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Absence of First-Order Phase Transitions for Antiferromagnetic Systems

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We consider a spin system with nearest-neighbor antiferromagnetic pair interactions in a two-dimensional lattice. We prove that the free energy of this system is differentiable with respect to the uniform external field h, for all temperatures and all h. This implies the absence of a first-order phase transition in this system.

KEY WORDS: Phase transition; antiferromagnet; Gibbs state; free energy; pressure; Ising model.

1. INTRODUCTION

We consider an antiferromagnetic system on a two-dimensional lattice Z^2 whose Hamiltonian is given by

$$\tilde{H}(\sigma) = \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_{i \in Z^2} \sigma_i$$

Here $\sigma_i = 1$ or -1 for all $i \in Z^2$ and $\langle i, j \rangle$ indicates that the sum is over nearest-neighbor pairs of lattice sites i and j.

Let μ^+ and μ^- represent the (extremal) Gibbs states corresponding to the two possible "chessboard" boundary configurations of 1's and -1's. Dobrushin[4] showed that if $|h| < 4$, $\mu^+ \neq \mu^-$ at sufficiently low temperatures. He also proved that if $|h| > 4$, there exists only one Gibbs state for all temperatures. Thus, the antiferromagnet experiences a phase transition in the sense that the number of Gibbs states is discontinuous in the phase plane.

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It has been conjectured that this system experiences a second-order phase transition (see, for example, refs. 5 and 8) and that the free energy P is therefore a differentiable function of h for all values of h and all temperatures.

In this paper, we prove the following:

Theorem 1.1. Let P be the free energy of the spin system with Hamiltonian $\tilde{H}$. Then dP/dh exists everywhere.

The absence of a first-order phase transition for the two-dimensional antiferromagnet may be contrasted with related models. It is well known that the Ising ferromagnet and the antiferromagnet with external uniform magnetic field h replaced by the (unphysical) staggered field experience first-order phase transitions. Unlike the ferromagnetic case, the antierromagnet has coexisting Gibbs states while the free energy is continuously differentiable.

The proof of Theorem 1.1 may be summarized as follows. A standard argument (given in Section 6 for the convenience of the reader) shows that the free energy is differentiable at h if and only if $M=\mu[\sigma_{(0,0)}+\sigma_{(1,0)}+\sigma_{(0,1)}+\sigma_{(1,1)}]$ is the same for any Gibbs state μ, invariant under reflections and two-step translations about coordinate axes. Let G_0 be the set of such invariant Gibbs states. The problem then reduces to proving that M is the same for all $\mu \in G_0$, for fixed temperature and external field. Since μ^+ and μ^- give the same value for M, P will be differentiable provided μ^+ and μ^- are the only extreme points in G_0. This follows if the probability of coexistence of two infinite chessboard clusters of opposite type is zero for any Gibbs state in G_0. By conditioning an arbitrary Gibbs state in G_0 on an appropriate invariant set D of configurations, we prove the impossibility of this coexistence in Section 5. Preliminary technical results are given in Section 3 and 4, while definitions and some basic properties of Gibbs states are given in Section 2.

For the two-dimensional ferromagnetic case, Aizenman[1] showed that the set of all Gibbs states has at most two extremal Gibbs states. Our situation here is different from that in refs. 1 and 9 for the lack of sign symmetries due to the presence of h. The problem of determining the structure of the set of all Gibbs states for the antiferromagnetic system remains open.

2. NOTATIONS, DEFINITIONS, AND BASIC PROPERTIES

Let Ω be the set of all configurations $\sigma=(\sigma_i,\ i\in Z^2)$, with $\sigma_i=1$ or -1. For any finite subset Λ of Z^2 and $\bar{\sigma}$, the finite-volume Gibbs state in

Λ with boundary condition $\bar{\sigma}$, corresponding to the Hamiltonian $\tilde{H}$, is the probability measure defined by

$$\tilde{\mu}_{\Lambda}^{\bar{\sigma}}(\sigma) = (1/\tilde{Z}_{\Lambda}^{\bar{\sigma}}) \exp\left(-\beta \sum_{\langle i,j\rangle \in \Lambda} \sigma_i \sigma_j + h\beta \sum_{i \in \Lambda} \sigma_i\right)$$

for $\sigma \in \Omega_{\Lambda}$. Here $\Omega_{\Lambda} = \{-1, 1\}^{\Lambda}$, $\langle i, j\rangle \in \Lambda$ means at least i or j must be in Λ, $|i-j| = 1$, and $\sigma_i = \bar{\sigma}_i$ if i is not in Λ. The positive number β is the inverse of the temperature, and $\tilde{Z}_{\Lambda}^{\bar{\sigma}}$ is the normalization constant.

It is well known that

$$P = -\lim \frac{\ln \tilde{Z}_{\Lambda}^{\bar{\sigma}}}{|\Lambda|} \qquad \text{as} \quad \Lambda \uparrow Z^2$$

where the limit is independent of $\bar{\sigma}$. P is called the free energy of the system.

It is convenient to consider the transformation $s_i = (-1)^{|i|}\sigma_i$, where $|i| = i_1 + i_2$ for $i = (i_1, i_2)$. Under this transformation, $\tilde{\mu}_{\Lambda}^{\bar{\sigma}}(\sigma)$ is equal to

$$\mu_{\Lambda}^{\bar{s}}(s) = (1/Z_{\Lambda}^{\bar{s}}) \exp\left[\beta \sum_{\langle i,j\rangle \in \Lambda} s_i s_j + h\beta \sum_{i \in \Lambda} (-1)^{|i|} s_i\right]$$

The free energy becomes

$$P = -\lim \frac{\ln Z_{\Lambda}^{\bar{s}}}{|\Lambda|} \qquad \text{as} \quad \Lambda \uparrow Z^2 \tag{2.1}$$

for all $\bar{s}$.

The set Ω is compact in the product topology of discrete topologies at each lattice site. For any continuous function f defined on Ω, let

$$\mu_{\Lambda}^{\bar{s}}(f) = \sum_{s \in \Omega_{\Lambda}} \mu_{\Lambda}^{\bar{s}}(s)\, f(s \wedge \bar{s})$$

where $(s \wedge \bar{s})_i = s_i$ for $i \in \Omega$ and equals $\bar{s}_i$ for $i \in \Omega^c$. Then $\mu_{\Lambda}^{\bar{s}}$ defines a measure on the Borel sets of Ω.

Let $\mathscr{B}_{\Lambda}$ be the σ-algebra generated by $\{s_i,\ i \in \Lambda\}$. A probability measure μ on the Borel sets of Ω is called a Gibbs state if

$$\mu(f \mid \mathscr{B}_{\Lambda})(\bar{s}) = \mu_{\Lambda}^{\bar{s}}(f), \qquad \mu\text{-a.s. } \bar{s} \tag{2.2}$$

for any bounded measurable function f on Ω.

For $s, s' \in \Omega$, we say that $s \leqslant s'$ if $s_i \leqslant s'_i$ for all $i \in Z^2$. A function f on Ω is said to be increasing if $f(s) \leqslant f(s')$ whenever $s \leqslant s'$. Let μ, ν be measures on the Borel sets of Ω. We say that $\mu \leqslant \nu$ if $\mu(f) \leqslant \nu(f)$, for all increasing functions f.

It is well known (see, e.g., ref. 7) that the following FKG inequalities hold. Let ν be a Gibbs state or finite-volume Gibbs state, f, g increasing functions on Ω. Then

$$\nu(fg) \geqslant \nu(f)\,\nu(g) \tag{2.3}$$

$$\mu_\Lambda^s \leqslant \mu_\Lambda^{s'} \qquad \text{for} \quad s \leqslant s' \tag{2.4}$$

Denote by μ_Λ^+ and μ_Λ^- the finite-volume Gibbs state in Λ with boundary conditions $s_i = 1$ and $s_i = -1$, respectively. It follows from the FKG inequalities that μ_Λ^+ decreases to a Gibbs state μ^+, and μ_Λ^- increases to a Gibbs states μ^-, as Λ increases to Z^2. Now we make a list of basic properties about Gibbs states (see, e.g., ref. 7 for the proofs).

(a) The set of all Gibbs states G is a compact convex set. μ^+, μ^- are extremal points of G.

(b) Any Gibbs state is Markovian.

(c) μ^+, μ^- are two-step translational invariant, reflectional invariant about each axis and rotational invariant by right angles.

(d) Let $\mathscr{B}_\infty = \bigcap_\Lambda \mathscr{B}_{\Lambda^c}$, where Λ runs over all finite subset of Z^2. Then $\mu(\cdot \mid B_\infty) \in G$, for all $\mu \in G$ and $B_\infty \in \mathscr{B}_\infty$ for which $\nu(B_\infty) \neq 0$.

(e) Let $\text{ext}(G)$ be the set of extremal points of G. If $\mu \in \text{ext}(G)$, then $\mu(B_\infty) = 0$ or 1 for all $B_\infty \in \mathscr{B}_\infty$.

(f) Let $\Lambda \in Z^2$ be a finite set. If $A \in \mathscr{B}_\Lambda$ and $A \neq \varnothing$, then $\mu(A) > 0$ for all $\mu \in G$.

(g) If $\mu \in \text{ext}(G)$, then $\mu(A) = 0$ or 1 for any event A which is invariant under any nontrivial subgroup of the translation group.

(h) Let θ be a one-step translation along either the 1-axis or 2-axis. Let $I\colon \Omega \to \Omega$ be the transformation $I(s) = -s$. Then $\theta\mu^+ = I\mu^-$.

(i) There exists only one Gibbs state if and only if $\mu^+(s_{(00)}) = \mu^-(s_{(00)})$ or equivalently $\mu^+(s_{(00)} + s_{(10)}) = 0$.

3. ERGODIC DECOMPOSITIONS

Let T_i be the two-step translation along the i axis. Let R_i be the reflection about the i axis. For $i = 1, 2$, we denote by H_i the group generated by T_i, R_1, R_2. The group generated by T_1, T_2, R_1, and R_2 is denoted by H_0. Let $\mathscr{H}_i$ be the set of H_i-invariant events and G_i the set of H_i-invariant Gibbs states. Let μ be a probability measure on Ω, and A an event. For the rest of this paper, we write μ^S and A^S for the transformations of μ and A, respectively, by a transformation S on Z^2.

Lemma 3.1. For $i=1, 2$, if $\nu \in \text{ext}(G_i)$, then there exists $\mu \in G$ such that μ is T_i-ergodic and

$$\nu = \tfrac{1}{4}\{\mu + \mu^{R_1} + \mu^{R_2} + \mu^{R_1 R_2}\} \tag{3.1}$$

Proof. Let J_i be the set of T_i-invariant Gibbs states. By the Choquet–Meyer theorem,[3] there exists a probability measure γ on $\text{ext}(J_i)$ such that

$$\nu = \int_{\text{ext}(J_i)} \omega \, d\gamma(\omega)$$

Since ν is H_i-invariant, it follows that

$$\nu = \tfrac{1}{4} \int_{\text{ext}(J_i)} [\omega + \omega^{R_1} + \omega^{R_2} + \omega^{R_1 R_2}] \, d\gamma(\omega)$$

Note that the integrand is G_i-valued. Since $\nu \in \text{ext}(G_i)$, the integrand must be a constant for γ-a.e. ω. This constant is equal to the right side of (3.1) for some $\mu \in \text{ext}(J_i)$. This proves the lemma since any element of $\text{ext}(J_i)$ is T_i-ergodic.

Let $i_k \in Z^2$, $k=1, 2,...$. We call $(i_1,..., i_n)$ a chain if i_k and i_{k+1} are nearest neighbor for all k. Let $i, j \in Z^2$, $W \subset Z^2$. We say that i and j are connected in W if there exists a chain $i_1,..., i_n$ in W such that $i_1 = i$ and $i_n = j$. We say that W is connected if any two elements of W are connected in W. A chain is called a circuit if all the points are different except that two endpoints are equal.

Given a configuration s and a subset W of Z^2, a connected component of $\{i \in W;\, s_i = 1\}$ is called a $(+)$-cluster in W and a connected component of $\{i \in W;\, s_i = -1\}$ is called a $(-)$-cluster in W. A chain in $\{i;\, s_i = 1\}$ is called a $(+)$-chain of s. Similar definitions apply to $(+)$-circuit, $(-)$-chain, etc. Let $z \in Z^2$, $V, W \subset Z^2$. We denote by $[z, V; W]$ the event that z is connected to some element of V by a $(+)$-chain in W. We also denote by $[z, \infty; W]$ the event that z is contained in an infinite $(+)$-cluster in W.

It follows essentially from the proof of the corollary after the "Multiple Ergodic Lemma" in ref. 6 that the following lemma holds.

Lemma 3.2. Let W be a subset of Z^2 and U, V finite subsets of Z^2. If the FKG inequalities hold for μ and μ is T_i-ergodic, then there exists a sequence of natural numbers N such that

$$\mu[z, \infty; W \backslash (T_i^{-N} U \cup T_i^N V)] \geqslant \mu[z, \infty; W]/2 \tag{3.2}$$

Lemma 3.3. Let W be a subset of Z^2 and U, V finite subsets of Z^2. If $\nu \in \text{ext}(G_i)$, then there exists a sequence of natural numbers N such that

$$\nu(A \cup A^{R_1} \cup A^{R_2} \cup A^{R_1 R_2}) \geqslant \nu(B \cap B^{R_1} \cap B^{R_2} \cap B^{R_1 R_2})/2$$

where $A = [z, \infty; W \backslash (T_i^{-N} U \cup T_i^N V)]$ and $B = [z, \infty; W]$.

Proof of Lemma 3,3, Let $\mu \in G$ such that μ is T_i-ergodic. Then by Lemma 3.2, there exists N such that

$$\mu(A \cup A^{R_1} \cup A^{R_2} \cup A^{R_1 R_2}) \geqslant \mu(A) \geqslant \mu(B)/2 \geqslant \mu(B \cap B^{R_1} \cap B^{R_2} \cap B^{R_1 R_2})/2 \qquad (3.3)$$

Now Lemma 3.3 follows from (3.3), Lemma 3.1, and the reflectional invariance of events on the left and right sides of (3.3) about each axis.

Let A, B be defined as in Lemma 3.3.

Corollary 3.4. Let $\nu \in \text{ext}(G_i)$. If A, B are R_1, R_2-invariant for all N, then there exists a sequence of natural numbers N such that

$$\nu(A) \geqslant \nu(B)/2 \qquad (3.4)$$

Proof. This is a direct consequence of Lemma 3.3.

Corollary 3.5. Let $\nu \in \text{ext}(G_i)$. Then there exists a sequence of natural numbers N such that

$$\nu(A) \geqslant [\nu(B)]^4/8 \qquad (3.5)$$

Proof. By Lemma 3.3 and the FKG inequalities, there exists a sequence N such that

$$\nu(A \cup A^{R_1} \cup A^{R_2} \cup A^{R_1 R_2}) \geqslant \nu(B)\, \nu(B^{R_1})\, \nu(B^{R_2})\, \nu(B^{R_1 R_2})/2$$

Now the corollary follows from the R_1, R_2-invariance of ν.

4. PERCOLATION IN STRIPS

Let $Q_N = \{(i_1, i_2);\ |i_2| \leqslant N\}$ and $K_N = \{(i_1, i_2);\ |i_1| \leqslant N\}$.

Lemma 4.1. Let $\mu \in G_0$. Then

$$\mu[z, \infty; Q_N] = 0 \quad \text{for all} \quad z \in Q_N \quad \text{for all } N \qquad (4.1)$$

$$\mu[z, \infty; K_N] = 0 \quad \text{for all} \quad z \in K_N \quad \text{for all } N \qquad (4.2)$$

Proof. $\mu \in G_0$ implies $\mu \in G_1$. By the Choquet–Meyer theorem,[3] there exists a probability measure α on $\text{ext}(G_1)$ such that

$$\mu = \int_{\text{ext}(G_1)} \nu \, d\alpha(\nu) \tag{4.3}$$

By the H_1-ergodicity of $\nu \in \text{ext}(G_1)$ and property (f) of Section 2, $\nu[z, \infty; Q_N] = 0$ for all $z \in Q_N$, for all N.

By (4.3), $\mu[z, \infty; Q_N] = 0$ for all $z \in Q_N$, for all N. The proof for the other direction is similar.

5. STRUCTURE OF G_0

Theorem 5.1. Let $\mu \in G_0$. Then

$$\mu = \lambda\mu^+ + (1-\lambda)\mu^-, \qquad 0 \leqslant \lambda \leqslant 1$$

To prove Theorem 5.1, we use the following lemmas, which are obtained essentially by following the proof of the theorem in ref. 6. Let $H^+ = \{i;\ i_2 \geqslant 0\}$ and $H^- = \{i;\ i_2 \leqslant 0\}$. Let $B = \{i = (i_1, i_2);\ |i_1| \leqslant n, |i_2| \leqslant n\}$, and let $\mathbf{B}$ be the event that the box B is surrounded by the $(+)$-circuit. From the "first part of the proof" in ref. 6, we have the following result.

Lemma 5.2. Suppose the FKG inequalities hold for μ, μ is H_2-invariant, and μ satisfies (4.1) and (3.5) with $i = 2$. If $\mu[0, \infty; H^+] = p > 0$, then $\mu(\mathbf{B}) \geqslant p^{16}/2^{18}$ for all B.

Let F_{j^-} be the event that $(0, j) \in Z^2$ is contained in an infinite $(+)$-cluster in $\{i_2 \leqslant j\}$. The event F_{j^+} is defined similarly with $i_2 \leqslant j$ replaced by $i_2 \geqslant j$. From the "second part of the proof" in ref. 6, we have the following result.

Lemma 5.3. Suppose the FKG inequalities hold for μ, μ is H_1-invariant, and μ satisfies (3.5) with $i = 1$. If $\mu[0, \infty; Z^2] = p > 0$, $\mu(F_{j^+}) = \mu(F_{j^-}) = 0$ for all j, then $\mu(\mathbf{B}) \geqslant p^{16}/2^{42}$ for any box B.

Remark. The conclusion of Lemmas 5.2 and 5.3 needed for our purpose is that $\mu(\mathbf{B})$ is uniformly bounded below by a positive number. Under the assumptions of Lemma 5.2, this can be proved rather easily using the results of Burton and Keane[2] as well as the methods of ref. 6.

Proof of Theorem 5.1. Let $\mu \in G_0$. Let

$$D = \bigcup_{j \text{ even}} \{C^+_{\geqslant j} \cup C^+_{\leqslant j}\}$$

where $C^+_{\geqslant j}$ is the event that there exists an infinite $(+)$-cluster in $\{i_2 \geqslant j\}$ and $C^+_{\leqslant j}$ is the event that there exists an infinite $(+)$-cluster in $\{i_2 \leqslant j\}$.

Case 1. Suppose $\mu(D) = 1$. Since $\mu \in G_2$, we have

$$\mu = \int_{\text{ext}(G_2)} v \, d\beta(v) \tag{5.1}$$

for some probability measure β on $\text{ext}(G_2)$.

By (4.1), for each z and N, $v[z, \infty; Q_N] = 0$ for β-a.s. v. This implies, for β-a.e. v, $v[z, \infty; Q_N] = 0$ for all $z \in Q_N$ for all N.

Therefore for β-a.e. v, v satisfies (4.1). By Corollary 3.5 (applied to G_2), v satisfies (3.5) with $i = 2$ for all $v \in \text{ext}(G_2)$.

By assumption $\mu(D) = 1$, we get $v(D) = 1$ for β-a.e. v. By the FKG inequalities and T_2-invariance of v, for β-a.e. v, $v[0, \infty; H^+] > 0$. By Lemma 5.2, there exists $\delta > 0$ such that $v(\mathbf{B}) \geqslant \delta$ for all B. This implies $v(\bigcap_B \mathbf{B}) \geqslant \delta$. Since $v \in \text{ext}(G_2)$ and $\bigcap_B \mathbf{B}$ is G_2-invariant, we get $v(\bigcap_B \mathbf{B}) = 1$. This implies $v(C^+ \cap C^-) = 0$ for β-a.e. v, where C^+ is the event that there exists an infinite $(+)$-cluster in Z^2 and C^- is the event that there exists an infinite $(-)$-cluster in Z^2. By (5.1), $\mu(C^+ \cap C^-) = 0$.

Case 2. Assume $\mu(D) = 0$. To prove $\mu(C^+ \cap C^-) = 0$, it is sufficient to consider the case $\mu(C^+) > 0$. By considering the conditioning on C^+, we may assume $\mu(C^+) = 1$. By the Choquet–Meyer theorem, there exists a probability measure α on $\text{ext}(G_1)$ such that

$$\mu = \int_{\text{ext}(G_1)} v \, d\alpha(v) \tag{5.2}$$

Then for α-a.e. v, $v(C^+) = 1$ and $v(D) = 0$. By the FKG inequalities and R_1-invariance of v, we have $v[0, \infty; Z^2] > 0$, $v(F_{j+}) = v(F_{j-}) = 0$, for all j, for α-a.e. v. By Corollary 3.5, v satisfies (3.5). By Lemma 5.3, there exists a δ such that $v(\bigcap_B \mathbf{B}) \geqslant \delta$. Since $v \in \text{ext}(G_1)$ and $(\bigcap_B \mathbf{B})$ is G_1-invariant, we have $v(\bigcap_B \mathbf{B}) = 1$, α-a.e. This implies $v(C^+ \cap C^-) = 0$ for α-a.e. v. By (5.2), we have $\mu(C^+ \cap C^-) = 0$.

Case 3. Assume $0 < \mu(D) < 1$. Consider

$$\mu(\cdot) = \mu(\cdot \mid D)\, \mu(D) + \mu(\cdot \mid D^c)\, \mu(D^c)$$

Note that D is H_0-invariant. Therefore both conditional probability measures are in G_0. They satisfy the assumptions in case 1 or case 2 and therefore $\mu(C^+ \cap C^-) = 0$.

The conclusions in cases 1–3 imply that

$$\mu(\cdot) = \mu(\cdot \mid (C^+)^c)\, \mu((C^+)^c) + \mu(\cdot \mid C^+ \cap (C^-)^c)\, \mu(C^+ \cap (C^-)^c)$$

By essentially the same proof as that of Lemma 1 in ref. 9, the first conditional probability measure equals μ^- and the second one equals μ^+. This proves Theorem 5.1.

6. PROOF OF THEOREM 1.1

Let $g = \frac{1}{4}[s_{(0,0)} - s_{(1,0)} - s_{(0,1)} + s_{(1,1)}]$. It follows from a general method using tangent functionals (see, e.g., ref. 6) that dP/dh exists if and only if there exists a constant M such that

$$M = \mu(g)$$

for all $\mu \in G_0$. This fact can be proved easily. We include a proof here for the convenience of the reader.

By Hölder inequalities and (2.1), $-P$ is the limit of convex functions $|\Lambda|^{-1} \ln Z_\Lambda^{\bar{s}}$ in h. Therefore $P'(h)$ exists for almost every h, $-P'$ is increasing in h, and when it exists, it can be evaluated by taking derivative inside the limit sign. Then

$$-P'(h) = \lim \frac{\beta \mu_\Lambda^{\bar{s}}(\sum_{i \in \Lambda} (-1)^{|i|} s_i)}{|\Lambda|} \qquad \text{as} \quad \Lambda \uparrow Z^2 \tag{6.1}$$

if $P'(h)$ exists.

Integrating both sides of (6.1) with respect to $d\mu(\bar{s})$, using (2.2) and the dominated convergence theorem, we get for all $\mu \in G_0$,

$$-P'(h) = \mu(g) \tag{6.2}$$

if $P'(h)$ exists.

Let h_0 be fixed. Choose h_n such that $P'(h_n)$ exists for each n and $h_n \downarrow h_0$. Then (6.2) holds for each n. Let μ_n be the Gibbs state in the right-hand side of (6.2) for each n. By Helley's theorem, there exists a convergent subsequence (μ_{n_l}) of (μ_n). Let μ be the limit of the subsequence. Then $\mu \in G_0$. Therefore we have

$$\lim_{h_n \downarrow h_0} -P'(h_n) = \mu(g) \tag{6.3}$$

for some $\mu \in G_0$. The same argument applies to the left derivative and it shows that the left derivative of P at h_0 is equal to the right-hand side of (6.3) with μ replaced by some Gibbs state $\nu \in G_0$. This proves the claim.

Now by Theorem 5.1, for any $\mu \in G_0$,

$$\mu(g) = \lambda \mu^+(g) + (1 - \lambda)\, \mu^-(g)$$

By property (h) of Section 2, the above is equal to $\mu^+(g)$. End of proof of Theorem 1.1.

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