Absence of Spontaneous Magnetic Order at Nonzero Temperature in One- and Two-Dimensional Heisenberg and XY Systems with Long-Range Interactions

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The Mermin-Wagner theorem is strengthened so as to rule out magnetic long-range order at T>0 in one- or two-dimensional Heisenberg and XY systems with long-range interactions decreasing as $R^{-\alpha}$ with a sufficiently large exponent α . For oscillatory interactions, ferromagnetic long-range order at T>0 is ruled out if $\alpha \geq 1(D=1)$ or $\alpha > 5/2(D=2)$. For systems with monotonically decreasing interactions, ferro- or antiferromagnetic long-range order at T>0 is ruled out if $\alpha \geq 2D$.

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 $H = -\sum_{\mathbf{R},\mathbf{R}'} [J'_{\mathbf{R}-\mathbf{R}'} S^{x}_{\mathbf{R}} S^{x}_{\mathbf{R}'} + J_{\mathbf{R}-\mathbf{R}'} (S^{y}_{\mathbf{R}} S^{y}_{\mathbf{R}'} + S^{z}_{\mathbf{R}} S^{z}_{\mathbf{R}'})] + K \sum_{\mathbf{R}} (S^{x}_{\mathbf{R}})^{2} - B \sum_{\mathbf{R}} S^{z}_{\mathbf{R}}.$ (2)

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In a seminal paper exploiting a thermodynamic inequality due to Bogoliubov [1], Mermin and Wagner proved the following important theorem [2]: "For one- or two-dimensional Heisenberg systems with isotropic interactions, and such that the interactions are short ranged, namely, which satisfy the condition

$$\sum_{\mathbf{R}} \mathbf{R}^2 |J_{\mathbf{R}}| < +\infty, \tag{1}$$

there can be no spontaneous ferro- or antiferromagnetic long-range order at T>0 [3]." In view of the fact that most of our knowledge of critical phenomena and phase transitions is based upon approximate theories, the few known rigorous results [4] such as the Mermin-Wagner theorem are of key importance, for they allow one to test the validity of approximate theories.

For interactions with a finite range or with an exponential decay, the condition (1) is trivially satisfied. For interactions with a power-law decay $|J_{\mathbf{R}}| \propto R^{-\alpha}$, condition (1) is satisfied provided that $\alpha > D + 2$, where D is the dimensionality. In metallic magnetic systems, the exchange interactions are of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type [5], which have a long-range oscillatory behavior for large R: $J_{\mathbf{R}} \propto R^{-D} \cos(q_0 R + \phi)$. It is obvious that the RKKY interactions do not satisfy the criterion of short rangedness (1), so that no conclusion on the magnetism one- and two-dimensional RKKY systems can be obtained from the Mermin-Wagner theorem. This situation is highly unsatisfactory, in view of the fact that most magnetic ultrathin films investigated experimentally consist of metals and alloys.

In the present paper, I extend the result of Mermin and Wagner to Heisenberg and XY systems with a *long-range interaction*, i.e., which do not satisfy the condition (1), with particular emphasis on systems with oscillatory interactions. Results for systems with monotonically decaying interactions are also presented. More specifically, I consider one- and two-dimensional systems described by the following Hamiltonian:

We also define the Fourier transform of the spin operator S_R , $S(\mathbf{k}) \equiv \sum_R S_R e^{-i\mathbf{k} \cdot \mathbf{R}}$, as well as $E(\mathbf{k}) \equiv \sum_R J_R (1 - e^{i\mathbf{k} \cdot \mathbf{R}}) = E(-\mathbf{k})$, and $\tilde{E}(\mathbf{k}) \equiv \sum_R |J_R| (1 - e^{i\mathbf{k} \cdot \mathbf{R}}) = \tilde{E}(-\mathbf{k})$. For K = 0 and $J_R' = J_R$, the above Hamiltonian corresponds to the isotropic Heisenberg model. In the general case, it corresponds to a system with uniaxial anisotropy of axis x, with a single-spin anisotropy (for $S \ge 1$) and/or a two-spin exchange anisotropy. Depending on the value of the anisotropy parameters K and $J_R' - J_R$, one therefore has either an isotropic system, an XY-like system with yz easy plane, or an Ising-like model with x easy axis (in the latter case, one merely shows that the spontaneous magnetization has to be along the x axis). For such systems (with arbitrary values of parameters J_R' and K), I prove the following results:

Theorem 1.—A *D*-dimensional (D = 1 or 2) Heisenberg or *XY* system for which one can find some numbers $k_0 > 0$ [with k_0 belonging to the first Brillouin zone (BZ)], $\alpha > 0$, $\beta \le 1$, such that, for $|\mathbf{k}| < k_0$ and $|\mathbf{k}'| < k_0$,

$$|E(\mathbf{k})| \le \alpha |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^{\beta}, \tag{3a}$$

$$|E(\mathbf{k}' - \mathbf{k}) + E(\mathbf{k}' + \mathbf{k}) - 2E(\mathbf{k}')|$$

$$\leq \alpha |\mathbf{k}|^{D} |\ln(|\mathbf{k}|^{-1})|^{\beta}, \tag{3b}$$

$$\frac{1}{A_D} \int d^D \mathbf{k}'' |E(\mathbf{k}'' - \mathbf{k}) + E(\mathbf{k}'' + \mathbf{k}) - 2E(\mathbf{k}'')|$$

$$\leq \alpha |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^{\beta}, \quad (3c)$$

cannot be ferromagnetic [6].

Corollary 1.—A *D*-dimensional (D = 1 or 2) Heisenberg or *XY* system with long-range oscillatory interactions of the form

$$J_{\mathbf{R}} \propto \frac{\cos(q_0 R + \phi)}{R^{\alpha}},$$
 (4)

with $q_0 \neq 0$ belonging to the first BZ and $\alpha \geq 1$ (D = 1), or $\alpha > 3/2 [D = 2, \sin(\phi + \pi/4) = 0]$, or $\alpha > 5/2 [D =$ $2, \sin(\phi + \pi/4) \neq 0$ cannot be ferromagnetic.

Theorem 2.—A *D*-dimensional (D = 1 or 2) Heisenberg or XY system satisfying

$$\frac{1}{A_D} \int d^D \mathbf{k} \frac{1}{\tilde{E}(\mathbf{k})} = +\infty, \tag{5}$$

where A_D is the measure of the first BZ, cannot be ferroor antiferromagnetic.

Corollary 2.—A *D*-dimensional (D = 1 or 2) Heisenberg or XY system with interactions monotonically decaying as $|J_{\mathbf{R}}| \propto R^{-\alpha}$ with $\alpha \geq 2D$ cannot be ferro- or antiferromagnetic.

Proof of Theorem 1.—As for the Mermin-Wagner theorem, the proof of Theorem 1 relies on using the Bogoliubov inequality to prove that the z component of the spontaneous magnetization $\lim_{B\to 0} |\langle S^z \rangle|$ vanishes for any finite temperature. The proof of Theorem 1 is, however, significantly more delicate than the Mermin-Wagner one.

Our proof proceeds by reductio ad absurdum. Let us assume that the system is ferromagnetic. This implies that one can find a temperature $T_0 > 0$ and a quantity $m_0 > 0$ such that, for any temperature $T \le T_0$, one has $|\langle S^z \rangle| \geq m_0.$

Bogoliubov inequality [1] $\langle \{A, A^{\dagger}\} \rangle \langle [[C, H], C^{\dagger}] \rangle \ge 2\hat{k}_B T |\langle [C, A] \rangle|^2$, where A and C are arbitrary operators, [A, B] is the commutator of A and B, $\{A, B\}$ is the anticommutator of A and B, and $\langle A \rangle$ is the thermodynamic average of A. The two factors on the left-hand side of the inequality are ≥ 0 . We use Bogoliubov's inequality for $A \equiv S^{y}(-\mathbf{k})$ and $C \equiv S^{x}(\mathbf{k})$. Straightforward algebra together with the inequality $\langle (S_{\mathbf{R}}^{y})^{2} \rangle \leq S^{2}$ then yield the following inequality:

$$S^{2} \ge \frac{1}{A_{D}} \int d^{D}\mathbf{k} \, \frac{k_{B}T\langle S^{z}\rangle^{2}}{B\langle S^{z}\rangle + 2\sum_{\mathbf{R}} J_{\mathbf{R}}[1 - \cos(\mathbf{k} \cdot \mathbf{R})]\langle S_{0}^{y}S_{\mathbf{R}}^{y} + S_{0}^{z}S_{\mathbf{R}}^{z}\rangle}.$$
(6)

with

Note that the above result is independent of $J'_{\mathbf{R}}$ and K, and depends only on $J_{\mathbf{R}}$. Thus far, our proof follows exactly the one of Mermin and Wagner. From this point, Mermin and Wagner proceed by stating that, if the condition (1) is satisfied, the (positive) denominator $\Delta(\mathbf{k})$ of the above equation can be majorated near $\mathbf{k} = 0$ by an expression of the form $|B|S + \alpha k^2$ (with $\alpha > 0$), from which they then easily show that the spontaneous magnetization vanishes.

In order to obtain a stronger theorem, i.e., to rule out ferromagnetism for a broader class of systems, one therefore needs to find a tighter majoration of $\Delta(\mathbf{k})$ than used by Mermin and Wagner. One can check easily that a majoration of the form $\Delta(\mathbf{k}) \leq |B|S + \gamma |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^\beta$ near $\mathbf{k} = 0$, with $\gamma > 0$ and $\beta \leq 1$, would be sufficient for our purpose.

To this aim, we rewrite the denominator $\Delta(\mathbf{k})$ of Eq. (6)

$$\Delta(\mathbf{k}) = B\langle S^z \rangle + 2\langle S^z \rangle^2 E(\mathbf{k})$$

$$+ \frac{1}{A_D} \int d^D \mathbf{k}' [E(\mathbf{k}' - \mathbf{k}) + E(\mathbf{k}' + \mathbf{k}) - 2E(\mathbf{k}')] F(\mathbf{k}'),$$
(7)

 $F(\mathbf{k}) \equiv \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} \langle S_0^y S_{\mathbf{R}}^y + \delta S_0^z \delta S_{\mathbf{R}}^z \rangle$ $= \frac{1}{N} \langle |S^{y}(\mathbf{k})|^{2} + |\delta S^{z}(\mathbf{k})|^{2} \rangle$ $= k_B T [\chi^{yy}(\mathbf{k}) + \chi^{zz}(\mathbf{k})],$

(8)

where we have introduced the longitudinal fluctuation $\delta S_{\mathbf{R}}^z \equiv S_{\mathbf{R}}^z - \langle S^z \rangle$ and the transverse and longitudinal **k**-dependent susceptibilities $\chi^{yy}(\mathbf{k})$ and $\chi^{zz}(\mathbf{k})$, respectively. Since we are assuming that the system has a long-range ferromagnetic order, one can argue that $F(\mathbf{k})$ has to be finite for $\mathbf{k} \neq 0$; otherwise the ferromagnetic order would be unstable against fluctuations of the nonzero wave vector. On the other hand, $F(\mathbf{k})$ certainly diverges for $\mathbf{k} = 0$ due to the divergence of the static transverse susceptibility of systems having a continuous rotational invariance. Nevertheless, one has

$$\frac{1}{A_D} \int d^D \mathbf{k} \, F(\mathbf{k}) = \langle (S^y)^2 + (S^z)^2 \rangle \le S(S+1). \tag{9}$$

In view of the above remarks concerning $F(\mathbf{k})$, there exists a number $F_0 > 0$ such that $0 \le F(\mathbf{k}) \le F_0$ for $|\mathbf{k}| > k_0$. Making use of conditions (3b) and (3c), one can therefore write, for $|\mathbf{k}| < k_0$,

$$A(\mathbf{k}) \equiv \frac{1}{A_D} \int d^D \mathbf{k}' |E(\mathbf{k}' - \mathbf{k}) + E(\mathbf{k}' + \mathbf{k}) - 2E(\mathbf{k}')|F(\mathbf{k}')$$

$$\leq \frac{1}{A_D} \int_{|\mathbf{k}'| < k_0} d^D \mathbf{k}' \alpha |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^\beta F(\mathbf{k}') + \frac{1}{A_D} \int_{|\mathbf{k}'| > k_0} d^D \mathbf{k}' |E(\mathbf{k}' - \mathbf{k}) + E(\mathbf{k}' + \mathbf{k}) - 2E(\mathbf{k}')|F_0$$

$$\leq \frac{1}{A_D} \int d^D \mathbf{k}' \alpha |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^\beta F(\mathbf{k}') + \frac{1}{A_D} \int d^D \mathbf{k}' |E(\mathbf{k}' - \mathbf{k}) + E(\mathbf{k}' + \mathbf{k}) - 2E(\mathbf{k}')|F_0$$

$$\leq [S(S+1) + F_0] \alpha |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^\beta. \tag{10}$$

137203-2 137203-2 Combining this result with condition (3a), we obtain

$$0 \le \Delta(\mathbf{k}) \le |B|S + \gamma |\mathbf{k}|^D |\ln(|\mathbf{k}|^{-1})|^{\beta}, \quad (11)$$

for $|\mathbf{k}| < k_0$, with $\gamma \equiv S^2 + S(S+1) + F_0 > 0$. Combining the above result with inequality (6), one obtains

$$S^{2} \geq \frac{1}{A_{D}} \int_{|\mathbf{k}'| < k_{0}} d^{D}\mathbf{k}' \frac{k_{B}T \langle S^{z} \rangle^{2}}{|B|S + \gamma |\mathbf{k}|^{D} |\ln(|\mathbf{k}|^{-1})|^{\beta}},$$
(12)

from which one shows immediately that $\lim_{B\to 0} |\langle S^z \rangle| = 0$ for T > 0, which is in contradiction with our hypothesis that the system is ferromagnetic. This completes the proof of Theorem 1 by *reductio ad absurdum*. \square

Proof of Corollary 1.—Consider interaction of the form of Eq. (4). To investigate the behavior of $E(\mathbf{k})$ in the vicinity of $\mathbf{k}=0$, we can substitute the discrete sum over \mathbf{R} by an integral. One can show easily that, for any value of α , $E(\mathbf{k})$ is analytical for all wave vectors except for $|\mathbf{k}|=q_0$. Therefore, for $\mathbf{k}\to 0$,

$$E(\mathbf{k}) \propto |\mathbf{k}|^2 \qquad (\forall \ \alpha), \tag{13}$$

and, for $\mathbf{k} \to 0$ and $|\mathbf{k}| < ||\mathbf{k}'| - q_0|$,

$$|E(\mathbf{k}' - \mathbf{k}) + E(\mathbf{k}' + \mathbf{k}) - 2E(\mathbf{k}')| \propto |\mathbf{k}|^2 \qquad (\forall \alpha).$$
(14)

The integral over \mathbf{k}'' in (3c) is dominated by the nonanalyticity of $E(\mathbf{k})$ in the vicinity of $|\mathbf{k}''| = q_0$. Let us therefore

study $\varepsilon(\kappa)$, the singular part of $E(\mathbf{k})$ for $\kappa \equiv |\mathbf{k}| - q_0 \rightarrow 0$. We get

$$\varepsilon(\kappa) \propto \begin{cases} \left[A + B \operatorname{sgn}(\kappa) \right] |\kappa|^{\alpha - 1} & (\alpha < 1) \\ A \ln|\kappa|^{-1} + B \operatorname{sgn}(\kappa) & (\alpha = 1) \\ B \operatorname{sgn}(\kappa) |\kappa|^{\alpha - 1} & (1 < \alpha < 2) & (15) \\ B \operatorname{sgn}(\kappa) |\kappa| \ln|\kappa|^{-1} & (\alpha = 2) \\ B \operatorname{sgn}(\kappa) |\kappa| & (\alpha > 2), \end{cases}$$

for D = 1, with $A \propto \cos \phi$ and $B \propto \sin \phi$, and

$$\varepsilon(\kappa) \propto \begin{cases} [A + B \operatorname{sgn}(\kappa)] |\kappa|^{\alpha - 3/2} & (\alpha < 3/2) \\ A \ln|\kappa|^{-1} + B \operatorname{sgn}(\kappa) & (\alpha = 3/2) \\ B \operatorname{sgn}(\kappa) |\kappa|^{\alpha - 3/2} & (3/2 < \alpha < 5/2) \\ B \operatorname{sgn}(\kappa) |\kappa| \ln|\kappa|^{-1} & (\alpha = 5/2) \\ B \operatorname{sgn}(\kappa) |\kappa| & (\alpha > 5/2), \end{cases}$$
(16)

for D=2, with $A \propto \cos(\phi + \pi/4)$ and $B \propto \sin(\phi + \pi/4)$. Let $C(\mathbf{k})$ be the left-hand side expression in Eq. (3c). We then get, for $\mathbf{k} \to 0$,

$$C(k) \propto \begin{cases} +\infty & (\alpha \leq 0) \\ |k|^{\alpha} & (0 < \alpha < 1) \\ |k| \ln|k|^{-1} & (\alpha = 1, \cos\phi \neq 0) \\ |k| & (\alpha = 1, \cos\phi = 0) \\ |k|^{2} & (\alpha > 1, \sin\phi = 0) \\ |k| & (1 < \alpha < 2, \sin\phi \neq 0) \\ |k|^{2} \ln|k|^{-1} & (\alpha = 2, \sin\phi \neq 0) \\ |k|^{2} & (\alpha > 2, \sin\phi \neq 0), \end{cases}$$
(17)

for D = 1, and

$$C(\mathbf{k}) \propto \begin{cases} +\infty & (\alpha \leq 1/2) \\ |\mathbf{k}|^{\alpha - 1/2} & (1/2 < \alpha < 3/2) \\ |\mathbf{k}| \ln |\mathbf{k}|^{-1} & (\alpha = 3/2, \cos(\phi + \pi/4) \neq 0) \\ |\mathbf{k}| & (\alpha = 3/2, \cos(\phi + \pi/4) = 0) \\ |\mathbf{k}|^{2} & (\alpha > 3/2, \sin(\phi + \pi/4) = 0) \\ |\mathbf{k}|^{\alpha - 1/2} & (3/2 < \alpha < 5/2, \sin(\phi + \pi/4) \neq 0) \\ |\mathbf{k}| \ln |\mathbf{k}|^{-1} & (\alpha = 5/2, \sin(\phi + \pi/4) \neq 0) \\ |\mathbf{k}|^{2} & (\alpha > 5/2, \sin(\phi + \pi/4) \neq 0), \end{cases}$$
(18)

for D=2. From Eqs. (13) and (14), it follows that conditions (3a) and (3b) are satisfied for all values of α . From Eqs. (17) and (18), one gets that condition (3c) is fulfilled for $\alpha \geq 1$ (D=1), and for $\alpha > 3/2$ [D=2, $\sin(\phi+\pi/4)=0$] or $\alpha > 5/2$ [D=2, $\sin(\phi+\pi/4)\neq 0$], which completes the proof of Corollary 1. \square

Proof of Theorem 2.—Theorem 2 is an immediate generalization of the Mermin-Wagner theorem. For the sake of simplicity, we detail the proof only for the case of ferromagnetism; the extension to the case of antiferromagnetism is immediate by introducing a staggered field and staggered magnetization as done by Mermin and Wagner.

The proof follows the one of Theorem 1 until Eq. (6). Then, by using $|\langle S_0^y S_{\mathbf{R}}^y + S_0^z S_{\mathbf{R}}^z \rangle| \le S(S+1)$,

$$\Delta(\mathbf{k}) \le |B|S + 2S(S+1)\tilde{E}(\mathbf{k}). \tag{19}$$

From condition (5) it follows immediately that $\lim_{B\to 0} |\langle S^z \rangle| = 0$ for T > 0, which is in contradiction with our hypothesis that the system is ferromagnetic. This completes the proof of Theorem 2 by *reductio ad absurdum*. \square

Proof of Corollary 2.—Let us consider the behavior of $\tilde{E}(\mathbf{k})$ in the vicinity of $\mathbf{k} = 0$ for $|J_{\mathbf{R}}| \propto R^{-\alpha}$. In this regime, the discrete sum over \mathbf{R} can be replaced by an integral, and one shows easily that, for $|\mathbf{k}| \to 0$,

$$\tilde{E}(\mathbf{k}) \propto \begin{cases}
|k|^{\alpha - D} & (D < \alpha < D + 2) \\
|k|^{2} \ln(|k|^{-1}) & (\alpha = D + 2) \\
|k|^{2} & (\alpha > D + 2).
\end{cases} (20)$$

It then follows immediately that condition (5) is satisfied if $\alpha \ge 2D$, which completes the proof of Corollary 2. \square

As for the Mermin-Wagner theorem, the above theorems and corollaries can be extended also to

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one-dimensional systems of arbitrary finite cross section and to two-dimensional systems of arbitrary finite thickness.

The importance of Theorem 1 and Corollary 1 is that the class of systems for which ferromagnetism is rigorously ruled out is significantly increased. In particular, we obtain interesting results for systems with RKKY interactions $(\alpha = D)$. For one-dimensional RKKY systems, ferromagnetism is rigorously ruled out. For twodimensional RKKY systems, the results are less satisfactory, since ferromagnetism can be strictly ruled out only for the particular case with $\sin(\phi + \pi/4) = 0$. For the general case $[\sin(\phi + \pi/4) \neq 0]$, it does not seem possible to rule out ferromagnetism for $\alpha = D = 2$ without analyzing in detail the behavior of $F(\mathbf{k})$ near $|\mathbf{k}| = q_0$. If one could prove that $F(\mathbf{k})$ has no singularity more singular than a square-root singularity at $|\mathbf{k}| = q_0$, then the absence of ferromagnetism would follow from Eq. (18). This situation is somehow puzzling. Indeed, within the (nonrigorous) linearized spin-wave theory, as well as the random phase approximation Green's function method, having $E(\mathbf{k}) \propto k^2$ is sufficient to rule out ferromagnetism in two dimensions, which implies that these theories rule ferromagnetism in systems with oscillatory interactions, for any value of α . In view of these considerations, I therefore propose the following result:

Conjecture 1.—A *D*-dimensional (D = 1 or 2) Heisenberg or *XY* system, for which there exists some finite **k** region with $E(\mathbf{k}) < 0$, or satisfying

$$\frac{1}{A_D} \int d^D \mathbf{k} \, \frac{1}{E(\mathbf{k})} = +\infty, \tag{21}$$

cannot be ferromagnetic.

From Eq. (13), it then follows immediately:

Corollary 3.—If Conjecture 1 is true, then a *D*-dimensional (D = 1 or 2) Heisenberg or *XY* system with long-range oscillatory interactions of the form (4) cannot be ferromagnetic, for any value of α .

Let us now discuss the results of Theorem 2 and Corollary 2. They essentially constitute an extension to XY systems of a result obtained earlier by Joyce [7]. For the one-dimensional (classical) Heisenberg and XY systems with positive (ferromagnetic) long-range interaction, Fröhlich et al. proved the existence of ferromagnetism

if $1 < \alpha < 2$ [8]. This is to be contrasted with onedimensional Ising with long-range interaction, for which ferromagnetism is ruled out if $\alpha > 2$ [9], whereas ferromagnetism exists for $1 < \alpha \le 2$ [10]. The Heisenberg and XY systems therefore differ only from the Ising system on the borderline $\alpha = 2$: there ferromagnetism is excluded for the Heisenberg and XY cases, but exists for the Ising case, illustrating the stronger tendency towards ordering displayed by the Ising model.

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