ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

ДУБНА

E4 - 7150

J.G.Brankov, A.S.Shumovsky, V.A.Zagrebnov

ON MODEL SPIN HAMILTONIANS INCLUDING LONG-RANGE FERROMAGNETIC INTERACTION

1973

ЛАБОРАТОРИЯ
ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

E4 - 7150

J.G.Brankov,* A.S.Shumovsky,** V.A.Zagrebnov

ON MODEL SPIN HAMILTONIANS INCLUDING LONG-RANGE FERROMAGNETIC INTERACTION

Submitted *to Physics Letters*

* On leave of absence from Institute for Nuclear Research and Nuclear Energetics, Bulgarian Academy of Sciences, Sofia, Bulgaria.

** Permanent address: Department of Quantum Statics, Moscow State University, Moscow, U.S.S.R.

Considerable interest has been expressed recently in the study of model Hamiltonians with competing short-range and infinitely long-range interactions [1,2]. It has been assumed, on physical grounds, that the long-range part of the Hamiltonian can be treated by a mean-field theory. This suggested the present rigorous investigation of a general spin $\frac{1}{2}$ system described by the Hamiltonian:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_L - N \sum_{a=1}^{3} h_a I_a . \tag{1}$$

Here $\mathcal{H}_S$ is an unspecified N -body Hamiltonian satisfying the condition:

$$\| [\mathcal{H}_S , I_a]_- \| \le K \qquad a = 1, 2, 3 . \tag{2}$$

where $\|...\|$ denotes the norm of the commutator, $K < \infty$ does not depend on N, and

$$I_a = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^a \qquad a = 1, 2, 3. \tag{3}$$

with Pauli matrices σ_i^a standing for the components of the spin-vector operator at i^{th} site, so that I_a obeys:

$$\| I_a \| \le 1 ; \qquad \| [I_a , I_\beta]_- \| \le \frac{2}{N} . \tag{4}$$

We assume the infinitely long-range part $\mathcal{H}_L$ of the Hamiltonian (1) to be of a ferromagnetic type and take it in the form:

$$\mathcal{H} = -\frac{1}{2} N \sum_{a=1}^{3} J_a I_a^2 , \tag{5}$$

where J_a are positive interaction parameters. The last term in the right-hand side of (1) is the magnetic energy of the system, placed in an external field $\{h_a\}$.

First we show how the Thermodynamically Equivalent Hamiltonian method /3,4/ can be rigorously applied to the present case *.

We introduce a set of variational parameters $\{C_a\}$ $(a = 1, 2, 3)$ into (1) and rewrite the Hamiltonian in the form:

$$\mathcal{H} = \mathcal{H}_0(\{C_a\}) + \mathcal{H}'(\{C_a\}), \qquad (6)$$

where:

$$\mathcal{H}_0(\{C_a\}) = \mathcal{H}_S - N \sum_a (h_a + J_a C_a) I_a + \frac{1}{2} N \sum_a J_a C_a^2, \qquad (7)$$

$$\mathcal{H}'(\{C_a\}) = -\frac{1}{2} N \sum_a J_a (I_a - C_a)^2. \qquad (8)$$

The canonical free energy per spin $f[\mathcal{H}]$, associated with $\mathcal{H}$, is defined by:

$$f[\mathcal{H}] = -\frac{1}{\beta N} \ln Tr\, e^{-\beta \mathcal{H}},$$

where $\beta = \frac{1}{\theta}$ is the inverse temperature.

In order to investigate the contribution from the residual Hamiltonian $\mathcal{H}'$ to the free energy of the system $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$ we use Bogolubov's theorem (see the proof in ref. /6/) which yields:

$$-\frac{1}{N} \langle \mathcal{H}' \rangle_0 \leq f[\mathcal{H}_0] - f[\mathcal{H}] \leq -\frac{1}{N} \langle \mathcal{H}' \rangle. \qquad (9)$$

Here $\langle \ldots \rangle_0$ and $\langle \ldots \rangle$ denote thermal average with respect to $\mathcal{H}_0$ and $\mathcal{H}$ correspondingly.

Due to the explicit form (8) of $\mathcal{H}'$, we have:

----

* It should be noted that a system given by $\mathcal{H}_L - N \sum_a h_a I_a$ has been treated rigorously in ref. /5/.

$$0 \leq f[\mathcal{H}_0(\{C_a\})] - f[\mathcal{H}] \leq \frac{1}{2} \sum_a J_a \langle (I_a - C_a)^2 \rangle. \qquad (10)$$

It is readily seen from (10) that the best approximation to the exact thermodynamic potential $f[\mathcal{H}]$ is obtained when trial parameters $\{C_a\}$ obey the condition for absolute minimum of $f[\mathcal{H}(\{C_a\})]$ with respect to $\{C_a\}$:

$$f[\mathcal{H}_0(\{\bar{C}_a\})] = \min_{\{C_a\}} f[\mathcal{H}_0(\{C_a\})]. \qquad (11)$$

This yields the following self-consistent field equations:

$$\bar{C}_a = \langle I_a \rangle_0 \qquad a = 1, 2, 3, \qquad (12)$$

where the thermal average is taken with $\mathcal{H}_0(\{\bar{C}_a\})$.

Now the essential problem is to prove rigorously that $\mathcal{H}_0(\{\bar{C}_a\})$ is thermodynamically equivalent to $\mathcal{H}$. To this end we make use of the majoration technique of N.N.Bogolubov (Jr.) /7/.

From (10) and (11) we see that:

$$0 \leq f[\mathcal{H}_0(\{\bar{C}_a\})] - f[\mathcal{H}] \leq f[\mathcal{H}_0(\{\langle I_a \rangle\})] - f[\mathcal{H}] \leq$$
$$\leq \frac{1}{2} \sum_a J_a \langle (I_a - \langle I_a \rangle)^2 \rangle. \qquad (13)$$

Hence, following ref. /7/, we find that the difference of the normalized free energies:

$$\Delta(\theta, \{h_a\}) \equiv f[\mathcal{H}_0(\{\bar{C}_a\})] - f[\mathcal{H}] \qquad (14)$$

is majorized by:

$$\frac{1}{2} \sum_a J_a \langle (I_a - \langle I_a \rangle)^2 \rangle \leq \frac{\theta}{2N} \sum_a J_a \left(-\frac{\partial^2 f[\mathcal{H}]}{\partial h_a^2}\right) +$$
$$+ \left(\frac{1}{2N}\right)^{2/3} \sum_a J_a \left(\| [\mathcal{H}, I_a]_- \|\right)^{2/3} \left(-\frac{\partial^2 f[\mathcal{H}]}{\partial h_a^2}\right)^{2/3} \qquad (15)$$

An upper bound on the average of $\Delta(\theta,\{h_a\})$ over a small region Ω_ℓ in (h_1, h_2, h_3)-space

$$\Omega_\ell = \underset{a}{\otimes} [h_a, h_a + \ell]$$

surrounding the point $\{\xi_a\} \in \Omega_\ell$ is then given by:

$$\Delta(\theta,\{\xi_a\}) = \frac{1}{\ell^3} \iiint\limits_{\Omega_\ell} \prod_\beta dt_\beta \Delta(\theta,\{t_a\}) \leq$$

$$\leq 3J_{max} \{\frac{\theta}{\ell N} + [\frac{K + 2(J_{max} - J_{min}) + 4(|h| + \ell)}{\ell N}]^{2/3}\} \quad (16)$$

if the following relations are used.

$$0 \leq \frac{1}{\ell^3} \iiint \prod dt \left(-\frac{\partial^2 f[\mathcal{H}]}{\partial t_a^2}\right) = \frac{1}{\ell^3} \iint \prod_{\beta \neq a} dt_\beta [\langle I_a \rangle|_{h_a + \ell} -$$

$$- \langle I_a \rangle|_{h_a}] \leq \frac{2}{\ell},$$

$$||[\mathcal{H}, I_a]_-|| \leq K + 2(J_{max} - J_{min}) + 4|h| \equiv L(h),$$

(where J_{max} (J_{min}) stands for the maximum (minimum) value of J_a) and applying Hölder's integral inequality to the last term in (15).

Now according to the majorization:

$$\Delta(\theta,\{h_a\}) \leq \sum_{a=1}^{3} \max |\frac{\partial \Delta}{\partial h_a}| \cdot |h_a - \xi_a| + \Delta(\theta,\{\xi_a\}) \leq$$

$$\leq 6\ell + \Delta(\theta,\{\xi_a\}) \quad (17)$$

we find combining it with (16):

$$|\Delta(\theta,\{h_a\})| \leq 6\ell + 3J_{max} [\frac{\theta}{\ell N} + (\frac{L(h)}{\ell N} + \frac{4}{N})^{2/3}].$$

Since the last inequality holds for all $\ell > 0$, the left-hand side being independent of ℓ, it can be optimized by the choice of ℓ. We choose:

$$\ell = \frac{J_{max}}{N^{2/5}}$$

and finally obtain the bound:

$$|\Delta(\theta,\{h_a\})| \leq \frac{3J_{max}}{N^{2/5}} [2 + (\frac{L(h)}{J_{max}} + \frac{4}{N^{2/5}})^{2/3}] \quad (18)$$

$$+ \frac{3\theta}{N^{3/5}}$$

which proves the uniform convergence of $f[\mathcal{H}_0(\{\bar{C}_a\})]$ to $f[\mathcal{H}]$ as $N \to \infty$ in any compact set in (θ, h_1, h_2, h_3)-space.

The authors wish to express their sincere gratitude to Prof. N.N.Bogolubov (Jr.) for valuable remarks and useful discussions.

References

1. J.F.Nagle. Phys.Rev., A2, 2124 (1970).
2. J.S.Hoye. Phys.Rev., B6, 4261 (1972).
3. G.Wentzel. Phys.Rev., 120, 1572 (1960).
4. M.Girardeau. J.Math.Phys., 3, 131 (1962).
5. J.G.Brankov, A.S.Shumovsky. JINR P4-6893, Dubna, 1973.
6. S.V.Tyablikov. The Methods of Quantum Theory of Magnetism (Nauka, Moscow, 1965).
7. N.N.Bogolubov (Jr.). A Method for Studying Model Hamiltonians (Pergamon Press, 1972).

Received by Publishing Department
on May 8, 1973.