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ON PROPERTIES OF THE SINGULARITY OF THE GROUND STATE IN CERTAIN CLASSICAL HEISENBERG MODELS

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Abstract: We prove that for both the classical ferro - and antiferromagnetic Heisenberg models the infinite volume limit of the ground state energy per unit volume of the system (Hamiltonian plus λ times an operator is not differentiable at zero in λ for some operators. This characterization of the singularity at T=0, which corresponds to Fisher's ([5]) for positive temperature, adds to a number of others, which are to some extent analogous to the several characterizations of phase transitions at T>0 (|8|). A comment is made upon a related open problem concerning the ground state of the quantum antiferro - magnetic Heisenberg chain.

As far as we know no explicit examples of Fisher's (|5|) characterization of a phase transition in terms of the nondifferentiability of certain infinite volume correlation functions with respect to external parameters exist. In this note we study the analogous characterization for T=0, in the case of some classical Heisenberg (anti-) ferromagnets [1] and prove that it holds. This result on ground states of classical systems (for general ground-state representations, see [9]) adds to some other features of the singularity at T=0, known for the one-dimensional chain with nearest-neighbour interactions, namely: divergence of the susceptibility χ_β as β^2 as $\beta \to \infty$ ([3]), existence of long-range order (|4|), (infinite) asymptotic degeneracy of the highest eigenvalue of the transfer matrix as $\beta \to \infty$ ([4]) [2], which are to some extent analogous to some of the several alternative determinations of a phase transition at T>0 (see, e.g., |8|). To display one more property in this set of alternate descriptions, whose interrelation is not entirely

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1) Some references on classical spin systems, to which we refer for additional literature, are [11], [12]..

2) The eigenvalues $\{\lambda_\ell(\beta)\}$ $\ell=0,1,2,\ldots$ of the transfer matrix, of which the largest $\lambda_0(\beta)$ is simple and the remainder ones are $(2\ell+1)$- fold degenerate, become all degenerate with the largest eigenvalue for ℓ odd, i.e., $\lim_{\beta\to\infty} |\lambda_\ell(\beta)/\lambda_0(\beta)| = (-1)^\ell$ ([4])

clear, and the clarification of which is a major problem in the theory of phase transitions, is the motivation of this paper . For notational simplicity, we write out the proof for the one dimensional case and nearest neighbour interactions. However, the result and proof of the forthcoming theorem hold in any number of dimensions, with a Hamiltonian for the region $\Lambda \subset \mathbb{Z}^{\nu}$ (ν arbitrary integer) given by

$$H_\Lambda = - \sum_{i,j \in \Lambda} J(i-j) \; \vec{t}_i \cdot \vec{t}_j \tag{1}$$

where $\vec{t}_i$, $i \in \Lambda$, are unit vectors, $\sum_{i \in} |J(i)| < \infty$ by stability ([10]), such that Λ may be divided into two "sublattices" A and B ($A \cup B = \Lambda$), with $J(i-j) \leq 0$ if i,j both belong to either A or B, and $J(i-j) \geq 0$ if $i \in A$ and $j \in B$ or vice-versa. If A is the set of nearest neighbours of B, the above conditions correspond to antiferromagnetism, and if A or B are empty we have a ferromagnetic system (see [2]).

Let $\underline{t}_i$, $i \in [0, N-1]$, be vectors in $S = \{\vec{x} \in \mathbb{R}^3 ; x^2 = 1\}$, with $\underline{t}_0 = \underline{t}_N$ (periodic boundary conditions), with components $(\Omega_i \equiv (\theta_i, \phi_i))$

$t_i^1(\Omega_i) = t_i^1 = \sin\theta_i \cos\phi_i \quad t_i^2(\Omega_i) = t_i^2 = \sin\theta_i \sin\phi_i$

$$t_i^3(\Omega_i) = t_i^3 = \cos\theta_i$$

$(0 \leq \theta_i < \pi , \; 0 \leq \phi_i < 2\pi)$

$$\text{On } \mathcal{H} = \bigotimes_{i=0}^{N-1} L^2(\mathcal{S}, d\Omega_i), \text{ with } d\Omega_i = \sin\theta_i d\theta_i d\phi_i,$$

$$\text{let } C_N^+(r, \Omega) = \sum_{i=0}^{N-1} t_i^3 \, t_{i+2r}^3 \tag{2a}$$

$$C_N^-(r, \Omega) = \sum_{i=0}^{N-1} t_i^3 \, t_{i+r}^3 \tag{2b}$$

$$H_N^{(\pm)}(\Omega) = \pm 2J \sum_{i=0}^{N-1} \underline{t}_i \cdot \underline{t}_{i+1} \quad , \underline{t}_0 = \underline{t}_N \, , \; J > 0 \tag{3}$$

with + (resp. -) corresponding to anti- (resp. ferro-) magnetism. The precise way in which a large class of classical spin systems (including (3) and the more general Hamiltonian (1)) is the limit, "as the spin tends to infinity", of the corresponding quantum spin systems is described in [7].

Let

$$g_{N,r}^{(\pm)}(\lambda) = \min_{\Omega \in \mathcal{S}^N} \frac{1}{N} \left[H_N^{(\pm)}(\Omega) + \lambda C_N^{(\pm)}(\Omega) \right] \tag{4}$$

$$\text{and let } g_r^{(\pm)}(\lambda) = \lim_{N \to \infty} g_{N,r}^{(\pm)}(\lambda) \tag{5}$$

For fixed r, this limit exists by a simple adaptation of the proof in ([9]).

Note that $g_{N,r}^{(\pm)}$ is a concave function of λ, Hence $g_r^{(\pm)}$ is also a concave function of λ, whence (e.g., [1]) it has both a right-hand derivative $\frac{d^+ g_r^{(\pm)}(\lambda)}{d\lambda}$ and a left-hand one $\frac{d^- g_r^{(\pm)}(\lambda)}{d\lambda}$.

Theorem $\dfrac{d^+ g_r^{(\pm)}(\lambda)}{d\lambda}(\lambda = 0) \neq \dfrac{d^- g_r^{(\pm)}(\lambda)}{d\lambda}(\lambda = 0)$.

Proof A possible choice for our "sublattices" is

$A = \{0,2,\ldots\ldots, N\}, \{B = 1,3,\ldots\ldots, (N-1)\}$ if N is even, or $A = \{0,2,\ldots, (N-1)\}$ and $B=\{1,3,\ldots,N\}$ if N is odd. Clearly, for all N,

$$g_{N,r}^{(\pm)}(0) = -2J$$

Now consider the state given by $t_i^2 = t_i^3 = 0$, $\forall i \in [0,N-1]$, and $t_i^1 = +1$ $\forall i \in [0,N-1]$ in the $-$ (ferromagnetic) case, and $t_i^1 = 1$ $\forall i \in A$ and $t_i^1 = -1$ $\forall i \in B$ in the $+$ (anti-ferromagnetic) case. In this state and any λ,

$\frac{1}{N}\left[H_N^{(\pm)}(\Omega) + \lambda C_N^{(+)}(r,\Omega)\right]$ takes the value $(-2J)$, hence

$g_{N,r}^{(\pm)}(\lambda) \leq -2J$ for any λ and for all N. Hence,

$$1/\lambda \left[g_{N,r}^{\pm}(\lambda) - g_{N,r}^{\pm}(0)\right] \leq 0 \ \forall \lambda > 0, \quad \forall N$$

Hence, $1/\lambda[g_r^{\pm}(\lambda)-g_r^{\pm}(0)] \leq 0$ $\forall \lambda > 0$, from which we get

$$\frac{d^+ g_r^{\pm}(\lambda)}{d\lambda}(\lambda=0) \leq 0 \tag{6}$$

Now, $\dfrac{d^- g_r^{(\pm)}(\lambda)}{d\lambda}(\lambda = 0) = \lim\limits_{\lambda\to 0}\left[g_r^{(\pm)}(0) - g_r^{(\pm)}(-\lambda)\right]/\lambda =$

$$= \lim_{\lambda\to 0_+} \frac{1}{\lambda}\left[\lim_{N\to\infty} \min_{\Omega\in\mathcal{S}^N}\left\{\frac{1}{N} H_N^{(\pm)}(\Omega)\right\} - \lim_{N\to\infty} \min_{\Omega\in}{}^{N}\left\{\left\{\frac{1}{N}\left[H_N^{(\pm)}(\Omega) - \lambda C_N^{(\pm)}(r,\Omega)\right]\right\}\right\}\right] \tag{7}$$

Now, we clearly have

$$\min_{\Omega \in \mathcal{S}^N} \frac{1}{N} \left[H_N^{(\pm)} \ (\Omega) \right] = -1 \qquad (8)$$

while

$$\frac{1}{N} \left[H_N^{(\pm)} (\Omega) \ - \lambda \ C_N^{(\pm)} (r, \Omega) \right] \ \geq -1 \ - \lambda \ ,$$

and this minimum value is attained, e.g., for

$t_i^1 = t_i^2 = 0 \ \ \forall \ i \in [0, \ N-1]$, and $t_i^3 = 1 \ \ \forall \ i \in [0, N-1]$ in the $-$ case, and $t_i^3 = 1 \ \ \forall \ i \in A$, and $t_i^3 = -1 \ \forall \ i \in B$, in the $+$ case. Hence, we have

$$\min_{\Omega \in \mathcal{S}^N} \ \frac{1}{N} \left[H_N^{(\pm)} (\Omega) - \lambda \ C_N^{(\pm)} (r, \Omega) \right] = -1- \lambda \qquad (9)$$

By (8) and (9) in (7) we get immediately

$$\frac{d^- g_r^{(\pm)} (\lambda)}{d \lambda} \ (\lambda = 0 \ ) \ = \ \lim_{\lambda \to 0} \frac{1}{\lambda} \ \left[-1-(-1-\lambda) \right] = 1 \qquad (10)$$

The results (6) and (10) imply the assertion of the theorem. ∎

<u>Remark</u> Consider the one-dimensional isotropic antiferromagnetic Heisenberg chain for spin S and periodic boundary conditions, described by the Hamiltonian (on $\mathcal{H} \ \bigotimes_{i=0}^{N-1} \mathbb{C}_i^{2S+1}$)

$$H_N^S = \frac{2J}{S^2} \sum_{i=0}^{N-1} (\underline{S}_i \cdot \underline{S}_{i+1}) \quad \underline{S}_0 = \underline{S}_N \quad S_i^{(k)} = \frac{1}{2} \cdot \sigma_i^{(k)}$$

$\sigma_i^{(k)}$ $k \in [1, 3]$, being spin matrices for spin S, and J>0.
The ground state Ω_N^S of H_N^S is unique ([2]), and we define

$$L_s \equiv \liminf_{r\to\infty} \ \liminf_{N\to\infty} \ (\Omega_N^s, \ S_0^3 \ S_{2r}^3 \ \Omega_N^s)/S^2$$

If $L_s \geq \gamma > 0$, we may take this to mean that the one-dimensional antiferromagnet exhibits "long-range order" in the ground state.

Define

$$C_N(r) = \sum_{i=0}^{N-1} S_i^3 \ S_{i+2r}^3 \qquad S_0 = S_N$$

$$C_N(\delta, r, \Omega) = \delta^2 \ C_N^{(1)}(r, \Omega)$$

$$H_N(\delta\ \Omega) = \delta^2 \ H_N^{(1)}(\Omega)$$

$$f_{N,r}(\lambda, \delta) = \min_{\Omega\in S^N} \left\{ \frac{1}{N} \left[H_N(\delta,\Omega) + \lambda\, C_N(\delta, r, \Omega) \right] \right\} - \min_{\Omega\in S^N} \frac{1}{N} H_N(1,\Omega)$$

Now $f_{N,r}(\lambda,\delta)$ is a double sequence of functions concave in λ.

Hence $f(\lambda,\delta) \equiv \liminf_{r\to\infty} \ \liminf_{N\to\infty} \ f_{N,r}(\lambda,\delta)$

is also concave in λ. Now, $f_{N,r}(\lambda,\delta)$ is uniformly continuous (in (r,N) as a function of δ. Hence,

$$f(\lambda) = f(\lambda) - f(0) \equiv \lim_{\delta\to 1} f(\lambda,\delta) = \liminf_{r\to\infty} \ \liminf_{N\to\infty} f_{N,r}(\lambda,1)$$

$$= \liminf_{r\to\infty} \ \liminf_{N\to\infty} \left[f_{N,r}(\lambda,1) - f_{N,r}(0,1) \right]$$

From the r.h.s. of inequality (6.5) of [7], transcribed to vacuum expectation values, we easily get

$$\liminf_{\beta\to\infty} \ \liminf_{r\to\infty} \ \liminf_{N\to\infty} (\Omega_N^S, \ \frac{C_N(r)}{N} \ \Omega_N^S)/S^2 \geq \lambda^{-1} f(\lambda) =$$

$$= \liminf_{r\to\infty} \ \liminf_{N\to\infty} \lambda^{-1} f_{N,r}(\lambda,1) = \liminf_{r\to\infty} \ \liminf_{N\to\infty} \ \lim_{\beta\to\infty} \lambda^{-1} f_{N,r,\beta}(\lambda,1)$$

where $f_{N,r,\beta}(\lambda,1) \equiv -\frac{1}{N\beta} \log \dfrac{\int d\Omega^N \ e^{-\beta[H_N(1,\Omega) + \lambda C_N(1,r,\Omega)]}}{\int d\Omega^N \ e^{-\beta H_N(1,\Omega)}}$

If $\lim_{\lambda \to 0_+} \liminf_{r \to \infty} \liminf_{N \to \infty} \lim_{\beta \to \infty} \lambda^{-1} f_{N,r,\beta}(\lambda, 1) \overset{(?)}{=}$

$\overset{(?)}{=} \liminf_{r \to \infty} \liminf_{N \to \infty} \lim_{\beta \to \infty} \lim_{\lambda \to 0_+} \lambda^{-1} f_{N,r,\beta}(\lambda, 1) = 1/3$

by Refs. [3], [4], which would follow if, e.g., for λ in a sufficiently small neighbourhood of zero one had

$$[\beta < (C_N(1,r,\Omega) - \langle C_N(1,r,\Omega)\rangle_\lambda)^2 >_\lambda]/ N \le \text{const.}$$

(independent of r, N, β) (13)

where

$$\langle A_N(r,\Omega)\rangle_\lambda \equiv \frac{\int d\Omega^N\, e^{-\beta[H_N(1,\Omega) + \lambda C_N(1,r,\Omega)]} A_N(r,\Omega)}{\int d\Omega^N\, e^{-\beta[H_N(1,\Omega) + \lambda C_N(1,r,\Omega)]}}$$

then we would clearly have $L_S \ge \gamma > 0$ for sufficiently large S, on putting (12) into (11). Unfortunately, we have been unable to prove (12) (or (13) to date. ∎

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