non-analyticity, singularity, first order phase transition, condensation, Pirogov-Sinai Theory, droplet model, Kac potential, van der Waals limit, Mayer theory.

INTRODUCTION

The first theory of condensation originated with the celebrated equation of state of van der Waals [1]:

$$\Big(p + \frac{a}{v^2}\Big)\big(v - b\big) = RT\,. \tag{1}$$

When complemented with the Maxwell Construction (or "equal area rule"), (1) leads to isotherms describing general characteristics of the liquid-vapor equilibrium, including the existence of a critical temperature. The isotherms obtained with the van der Waals-Maxwell Theory have a very simple analytic structure: they are analytic in a pure phase and have analytic continuations along the liquid and gas branches, through the transition points. These analytic continuations, which were originally interpreted as describing the pressure of metastable states, are provided by the original isotherm given in (1).

The theoretical question of knowing whether the results predicted by the van der Waals Theory can be derived from first principles of Statistical Mechanics remained a longstanding problem during a large part of the twentieth century. The theories of Mayer [2] and Yang-Lee [3] were decisive contributions to the theory of phase transitions, but didn't give an answer concerning the delicate question of the analytic continuation at transition points. With regard to this latter property, two scenarios were discussed in the fifties and sixties.

The first one was essentially based on the mean field (or Bragg-Williams) approximation [4]. In the Ising set-up mean field theory is usually described as the Curie-Weiss model. In this approach, the interaction is replaced by an infinite range and infinitely weak potential. The central characteristic of the effective model obtained after this approximation is that the spatial positions of the particles don't play any role. As a consequence, an exact computation of the partition function leads to the same behaviour as in the van der Waals-Maxwell Theory: at low temperature, thermodynamic potentials are analytic in a pure phase, and have analytic continuation at transition points. Katsura [5] conjectured that this scenario holds also for short range models, like the Ising model (see also the discussion below).

The second argument, totally different in spirit, originated with the so called "droplet mechanism" of the condensation phenomenon, proposed by Andreev [6], Fisher [7] and Langer [8]. This mechanism, as opposed to the mean field approximation, predicts that the finiteness of the range of interaction plays a crucial role in the analytic properties of the thermodynamic potentials. Namely, when the range of interaction is finite, droplets of any size are stable at the condensation point, and although the probability of occurrence of *large* droplets is very small, it is their stability that yields a contribution of the order $k!^{\frac{d}{d-1}}$ to the k-th derivative of the pressure, which prevents an analytic continuation. Kunz

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and Souillard were led to the same conclusions after having studied a similar model, related to percolation [9].

Subsequent papers on the subject, in which no definite answer was given, include [10], [11], [12]. More recent studies can also be found in [13], [14], [15].

RIGOROUS RESULTS

Isakov (1984): *In dimension $d \geq 2$, at low enough temperature, the pressure of the Ising model in a magnetic field λ, $p = p(\lambda)$, is infinitely differentiable at $\lambda = 0^{\pm}$, but has no analytic continuation from $\{\lambda < 0\}$ to $\{\lambda > 0\}$ across $\lambda = 0$, or vice versa.*

Isakov proved that the Taylor series of the pressure at $\lambda = 0^{\pm}$ have zero convergence radius, by proving that

$$p^{(k)}(0^{\pm}) \sim C^k k!^{\frac{d}{d-1}} . \tag{2}$$

In a second paper [17], Isakov tried to extend this result to general two phase lattice models. He had, however, to introduce hypotheses that are not easy to verify in concrete models. Weaker but conceptually related results, on the absence of thermodynamic "metastable states", have been proved by Lanford and Ruelle [18]. Nowadays metastability is treated as a dynamical phenomenon. In this respect we mention an important paper by Schonmann and Shlosman [19]. We now present our results.

Two Phase Models. Consider a lattice model with finite state space at each site of $\mathbb{Z}^d$, $d \geq 2$. Let H_0 be a hamiltonian with finite range periodic interaction, having two periodic ground states ψ_1, ψ_2. We assume furthermore that the Peierls Condition is satisfied [20]. Let V be a periodic potential with finite range interaction, so that the perturbed hamiltonian

$$H_\lambda = H_0 + \lambda V \tag{3}$$

splits the degeneracy of H_0. That is, H_λ has a single ground state ψ_2 when $\lambda < 0$ and a single ground state ψ_1 when $\lambda > 0$. Denote by $p = p(\lambda)$ the pressure of the model (at inverse temperature β). Let $\delta > 0$. The general theory of Pirogov-Sinai [21] guarantees that if β is large enough, then there exists $\lambda^*(\beta) \in (-\delta, +\delta)$ such that the pressure has a first order phase transition at $\lambda^*(\beta)$. Our first result [22] is the following:

Theorem 1 *There exists $\beta_0 > 0$ such that for all $\beta \geq \beta_0$, the pressure is analytic in λ on $(-\delta, \lambda^*(\beta))$ and $(\lambda^*(\beta), +\delta)$, but has no analytic continuation from $(-\delta, \lambda^*(\beta))$ to $(\lambda^*(\beta), +\delta)$ across $\lambda^*(\beta)$ or vice-versa.*

Kac Potentials and the van der Waals Limit. Consider an Ising ferromagnet, with a spin $\sigma_i \in \{+1, -1\}$ at each site of $\mathbb{Z}^d$, $d \geq 2$. Let $\varphi : \mathbb{R}^d \to \mathbb{R}^+$, supported by the cube $[-1, +1]^d$, such that

$$\int \varphi(x) \mathrm{d}x = 1 . \tag{4}$$

Let $0 < \gamma < 1$ be a small scaling parameter, and consider the Kac potential $J_\gamma(x) = \gamma^d \varphi(\gamma x)$, together with the hamiltonian

$$H = -\frac{1}{2} \sum_{i \neq j} J_\gamma(i-j) \sigma_i \sigma_j . \tag{5}$$

Let $f_\gamma = f_\gamma(m)$ denote the free energy of this model, with fixed magnetization $m \in [-1, +1]$. The Theorem of Lebowitz-Penrose [23] gives a closed form to the free energy in the van der Waals limit $\gamma \searrow 0$ (called sometimes the Kac or mean field limit), and justifies the Maxwell construction. Let $f_0(m) = \lim_{\gamma \searrow 0} f_\gamma(m)$. Then (see Figure 1)

$$f_0(m) = \text{convex envelope of } \Big\{ -\frac{1}{2} m^2 - \frac{1}{\beta} I(m) \Big\} , \tag{6}$$

where $I(m)$ equals

$$I(m) = -\frac{1-m}{2} \log \frac{1-m}{2} - \frac{1+m}{2} \log \frac{1+m}{2} . \tag{7}$$

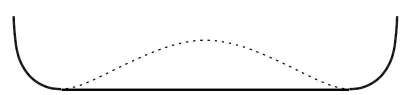

FIG. 1: The free energy in the van der Waals Limit.

When $\beta > 1$, $f_0(m)$ has a plateau $[-m^*(\beta), +m^*(\beta)]$, where $m^*(\beta)$ is the positive solution of the mean field equation $m = \tanh(\beta m)$. As a consequence of the Lebowitz-Penrose Theorem, all the analytic properties of the free energy are known explicitly after the van der Waals limit: f_0 is analytic on the branches $(-1, -m^*(\beta))$ and $(+m^*(\beta), +1)$, and has analytic continuation along the paths $m \nearrow -m^*(\beta)$, $m \searrow +m^*(\beta)$. The analytic continuation, which is unique, is given by the mean field free energy $-\frac{1}{2}m^2 - \frac{1}{\beta}I(m)$. After the van der Waals limit, the scenario is thus the same as in the van der Waals-Maxwell Theory.

Consider the specific choice $\varphi(x) = 2^{-d} 1(x)$, where $1(\cdot)$ is the indicator of the cube: $1(x) = 1$ if $x \in [-1, +1]^d$, 0 otherwise. For a fixed $0 < \gamma < 1$, J_γ is finite range and Theorem 1 can be used, but only for temperatures $\beta \geq \beta_0(\gamma)$, with $\lim_{\gamma \searrow 0} \beta_0(\gamma) = +\infty$. Our result [24] is given hereafter. It holds at low temperature, uniformly in the range of interaction.

Theorem 2 *There exists β_0, independent of γ, such that for all $\beta \geq \beta_0$ and all $0 < \gamma < 1$, the free energy f_γ is analytic on $(-1, -m^*(\beta,\gamma))$ and $(+m^*(\beta,\gamma), +1)$, but has no analytic continuation along the real paths $m \nearrow -m^*(\beta,\gamma)$, $m \searrow +m^*(\beta,\gamma)$.*

As opposed to the mean field behaviour, finite range interactions, even of very long range, imply absence of analytic continuation at transition points. A crucial ingredient for the proof of Theorem 2 is the use of the coarse-graining technique of Bovier and Zahradník [25].

We study the pressure $p_\gamma = p_\gamma(\lambda)$, in which the constraint on the magnetization is replaced by a magnetic field λ. The pressure and free energy are related by a Legendre transform:

$$f_\gamma(m) = \sup_\lambda \big(hm - p_\gamma(\lambda)\big)\,. \tag{8}$$

By the Theorem of Yang-Lee, p_γ is analytic in λ on $\{\lambda < 0\}$ and $\{\lambda > 0\}$. Our main result is a precise characterization of the properties of p_γ along the path $\lambda \searrow 0$ (using symmetry, we need only consider fields $\lambda > 0$).

Theorem 3 *There exists β_0, independent of γ, such that for all $\beta \geq \beta_0$ and all $\gamma > 0$, all the limits $p_\gamma^{(k)}(0^+) = \lim_{\lambda\searrow 0} p_\gamma^{(k)}(\lambda)$ exist, but the pressure has no analytic continuation from $\{\lambda > 0\}$ to $\{\lambda < 0\}$ across $\lambda = 0$. More precisely, there exists integers $k_1(\gamma)$, $k_2(\gamma)$, $k_1(\gamma) < k_2(\gamma)$, with $\lim_{\gamma\searrow 0} k_i(\gamma) = +\infty$, such that*

$$|p_\gamma^{(k)}(0^+)| \leq C_1^k k! \qquad \text{when } k \leq k_1(\gamma)\,, \tag{9}$$

$$|p_\gamma^{(k)}(0^+)| \geq C_2^k k!^{\frac{d}{d-1}} \qquad \text{when } k \geq k_2(\gamma)\,. \tag{10}$$

The constant C_1 is independent of γ and k, $C_2 = C_2(\gamma,\beta) > 0$, and $k_1(\gamma) = \gamma^{-d}$.

That is, the large order derivatives reveal the non-analytic feature of the singularity, although a signature of the mean field (analytic) behaviour can be detected in the low order derivatives. We have illustrated this crossover on Figure 2.

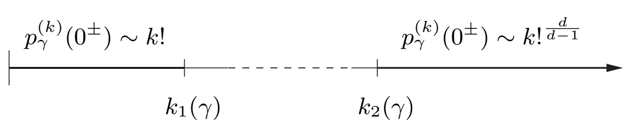

FIG. 2: The crossover in the derivatives of the pressure.

METHOD

The pressure has a singularity only in the thermodynamic limit. However, we study the system in large finite volumes, and obtain bounds on the derivatives that are uniform in the volume. At the end we prove that it is possible to interchange the operations of taking the derivative and the thermodynamic limit.

The method used to obtain lower bounds on the derivatives of the pressure at finite volume is inspired by the technique of Isakov. Let Λ be a finite cube in $\mathbb{Z}^d$ with a fixed boundary condition, and $Z(\Lambda)$ be the corresponding partition function. One enumerates all possible contours [26] inside Λ: $\Gamma_1, \Gamma_2, \ldots, \Gamma_n$, in such a way that $V(\Gamma_i) \leq V(\Gamma_j)$ when $i \leq j$ ($V(\Gamma_i)$ denotes the volume of the interior of the contour Γ_i). One then defines the restricted partition functions $Z_i(\Lambda)$, $i = 0, \ldots, n$. By definition, $Z_0(\Lambda)$ is the partition function computed for a system containing no contours, and $Z_i(\Lambda)$ is the partition function computed for a system containing no contour Γ_j with $j > i$. Obviously,

$$Z(\Lambda) = Z_0(\Lambda) \prod_{i=1}^n \frac{Z_i(\Lambda)}{Z_{i-1}(\Lambda)}\,. \tag{11}$$

For the proof of Theorem 1, there is only the ground state configuration contributing to $Z_0(\Lambda)$. For the proof of Theorem 2, $Z_0(\Lambda)$ is the partition function of a restricted phase, describing small local fluctuations of the ground state. Let

$$u_\Lambda(\Gamma_i) = \log \frac{Z_i(\Lambda)}{Z_{i-1}(\Lambda)}\,. \tag{12}$$

Notice that we have the fundamental relation

$$Z_i(\Lambda) = Z_{i-1}(\Lambda) + Z_{i-1}^*(\Lambda)\,, \tag{13}$$

where the contour Γ_i appears in each configuration contributing to $Z_{i-1}^*(\Lambda)$. A precise analysis of the phase diagram shows that $\lambda \mapsto u_\Lambda(\Gamma_i)(\lambda)$ is analytic in a disc $\mathcal{U}_i$ centered at $\lambda = \lambda^*(\beta)$ (resp. $\lambda = 0$ for the Kac ferromagnet), with a radius of order $V(\Gamma_i)^{-\frac{1}{d}}$. In the domain $\mathcal{U}_i$, $u_\Lambda(\Gamma_i)$ can be represented as follows:

$$u_\Lambda(\Gamma_i) = \log\Big(1 + \frac{Z_{i-1}^*(\Lambda)}{Z_{i-1}(\Lambda)}\Big) \equiv \log(1 + e^{g_\Lambda(\Gamma_i)})\,. \tag{14}$$

The dependence of $g_\Lambda(\Gamma_i)$ on the volume Λ is weak. Moreover, $g_\Lambda(\Gamma_i)$ can be decomposed into a surface term and a volume term, like in the droplet model. Then, by choosing a path of integration $\mathcal{C} \subset \mathcal{U}_i$,

$$u_i(\Lambda)^{(k)}(\lambda^*) = \frac{k!}{2\pi i} \int_{\mathcal{C}} \frac{u_i(\Lambda)(\lambda)}{(\lambda - \lambda^*)^{k+1}} \mathrm{d}\lambda\,. \tag{15}$$

The observation of Isakov is that $u_\Lambda(\Gamma_i) \simeq e^{g_\Lambda(\Gamma_i)}$ on $\mathcal{U}_i$, and that for a given large enough k, one can estimate precisely the Cauchy integral (15), for all large enough contours, by a stationary phase method, choosing suitably the path of integration $\mathcal{C}$. In this way one gets a contribution to the k-th derivative of the pressure of order $A^k k!^{\frac{d}{d-1}}$. For the other contours, only an upper bound can be obtained on the integral, of the same order $B^k k!^{\frac{d}{d-1}}$. The crucial point is therefore to have large enough neighbourhoods $\mathcal{U}_i$, in order to show that $A > B$.

DISCUSSION

In the framework of Kac potentials, the role played by the range of interaction in the analyticity properties of the pressure can be clarified by the following discussion. When $\lambda \geq 0$, our analysis allows to decompose the pressure in two distinct parts: $p_\gamma = r_\gamma + q_\gamma$. On one hand, r_γ is constructed with the partition function $Z_0(\Lambda)$ of (11), and describes a homogeneous phase with positive magnetization, containing no droplets of the $-$ phase. When $\gamma \searrow 0$, r_γ converges to the pressure of the mean field model. On the other hand, q_γ contains the contributions from the droplets of the $-$ phase, which are all stable at $\lambda = 0$, and $q_\gamma = O(e^{-\beta\gamma^{-d}})$. Namely, the main contribution to q_γ comes from the smallest droplets, which live on a coarse-grained lattice whose cells have side length γ^{-1}. Then, the pressure r_γ behaves analytically at $\lambda = 0$, i.e. ${r_\gamma}^{(k)}(0^\pm) \sim k!$ for all k, but q_γ is responsible for the absence of analytic continuation at $\lambda = 0$, since ${q_\gamma}^{(k)}(0^\pm) \sim k!^{\frac{d}{d-1}}$ for large enough k. The combination of these two behaviours leads to a crossover in the derivatives, as was shown in Theorem 3.

Our results also have an important consequence regarding the theory of condensation initiated by Mayer [2]. In this theory, the pressure of a non-ideal gas is described, near $z = 0$ (z is the fugacity), by a convergent Taylor expansion, given by the Mayer series:

$$\beta p(z) = \sum_{l \geq 1} b_l z^l \quad (b_l \text{ are the cluster coefficients})\,. \quad (16)$$

The condensation point is defined to be the first singularity, say z_M^*, encountered when (16) is continued analytically along the positive real line $z > 0$. It was suggested [4] that this method could actually lead to a wrong determination of the condensation point: the analytic continuation of the Mayer series might not "see" the real transition point z_c^*, situated somewhere between 0 and z_M^*: $0 < z_c^* < z_M^*$. This is indeed the case in the mean field approximation: the system does not "see" the condensation point, since there are no droplets of the liquid phase inside the gaseous phase. We saw that if one suppresses the condensation mechanism by retaining, in $p_\gamma = r_\gamma + q_\gamma$, only the term r_γ, then there is an analytic continuation of the pressure. Our analysis shows that the method initiated by Mayer for determining the condensation point gives the correct result for a large class of lattice gas models.

To conclude, we mention that the problem of knowing whether the pressure can be continued analytically around the singularity, in the complex plane, remains open. It is not clear, in this case, whether the droplet models can be used as a guiding mechanism, even to give a heuristic description [27].

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[20] Without restricting the generality we can assume that the energy $E_0(\psi_i)$ (associated to H_0) of each ground state ψ_i is zero. Let $y \in \mathbb{Z}^d$, $l_0 > R$ (R denotes the range of interaction), and $C_y = \{x \in \mathbb{Z}^d : |x_i - y_i| \leq l_0, i = 1, \dots, d\}$. Given a spin configuration ω, which differs from a ground state configuration only at finitely many points, we say that y is correct if the configuration ω, restricted to C_y, coincides with one of the ground states. Let $I(\omega)$ denote the set of points that are not correct. The Peierls Condition means that there exists a constant $\rho > 0$ such that $E_0(\omega) \geq \rho|I(\omega)|$. That is, regions of incorrect points are energy barriers.
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[26] For Theorem 1 contours are connected components of incorrect points (see [20]). For Theorems 2 and 3 we use a more elaborate notion of contours based on the coarse-graining technique of Bovier and Zahradník [25].
[27] See the discussion in [14], p.274, before Theorem 1.