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On the phase transition in XY- and Heisenberg models[1])

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Abstract. For the free energy and susceptibility of the quantum XY- and Heisenberg models singular lower and upper bounds have been constructed in d dimensions. The bounds are given by the Ising model free energies and susceptibilities which prove the onset of continuous phase transition in d dimensions, $d \geq 2$.

1. Introduction

Continuous phase transition and symmetry breaking in statistical mechanics are interesting and deep problems. It is especially hard to understand them in the quantum XY- and Heisenberg models. If one would like to understand the phenomenon of continuous phase transition in these models, one must be clear about its characterization, which can be given by a singular behaviour in different quantities as the susceptibility, specific heat, etc., at the transition temperature T_c and by the appearance of a from-zero different magnetization below T_c in the case of magnetic systems. Here, we take up the idea of singularity in the above mentioned quantities.

The idea is to construct lower and upper bounds to the susceptibilities of the quantum XY- and Heisenberg models which do diverge. This can be achieved by constructing lower and upper bounds given by the Ising susceptibility, which does diverge, and therefore the susceptibilities of the quantum XY- and Heisenberg models must also do so. This fact characterizes the onset of continuous phase transition in the quantum XY- and Heisenberg models. The order parameter exists below T_c. In dimension $d = 2$ its existence is proved by these inequalities and by the theorem of Szegö and Kac. It is believed that the two dimensional quantum XY- and Heisenberg models do not show continuous phase transition [1] contrary to our finding. See the appendix for discussions. For higher dimensionality such as $d = 2$ some progress has been made. In three dimensions, Fröhlich *et al.* [2] and Dyson *et al.* [3] proved continuous phase transition which is supported by our ideas also. Now we turn to the technicalities.

Our considerations are based on the theorem of Golden [4] and Thompson [5]: if A and B are two hermitian square matrices, then

$$\mathrm{Tr}\,\{e^{-(A+B)}\} \leq \mathrm{Tr}\,\{e^{-B/2}\, e^{-A}\, e^{-B/2}\}, \quad (-A,\, -B \geq 1) \tag{1}$$

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holds. If A and B commute then the equality is valid. This theorem has been generalized by Segal [6] to certain selfadjoint operators A and B. Because we will work at first in finite volume and then take the thermodynamic limit, it is enough for us to work first with finite matrices, e.g., with the theorem of Golden and Thompson. From equation (1) it follows

$$\operatorname{Tr}\{e^{-(A+B)}\} \leq [\operatorname{Tr}\{e^{-2A}\}]^{1/2}[\operatorname{Tr}\{e^{-2B}\}]^{1/2} \leq \operatorname{Tr}\{e^{-2A}\} \operatorname{Tr}\{e^{-2B}\} \tag{2}$$

by Schwartz inequality for symmetric and bounded A and B. This inequality will now be used to discuss the upper and lower bounds of the partition functions belonging to the quantum mechanic XY- and Heisenberg models. We make no restriction on the space dimension d at first, but we will refer to the solution of the two-dimensional Ising model.

2. XY-model

The model Hamiltonian is

$$H_{xy}(v) = \sum_{\mathbf{q};\,\alpha=x,y} -v_{\mathbf{q}}\hat{\sigma}^{\alpha}_{\mathbf{q}}\hat{\sigma}^{\alpha}_{-\mathbf{q}} = H_x(v) + H_y(v). \tag{3}$$

$\hat{\sigma}^{\alpha}_{\mathbf{q}}$are the Fourier transforms of the Pauli spin operators σ^{α}_{i}. The operators $-H_{xy}(v)$ and $-H_{\alpha}(v)$ are positive definite operators and fulfil the relations

$$-H_{xy}(v) \geq -H_{\alpha}(v) \geq 0, \quad \alpha = x, y \tag{4}$$

by unitary equivalence of $H_x(v)$ and $H_y(v)$, $H_{\alpha} = H^{+}_{\alpha}$ and $H_{xy} = H^{+}_{xy}$.

To construct upper and lower bounds to the partition function of the XY-model we make the following choices for A and B of equation (2):

$$A + B = H_{xy}, \quad B = H_y \tag{5a}$$

$$A + B = \frac{1}{2}H_x, \quad B = -\frac{1}{2}H_y. \tag{5b}$$

Equations (2) and (5) give the inequalities

$$Z_x\left(\frac{1}{2}v\right) \leq Z^{1/2}_{xy}(v)Z^{1/2}_{x}(-v) \leq Z_x(2v)Z^{1/2}_{x}(-v) \tag{6a}$$

or

$$\frac{1}{N}\ln Z_x\left(\frac{1}{2}v\right) \leq \frac{1}{2N}[\ln Z_{xy}(v) + \ln Z_x(-v)] \leq \frac{1}{2N}[2\ln Z_x(2v) + \ln Z_{\alpha}(-v)] \tag{6b}$$

with definitions

$$Z_{\alpha}(\gamma v) = \operatorname{Tr}\{\exp[-\gamma H_{\alpha}(v)]\}, \quad \gamma = -1, \frac{1}{2}, 2,$$

$$Z_{xy}(v = \operatorname{Tr}\{\exp[-H_{xy}(v)]\}$$

for the partition functions. In equation (6b) the number of lattice sites N has been introduced to perform the thermodynamic limit. On the other hand $\ln Z_\alpha(\gamma v)$ can be written as

$$\frac{1}{N}\ln Z_\alpha(\gamma v) = -\int_0^1 \frac{d\lambda}{\lambda}\,\mathrm{Tr}\,\{\rho_\alpha(\lambda\gamma v)H_\alpha(\lambda\gamma v)\} + \ln 2 \tag{7}$$

and a similar expression for $Z_{xy}(v)\cdot\rho_\alpha$ is the density operator of the Ising model. The positive definiteness of the operators

$$\exp\left[-H_{xy}(v)\right] - \exp\left[-\frac{1}{2}H_x(v) - \ln 2\right] \geq 0 \tag{8a}$$

$$\exp\left[-2H_\alpha(v)\right] - \exp\left[-H_{xy}(v) - \ln 2\right] \geq 0 \tag{8b}$$

implies with the help of (6b) and (7) the following inequalities

$$\frac{1}{2}\chi_x\left(\frac{1}{2}v|\mathbf{q}\right) \leq \frac{1}{2}\chi_{xy}(v|\mathbf{q}) \leq 2\chi_x(2v|\mathbf{q}) \tag{9}$$

by neglecting the antiferro correlation function originated from $Z_x(-v)$ and terms given by ln 2. Further we assume the existence of the thermodynamic limit in (6b) and (9). The correlation functions of equation (9) are defined as

$$\chi_\alpha(\gamma v|\mathbf{q}) = \mathrm{Tr}\,\{\rho_\alpha(\gamma v)\hat{\sigma}^\alpha_{\mathbf{q}}\hat{\sigma}^\alpha_{-\mathbf{q}}\},\quad \gamma = 1, 2, \tag{10a}$$

$$\chi_{xy}(v|\mathbf{q}) = \mathrm{Tr}\,\{\rho_{xy}(v)\sum_{\alpha=x,y}\hat{\sigma}^\alpha_{\mathbf{q}}\hat{\sigma}^\alpha_{-\mathbf{q}}\}. \tag{10b}$$

If the dimensionality of the system is two, $d = 2$, then we know from the Onsager solution of the two-dimensional Ising model [7] that the upper and lower bounds of equations (6b) and (9) do exist. Further we can show that $1/N \ln Z_{xy}(v)$ is a monotonically increasing function of N and therefore the free energy and the correlation function of the XY-model in equations (6b) and (9) exist as for the two-dimensional Ising model [7]. We assumed the existence of the thermodynamic limit for $d > 2$.

The key result is the inequality equation (9) which states that the correlation function of the XY-model must diverge because the lower bound does so, as the temperature T goes from above to the transition temperature, $T^+ \to T_c$, and $\mathbf{q} \to 0$. This fact proves the onset of instability to second order phase transition in d dimensions for the XY-model, because the Ising model exhibits second-order phase transition. In two dimensions, $d = 2$, the latter case is surprising because of the existence of long-range order in the Ising model and of the belief that the two dimensional XY- and Heisenberg models exhibit no second order phase transition.

3. Heisenberg-model

For the Heisenberg-model,

$$H(v) = \sum_{\mathbf{q},\alpha} -v_{\mathbf{q}}\hat{\sigma}^\alpha_{\mathbf{q}}\hat{\sigma}^\alpha_{-\mathbf{q}},\quad \alpha = x, y, z, \tag{11}$$

we get to (6) similar free energy inequality:

$$\frac{1}{N}\left[\ln Z_x\left(\frac{1}{2}v\right) - \frac{1}{2}\ln Z_{xy}(-v)\right] \leq \frac{1}{2N}\ln Z(v) \leq \frac{1}{2N}[\ln Z_{xy}(2v) + \ln Z_x(2v)], \tag{12}$$

with the help of equation (1), the Schwartz inequality and the following choice of A and B in equation (1): $H(v) = A + B$, $B = H_{xy}$ and $H_x(v) = 2(A + B)$, $2B = -H_{xy}(v)$. $Z(v)$ in equation (12) is the partition function of the Heisenberg-model. Similar operator inequalities, as used for the XY-model, are fulfilled again, namely:

$$-H(v) \geq -H_\alpha(v) \geq 0, \quad \alpha = x, y, z, \tag{13a}$$

$$\exp[-H(v)] - \exp\left[-\frac{1}{2}H_x(v)\right] \geq 0, \tag{13b}$$

$$\exp[-2H_{xy}(v) + \ln 4] + \exp[-2H_x(v) + \ln 2] - \exp[-H(v) + \ln 3] \geq 0 \tag{13c}$$

which imply that the Heisenberg correlation function

$$\chi(v|\mathbf{q}) = \mathrm{Tr}\,\{\rho \sum_\alpha \hat{\sigma}^\alpha_{\mathbf{q}}\hat{\sigma}^\alpha_{-\mathbf{q}}\}$$

is bounded from above and from below:

$$\chi_x\left(\frac{1}{2}v|\mathbf{q}\right) \leq \chi(v|\mathbf{q}) \leq 2\chi_{xy}(2v|\mathbf{q}) + 2\chi_x(2v|\mathbf{q}). \tag{14}$$

This inequality has been obtained by using the definition equation (7) and neglecting the antiferro correlation function $\chi_{xy}(-v|\mathbf{q}) \geq 0$ and terms given by ln 2. (9) in (14) gives further

$$\chi_x\left(\frac{1}{2}v|\mathbf{q}\right) \leq \chi(v|\mathbf{q}) \leq 6\chi_x(2v|\mathbf{q}) \tag{15}$$

Again, the Heisenberg correlation function $\chi(v|\mathbf{q})$ is bounded from below as well as from above by the Ising model correlation function with different coupling constants. The singular behaviour of $\chi_x(\frac{1}{2}v|\mathbf{q})$ indicates again the onset of second order phase transition in the Heisenberg model with dimensions $d \geq 2$.

Note that for quantum-mechanical models the susceptibility is described by the Duhamel two point function

$$(A, B) = \mathrm{Tr}\left\{\rho\int_0^\beta d\lambda A^+(i\lambda)B\right\}$$

which fulfills the inequality of Roepstorff [8]

$$\frac{1}{2}\langle\{A^+, A\}_+\rangle\frac{1 - e^{-c}}{c} \leq (A, A) \leq \frac{1}{2}\langle\{A^+, A\}_+\rangle. \tag{16}$$

See also Naudts and Verbeure [9]. The lower bound of equation (16) is due to Roepstorff for $A^+ = A$. The generalized case, $A^+ \neq A$, is treated in reference [9]. In the case of the XY-model we can use the inequalities, equation (9), for the correlation function

$\langle\{A^+, A\}\rangle$ and equation (15) for the Heisenberg model. In both cases we find divergent lower bounds for dimensions $d \geq 2$. That means the Duhamel two point function does diverge for these two models. Again the onset of phase transition is announced by this singular behaviour. Now, we may allow that the coupling constant of the Ising model takes values below T_c for the lower bound. In this case a δ-function appears in Fourier space due to long range order, which forces a δ-function in the Duhamel two point function or in the correlation function of the XY- or Heisenberg models. This indicates long range order in these two models.

Similar inequalities as equations (8) and (13) can be used immediately in equation (16) with entirely different coupling constants for the XY- and Ising models, with the restriction $v_{xy} > v_J$, or also for the Heisenberg model susceptibility.

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Appendix

Using the Heisenberg model Hamiltonian, as in the work of Mermin and Wagner (MW) [1], with constant nearest neighbour coupling, we discuss here their inequality

$$\frac{\beta}{2}\langle\{S_+(\mathbf{k}), S_-(-\mathbf{k})\}_+\rangle\cdot(B, B) \geq M^2 \tag{A.1}$$

in the ferromagnetic case, where

$$(B, B) = \frac{1}{N}\sum_{\mathbf{q}}[J(\mathbf{q}) - J(\mathbf{q} - k)].\ \langle S_z(\mathbf{q})S_z(-\mathbf{q}) + \tfrac{1}{4}\{S_+(\mathbf{q}), S_-(-\mathbf{q})\}_+\rangle + \tfrac{1}{2}hM \tag{A.2}$$

and M is the magnetization $M = 1/N\sum_{\mathbf{R}}\langle S_z(\mathbf{R})\rangle$. We restrict the space dimension $d = 2$. In this case (B, B) can be written as

$$(B, B) = \frac{4J}{N}\sum_{\mathbf{q}}\left[\cos(q_x a)\sin^2\left(\frac{k_x a}{2}\right)\cdot + \cos(q_y a)\sin^2\left(\frac{k_y a}{2}\right)\right] * \langle S_z(-\mathbf{q})S_z(\mathbf{q}) + \tfrac{1}{4}\{S_+(\mathbf{q}), S_-(-\mathbf{q})\}_+ \rangle + \tfrac{1}{2}hM, \tag{A.3}$$

where we used the invariance of the correlation function with respect to space reflection to get equation (A.3). The sum over $\mathbf{q}$ can be performed formally by interchanging q_y and q_x in the second summand. One gets

$$(B, B) = \left[\sin^2\left(\frac{k_x a}{2}\right) + \sin^2\left(\frac{k_y a}{2}\right)\right]4F(h, T) + \tfrac{1}{2}hM \geqslant 0, \tag{A.4}$$

$$F(h, T) = \frac{J}{N}\sum_{\mathbf{q}}\cos(q_x a)\langle S_z(\mathbf{q})S_z(-\mathbf{q}) + \tfrac{1}{4}\{S_+(\mathbf{q}), S_-(-\mathbf{q})\}\rangle > 0. \tag{A.5}$$

The function $F(h, T)$ is essentially a spin-spin correlation function of nearest neighbour spins and is related to the expectation value of the model Hamiltonian. Furthermore, $F(h, T)$ is a bounded function and therefore the first term in equation (A.4) is bounded in the first Brillouin zone (BZ).

From the form of (B, B) one sees immediately that the division of equation (A.1) by (B, B) is not without problems, because $(B, B)^{-1}$ for $h = 0$ does diverge as k^{-2} $(k \to 0)$. Therefore the multiplication of equation (A.1) by $(B, B)^{-1}$ and the following integration over (BZ) result an inequality

$$\frac{\beta}{2} \int_{\mathrm{BZ}} d^2k \, \langle \{S_+(\mathbf{k}), S_-(-\mathbf{k})\}_+ \rangle \geq M^2 \int_{\mathrm{BZ}} d^2k (B, B)^{-1} \tag{A.6}$$

in which one may not put the explicit magnetic field dependence equal zero, because the lower bound would diverge by fixed magnetization M. On the other hand one may integrate over a smaller region as the BZ, e.g. $[2\pi/3, \pi/3; 2\pi/3, \pi/3]$. In this case the lower bound is explicitly given, and remains finite and > 0 at $h = 0$, if M is fixed. One sees in this manner that the method can not give any conclusion about the existence of finite magnetization at $h = 0$, because $F(0, T)$ is bounded. Another possibility is to multiply equation (A.1) by

$$\sin^2\left(\frac{k_x a}{2}\right) \cos\left(\frac{k_x a}{2}\right) \cdot (B, B)^{-1} \tag{A.7}$$

and to integrate over BZ. One gets

$$\begin{aligned} f(h, T) &= \frac{\beta}{2} \int_{\mathrm{BZ}} d_k^2 \, \langle \{S_+(\mathbf{k}), S_-(-\mathbf{k})\}_+ \rangle \sin^2\left(\frac{k_x a}{2}\right) \cos\left(\frac{k_x a}{2}\right) \\ &\geq \frac{\pi M^2}{2^{5/2}} \int_{z_1}^{z_3} dz \sqrt{ch(z) - 1 - 2c} \end{aligned} \tag{A.8}$$

$f(h, T)$ is a bounded function, $c = (\frac{1}{2} hM)/F(h, T)$ and $z_k = \mathrm{Arch}\,(k + 2c)$.

From this equation it follows again that one can not make any conclusion about the existence of the magnetization M.

The origin of the theorem of MW is the divergent behaviour of $(B, B)^{-1}$. Recapitulating one can say that this ambiguous division requires $h > 0$ and the inequality of MW can not be conclusive as we have demonstrated. On the right hand side of equation (A.6) the situation is very similar to the problem of the Fourier-transform of the susceptibility in the Ornstein-Zernike theory.

REFERENCES

[1] N. D. MERMIN and H. WAGNER, Phys. Rev. Lett. *17*, 1133 (1966).
[2] J. FRÖHLICH, B. SIMON and T. SPENCER, Phys. Rev. Lett. *36*, 804 (1976).
[3] F. J. DYSON, E. H. LIEB and B. SIMON, Phys. Rev. Lett. *37*, 120 (1976).
[4] S. GOLDEN, Phys. Rev. *137*, B1127 (1965).
[5] C. J. THOMPSON, J. Math. Phys. *6*, 1812 (1965); Ind. Univ. Math. J. *21*, 469 (1971); see also A. LENARD, Ind. Univ. Math. J. *21*, 457 (1971).
[6] J. SEGAL, Bull. Amer. Math. Soc. *75*, 1390 (1969).
[7] L. ONSAGER, Phys. Rev. *65*, 117 (1944); see also T. D. SCHULTZ, D. C. MATTIS and E. H. LIEB, Rev. Mod. Phys. *36*, 856 (1964).
[8] G. ROEPSTORFF, Comm. Math. Phys. *46*, 253 (1976).
[9] J. NAUDTS and A. VERBEURE, J. Math. Phys. *17*, 419 (1976).