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Phase transitions in quantum XY- and Heisenberg models: Critique of N. Szabo's discussion

by

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Abstract. We criticize three recent papers by Szabo which, among other results, claim to prove the existence of spontaneous magnetization at finite temperature in the two-dimensional quantum XY- and Heisenberg models with nearest neighbor interactions, in contradiction to the Mermin-Wagner theorem. We identify the errors in Szabo's arguments and show, in particular, why his discussion of the Mermin-Wagner proof is inadequate.

1. Introduction

About twelve years ago, Mermin and Wagner [1] proved the absence of spontaneous magnetization at any finite temperature in the two-dimensional quantum Heisenberg model with interactions decreasing sufficiently rapidly at infinity. Since then, there have been many adaptations and extensions of their theorem (see, for example, [2–4]) and, although there is ample evidence of the existence of a subtler type of phase transitions in two-dimensional XY- and Heisenberg models [5–7], there is no doubt that the original Mermin-Wagner's argument is correct.

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In three recent papers, however, (hereafter referred to as I, II, and III) N. Szabo has, in particular, claimed to prove the existence of spontaneous magnetization at non zero temperature in the quantum XY- and Heisenberg models with short-range interactions for a lattice dimension $d \geqslant 2$ [8]. This clearly contradicts the Mermin-Wagner theorem which, however, in the appendix of I, Szabo claims to refute. We quote his judgement: "... the inequality of MW (Mermin-Wagner) *can not* be conclusive as we have demonstrated" (I, p. 762).

After careful study of Szabo's arguments we have concluded that many of the statements in I, II, and III are erroneous, that most of the theorems are false, and that the discussion of the Mermin-Wagner argument is totally misleading. Our goal in this note is to point out the most important mistakes we have found in Szabo's work. In Section 2, we discuss briefly the Mermin-Wagner argument and show that the discussion in I casts no doubt on their validity. In Sections 3 and 4 we indicate the basic error common to all Szabo's proofs, specifically we show that his derivations of inequalities for the correlation functions are erroneous. Thence the arguments for the existence of spontaneous magnetization are incorrect. Section 5 is devoted to some concluding remarks.

2. Recapitulation of the Mermin-Wagner argument

We will not, of course, present all details, but will rather mention the original paper [1] and Ruelle's book [9] as references. We consider the Hamiltonian

$$-H_\Lambda = \sum_{r, r' \in \Lambda} J(r-r') \sum_{\alpha = x, y, z} S_r^\alpha S_{r'}^\alpha + h \sum_{r \in \Lambda} S_r^z \tag{2.1}$$

where $\Lambda \subset \mathbb{Z}^d$ is a finite region in the d-dimensional cubic lattice $\mathbb{Z}^d$; H_Λ acts on the $(2S+1)^{|\Lambda|}$-dimensional Hilbert space $\mathcal{H}_\Lambda = \otimes_{r \in \Lambda} \mathbb{C}^{(2S+1)}$, where $S = \frac{1}{2}, 1, \frac{3}{2}$, (spin-magnitude) and where $|\Lambda| < +\infty$ stands for the number of lattice sites in Λ. In (2.1) we have $J(-r) = J(r)$, $J(0) = 0$ and $h \in \mathbb{R}$, while the S^{α}'s are the spin operators obeying the usual commutation relations. The Bogoliubov inequality ([1], [9])

$$\frac{\beta}{2} \langle [A, A^*]_+ \rangle_\Lambda \langle [[C, H_\Lambda]_-, C^*]_- \rangle_\Lambda \geqslant |\langle [C, A]_- \rangle_\Lambda|^2 \tag{2.2}$$

is then valid for all linear operators A and C on $\mathcal{H}_\Lambda$. here $\langle\,\rangle_\Lambda$ denotes the thermal average at inverse temperature $\beta > 0$, and $[\,,\,]_{(\pm)}$ denotes (anti-) commutators. For a suitable choice of A and C one can get ([1], [9])

$$\frac{\beta}{2} \langle [S^+(k), S^-(-k)]_+ \rangle_\Lambda \langle [[C, H_\Lambda]_-, C^*]_- \rangle_\Lambda \geqslant |\Lambda|^2 m_\Lambda^2(h) \tag{2.3}$$

where

$$S^\pm(k) = \sum_{r \in \Lambda} \exp\left[-i \sum_{j=1}^{d} k_j r_j\right] S_r^\pm \tag{2.4}$$

$$S^\pm = S^x \pm i S^y \tag{2.5}$$

and

$$m_\Lambda(h) = |\Lambda|^{-1} \sum_{r\in\Lambda} \langle S_r^z \rangle_\Lambda \tag{2.6}$$

denotes the magnetization. The inequality (2.3) is the starting point of Szabo's considerations, and we are now going to discuss his errors. First of all, as far as the existence of *spontaneous order* defined by

$$m_S \equiv \lim_{h\to 0} \lim_{\Lambda\nearrow\mathbb{Z}^d} m_\Lambda(h) \tag{2.7}$$

is concerned, nobody has ever said that one should put $h = 0$ in (2.3) and then divide by $\langle[[C, H_\Lambda]_-, C^*]_-\rangle_\Lambda$ ($=(B, B)$ is Szabo's notation, see also [9]) both sides of the inequality; indeed, the basic idea behind the argument rests on Bogoliubov's concept of *quasi-averages* [10], and a symmetry breaking term like $h \sum_{r\in\Lambda} S_r^z$ should thus clearly be kept fixed through the whole procedure, including the infinite-volume limit; and, on the other hand, the relevance of the argument depends heavily on a suitable *strictly positive* upper bound for $\langle[[C, H_\Lambda]_-, C^*]_-\rangle_\Lambda$, having the right infrared behaviour; that bound is usually of the form

$$\langle[[C, H_\Lambda]_-, C^*]_-\rangle_\Lambda = (B, B) \leq |\Lambda|(ak^2 + |h|b)$$

with *strictly positive* a and b provided $\sum_{r\in\mathbb{Z}^d} r^2|J(r)| < +\infty$ (not too long range interactions), and we have then

$$\frac{\beta}{2}|\Lambda|\langle[S^+(k), S^-(-k)]_+\rangle\,(ak^2 + b|h|) \geq |\Lambda|^2 m_\Lambda^2(h)$$

from (2.3), or

$$\frac{\beta}{2}\langle[S^+(k), S^-(-k)]_+\rangle_\Lambda \geq |\Lambda| \frac{m_\Lambda^2(h)}{ak^2 + b|h|} \tag{2.8}$$

There is, therefore, no "ambiguous division by (B, B)" (I, loc. cit.) in those considerations, and standed manipulations, including indeed an integration over a suitable smaller region of the Brillouin zone than the Brillouin zone itself, then lead to the perfectly correct statement

$$m_S \equiv 0 \tag{2.9}$$

whenever $d = 1, 2$.

To illustrate the preceding considerations, one can start in particular from Szabo's formula (A.4) giving (B, B) for a two-dimensional square lattice of parameter $\tilde{a}$ and nearest-neighbor coupling J namely

$$(B, B) = \left[\sin^2\left(\frac{k_x\tilde{a}}{2}\right) + \sin^2\left(\frac{k_y\tilde{a}}{2}\right)\right] 4F(h; T) + \tfrac{1}{2} h m_\Lambda(h)$$

with

$$F(h; T) = |\Lambda|^{-1} J \sum_q \cos(q_x\tilde{a}) \langle S^z(q) S^z(-q) + \tfrac{1}{4}[S^+(q), S^-(-q)]_+\rangle_\Lambda$$

On the one hand, $F(h; T)$ is uniformly bounded in h and T by a strictly positive constant depending on S and J; on the other hand, $|m_\Lambda(h)| \leq S$ and since $\sin^2 x \leq x^2$ for all x, one gets the upper bound

$$\begin{aligned}(B, B) &\leq \tilde{a}^2 F(h; T)|k|^2 + S\,|h| \\ &\equiv \tilde{a}^2 F(h; T)|k|^2 + b\,|h| \\ &\leq a|k|^2 + b|h|\end{aligned}$$

Starting then from (2.8) and applying the standard considerations mentioned above, one ends up with an integral over the Brillouin zone that can still be bounded below by an integration over a *suitable* smaller region, in that case the sphere of radius π centered at the origin, suitable in the sense that the corresponding lower bound is explicit: we have indeed

$$(2\pi)^{-1} \int_{-\pi}^{+\pi} \frac{dk_x\, dk_y}{a\,|k|^2 + b\,|h|} \geq \int_0^{\pi} \frac{k\, dk}{a\,|k|^2 + b\,|h|} = (2a)^{-1} \log\left(1 + \frac{a\pi^2}{b\,|h|}\right) \tag{2.10}$$

which has the suitable *divergent behaviour* when $|h| \downarrow 0$: *even though $F(h; T)$ is bounded when $|h| \downarrow 0$, the explicit lower bound* (2.8) *does not lead to a finite value in that limit*, contrary to Szabo's statement claiming that "one may integrate over a smaller region as the BZ (Brillouin zone), 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." (loc. cit.).

Whereas it is true that one can also introduce a notion of *long-range order* that does not require $h \neq 0$ throughout (see for example the papers by Jasnow and Fisher [11] and McBryan and Spencer [12]), Mermin and Wagner never claimed to prove anything else than (2.9), which *does* require $h \neq 0$ according to the definition (2.7). In the next two sections, we shall discuss Szabo's correlation functions inequalities.

3. Correlation function inequalities

We have seen that all Szabo's results for the two-dimensional quantum XY- and Heisenberg models are in contradiction with the Mermin-Wagner theorem, and we now have to show where and why his proofs are incorrect.

The basic scheme of Szabo's arguments is essentially the same in I, II, and III. the partition function or the free energy of the models of interest (d-dimensional Ising-, XY- or Heisenberg models) is shown to be bounded in terms of the partition function or the free energy of the two-dimensional Ising model. On this basis, Szabo claims to derive inequalities for the corresponding correlation functions or their Fourier transforms. Using these inequalities, he finally concludes to the existence of long range order or spontaneous magnetization, using the established fact of the existence of long range order in the two-dimensional Ising model. His argument is particularly explicit in III which deals with spatially anisotropic interactions but contains the isotropic model as a particular case. In

Section 2 of III the method of I is used to obtain upper and lower bounds for the free energies of the d-dimensional quantum XY- and Heisenberg models in terms of the free energy of the Ising model of the same dimensionality, but with different interaction strength (see equations (14) and (18) of III). Szabo then correctly observes that these inequalities still hold if a positive contribution $\lambda\sigma_r^x\sigma_{r'}^x$ is added to the Hamiltonian in each term. From the monotonicity and the convexity of the free energies with respect to λ, Szabo then concludes that the inequalities are preserved for the derivatives with respect to λ; from this he directly obtains, therefore, bounds for the correlation functions! (See equations (19) and (20) of (III)). Whereas we believe that the inequalities (14) and (18) of (III) are correct, it is clear that the argument leading to the equations (19) and (20) of (III) is quite fallacious: monotonicity and convexity in λ do not imply that an inequality between functions holds for their derivatives as well. As a counter example, consider the two simple functions

$$f(\lambda)=\lambda^4+6a^2\lambda^2+a^4+b \tag{3.1}$$

$$g(\lambda)=4a\lambda^3+4a^3\lambda \tag{3.2}$$

with positive a and b. It is easy to check that f and g are both monotone increasing and convex for $\lambda>0$. Moreover

$$f(\lambda)-g(\lambda)=(\lambda-a)^4+b>0 \tag{3.3}$$

for *all* real λ, so that $f>g$. Nevertheless we have

$$f'(\lambda)-g'(\lambda)=4(\lambda-a)^3<0 \tag{3.4}$$

for $\lambda<a$, so that $f'<g'$ in this case. In Section 1 of III, the same false argument is used to derive inequalities between the correlation functions of Ising models on lattices of different dimensionalities (equations (12) and (13)). We note that, although the derivation is misleading (even equation (11) does not hold), the result is correct provided one does not require strict inequalities; indeed it is a simple consequence of the Griffiths-Kelly-Sherman (GKS) inequalities [13].

The error is repeated in Section 3 of I (see the proofs of lemma 1, lemma 2 and of the resulting theorem), where the equivalence between the spontaneous magnetization and the long-range order is discussed. In I and II, Szabo derives inequalities between free energies (equations (6) and (12) of (I); equations (3.4) and (3.17) of (II)). The free energies are then expressed as integrals over the correlation functions (equation (7) of (I); equation (3.18) of (II)). However, from the inequalities for the integrals, Szabo finally claims the validity of the corresponding inequalities for the integrands. That is clearly an unjustifiable argument.

At this stage, we have shown that the proofs of the correlation inequalities (equations (9) and (14) in (I); equations (3.5), (3.9), (3.10), (3.21) of II; equations (12), (13), (19), (20), (28) of III) are incorrect. In the case of the Ising model, the wrong argument leads nevertheless to a true result: for instance it is a classical application of the GKS theorems [13] to derive inequalities between the correlation functions of Ising models with different dimensionalities, provided however, that one *does not* require *strict* inequalities. In the case of the quantum XY- and Heisenberg models in two-dimensions, however, inequalities like (19) and (20) of (III) lead to results that are in direct contradiction to the Mermin-Wagner theorem [1], and, thus, cannot be valid. We shall examine this further in the next section.

4. Susceptibility inequalities and functions of positive type

In the Section (4) of II indeed, Szabo derives new correlation inequalities and susceptibility inequalities (equations (4.4) and (4.9) of II) in direct space from the corresponding inequalities in the reciprocal space (equations (3.5), (3.21), (4.7) and (4.8) of II).

Unfortunately, his derivation based on Bochner's theorem characterizing functions of positive type, or positive definite functions [14], is again quite fallacious. The error is based on the fact that the expression "positive definite" is used to describe two entirely different concepts in Szabo's formulation, which makes already his quotation of Bochner's theorem erroneous (theorem 4.1 of II): the "positive definiteness" of $\hat{p}$, in that formulation, actually means that $\hat{p}$ is non-negative as a function on the Brillouin zone, namely $\hat{p}(q) \geqslant 0$ for all q. That is indeed the only possible reader's interpretation to get consistency with the original Bochner's theorem [14]; the "positive definiteness" of f, however, means that the quadratic form on $\mathbb{C}^n$ with matrix elements $A_{\alpha\beta} = f(\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta)$ is hermitean positive for all $\boldsymbol{x}_\alpha, \boldsymbol{x}_\beta \in \mathbb{R}^d$, namely

$$\sum_{\alpha,\beta=1}^{n} C_\alpha \bar{C}_\beta f(\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta) \geqslant 0 \qquad (4.1)$$

for all $C_\alpha \in \mathbb{C}$ and $n \in \mathbb{N}$; obviously, as follows from elementary linear algebra, condition (4.1) does not imply $f(\boldsymbol{x}_\alpha) \geqslant 0$ for all $\boldsymbol{x}_\alpha \in \mathbb{R}^d$, nor does this last non-negatively condition imply (4.1). It is, nonetheless, this confusion that led, as we shall see, to the other erroneous statements of Section 4 of II. Consider indeed the Ising Hamiltonian

$$-h_\Lambda = J \sum_{\langle \boldsymbol{x},\boldsymbol{y}\rangle \in \Lambda} \sigma_{\boldsymbol{x}} \sigma_{\boldsymbol{y}} \qquad (4.2)$$

In a finite square region Λ around the origin with periodic boundary conditions, with nearest neighbor ferromagnetic coupling $J > 0$ and $\sigma_{\boldsymbol{x}} = \mp 1$ for all $\boldsymbol{x}$. Define the two-point correlation function

$$f_d(x) = \langle \sigma_{(x, x_2, \ldots, x_d)} \sigma_{(0, x_2 \cdots x_d)} \rangle_\Lambda(J) \qquad (4.3)$$

where $x_2, \ldots, x_d \in \mathbb{Z}$ are kept fixed once and for all; here $\langle\,\rangle_\Lambda$ stands for the thermal average at inverse temperature $\beta > 0$ defined from (4.2). Defining similarly

$$f_{d-1}(x) = \langle \sigma_{(x, x_2 \cdots x_{d-1})} \sigma_{(0, x_2 \cdots x_{d-1})} \rangle_{\Lambda'}(J) \qquad (4.5)$$

where Λ' is Λ restricted to $\mathbb{Z}^{d-1}$ considered as the hyperplane of $\mathbb{Z}^d$ orthogonal to the d^{th} direction, Szabo claims to show through Bochner's theorem that

$$d\langle \sigma_{(x, x_2 \ldots, x_d)} \sigma_{(0, x_2 \cdots x_d)} \rangle_\Lambda(J) \geqslant (d-1) \langle \sigma_{(x, x_2 \cdots x_{d-1})} \sigma_{(0, x_2 \cdots x_{d-1})} \rangle_{\Lambda'}(J) \qquad (4.6)$$

holds for all x (equation (4.4) in II), whenever

$$d\hat{\chi}_d(q;J) \geq (d-1)\hat{\chi}_{d-1}(q;J) \tag{4.7}$$

is valid for all q of the Brillouin zone (equation (3.5) in II), providing the relations

$$\hat{\chi}_d(q;J) = |\Lambda''|^{-1} \sum_{x\in\Lambda''} \exp[iqx] f_d(x) \tag{4.8}$$

$$\hat{\chi}_{d-1}(q;J) = |\Lambda''|^{-1} \sum_{x\in\Lambda''} \exp[iqx] f_{d-1}(x) \tag{4.8'}$$

where Λ'' is Λ restricted to the first direction $\mathbb{Z}$ (equation (3.6) of II, up to a temperature factor; actually, Szabo claims to show much more, namely a strict inequality in (4.6) from a strict inequality in (4.7)!). Unfortunately, his argument if *false*: the inequality (4.6) cannot be "the direct consequence of the above theorem (Bochner's theorem)" (p. 913 of II, following theorem (4.9)). From (4.8), (4.8′), we have indeed

$$df_d(x) - (d-1)f_{d-1}(x) \equiv F_d(x)$$
$$= \sum_{q\in\Delta} \exp[-iqx]\{d\hat{\chi}_d(q;J) - (d-1)\hat{\chi}_{d-1}(q;J)\} \tag{4.9}$$

Since $d\hat{\chi}_d(q;J) - (d-1)\hat{\chi}_{d-1}(q;J) \geq 0$ according to (4.7), the function F_d is obviously of positive type in the sense of (4.1) since

$$\sum_{\alpha,\beta=1}^{n} C_\alpha \bar{C}_\beta F_d(x_\alpha - x_\beta) = \sum_q \left| \sum_{\alpha=1}^{n} C_\alpha e^{iqx_\alpha} \right|^2 \{d\hat{\chi}_d(q;J) - (d-1)\hat{\chi}_{d-1}(q;J)\} \geq 0 \tag{4.10}$$

for all x_α, $x_\beta \in \mathbb{Z}$ and all $C_\alpha \in \mathbb{C}$; as we mentioned above, however, this *does not* imply $F_d(x) \geq 0$ for all x, namely

$$df_d(x) \geq df_{d-1}(x) \tag{4.11}$$

which is nevertheless Szabo's statement in corollary (4.2) (our inequality 4.6). (Counterexample: $F(x) = \cos x$ is positive definite in the sense of (4.1), but has negative parts!)

5. Conclusion

We have identified many errors in Szabo's papers and shown why his discussion of the Mermin-Wagner theorem is inadequate; there is no doubt whatsoever regarding the validity of that theorem. On the other hand, the existence of spontaneous magnetization at finite temperature for a class of classical and quantum XY- and Heisenberg models for $d \geq 3$ has been proved in

[15] and [16]. The problem is still open, however, for the *ferromagnetic quantum* Heisenberg model with $d \geqslant 3$, for which Szabo's discussion does not help anything.

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REFERENCES

[1] N. D. MERMIN and H. WAGNER, Phys. Rev. Lett. *17*, 1133 (1966).
[2] N. D. MERMIN, J. Math. Phys. *8*, 1061 (1967).
[3] P. A. VUILLERMOT and M. V. ROMERIO, Commun. Math. Phys. *41*, 281 (1975).
[4] P. A. VUILLERMOT, J. Phys. A: Math. Gen. *10*, 1319 (1977).
[5] H. E. STANLEY and T. A. KAPLAN, Phys. Rev. Lett. *17*, 913 (1966).
[6] J. M. KOSTERLITZ and D. J. THOULESS, J. Phys. C*6*, 1181 (1973); J. M. KOSTERLITZ, J. Phys. C7, 1046 (1974).
[7] J. V. JOSE, L. P. KADANOFF, S. KIRKPATRICK and D. R. NELSON, Phys. Rev. B*16*, 1217 (1977).
[8] N. SZABO, I. Helv. Phys. Acta *50*, 757 (1977); II *ibid. 50*, 905 (1977); III *ibid 51*, 167 (1978).
[9] D. RUELLE, *Statistical Mechanics, Rigorous Results*, (Benjamin, N.Y. 1969).
[10] N. N. BOGOLIUBOV JR., *A Method for Studying Model Hamiltonians*; *A Minimax Principle for Problems in Statistical Physics*, (Pergamon, N.Y. 1972). See the introduction p. 16–24.
[11] D. JASNOW and M. E. FISHER, Phys. Rev. B*3*, 895 (1971); M. E. FISHER and D. JASNOW, Phys. Rev. B*3*, 907 (1971).
[12] O. A. MCBRYAN and T. SPENCER, Commun Math. Phys. *53*, 299 (1977).
[13] R. B. GRIFFITHS, J. Math. Phys. *8*, 478 (1967); D. G. KELLY and S. SHERMAN, J. Math. Phys. *9*, 466 (1968). See also R. B. GRIFFITHS, in Phase Transitions and Critical Phenomena, edited by C. Domb and M. S. Green (Academic, London, 1972). Vol. 1, p. 7.
[14] S. BOCHNER, "Lectures on Fourier Integrals", Annals of Mathematical Studies No. 42 (Princeton University Press, Princeton, N.J. 1959).
[15] J. FRÖHLICH, B. SIMON and T. SPENCER, Commun. Math. Phys. *50*, 79 (1976).
[16] F. J. DYSON, E. H. LIEB and B. SIMON, Phys. Rev. Lett. *37*, 120 (1976); J. Stat. Phys. *18*, 335 (1978).