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The phase diagram is analyzed rigorously, and in particular the wetting transition is discussed.

KEY WORDS: Ising model; wetting transition; correlation inequalities.

1. INTRODUCTION

In this paper I report on new rigorous results for the half-infinite Ising model, which I have obtained in collaboration with Jürg Fröhlich.^(1,2) The plan of the paper is as follows. In Section 2, I review the known results for two dimensions and state my main results. Section 3 treats the surface free energy, and Sections 4–6 treat, respectively, the phase diagram in the absence of external fields, with a boundary external field (the wetting transition), and with a boundary field and a bulk external field.

2. INTRODUCTION

We study the Ising model on the half-infinite lattice $\mathbb{L} = \mathbb{Z}^{d-1} \times \mathbb{Z}^+$, whose points are denoted by *i*, *j*,... or by i = (x, z), $x \in \mathbb{Z}^{d-1}$, $z \in \mathbb{Z}^+$. The boundary layer, or first layer, of the lattice is Σ ,

$$\Sigma = \{i \in \mathbb{L}; i = (x, 1)\}$$

$$(2.1)$$

For each lattice point *i* we have an Ising spin $\sigma(i) = \sigma(x, z) = \pm 1$, and the Hamiltonian is formally given by

$$H = -\sum_{\langle ij \rangle \subset \mathbb{L}} K(i,j) \,\sigma(i) \,\sigma(j) - \lambda \sum_{i \in \mathbb{L}} \sigma(i) - h \sum_{i \in \Sigma} \sigma(i)$$
(2.2)

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where $\langle ij \rangle$ denotes a pair of nearest neighbor points. Our choice of the coupling constant is

$$K(i, j) = J > 0, \qquad i \in \Sigma, \quad j \in \Sigma$$

$$K(i, j) = K > 0, \qquad \text{otherwise}$$
(2.3)

We always choose $h \ge 0$, but the bulk field λ is arbitrary.

The model with $\lambda = 0$ and dimension d = 2 was investigated by McCoy and Wu⁽³⁾ when J = K and by Au-Yang⁽⁴⁾ when $J \neq K$. In these works, the surface free energy is computed as a function of the temperature and the field h. The surface free energy F^p is defined with *periodic boundary con*dition (b.c.). It is an analytic function of h and β (the inverse temperature) when $h \neq 0$. At h = 0, it has a singularity at $\beta_c(2)$, the inverse critical temperature of the two-dimensional model with coupling constant K. Above $\beta_c(2)$ and at h = 0, the symmetry of the model is broken, and

$$\lim_{h \downarrow 0} -\frac{\partial F^{p}}{\partial h} \neq \lim_{h \downarrow 0} -\frac{\partial F^{p}}{\partial h}$$
(2.4)

The critical exponents of the transition at β_c are $\gamma = 0$, $\alpha = 1$, $\beta = 1/2$, $\nu = 1$. These exponents are quite different from the exponents of the twodimensional model.

However, these results do not give the phase diagram at $\lambda = 0$, since they do not describe the wetting transition, which occurs for nonzero h. This transition was rigorously established by Abraham⁽⁵⁾ for d=2 and J = K. In order to explain these results, let us interpret the model as a model of a binary mixture, with phases plus and minus, in the presence of a substrate. The field h and coupling J describe the interaction of the substrate with the binary mixture. Since h is positive, the substrate adsorbs preferentially the plus phase. Let J and K be given, and let $\lambda = 0$. We also suppose that the temperature is low enough so that the two-dimensional Ising model with coupling K is in the coexistence region. Far from the substrate we suppose that the system is in the minus phase. Since h is positive, there is formation of a film of the plus phase near the substrate. Two situations are possible. The thickness of this film is microscopic or macroscopic. In the former case, the plus phase wets partially the substrate, and in the latter case, we have complete wetting. The wetting transition is the transition from partial wetting to complete wetting. This transition can be detected by computing the magnetization profile $\langle \sigma(0,z) \rangle^{-}$ as a function of $z \ge 1$. The index minus indicates that the system is in the minus phase in the bulk. This is the method used by Abraham.⁽⁵⁾ Usually this transition is described in terms of surface tension. Let J, K, and β be fixed.

If $\lambda \neq 0$, the *d*-dimensional Ising model has only one phase and it is expected that the surface free energy is well defined, i.e., is a well-defined function of the parameters of the model. Equivalently, we can say that the surface free energy is independent of the b.c. Thus, we have a function $F(\beta; J, K, h, \lambda)$. However, when $\lambda = 0$ and β is large enough, the bulk system has two different phases, and it is no longer true that the surface free energy is a function of the parameters of the model only. Indeed, if $\lambda \downarrow 0$, we have the plus phase in the bulk, and if $\lambda \uparrow 0$, we have the minus phase in the bulk. In this last case we have seen that there is formation of a film of the plus phase between the minus phase and the substrate. The interface between the minus phase and the film gives a nonzero contribution to the surface free energy. To summarize, the surface free energy depends on the nature of the phase in the bulk, and we must consider

$$F^{+}(\beta; J, K, h, 0) = \lim_{\lambda \downarrow 0} F(\beta; J, K, h, \lambda)$$
(2.5)

respectively,

$$F^{-}(\beta; J, K, h, 0) = \lim_{\lambda \uparrow 0} F(\beta; J, K, h, \lambda)$$
(2.6)

It is also possible to define F^+ , resp. F^- , by taking directly $\lambda = 0$, and by using +b.c., resp. -b.c. This is what we do in Section 3. In the physics literature F^+ is called the surface tension of the plus phase against the substrate and F^- is the surface tension of the minus phase against the substrate. Let $\tau^{\pm}(\beta; K)$ be the surface tension between the plus phase and the minus phase when there is no substrate.

From the above discussion, we must have $F^- > F^+$. Let us suppose that we have complete wetting. In this case

$$F^{-}(\beta; J, K, h, 0) = F^{+}(\beta; J, K, h, 0) + \tau^{\pm}(\beta; K)$$
(2.7)

Indeed, the difference between F^- and F^+ is the free energy due to the interface between the minus phase in the bulk and the adsorbed film. But this film is macroscopic, meaning that this interface is far from the substrate. Consequently, the interface free energy is τ^{\pm} . Relation (2.7) is Antonov's rule. It characterizes the complete wetting regime. For thermodynamic reasons, we must have

$$F^{-}(\beta; J, K, h, 0) \leqslant F^{+}(\beta; J, K, h, 0) + \tau^{\pm}(\beta; K)$$
(2.8)

The partial wetting regime is characterized by $F^- < F^+ + \tau^{\pm}$. We prove in Section 5 that Antonov's rule is equivalent to the existence of a unique

equilibrium state. For $\lambda = 0$ it is possible to show that there is a unique equilibrium state if and only if

$$\langle \sigma(0,1) \rangle^+ = \langle \sigma(0,1) \rangle^- \tag{2.9}$$

Here $\langle (\cdot) \rangle^+$ [resp. $\langle (\cdot) \rangle^-$] are the equilibrium states of the model defined with +b.c. [resp. -b.c.].

Let us come back to the work of McCoy and Wu. We can show that their definition of the surface free energy F^p coincides with F^+ for $h \ge 0$. By symmetry, $F^p = F^-$ for $h \le 0$. In particular,

$$-\frac{\partial F^{p}}{\partial h} = -\frac{\partial F^{+}}{\partial h} = \langle \sigma(0,1) \rangle^{+}(h), \qquad h > 0$$
(2.10)

and

$$-\frac{\partial F^{p}}{\partial h} = -\frac{\partial F^{-}}{\partial h} = \langle \sigma(0,1) \rangle^{-}(h), \qquad h < 0$$
(2.11)

Relation (2.4) can be rewritten as

$$\langle \sigma(0,1) \rangle^{-}(h=0) \neq \langle \sigma(0,1) \rangle^{+}(h=0)$$
(2.12)

In order to discuss the wetting transition we need $\langle \sigma(0, 1) \rangle^{-}(h)$ for h > 0[or $\langle \sigma(0, 1) \rangle^{+}(h)$, h < 0]. It is interesting to notice that McCoy and Wu computed indirectly $\langle \sigma(0, 1) \rangle^{-}(h)$ for h > 0 (although we did not check this explicitly). For h < 0, $\langle \sigma(0, 1) \rangle^{-}(h)$ is an analytic function of h. They found that there is an analytical continuation of this function for h > 0. (In the *d*-dimensional Ising model, such an analytical continuation is impossible.⁽⁶⁾). This analytical continuation is simply the expected value of $\sigma(0, 1)$ in the equilibrium state $\langle (\cdot) \rangle^{-}(h)$ with h > 0. Therefore we have $\langle \sigma(0, 1) \rangle^{-}(h)$, h > 0. We have seen above that the complete wetting regime coincides with the region where we have a unique equilibrium state. Using the analytical continuation of $\langle \sigma(0, 1) \rangle^{-}(h)$, we can determinate the wetting transition [see (2.9)], and it is not difficult to check that we get the same result as in Ref. 5.

Before ending this introduction, we give a precise definition of the equilibrium states $\langle (\cdot) \rangle^+$ and $\langle (\cdot) \rangle^-$. Let

$$A(L, M) = \{(x, z): |x^k| \le L, k = 1, ..., d-1; 1 \le z \le M\}$$
(2.13)

We fix the values of the spins for all $i \in \mathbb{L} \setminus A(L, M)$: $\sigma(i) = 1$. This is by definition the +b.c. [The -b.c. corresponds to $\sigma(i) = -1$ for all $i \in \mathbb{L} \setminus A(L, M)$.] If we restrict the summation in (2.2) over all pairs $\langle ij \rangle$

such that $\{i, j\} \cap A(L, M) \neq \emptyset$, then we get a Hamiltonian $H^+_{L,M}$. The corresponding partition function and finite-volume Gibbs state are denoted by $Z^+(L, M)$ and $\langle (\cdot) \rangle^+_{L,M}$. By taking the limit $L \to \infty$ and $M \to \infty$, we get an equilibrium state for the infinite system in \mathbb{L} ,

$$\langle (\cdot) \rangle^{+} = \lim_{L, M \to \infty} \langle (\cdot) \rangle_{L, M}^{+}$$
(2.14)

In a similar way we define $\langle (\cdot) \rangle^{-}$. The main properties of these states are summarized as follows:

- 1. They are extremal equilibrium states.
- 2. They are Σ -invariant, i.e., invariant under all lattice translations of the type $(x, z) \mapsto (x + a, z), a \in \mathbb{Z}^{d-1}$.
- 3. $\langle (\cdot) \rangle^+$ [resp. $\langle (\cdot) \rangle^-$] are right-continuous [resp. left-continuous] in h and in λ .
- 4. There is a unique equilibrium state in the model if and only if $\langle \sigma(i) \rangle^+ = \langle \sigma(i) \rangle^- \quad \forall i \in \mathbb{L}.$

The above results are valid for $h \in \mathbb{R}$ and $\lambda \in \mathbb{R}$, and are consequences of the FKG inequality. If we consider only $h \ge 0$ and $\lambda \ge 0$, then we can improve property 4:

5. Let $\langle (\cdot) \rangle$ be any equilibrium state. If $\langle \sigma(i) \rangle^+ = \langle \sigma(i) \rangle$ for some $i \in \mathbb{L}$, then $\langle (\cdot) \rangle^+ = \langle (\cdot) \rangle$. In particular, there is a unique equilibrium state if $\langle \sigma(0, 1) \rangle^+ = \langle \sigma(0, 1) \rangle^-$.

Proofs can be found in Ref. 1. Let us finally remark that we use the method of correlation inequalities and our results are not restricted to the dimension d=2.

3. SURFACE FREE ENERGY

We define precisely $F^+(\beta; J, K, h, \lambda)$, the surface free energy with + b.c., and $F^-(\beta; J, K, h, \lambda)$ is defined in a similar way. Then we prove the basic relation (2.8).

Let $Z^+(L, M)$ be the partition function of the model in $\Lambda(L, M)$ with + b.c. We introduce a second copy of this model in the box $\Lambda'(L, M)$ obtained by a reflection at the plane z = 1/2. If

$$\Omega(L, M) = \{i \in \mathbb{Z}^d : |i^k| \leq L, 1 \leq k \leq d-1, -M < i^d \leq M\}$$

then $\Lambda'(L, M) = \Omega(L, M) \setminus \Lambda(L, M)$. Let $Q^+(L, M)$ be the partition function of the Ising model

$$-K\sum_{\langle ij\rangle \subset \mathbb{Z}^d} \sigma(i) \,\sigma(j) - \lambda \sum_{i \in \mathbb{Z}^d} \sigma(i) \tag{3.1}$$

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in the box $\Omega(L, M)$ with +b.c. By definition

$$F^{+} = \lim_{\substack{L \to \infty \\ M \to \infty}} \frac{-1}{2\beta |\Sigma(L)|} \ln \frac{(Z^{+}(L, M))^{2}}{Q^{+}(L, M)}$$
(3.2)

where $|\Sigma(L)|$ is the cardinality of the set $\Sigma \cap \Lambda(L, M) \equiv \Sigma(L)$. In (3.2) we can choose $M = L^{\alpha}$, $\alpha > 0$. Using the FKG inequality, we can show that the limit (3.2) is well-defined for $h \in \mathbb{R}$ and $\lambda \in \mathbb{R}$ and that it is independent of $\alpha > 0$.

Let $\lambda = 0$. By symmetry we have $Q^+(L, M) = Q^-(L, M)$. Therefore, we can express $\tau_s^{\pm} \equiv F^-(\lambda = 0) - F^+(\lambda = 0)$ as the limit

$$\lim_{\substack{L \to \infty \\ M \to \infty}} \frac{-1}{\beta |\Sigma(L)|} \ln \frac{Z^{-}(L, M)}{Z^{+}(L, M)}$$
(3.3)

Let us modify the -b.c. as follows: instead of taking $\sigma(x, z) = -1$ for all $(x, z) \notin \Lambda(L, M)$, we take $\sigma(x, z) = 1$ for all $(x, z) \notin \Lambda(L, M)$ with $0 \le z \le M/2$, and $\sigma(x, z) = -1$ for all $(x, z) \notin \Lambda(L, M)$ with z > M/2. The new partition function is denoted by $Z^{\pm}(L, M)$. It is easy to see that

$$\frac{Z^{\pm}(L,M)}{Z^{+}(L,M)} = \exp O(L^{d-2+\alpha})$$
(3.4)

when $M = L^{\alpha}$. By choosing $0 < \alpha < 1$, we see that the limit of

$$\frac{-1}{\beta |\Sigma(L)|} \ln \frac{Z^{\pm}(L,M)}{Z^{+}(L,M)}$$
(3.5)

is equal to (3.3). The quantity (3.5) is a positive, monotone increasing function of h, for $h \ge 0$ (GKS inequality). We get an upper bound for (3.5) by taking the limit $h \uparrow \infty$,

$$\frac{-1}{\beta |\Sigma(L)|} \ln \frac{Z^{\pm}(L, M-1)}{Z^{+}(L, M-1)}$$
(3.6)

where we recognize the usual definition of the finite-volume surface tension of the Ising model (3.1) with $\lambda = 0$ (see e.g., Ref. 7). By taking the limit $L \rightarrow \infty$, we have proved the basic relation

$$F^- \leqslant F^+ + \tau^{\pm} \tag{3.7}$$

provided that we may take $M = L^{\alpha}$, $0 < \alpha < 1$, in the definition of the surface tension. This is an important, but technical point, which is proved in

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Refs. 1 and 2. It is not difficult, using correlation inequalities, to establish the following properties for $\tau_s^{\pm}(\beta; J, K, h)$:

- 1. It is a monotone increasing function of J, K, and h, and $\tau_s^{\pm}(h=0) = 0$. It is a concave function of h, $h \ge 0$.
- 2. $\tau_s^{\pm}(\beta) = \tau^{\pm}(\beta)$ if $J \ge K$ and $h \ge K$.
- 3. $\lim_{h \uparrow \infty} \tau_s^{\pm}(\beta; J, K, h) = \tau^{\pm}(\beta; K).$

Proofs are given in Ref. 2. Using these results, we define

$$h_{w}(\beta; J, K) = \inf\{h: F^{-}(\beta; J, K, h, 0) - F^{+}(\beta; J, K, h, 0) = \tau^{\pm}(\beta; K)\} \quad (3.8)$$

Partial wetting corresponds to $h < h_w$, and complete wetting corresponds to $h > h_w$. From the above results, we see that there is a wetting transition at h_w , $0 < h_w \le K$, when $J \ge K$. We prove in Section 5 the lower bound, which is valid for all J and K,

$$h_w(\beta; J, K) \ge \frac{1}{2}\tau^{\pm}(\beta; K) \tag{3.9}$$

4. PHASE DIAGRAM AT $h = \lambda = 0$

We set $\beta = 1$, $h = \lambda = 0$, and we consider the phase diagram in the (J, K) plane for dimensions $d \ge 3$. The results are summarized in Fig. 1,



Fig. 1

which we have divided into three regions, R_1 , R_2 , and R_3 . The high-temperature region is R_1 . It is defined by

$$\left\{ (J, K): \chi_{\Sigma} \equiv \sum_{x \in \mathbb{Z}^{d-1}} \left\langle \sigma(0, 1) \, \sigma(x, 1) \right\rangle^+ < \infty \right\}$$
(4.1)

Inside region R_1 , $\langle \sigma(0, 1) \rangle^+ = 0$, and this implies that there is a unique equilibrium state. We can show that the parallel correlation length ξ_{Σ} is finite, where ξ_{Σ} is by definition

$$\xi_{\Sigma}^{-1} = \lim_{L \to \infty} -\frac{1}{L} \ln \langle \sigma(0, 1) \sigma(x_L, 1) \rangle^+$$
(4.2)

with $x_L = (L, 0, ..., 0)$. Moreover, the boundary of the high-temperature region is critical, since $\xi_{\Sigma}^{-1}(J, K)$ is a continuous function of J and K. Inside R_1 , the transverse correlation length ξ_{\perp} is finite,

$$\xi_{\perp}^{-1} = \lim_{z \to \infty} -\frac{1}{z} \ln \langle \sigma(0, 1); \sigma(0, z) \rangle^{+}$$
(4.3)

In the regions R_2 and R_3 the symmetry of the model is broken, $\langle \sigma(0,1) \rangle^+ > 0$. These regions are separated by a critical line $K = K_c(d)$. We can show, for $\lambda = 0$ and $K \leq K_c(d)$, that

$$\xi_{\perp}(J, K, h, 0) = \xi_{\rm Is}(K) \tag{4.4}$$

where ξ_{Is} is the correlation length of the *d*-dimensional Ising model. In particular, the critical exponent v_{\perp} is equal to the exponent v of the Ising model. In region R_2 the bulk is still disordered. From these results we could conclude that there is no intermediate phase between regions R_1 and R_2 . Although this is most likely the case, we have not be able to prove it. In the intermediate phase $\langle \sigma(0, 1) \rangle^+$ would be zero and χ_{Σ} would diverge.

5. THE WETTING TRANSITION

In this section $\lambda = 0$ and h > 0. The case h < 0 is obtained by symmetry. In Section 3 we established the existence of a wetting transition at h_w on the basis of the thermodynamics. We now wish to explain the connection with equilibrium states. This connection is made through the formula

$$\tau_s^{\pm}(h) = \int_0^h dh' \left[\langle \sigma(0, 1) \rangle^+(h') - \langle \sigma(0, 1) \rangle^-(h') \right]$$
(5.1)

which follows from property 1 of Section 3. The integrand in (5.1) is a nonnegative, monotone decreasing function of h'. From (5.1) we get immediately the lower bound (3.9): at $h = h_w$, $\tau_s^{\pm}(h_w) = \tau^{\pm}$, and the integrand in (5.1) is bounded by 2. If $h > h_w$, $\tau_s^{\pm}(h) = \tau^{\pm}$. Therefore the integrand in (5.1) must be zero for all $h' > h_w$. This implies the unicity of the equilibrium state for those values of h. If $h < h_w$, we have, by definition of h_w , $\tau_s^{\pm}(h) < \tau^{\pm}$. Since we know that $\lim_{h\uparrow\infty} \tau_s^{\pm}(h) = \tau^{\pm}$, we must have $\langle \sigma(0, 1) \rangle^+(h) \neq \langle \sigma(0, 1) \rangle^-(h)$. These results show that $h_w(\beta; J, K)$ can also be defined by

$$h_{w}(\beta; J, K) = \inf\{h: \langle \sigma(0, 1) \rangle^{+}(\beta; h) = \langle \sigma(0, 1) \rangle^{-}(\beta; h)\}$$
(5.2)

Thus, complete wetting corresponds to unicity of the equilibrium state. This is a precise formulation of the fact that the thickness of the adsorbed phase is macroscopic in the complete wetting regime. At $h = h_w$, one may find a unique state or several states. The phase diagram in the (h, T) plane for a model with $J/K \ge 1$ and $d \ge 3$ is shown in Fig. 2. The temperature T_s is the temperature of the surface phase transition. The line $T = T_c(d)$ is a critical line, in the sense that ξ_{\perp} diverges when $T \downarrow T_c(d)$ [see (4.4)]. However, if $T = T_c(d)$ and $h \ne 0$, the surface free energy is analytic in h and

$$\chi_{\Sigma} = -\frac{\partial^2}{\partial h^2} F(h)$$

is finite.



Fig. 2

Using the equivalence between the definitions of h_w , (3.8) and (5.2), it is possible to prove the existence of several equilibrium states in some situations. For example, we can show that there is a unique equilibrium state for any finite temperature and any dimension d when J = K = h. However, if $d \ge 2$, K = h, but J < K, then there is a finite function $\beta^*(J; d)$ such that for $\beta > \beta^*(J; d)$, $\tau_s^{\pm}(\beta; J, K, h) < \tau^{\pm}(\beta; K)$. This implies that $h_w(\beta; J, K) > K$, and also the existence of several equilibrium states when $\beta > \beta^*(J; d)$.

6. A LAYERING TRANSITION

We now consider $h \neq 0$ and $\lambda \neq 0$. We suppose that $F^+ = F^-$ for $\lambda \neq 0$. From this assumption, it follows that there is a unique equilibrium state for h > 0 and $\lambda > 0$. The case h > 0 and $\lambda < 0$ is more interesting. Let $d \ge 3$ and K < 2J be given. If β is fixed and large enough, and if $\lambda < 0$, then we can find a function of λ , $h_{p.w.}(\lambda)$, with the following properties: $0 < h_{p.w.}(\lambda) \le K - \lambda$; there exists a positive constant $C(\beta)$, independent of λ , such that

$$\langle \sigma(0,1) \rangle^{-}(h,\lambda) \leq -C(\beta), \qquad 0 \leq h \leq h_{\text{p.w.}}(\lambda) \langle \sigma(0,1) \rangle^{-}(h,\lambda) \geq C(\beta), \qquad h \geq h_{\text{p.w}}(\lambda)$$

$$(6.1)$$

The function $h_{p.w.}(\lambda)$ is decreasing in λ , and $\lim_{h \uparrow 0} h_{p.w.}(\lambda) = h^*$ with $0 < h^* \le K$. Since $\langle (\cdot) \rangle^-$ is left-continuous in λ , relations (6.1) still hold for $\lambda = 0$ and $h_{p.w.}(0) = h^*$. The transition at $h_{p.w.}(\lambda)$ is a first-order layering transition. It is an open question to know whether h^* coincides with h_w or not. We only know that, for J < K and β large enough, we have cases with $h^* \le K < h_w(J, K)$ (see Section 5). Figure 3 shows this layering transition line.



It is interesting to notice that the line $h_{p.w.}(\lambda)$ is asymptotically given by $h = K - \lambda$ when $\beta \uparrow \infty$. The line $h = K - \lambda$, with $h \ge 0$ and $\lambda \le 0$, separates two kinds of ground states. Below the line the ground state is unique for $\lambda < 0$ and $\sigma(i) \equiv -1$. Above the line, the ground state is also unique for $\lambda < 0$, but now $\sigma(x, 1) = 1$ and $\sigma(x, z) = -1$ for $z \ge 2$. On the line itself there is coexistence of the two kinds of ground states. In the mean-field treatment of the model on a lattice one can show the existence of several layering transitions (see, e.g., the review in Ref. 8). Y. Sinai and S. Shlosman have informed us that A. G. Basuev claims to have recently proved the existence of several first-order transitions for the Ising model with h = J = K when λ , negative, tends to zero at fixed low temperature. The transition line defined above would correspond to the first transition found by Basuev when λ tends to zero.

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