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Rigorous study of the spin- $\frac{1}{2}$ Ising model in a layered magnetic field at low temperatures

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Abstract. We investigate the low-temperature phase diagram of the three-dimensional Ising model under an external layered magnetic field, *h*. For h = 2 we observe that there exists an infinite number of layered ground states and we prove that, at low temperatures, the external Gibbs state (the 'bilayer' phase) is unique. For h < 2 there exists two ferromagnetic ground states. Moreover, there exists in the plane (T, h) an open line of phase coexistence between the 'bilayer' phase and the '+' and '-' ferromagnetic phases.

1. Introduction

The spin- $\frac{1}{2}$ Ising model under a layered magnetic field has been used to study the observed features of ⁴He crystal shape evolution [3]. The model is described by the usual Ising Hamiltonian combined with a term representing the layered magnetic field. Namely,

$$H = H_0 + H_\mu = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \left[\sum_{i \in \Lambda_1} \sigma_i - \sum_{i \in \Lambda_2} \sigma_i \right]$$
(1.1)

where

$$H_0 = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j - 2 \left[\sum_{i \in \Lambda_1} \sigma_i - \sum_{i \in \Lambda_2} \sigma_i \right] \quad \text{and} \quad H_\mu = -\mu \left[\sum_{i \in \Lambda_1} \sigma_i - \sum_{i \in \Lambda_2} \sigma_i \right]$$

where, $\mu = h - 2$ and the site $i \equiv (x^i, y^i, z^i) \in \mathbb{Z}^3$ and Λ_1 (resp. Λ_2) is defined by the set of sites *i* for which z^i is odd (resp. even) and $\sigma_i = \pm 1$ are the Ising spins. The first sum in (1.1) is over all nearest neighbours and the two last sums are over sites of the two different sublattices with opposite magnetic fields. We observe that the model under study is similar to the anisotropic nearest neighbour Ising (ANNI) model already studied, in the case of ferromagnetic interactions by Fisher [1], and Griffiths and Weng [2]. Indeed the ANNI model with competing interactions can be obtained from the formula (1.1) by using the transformation:

$$\{\sigma_i\}_{i\in\Lambda_2}$$
 to $\{-S_i\}_{i\in\Lambda_2}$ and $\{\sigma_i\}_{i\in\Lambda_1}$ to $\{S_i\}_{i\in\Lambda_1}$.

Namely,

$$H = -\sum_{\langle i,j\rangle \in \Lambda_1 \text{ or } \Lambda_2} S_i S_j + \sum_{\langle i,j\rangle/i \in \Lambda_1 \text{ and } j \in \Lambda_2} S_i S_j - h \sum_{i \in \Lambda} S_i.$$

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We recall that the two-dimensional spin- $\frac{1}{2}$ Ising model in a layered magnetic field was studied in [4], by using the finite size scaling analysis, where the phase diagram contains the two coexistence ferromagnetic phases ('+' and '-') and the bilayer phase (which corresponds to the spin in successive layers being alternatively '+' and '-', i.e. $+ - + - + - + - \cdots$). On this phase diagram a *second*-order phase transition line between the ferromagnetic phases and the bilayer phase was shown.

Our purpose in this paper is to study the three-dimensional case by the low-temperature rigourous methods and to prove that the model exhibits a low-temperature *first*-order phase transition line between the ferromagnetic ('+' and '-') phases and the 'bilayer' phase.

We first notice that the Hamiltonian H_0 has an infinite number of ground states. For example, if we take the (+)-ground state (corresponding to site $\sigma_i = +1$, $\forall i \in \Lambda_1 \cup \Lambda_2$) and flipping all the spins in an arbitrary number of planes of type Λ_2 we get another ground state (cf figures 1(*a*) and (*b*)). The number of degeneracy is $[2.2^{(L/2)} - 1]$ where *L* is the size of the lattice. The reason is that, if all the spins of a plane of kind Λ_1 are up (resp. if those of kind Λ_2 are down) the spin of the two planes setting strictly over and under and which are of kind Λ_1 (resp. which are kind Λ_2) are arbitrary. The term '-1' appeared in the number of degeneracy because of the bilayer structure. Therefore the question is: How many phases does the model, with the Hamiltonian H_0 , have at non-zero temperatures? A partial answer will be given by considering the single-site excitations which are obtained



Figure 1. A type of ground state of the model for h = 2: taking a (+)-ground state (resp. (-)-ground state) and changing any plan of (+)-spins of kind Λ_2 (resp. any plan of (-)-spins of kind Λ_1) do not cost any energy. The 'bilayer' ground state is illustrated in (*b*).

		Type of a single-site excitation	Energy of the excitation
Type 1	z-axis ↑	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	<i>e</i> ¹ = 16
Type 2	z-axis ↑	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$e_2 = 8$
Type 3	z-axis ↑	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$e_3 = 8$
Type 4	z-axis ↑	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$e_4 = 8$

Table 1. Single-site excitations.

by flipping a spin + (resp. -) in the Λ_2 -plane (resp. Λ_1 -plane) (see table 1 where all the possible single-site excitations of the ground states are pictured). Hence for T > 0the degeneracy is lifted because different arrangements of the layer magnetizations have different entropies. Moreover, the bilayer ground state is the unique ground state which has a largest number of lowest-energy excitations and then more entropies. Therefore, it will be expected that it is the unique dominant ground state (here the domination means that there is a finite family of ground states having a greater number of lowest-energy excitations, and then the minimal free energy, than all the other ground states). In the case under our investigation, the domination means the existence of a unique pure phase 'bilayer phase' at low temperatures. We notice that whenever one gets a good control of the contribution of all the lowest-energy excitations (elementary excitations) then the contribution of all the higherorder excitations would not qualitatively change the picture. Clearly, in dimension two, if we consider the (+)-ground state and flip a segment with an arbitrary length of up spins on Λ_2 ; one observes that we only have an energy equal to that corresponding to a single-site excitation. Then it is obvious that a control of the lowest-energy excitations is lacking and the model is said to be irregular (the regularity means that the energy of an excitation increases with the size of its support [5]). It follows that in the two-dimensional case the nature of the phase transition between the ferromagnetic phases and the bilayer phase is still an open problem.

For the three-dimensional case one can easily see that the model is regular but the energy cost may be only proportional to the perimeter of the surface delimiting the domains containing two different coexisting ground states. Then the Peierls condition [5], which is verified for a large class of models with a *finite* number of ground states, is lacking for our Hamiltonian H_0 .

To resolve the problem we use the earlier extension of the Pirogov–Sinai (PS) theory of first-order phase transitions [6] to certain models with an infinite number of ground states. This extension was performed by Bricmont and Slawny (BS) [7] under two assumptions satisfied by our Hamiltonian H_0 . Namely,

• the ground states have layered structures, then the so-called condition *L* in [7] (or the layered condition which means that the ground states of the model is not relatively too large) is satisfied;

• a configuration which is 'excited' in a small region of the lattice surrounded by a region with a configuration having the lowest possible energy can be exchanged ('retouched') in this region in a unique way so that the energy has the lowest possible value everywhere (this is the retouch property in [7], see figure 3 for an example).

2. Ground states of the model

To define more precisely the structure of the ground states of the model we write the Hamiltonian H in terms of a potential, Φ , such that,

$$H = \sum_{c} \Phi_{c}$$
 $H_{0} = \sum_{c} \Phi_{0,c}$ $H_{\mu} = \sum_{c} \Phi_{\mu,c}$ (2.1)

where,

$$\Phi_{0,c} = -\frac{1}{4} \left[\sum_{\langle i,j \rangle \subset c} \sigma_i \sigma_j \right] - \frac{1}{4} \left[\sum_{i \in \Lambda_1 \cap c} \sigma_i - \sum_{i \in \Lambda_2 \cap c} \sigma_i \right] \quad \text{and} \\ \Phi_{\mu,c} = -\frac{\mu}{8} \left[\sum_{i \in \Lambda_1 \cap c} \sigma_i - \sum_{i \in \Lambda_2 \cap c} \sigma_i \right]$$

and *c* is an elementary cube of the lattice Z^3 . We verify that there exists a configuration *Y* such that $\Phi_c(Y) = \phi_c = \min_X(\Phi_c(X))$ for any cube *c*. It is the *m*-potential condition in [5].

The structure of the ground states of the Hamiltonian H_0 is simply given by comparing the energies corresponding to different configurations on a given cube, c. We obtain that the only configurations which give rise to a ground state are those in figure 2. We denote F-ground states (G^F) (corresponding to '+' and '-' ferromagnetic ground states) the configurations in which all the cubes are of kind F. The B-ground state (G^B) (corresponding to the bilayer ground state) is the configuration in which all the cubes are of kind B. Hence, when $\mu < 0$ the model only has the two F-ground states (related by spin-flip symmetry of the Hamiltonian for translation invariant states). For $\mu > 0$ there is only one ground state (bilayer ground state). But for $\mu = 0$ the model exhibits an infinite number of ground states.



Figure 2. The three regular cubes; all other cubes are irregular. (Here the full (resp. empty) circles denote the (+)-spin (resp. the (-)-spin).



Figure 3. (*a*) A type of a removable excitation; the hatched cubes set the support of this elementary excitation. (*b*) A type of non-removable excitation; there is no global ground state equal to (-) and (+) on their repective domains. The dotted cubes set the support of this elementary excitation (resp. to BS theory).

3. The low-temperature phase diagram

To construct the low-temperature phase diagram of the model in the parameter space (T, μ) for μ small enough $(\mu = h - 2)$, one proceeds as follows.

• We consider an excitation of a given ground state, G, and we define the set of its elementary excitations as the family of disjoint-connected components having an energy greater than the energy of G.

• We fix a cut-off energy E and we consider all the excitations whose energy (relative to G) does not exceed E. Since the model is regular, the set of all these excitations (we call the *G*-restricted ensemble) forms a gas of elementary excitations with a finite number of species interacting via a hard-core exclusion potential [5]. Namely, let $\chi_{\Lambda}^{G,E}$ be the *G*-restricted ensemble, then the partition function with a boundary condition *G* is given by:

$$Z_E(\Lambda/G) = \sum_{X \in \chi_\Lambda^G} \exp\bigg(-\beta \sum_{c \cap \Lambda \neq \emptyset} \Phi_c(X)\bigg).$$
(3.1)

To compute the restricted free energy, $f_R^E(G)$, we need the following algebraic formalism.

• We introduce a formal Hamiltonian $H(\vartheta) = \sum_X \vartheta(X)H(X)$. Here ϑ is a multiplicity function defined on the set of all the elementary excitations of G such that $\vartheta(X) = \{0, 1, 2, \ldots\},\$

• To any configuration, $Z \in \chi_{\Lambda}^{G,E}$, we associate the characteristic multiplicity function,

 ϑ_Z , defined on the set of elementary excitations of Z, such that:

$$\vartheta_Z(X) = \begin{cases} 1 & \text{if } X \text{ is a component of } Z \\ 0 & \text{otherwise.} \end{cases}$$

• Finally, on the set of multiplicity functions, we define the weight $\phi_E(\vartheta, G)$

$$\phi_E(\vartheta, G) = \begin{cases} \exp(-\beta H(\vartheta)) & \text{if } \vartheta = \vartheta_Z \text{ for some } Z \in \chi_\Lambda^{G, E} \\ 0 & \text{otherwise.} \end{cases}$$

Then, the partition function of the G-restricted ensemble is given by:

$$Z_E(\Lambda, G) = \exp\left[-\beta \sum_{C \cap \Lambda \neq \emptyset} \Phi_C(G)\right] \sum_{\vartheta/H_0(\vartheta) \leqslant E} \phi_E(\vartheta, G)$$
(3.2)

and the cluster expansion [7] gives

$$\log(Z_E(\Lambda, G)) = -\beta \sum_{C \cap \Lambda \neq \emptyset} \Phi_C(G) + \sum_{\vartheta/H_0(\vartheta) \leqslant E} \phi_E^T(\vartheta, G).$$
(3.3)

We recall that the Ursell functions, $\phi_E^T(\vartheta, G)$, are nonzero (and equal, up to a combinatorial factor, to $e^{-\beta H(\vartheta)}$) only for 'connected' ϑ (i.e. the elementary excitations, for which ϑ is nonzero, are vertices of a connected graph).

We notice that for a translation invariant, G, by vectors of a subgroup $\hat{Z}^3 \subset Z^3$, the convergent cluster expansion (3.3) is given by

$$\log(Z_E(\Lambda/G)) = -|\Lambda| f_R^E(G) + O(|\partial\Lambda|)$$

where $|\partial \Lambda|$ is the number of sites in the boundary $\partial \Lambda$ of Λ , and

$$f_R^E(G) = \beta e_G - |Z^3/\hat{Z}^3|^{-1} \sum_{\vartheta \pmod{\hat{Z}^3}/H_0(\vartheta) \leqslant E} \phi_E^T(\vartheta, G)$$
(3.4)

where

$$e_G = \sum_{c \subset \Lambda} \phi_c(G)$$

and $|Z^3/\hat{Z}^3|$ is the number of classes of the quotient group Z^3/\hat{Z}^3 .

As we discussed in the preceding sections, there exists ground states of H_0 which are non-periodic, then we need a local version of the formulae (3.4) by introducing the notion of the effective *potential* which reaches its minimum value only for the dominant ground states.

More precisely, we let the weight functions $\mathbb{C} \to \chi(c, \mathbb{C})$ and $\vartheta \to \chi(c, \vartheta)$ on the sets of cubes and multiplicity functions respectively such that for each *D* and ϑ we have

$$\sum_{c} \chi(c, \mathbb{C}) = 1 \qquad \sum_{c} \chi(c, \vartheta) = 1$$

then it follows that the energy of the ground state per cube is

$$e_G(c) = \sum_{\mathbb{C}} \chi(c, \mathbb{C}) \Phi_{\mathbb{C}}(G)$$

and we define the effective potential as

$$f_R^E(G,c) = \beta e_G(c) - \sum_{\vartheta/H_0(\vartheta) \leqslant E} \chi(c,\vartheta) \phi_E^T(\vartheta,G).$$
(3.5)

We notice that global free energy, $f_R^E(G)$ is a sum of local contributions. Since here, we only consider the elementary excitations in the *G*-restricted ensemble i.e. $\vartheta = \vartheta_X$, where *X* is the elementary excitation, then it follows from (3.4) that

$$\phi_E^T(\vartheta_X, G) = \phi_E(\vartheta_X, G) = e^{-\beta H(\vartheta_X)}$$
 and $\chi(c, \vartheta_X) = 1/n_c(X)$

where $n_c(X)$ is the number of excitations of kind X intersecting the cube c. Thus, we obtain

$$f_R^{E=E_1}(G,c) = \beta e_G(c) - (\frac{1}{8})n_1(G,c)e^{-\beta E_1} + O(e^{-\beta E_2})$$
(3.6)

here the contributions of μ are neglected in the exponents, because the phase diagram is only given in the neighbourhood of $\mu = 0$.

The term $n_1(G, c)$ is the number of excitations of type 2, 3 or 4 (see table 1) in the ground state G intersecting the cube c, and the energy is

$$e_G(c) = \sum_{\mathbb{C}ic} (\frac{1}{27}) \Phi_{\mathbb{C}}(G)$$

the sum is over all cubes C intersecting the cube c. Finally, we find the low-temperature phase diagram by comparing the effective potentials associated to the different ground states. The main results of the (BS) theory or contained in theorems A and B

The main results of the (BS) theory are contained in theorems A and B.

Theorem A. When H_0 has the retouch property and the condition L and that there is a finite family ζ^* of dominant ground states, all equivalent under symmetries of H_0 . Then for low temperatures there are exactly $|\zeta^*|$ different pure phases ($|\zeta^*|$ is the number of elements in the family ζ^*), each of them being a small perturbation of the corresponding ground states.

Theorem B. The coexistence line of the pure phases corresponding to dominant ground states from the asymptotic one up to order $\exp(-\beta E_D)$ where D is the order yielding domination.

More precisely let $\mu(T)$ be the coexistence line in the phase space (T, μ) and $\mu_D(T)$ its asymptotic line up to order *D*, then by theorem B,

$$\frac{1}{T}[\mu(T) - \mu_D(T)] = O(e^{-\frac{E_{D+1}}{T}})$$

To apply these results let us introduce the *structure constants* $n_{ic}(G, c)$, (i = 1, 2, 3), which determine completely the ground state G in the set of cubes intersecting a given cube c. We define $n_{ic}(G, c)$ for i = 1, 2 such that,

$$n_{1c}(G,c) = \begin{cases} 1 & \text{if } c \text{ is a } B\text{-cube} \\ 0 & \text{otherwise} \end{cases} \text{ and } n_{2c}(G,c) = \begin{cases} 1 & \text{if } c \text{ is an } F\text{-cube} \\ 0 & \text{otherwise.} \end{cases}$$

To define $n_{3c}(G, c)$ we consider a family of three cubes $\{c_+, c, c_-\}$ such that c_+ (resp. c_-) is a cube sitting exactly over (resp. under) the cube c. Then the number of *B*-cubes in such a family $\{c_+, c, c_-\}$ is equal to $n_{3c}(G, c)$.

In terms of these structure constants we rewrite the effective potential in (3.6) up to first order and we get,

$$f_R^{E=E_1}(G,c) = -\beta \left[3 + \frac{\mu}{3} n_{3c}(G,c) \right] - \frac{1}{2} [n_{3c}(G,c) + n_{2c}(G,c) - n_{1c}(G,c)] e^{-\beta E_1}.$$
 (3.7)

Setting $\mu = 0$, one obtains

$$f_R^{E=E_1}(G,c) = -3\beta - \frac{1}{2}[n_{3c}(G,c) + n_{2c}(G,c) - n_{1c}(G,c)]e^{-\beta E_1}.$$

The dominant ground states are those for which the number $\{n_{3c}(G, c) + n_{2c}(G, c) - n_{1c}(G, c)\}$ is maximal. Thus the bilayer ground state is the unique dominant ground state. Hence, by theorem A, at h = 2 there is exactly one pure phase at low temperatures

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corresponding to the bilayer ground state. Now, by setting $f_R^{E=E_1}(G^F, c) = f_R^{E=E_1}(G^B, c)$ one obtains $\mu_{D=1}^{F,B} = -\frac{T}{2}e^{\frac{-E_1}{T}}$. Therefore, by theorem B, there exists a line $T \to \mu^{F,B}(T)$ defined for T small enough such that

$$\frac{1}{T}[\mu^{F,B}(T) - \mu^{F,B}_{D=1}(T)] = O(e^{-\frac{E_2}{T}})$$

and then the low temperature phase diagram is as follows.

For any temperature T,

- if $\mu > \mu^{F,B}(T)$, the Gibbs state of the model is the unique bilayer phase,
- if $\mu < \mu^{F,B}(T)$ the phase diagram exhibits the coexistence of two ferromagnetic phases.

Finally, at $\mu = \mu^{F,B}(T)$ all these three phases coexist (see figure 4).

Figure 4. The low-temperature phase diagram of the layered field Ising model.

4. Conclusion

The low-temperature phase diagram of the three-dimensional Ising model in a layered magnetic field is found in which we pass from the ferromagnetic phases to the bilayer phase by a first-order transition as we vary the layered magnetic field. Further, we have determined the characteristic of the transition line at low temperature.

Moreover, the model in two dimensions is studied in [4] using the finite size scaling approximation method where the phase diagram shows a second-order phase transition line between the ferromagnetic phases and the bilayer phase. In this paper, we have proved, using the BS theory, that in three dimensions the phase transition is of first order.

Appendix. The retouch property of the model

To prove the retouch property we need to introduce some definitions. Namely, for a nonnegative number, l; and for a domain Λ , we define an l-boundary, $\partial_l \Lambda$, of Λ such that $\partial_l \Lambda = \{a \in \Lambda : \operatorname{dist}(a, \Lambda^C) \leq l\}$ and we also define an l-neighbourhood, $[\Lambda, l]$, of Λ such that $[\Lambda, l] = \{a \in Z^3 : \operatorname{dist}(a, \Lambda) \leq l\}$. Here $\operatorname{dist}(a, \Lambda) = \min_{b \in \Lambda} (\operatorname{dist}(a, b))$ and $\operatorname{dist}(a, b) = \max_i |a_i - b_i|$.

For a finite subset Λ in Z^3 , we define the set of partial configurations, χ_{Λ} , as the set of configurations, X, whose domain $(\operatorname{dom}(X))$ is Λ . The subsets of the configurations, X, in χ_{Λ} satisfying $\Phi_c(X) = \phi_c$, $c \subset \Lambda$; (with $\phi_c = \min_X(\Phi_c(X))$) are called local ground states. For Z^3 the local ground states lead to the usual global ground states.

A partial configuration, X, is an excitation of a local ground state, G, if its restriction to the *l*-boundary of its domain corresponds to the local ground state, G. We say that a

Figure A1. Diagram for a proof of the retouch property of the model.

partial configuration X is contained in a partial configuration Y, $X \subset Y$ if Y is equal to X on dom(X). An excitation which does not properly contain another one is an elementary excitation.

To an excitation, X, we associate its energy (relative to a local ground state),

$$H_0(X) = \sum_{c \in \text{dom}(X)} [\Phi_{0,c}(X) - \phi_{0,c}].$$

We define the support of X, (supp(X)), as the set of cubes (contained in the domain of X) for which the term, $\Phi_{0,c}(X) - \phi_{0,c}$, is strictly positive.

Finally we recall that a model has the retouch property if for any energy, E > 0, there exists l(E) such that for all l > l(E) all the elementary excitations with energy smaller than E are removable. It means that the ground states extend uniquely from the boundaries.

Let us consider a parallelepiped formed by the union of elementary cubes and define the *level* of a cube c in that parallelepiped as $z_0(c) = \min_z(z(M \in c))$, where M is a lattice site with a coordinate, z(M), on the z-axis.

Since the ground states have layered structures perpendicular to the z-axis, we remark that all the cubes with the same level in the parallelepiped are of the same type (F- or B-cubes in figure 2).

Since our model is regular then for a given elementary excitation whose energy $H_0(X) < E$, there exists a finite l(E) such that the support of X is contained in a smaller parallelepiped, P_0 , which in turn is contained in the interior of another parallelepiped which we denote $\tilde{\lambda}$, contained in dom(X) (figure A1).

Now we consider a domain Λ defined as the complement of P_0 in $\widetilde{\Lambda}$ (i.e. a domain consisting of the parallelepiped $\widetilde{\Lambda}$ with a cut-out smaller parallelepiped P_0). One obtains that Λ is the union of six overlapping parallelepipeds ($\Lambda_{xi}, \Lambda_{yi}, \Lambda_{zi}; i = +, -$).

First suppose that all the cubes of Λ are *F*-cubes, i.e. the surrounding ground state is the *F*-ground state, then one can uniquely extend the ground state of Λ to the ground state of $\tilde{\Lambda}$. Second, suppose that one cube of Λ is a *B*-cube of level z_0 and suppose that it is contained in $\Lambda_{x,+}$, then all the cubes of $\Lambda_{x,+}$ with level z_0 are *B*-cubes. Because of the overlapping between the parallelepipeds of $\Lambda_{x,+}$ and $\Lambda_{y,i}(i = +, -)$ there exists a family of *B*-cubes of level z_0 contained in both of them. Therefore, all the cubes of level z_0 in $\Lambda_{y,i}(i = +, -)$ are *B*-cubes. Now, starting by *B*-cubes with level z_0 in $\Lambda_{y,i}$ and since

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they overlap with $\Lambda_{+,-}$ then, by the preceding remark, one can easily show that all the cubes of level z_0 of the parallelepiped $\Lambda_{x,-}$ are *B*-cubes. Hence, all the cubes of level z_0 of the parallelepiped Λ are *B*-cubes. That implies that the extension of the ground state of Λ to that of $\tilde{\Lambda}$ is unique. Finally if there are many levels with *B*-cubes occurring in Λ one can, in the same manner as above, prove the uniqueness of the extension to a unique ground state and then conclude the proof.

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