The Mermin-Wagner Theorem

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Conclusion

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In one and two dimensions, continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions.

Contents

For systems in statistical equilibrium the expectation value of an operator A is given by

$$\langle A \rangle = \lim_{V \to \infty} tr\left(e^{-\beta\mathcal{H}} A\right)$$

If the Hamiltonian displays a continuous symmetry $\mathcal{S}$ it commutes with the generators $\Gamma^i_{\mathcal{S}}$ of the corresponding symmetry group

$$\left[\mathcal{H}, \Gamma^i_{\mathcal{S}}\right]_- = 0$$

If some operator is not invariant under the transformations of $\mathcal{S}$,

$$\left[B, \Gamma^i_{\mathcal{S}}\right]_- = C^i \neq 0$$

the average of the commutator C^i vanishes:

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It turns out that such averages may be unstable under an infinitesimal perturbation of the Hamiltonian

$$\mathcal{H}_\nu = H + \nu H' - \mu \hat{N}$$

one can define the *quasi-average*:

$$\langle A \rangle_q = \lim_{\nu \to 0} \lim_{V \to \infty} tr\left(e^{-\beta \mathcal{H}_\nu} A\right)$$

The quasi-average does not need to coincide with the normal average

$$\left\langle C^i \right\rangle_q = \lim_{\nu \to 0} tr\left(e^{-\beta \mathcal{H}_\nu} \left[\mathcal{H}, \Gamma^i_{\mathcal{S}}\right]_-\right) \neq 0$$

An Example:

$$H = -\sum_{ij} J_{ij} \mathbf{S_i} \cdot \mathbf{S_j}$$

it is invariant under rotations in spin-space

$$[H, \mathbf{S}]_- = 0$$

from

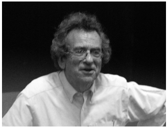
$$\left\langle \left[S^\alpha, S^\beta \right]_- \right\rangle = 0 \quad \text{and} \quad [S^x, S^y]_- = i\hbar S^z$$

we find that the conventional average of the magnetization vansihes.

Adding a symmetry breaking field

$$\mathbf{B_0} = B_0 \mathbf{e_z}$$

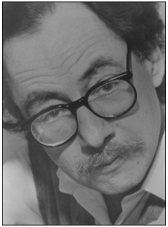
we may study quasi-averages and find spontaneous symmetry breaking.



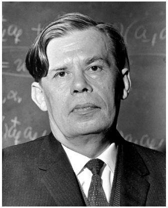
David Mermin (1935)

Herbert Wagner (1935)

Pierre Hohenberg (1934)



Sidney Coleman (1937-2007)



Nikolai Bogoliubov (1909-1992)

For the proof of the Mermin-Wagner Theorem we will use the Bogoliubov inequality

$$\frac{1}{2}\beta \left\langle \left[A, A^{\dagger}\right]_{+} \right\rangle \left\langle \left[[C, H]_{-}, C^{\dagger}\right]_{-} \right\rangle \geq \left|\langle [C, A]_{-} \rangle\right|^{2}$$

The idea for proofing the Bogoliubov inequality is to define an appropriate scalar product and then exploit the Schwarz inequality:

$$(A, B) = \sum_{n \neq m} \left\langle n \right| A^{\dagger} \left| m \right\rangle \langle m | B | n \rangle \frac{W_m - W_n}{E_n - E_m}$$

with

$$W_n = \frac{e^{-\beta E_n}}{Tr\left(e^{-\beta H}\right)}$$

A scalar product has four defining axioms:

1. $$(A, B) = (B, A)^*$$

   This is valid since

$$\left(\left\langle n \right| B^{\dagger} \left| m \right\rangle \langle m | A | n \rangle\right)^* = \left\langle n \right| A^{\dagger} \left| m \right\rangle \langle m | B | n \rangle$$

2. The linearity follows directly from the linearity of the matrix element
3. It is also obvious that

$$(A, A) \geq 0$$

4. From $A = 0$ it naturally follows that $(A, A) = 0$. The converse is not necessarily true

In conclusion this shows that we have constructed a semidefinite scalar product.

To exploit the Schwarz inequality, we calculate the terms occurring in it:

$$|(A, B)|^2 \leq (A, A)\,(B, B)$$

We now choose

$$B = \left[C^\dagger, H\right]_-$$

First we calculate

$$\begin{aligned}
(A,B) &= \sum_{n\neq m} \left\langle n \right| A^\dagger \left| m \right\rangle \left\langle m \right| \left[C^\dagger, H\right]_- \left| n \right\rangle \frac{W_m - W_n}{E_n - E_m} \\
&= \sum_{n,m} \left\langle n \right| A^\dagger \left| m \right\rangle \left\langle m \right| C^\dagger \left| n \right\rangle (W_m - W_n) \\
&= \sum_m W_m \left\langle m \right| C^\dagger A^\dagger \left| m \right\rangle - \sum_n W_n \left\langle n \right| A^\dagger C^\dagger \left| n \right\rangle \\
&= \left\langle C^\dagger A^\dagger - A^\dagger C^\dagger \right\rangle = \left\langle \left[C^\dagger, A^\dagger\right]_- \right\rangle
\end{aligned}$$

Substituting $B = \left[C^\dagger, H\right]_-$, we find

$$(B,B) = \left\langle \left[C^\dagger, [H,C]_-\right]_- \right\rangle \geq 0$$

For (A, A) we use the following approximation:

$$\begin{aligned} 0 &< \frac{W_m - W_n}{E_n - E_m} \\ &= \left(Tr\left(e^{-\beta H}\right)\right)^{-1} \frac{e^{-\beta E_m} + e^{-\beta E_n}}{E_n - E_m} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{e^{-\beta E_m} + e^{-\beta E_n}} \\ &= \frac{W_m + W_n}{E_n - E_m} \tanh\left(\frac{\beta}{2}(E_n - E_m)\right) \end{aligned}$$

Since $\tanh x < x$ for $x > 0$, we find that

$$0 < \frac{W_m - W_n}{E_n - E_m} < \frac{\beta}{2}(W_n + W_m)$$

We can now estimate the scalar product:

$$\begin{aligned}(A,A) &< \frac{\beta}{2}\sum_{n\neq m}\left\langle n\right| A^\dagger \left|m\right\rangle \langle m| A |n\rangle (W_n + W_m) \\ &\leq \frac{\beta}{2}\sum_{n,m}\left\langle n\right| A^\dagger \left|m\right\rangle \langle m| A |n\rangle (W_n + W_m) \\ &= \frac{\beta}{2}\sum_{n} W_n \left(\left\langle n\right| A^\dagger A \left|n\right\rangle + \left\langle n\right| A A^\dagger \left|n\right\rangle\right)\end{aligned}$$

This finally leads to

$$(A,A) \leq \frac{\beta}{2}\left\langle \left[A, A^\dagger\right]_+ \right\rangle$$

Putting what we found in the Schwarz inequality, we find that we proofed the Bogoliubov inequality

$$\frac{1}{2}\beta \left\langle \left[A, A^{+}\right]_{+} \right\rangle \left\langle \left[[C, H]_{-}, C^{+}\right]_{-} \right\rangle \geq \left|\left\langle [C, A]_{-} \right\rangle\right|^{2}$$

We now want to find out whether the isotropic Heisenberg model gives a spontaneous magnetization. The starting point is the Hamiltonian

$$H = -\sum_{i,j} J_{ij} \mathbf{S_i} \cdot \mathbf{S_j} - b \sum_i S_i^z e^{-i\mathbf{K}\cdot\mathbf{R_i}}$$

We are interested in the magnetization

$$M_s(T) = \lim_{B_0 \to 0} g_J \frac{\mu_B}{\hbar} \sum_i e^{-i\mathbf{K}\cdot\mathbf{R_i}} \langle S_i^z \rangle_{T,B_0}$$

For the following analysis, we assume that the exchange integrals J_{ij} decrease sufficiently fast with increasing distance $|\mathbf{R_i} - \mathbf{R_j}|$ so that the quantity

$$Q = \frac{1}{N} \sum_{i,j} |\mathbf{R_i} - \mathbf{R_j}|^2 \, |J_{ij}|$$

remains finite.

We will now prove the Mermin-Wagner Theorem by using the Bogoliubov inequality for the operators

$$\begin{aligned} A = S^{-}(-\mathbf{k}+\mathbf{K}) \quad &\Rightarrow \quad A^{\dagger} = S^{+}(\mathbf{k}-\mathbf{K}) \\ C = S^{+}(\mathbf{k}) \quad &\Rightarrow \quad C^{\dagger} = S^{-}(-\mathbf{k}) \end{aligned}$$

Where the spin operators in **k**-space are defined by

$$S^{\alpha}(\mathbf{k}) = \sum_i S_i^{\alpha} e^{-i\mathbf{k}\mathbf{R_i}}$$

From this we find the commutation relations

$$\begin{aligned} \left[S^{+}(\mathbf{k_1}), S^{-}(\mathbf{k_2})\right]_{-} &= 2\hbar S^{z}(\mathbf{k_1}+\mathbf{k_2}) \\ \left[S^{z}(\mathbf{k_1}), S^{\pm}(\mathbf{k_2})\right]_{-} &= \pm\hbar S^{\pm}(\mathbf{k_1}+\mathbf{k_2}) \end{aligned}$$

We now evaluate the three individual terms of the Bogoliubov inequality

$$\begin{aligned}\left\langle [C,A]_- \right\rangle &= \left\langle \left[S^+(\mathbf{k}), S^-(-\mathbf{k}+\mathbf{K})\right]_- \right\rangle \\ &= 2\hbar \left\langle S^z(\mathbf{K}) \right\rangle \\ &= 2\hbar \sum_i e^{-i\mathbf{K}\mathbf{R_i}} \left\langle S_i^z \right\rangle \\ &= \frac{2\hbar^2 N}{g_J \mu_B} M(T, B_0)\end{aligned}$$

$$
\begin{aligned}
\sum_{\mathbf{k}} \left\langle \left[A, A^{\dagger}\right]_{+} \right\rangle &= \sum_{\mathbf{k}} \left\langle \left[S^{-}(-\mathbf{k}+\mathbf{K}), S^{+}(\mathbf{k}-\mathbf{K})\right]_{+} \right\rangle \\
&= \sum_{\mathbf{k}} \sum_{i,j} e^{i(\mathbf{k}-\mathbf{K})(\mathbf{R_i}-\mathbf{R_j})} \left\langle S_i^{-} S_j^{+} + S_j^{+} S_i^{-} \right\rangle \\
&= 2N \sum_{i} \left\langle (S_i^{x})^2 + (S_i^{y})^2 \right\rangle \\
&\leq 2N \sum_{i} \left\langle \mathbf{S}_i^2 \right\rangle \\
&= 2\hbar^2 N^2 S(S+1)
\end{aligned}
$$

Now we calculate the double commutator

$$\left\langle \left[[C, H]_, C^\dagger \right]_- \right\rangle$$

First we will evaluate

$$\left[S_m^+, H \right]_- = -\hbar \sum_i J_{im} \left(2S_i^+ S_m^z - S_i^z S_m^+ - S_m^+ S_i^z \right) + \hbar b S_m^+ e^{-i\mathbf{K}\mathbf{R_m}}$$

Using this, we evaluate the double commutator

$$\begin{aligned} \left[\left[S_m^+, H \right]_-, S_p^- \right]_- &= 2\hbar^2 \sum_i J_{ip} \delta_{mp} \left(S_i^+ S_p^- + 2S_i^z S_p^z \right) \\ &- 2\hbar^2 J_{mp} \left(S_m^+ S_p^- + 2S_m^z S_p^z \right) + 2\hbar^2 b \delta_{mp} S_p^z e^{-i\mathbf{K}\mathbf{R}_p} \end{aligned}$$

This leads to the following intermediate result for the expectation value we are looking for

$$\begin{aligned}
\left\langle \left[[C, H]_, C^\dagger \right]_- \right\rangle &= \sum_{m,p} e^{i\mathbf{k}(\mathbf{R}_m - \mathbf{R}_p)} \left\langle \left[\left[S_m^+, H \right]_- , S_p^- \right]_- \right\rangle \\
&= 2\hbar^2 b \sum_p \left\langle S_p^z \right\rangle e^{-i\mathbf{K}\mathbf{R}_p} \\
&+ 2\hbar^2 \sum_{m,p} J_{mp} \left(1 - e^{-i\mathbf{k}(\mathbf{R}_m - \mathbf{R}_p)} \right) \left\langle S_m^+ S_p^- + 2 S_m^z S_p^z \right\rangle
\end{aligned}$$

To find a simple upper bound we may add to the right-hand side the same expression with $\mathbf{k}$ replaced by $-\mathbf{k}$:

$$\begin{aligned}
&\left\langle \left[[C, H], C^\dagger \right]_- \right\rangle \\
\leq\ & 4\hbar^2 b \sum_p \left\langle S_p^z \right\rangle e^{-i\mathbf{K}\mathbf{R}_p} \\
+\ & 4\hbar^2 \sum_{m,p} J_{mp} \left(1 - \cos\left(\mathbf{k}\left(\mathbf{R}_m - \mathbf{R}_p\right)\right)\right) \left\langle \mathbf{S}_m \mathbf{S}_p + S_m^z S_p^z \right\rangle
\end{aligned}$$

We can simplify the right hand side using the triangle inequality

$$\begin{aligned}
&\left\langle \left[[C, H], C^\dagger \right]_- \right\rangle \\
\leq\ & 4\hbar^2 bN \left|\left\langle S_p^z \right\rangle\right| \\
+\ & 4\hbar^2 \sum_{m,p} |J_{mp}| \left|(1 - \cos\left(\mathbf{k}\left(\mathbf{R}_m - \mathbf{R}_p\right)\right))\right| \left(\left|\langle \mathbf{S}_m \mathbf{S}_p \rangle\right| + \left|\left\langle S_m^z S_p^z \right\rangle\right|\right) \\
\leq\ & 4\hbar^2 bN \left|\left\langle S_p^z \right\rangle\right| \\
+\ & 4\hbar^2 \sum_{m,p} |J_{mp}| \left|1 - \cos\left(\mathbf{k}\left(\mathbf{R}_m - \mathbf{R}_p\right)\right)\right| \left(\hbar^2 S(S+1) + \hbar^2 S^2\right) \\
\leq\ & 4\hbar^2 bN \left|\left\langle S_p^z \right\rangle\right| \\
+\ & 8\hbar^2 S(S+1) \sum_{m,p} |J_{mp}| \left|1 - \cos\left(\mathbf{k}\left(\mathbf{R}_m - \mathbf{R}_p\right)\right)\right|
\end{aligned}$$

Therewith we have found

$$
\begin{aligned}
&\left\langle \left[[C, H]_{,} C^{\dagger} \right]_{-} \right\rangle \\
\leq\ & 4\hbar^2 \left| B_0 M(T, B_0) \right| \\
+\ & 8\hbar^2 S(S+1) \sum_{m,p} \frac{|J_{mp}|}{2} k^2 \left| \mathbf{R}_m - \mathbf{R}_p \right|^2 \\
\leq\ & 4\hbar^2 \left| B_0 M(T, B_0) \right| + 4Nk^2\hbar^4 QS(S+1)
\end{aligned}
$$

Substituting what we have found in the Bogoliubov inequality and summing over all the wavevectors of the first Brillouin zone we get:

$$\beta S(S+1) \geq \frac{M^2}{N^2 g_j^2 \mu_B^2} \sum_{\mathbf{k}} \frac{1}{|B_0 M| + k^2 \hbar^2 NQS(S+1)}$$

We are finally ready to prove the Mermin-Wagner Theorem. In the thermodynamic limit we find:

$$S(S+1) \geq \frac{m^2 v_d \Omega_d}{\beta (2\pi)^d g_j^2 \mu_B^2} \int_0^{k_0} \frac{k^{d-1} dk}{|B_0 M| + k^2 \hbar^2 QS(S+1)}$$

All that is left to do is to evaluate the integrals. This can be done exactly; in one dimension we find:

$$S(S+1) \geq \frac{m^2 v_1}{\beta 2\pi g_j^2 \mu_B^2} \frac{\arctan\left(k_0 \sqrt{\frac{Q\hbar^2 S(S+1)}{|B_0 m|}}\right)}{\sqrt{Q\hbar^2 S(S+1)\,|B_0 m|}}$$

We are specifically interested in the behaviour of the magnetization for small fields B_0:

$$|m(T, B_0)| \leq const. \frac{B_0^{1/3}}{T^{2/3}}, \quad \text{as } B_0 \to 0$$

For a two-dimensional lattice we find:

$$S(S+1) \geq \frac{m^2 v_2}{\beta 2\pi g_j^2 \mu_B^2} \frac{\ln\left(\sqrt{\frac{Q\hbar^2 S(S+1)k_0^2 + |B_0 m|}{|B_0 m|}}\right)}{2Q\hbar^2 S(S+1)}$$

from which for small fields we get

$$|m(T, B_0)| \leq const. \left(T \ln\left(\frac{const.' + |B_0 m|}{|B_0 m|}\right)\right)^{-1/2}$$

From the previous two expressions we conclude that there is no spontaneous magnetization in one and two dimensions:

$$m_{sp} = \lim_{B_0 \to 0} m(T, B_0) = 0 \text{ for } T \neq 0$$

Thus, the Mermin-Wagner Theorem is proved.

1. The proof is valid only for $T > 0$. For $T = 0$ our inequalities make no predictions.
2. Via the factor $e^{-i\mathbf{K}\mathbf{R}_\mathbf{i}}$ the proof also forbids long-range order in antiferromagnets.
3. We cannot make any predictions for $d > 2$, but Roepstroff strengthened the proof to find an upper bound for the magnetization in $d \geq 3$.

4. The theorem is valid for arbitrary spin S.
5. The theorem is valid only for the isotropic Heisenberg model. The proof is not valid even for a weak anisotropy. This explains the existence of a number of two-dimensional Heisenberg ferromagnets and antiferromagnets like K_2CuF_4.
6. The theorem is restricted only to the non-existence of spontaneous magnetization. It does not necessarily exclude other types of phase transitions. For example the magnetic susceptibility may diverge.

This is the end of my presentation

Thank you for your attention.

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