

MAGNETIC ORDERING IN ONE AND TWO-DIMENSIONAL SYSTEMS

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The Mermin-Wagner inequalities^[2] are extended to the anisotropic case. The impossibility of magnetic order in the anisotropic Heisenberg model is proved in the one-dimensional case. In the case of two-dimensional systems the Mermin-Wagner inequality imposes a restriction on the transition temperature.

1. The number of exact results referring to the theory of phase transitions has until recently been small. However, several years ago Hohenberg^[1] rigorously derived Bogolyubov's inequality (see below) and it became possible to set up a series of exact relations. Hohenberg himself proved that the presence of nonzero anomalous pairing or of quasi-averages (a gap Δ in the case of superconductivity and a condensate density n_0 in the case of superfluidity) in one- and two-dimensional cases contradicts the Bogolyubov inequality. It follows hence that superconductivity and superfluidity are impossible in one- and two-dimensional systems. An analogous treatment was carried out by Mermin and Wagner^[2] for an isotropic Heisenberg model. They proved that in an external field h directed along the z axis the projection of the magnetization vector on the field direction satisfies the following inequalities:

$$S_z < \frac{\text{const}}{T^{1/2}} |h|^{1/2} \quad (\text{one-dimensional case}), \quad (1)$$

$$S_z < \frac{\text{const}}{T^{1/2}} \frac{1}{\gamma |n| |h|} \quad (\text{two-dimensional case}). \quad (2)$$

It follows hence directly that ferromagnetism and antiferromagnetism in one- and two-dimensional systems are impossible for such a model. These results would, of course, also follow from the theory of spin waves, however, the existence of spin waves in such systems has itself not been established. It is analogously readily shown that the spin correlation function of the spins

$$\chi(\mathbf{k}, \omega) = \sum_j e^{i\mathbf{k}\cdot\mathbf{j}} \langle S_j(t) S_j(0) \rangle_\omega$$

also diverges for such systems; $\langle \dots \rangle_\omega$ denotes the Fourier transform in time. From this formula it is seen that

$$\langle S_i(t) S_i(0) \rangle_\omega = \frac{1}{(2\pi)^d} \int \chi(\mathbf{k}, \omega) d\mathbf{k}.$$

Taking also into account that for $\omega = 0$, $\chi(\mathbf{k}, 0) \sim 1/\omega_{\mathbf{k}}$, where for the isotropic model

$$\omega_{\mathbf{k}} = [J(0) - J(k)] \sim k^2,$$

we obtain the above-mentioned divergence of the correlation function.

However, it is clear that for an anisotropic Heisenberg model the preceding inequalities should change. This is also apparent from the fact that, as is well known, the two-dimensional Ising model admits the ex-

istence of a phase transition and the Ising model can be considered as the limiting case of the anisotropic Heisenberg model.

2. In order to derive our inequalities we write down the Bogolyubov relation

$$\langle \{A, A^+\} \times [CHC^+] \rangle \geq T |\langle [C, A] \rangle|^2. \quad (3)$$

Here the Hamiltonian \hat{H} is chosen in the following form:

$$\hat{H} = - \sum_{\mathbf{R}, \mathbf{R}'} J(\mathbf{R} - \mathbf{R}') S(\mathbf{R}) S(\mathbf{R}') + \sum_{\mathbf{R}, \mathbf{R}'} \alpha(\mathbf{R} - \mathbf{R}') S_z(\mathbf{R}) S_z(\mathbf{R}'),$$

α is the anisotropy energy, A and C are arbitrary operators, the curly brackets denote an anticommutator and the square brackets—a commutator.

Following Mermin and Wagner, we choose in the Bogolyubov inequality

$$A = S_-(-\mathbf{k}); \quad C = S_+(\mathbf{k}),$$

where

$$S_i(\mathbf{k}) = \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} S_i(\mathbf{R})$$

is the Fourier component of $S_i(\mathbf{R})$. The results of simple commutation are completely analogous to those of Mermin and Wagner^[2]:

$$\langle \{A, A^+\} \rangle = 2(S_x^2(0) + S_y^2(0)) = 2 \sum_{\mathbf{R}} S_x^2(\mathbf{R}) + S_y^2(\mathbf{R}) < 2S(S+1)$$

(here we imply successive integration over \mathbf{k})

$$\begin{aligned} \langle [CHC^+] \rangle &\leq \left\langle \sum_{\mathbf{R}} \left[J(\mathbf{R}) (1 - e^{i\mathbf{k}\cdot\mathbf{R}}) S(S+1) \right. \right. \\ &\quad \left. \left. + \alpha(\mathbf{R}) S_x^2 - \alpha(\mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}} \frac{1}{2} \{S_+, S_-\} \right] \right\rangle \end{aligned}$$

$$[C, A] = 2S_z(0) = 2 \sum_{\mathbf{R}} S_z(\mathbf{R}).$$

Introducing the notation

$$\Gamma = \sum_{\mathbf{R}} [J(\mathbf{R}) + \alpha(\mathbf{R})] R^2 S(S+1), \quad \gamma = \sum_{\mathbf{R}} \alpha(\mathbf{R})$$

and substituting the cited results in the new notation into Bogolyubov's inequality, we obtain

$$S(S+1) > \frac{T}{\rho(2\pi)^d} \int \frac{S_z^2}{|\Gamma|k^2 + |\gamma|S_z^2}, \quad (4)$$

where ρ^{-1} is the volume per spin.

Integrating over \mathbf{k} (assuming the volume to be infinite, we replace the summation by integration) over the first Brillouin zone, which can only make inequality (3) stronger, we obtain:

in the one-dimensional case

$$T < 2\pi \frac{\sqrt{|\Gamma\gamma|}}{|S_z|} S(S+1) \left/ \arctg \frac{k_0}{|S_z|} \sqrt{\frac{|\Gamma|}{|\gamma|}} \right.; \tag{5}$$

and in the two-dimensional case

$$T < (2\pi)^2 \frac{|\Gamma|}{S_z^2} S(S+1) \left/ \ln \left(1 + \frac{k_0^2 |\Gamma|}{|\gamma| S_z^2} \right) \right. \tag{6}$$

Here k_0 is the Brillouin zone boundary. For an anisotropy energy $\alpha \rightarrow 0$ formulas (5) and (6) go over into the inequalities (1) and (2) of Mermin and Wagner. When $J \rightarrow 0$ the Hamiltonian H corresponds to the Ising model. For $\Gamma \rightarrow 0$ we obtain the so-called X–Y model. For this model the inequalities (5) and (6) yield

$$T < 2\pi |\gamma| S(S+1) / k_0 \quad \text{in the one-dimensional case,}$$

$$T < (2\pi)^2 |\gamma| S(S+1) / k_0^2 \quad \text{in the two-dimensional case.}$$

Thus, in the form of Mermin and Wagner the inequalities (5) and (6) do not forbid ferromagnetism in one-dimensional systems, i.e., for such systems there is not sufficient ‘‘accuracy’’ for this inequality. Our mention of the X–Y model here is not accidental. As is well known, in the spin model of superconductivity (and superfluidity) it is precisely this model which corresponds to the BCS theory. We shall see below that the presence of the polarization S_z contradicts the Bogolyubov inequality only in the one-dimensional case (for an anisotropic system). However, here there is no lack of correspondence with Hohenberg’s results,^[1] since in the X–Y model the polarization S_x corresponds to a gap and for the former one can readily obtain the inequality

$$S_x^2 < \frac{S(S+1)}{T} \int \frac{dk}{(2\pi)^d} \frac{1}{|\Gamma|k^2}$$

Thus the choice of the operators A and C in the form of Mermin and Wagner for the anisotropic model is unfortunate. This is also clear from the fact that in this case

$$\omega_k = [J(0)(J(0) - J(k))]^{1/2} \propto k,$$

whence it follows that in the one-dimensional case the spin correlation function diverges.

Choosing now in the appropriate normalization

$$C = S_z + iS_y, \quad A = S_-(-k),$$

we obtain the following inequality:

$$|S_z|^2 < \frac{S(S+1)}{T} (2\pi)^d \int \frac{dk}{|\gamma|k}$$

Thus, while the introduction of an arbitrarily small anisotropy permits ordering in the two-dimensional case, in the one-dimensional case the anisotropy does not ‘‘save’’ the situation. It is interesting to note that one can also derive certain limitations on the quantity S_z from below which immediately clarify the situation in the one-dimensional case. To this end we choose

$$C = S_+(k); \quad A = S_z(-k)$$

and introduce the additional notation

$$\delta = \langle S_+ \rangle^2.$$

The result of commutation then yields the following inequality:

$$S_z^2 (|\Gamma|k^2 + |\gamma|S_z^2) \geq T\delta.$$

Since we are interested in the case of small S_z (in the vicinity of the transition temperature), at a finite temperature this inequality is equivalent to

$$S_z > \sqrt{T} \int \frac{\text{const}}{k} dk. \tag{7}$$

It follows from (7) and (5) that in the one-dimensional case ferromagnetism is also impossible for an anisotropic Heisenberg model.

Of course, if one retains in (7) the quantity $|\gamma|S_z^2$ in the numerator, then the derivation of the contradiction of this inequality in the one-dimensional case remains. If one takes into account the possibility that $\delta = 0$, then substituting this condition in (3) and taking into account the fact that $\langle \{A, A^*\} \rangle \sim \delta$, we also obtain $S_z = 0$. We note that analogous inequalities can also be obtained for $\chi(k, \omega)$.

3. In conclusion, we make several remarks.

1) One can easily include in our treatment an external magnetic field h parallel to the z axis. This adds to the Hamiltonian the term

$$H' = -h \sum_{\mathbf{R}} S_z(\mathbf{R}), \tag{8}$$

and in all the results a term $|hS_z|$ is added to $|\gamma|S_z^2$.

2) One can take into account the presence of antiferromagnetism by introducing into expression (8) the factor $\exp(i\mathbf{k} \cdot \mathbf{R})$ which takes on values of ± 1 depending on the sublattice to which \mathbf{R} belongs.

3) Bogolyubov’s inequality in its complete form has the following appearance:

$$\langle \{A - \langle A \rangle, A^+ - \langle A^+ \rangle\} \rangle \langle [CH]C^+ \rangle \geq T \langle [C, A] \rangle^2.$$

Formula (3) is hence obtained under the assumption that the averages $\langle A \rangle$ and $\langle A^+ \rangle$ in the left-hand side of the inequality are negligibly small. This is admissible for proving that the existence of quasi-averages is impossible; however, for accurate estimates of the transition temperature one must use the complete form of Bogolyubov’s inequality.

4) Inequalities analogous to those of Hohenberg^[1] can be proved for systems finite in one or two dimensions. This proof is carried out for quantities integrated over the ‘‘cross section’’ or by using the complete system of functions depending not only on k but also on the integer n which numbers the bands that appear as a result of the quantization of the transverse dimension. A derivation analogous to that of Hohenberg^[1] then leads to the absence of anomalous pairing in each band (their presence would contradict Bogolyubov’s inequality).

5) In order for the above treatment to be valid one requires a finite radius of interaction or, more accurately, that the series for Γ and γ converge.

6) In transforming the inequalities, we have made them weaker; this leads to a change in the numerical coefficients but does not change the dependence of S_z on the temperature, the magnetic field, and the anisotropy energy.

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²N. Mermin and G. Wagner, Phys. Rev. Letters 17, 1133 (1966).

¹P. C. Hohenberg, Phys. Rev. 158, 383 (1967).

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