The Heisenberg Model and The Mermin-Wagner Theorem

About the possibility of spontaneous symmetry breaking in low-dimensional systems

Robert Rüger

Institut für **T**heoretische **P**hysik
Goethe-Universität Frankfurt

January 18$^{\text{th}}$, 2012

Contents

Contents

The Heisenberg model

... the model hamiltonian

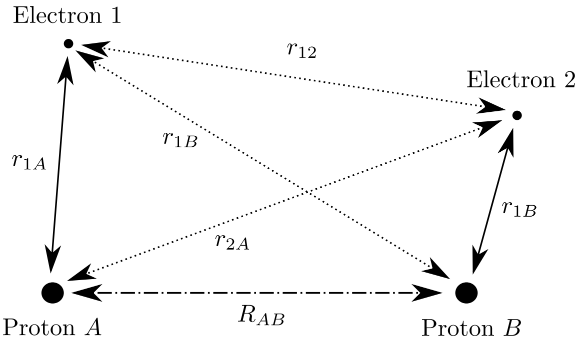
The Heisenberg model's hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \frac{g\mu_B}{\hbar} \sum_i \vec{B} \cdot \vec{S}_i$$

- This is a quantum mechanical model! H and $\vec{S}_k$ are operators and $\vec{S}_i \cdot \vec{S}_j = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_i^z$.
- $\sum_{\langle i,j \rangle}$ is the sum over nearest neighbours.
- In addition to the hamiltonian one also has to specify the spin positions (e.g. lattice).
- J is called the coupling constant. $J > 0$ is called ferromagnetic and $J < 0$ antiferromagnetic coupling.

The Heisenberg model

... a quick motivation



Hamiltonian in Born-Oppenheimer approximation:

$$H = -\frac{\hbar^2}{2m_e}\left(\vec{\nabla}_1^2 + \vec{\nabla}_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{1A}} + \frac{1}{r_{2B}} + \frac{1}{r_{1B}} + \frac{1}{r_{2A}} + \frac{1}{R_{AB}}\right)$$

The Heisenberg model
... a quick motivation

What is the ground state for this system?

Hamiltonian in Heitler-London approximation:

$$H' = -\frac{\hbar^2}{2m_e}\left(\vec{\nabla}_1^2 + \vec{\nabla}_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_{1A}} + \frac{1}{r_{2B}}\right) = H'_{1A} + H'_{1B}$$

This is just the hamiltonian for two hydrogen atoms that have no interaction. The solution to this problem is well known! E.g.

$$\left(-\frac{\hbar^2}{2m_e}\vec{\nabla}_1^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r_{1A}}\right)\phi_A(\vec{r}_1) = E_0\phi_A(\vec{r}_1)$$

Here $\phi_A(\vec{r}_1)$ is the hydrogen ground state orbital.

The Heisenberg model

... a quick motivation

Watch out: Our electrons 1 and 2 are identical fermions!

$$\psi\left(\vec{r}_1, \vec{r}_2\right) \neq \phi_A(\vec{r}_1)\phi_B(\vec{r}_2)$$

This is where is the spin becomes important ...

Pauli principle:

$$\psi\left(\vec{r}_1, s_1, \vec{r}_2, s_2\right) = -\psi\left(\vec{r}_2, s_2, \vec{r}_1, s_1\right)$$

There are two ways of constructing antisymmetric wavefunctions: Antisymmetry in either position or spin space!

Antisymmetric wavefunctions:

$$\psi_+\left(\vec{r}_1, s_1, \vec{r}_2, s_2\right) = N_+\Big(\phi_A(\vec{r}_1)\phi_B(\vec{r}_2) + \phi_A(\vec{r}_2)\phi_B(\vec{r}_1)\Big)\chi_a(s_1, s_2)$$

$$\psi_-\left(\vec{r}_1, s_1, \vec{r}_2, s_2\right) = N_-\Big(\phi_A(\vec{r}_1)\phi_B(\vec{r}_2) - \phi_A(\vec{r}_2)\phi_B(\vec{r}_1)\Big)\chi_s(s_1, s_2)$$

The Heisenberg model

... a quick motivation

Definition of the coupling strength J:

What is the difference in energy between ψ_+ and ψ_- in Born-Oppenheimer approximation?

$$J \equiv \langle\psi_+| H |\psi_+\rangle - \langle\psi_-| H |\psi_-\rangle$$

Let's think about the signs:

- Assume $\langle\psi_+| H |\psi_+\rangle > \langle\psi_-| H |\psi_-\rangle \Leftrightarrow J > 0$
- Then $|\psi_-\rangle$ is energetically favoured
- $|\psi_-\rangle$ is antisym. in position space and sym. in spin space
- Spin alignment is energetically favoured: ferromag. coupling

The Heisenberg model

... a quick motivation

Model hamiltonian for two spins

$$H_{\text{heisenberg}} = -J\ \vec{S}_1 \cdot \vec{S}_2$$

- This is an approximation (hence Heisenberg **model**)!
- Its usefulness stems from the fact, that lives only in spin space and leaves out position space completely. **Simple**!

More than two spins + external magnetic field

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \frac{g\mu_B}{\hbar} \sum_i \vec{B} \cdot \vec{S}_i$$

Contents

Spontaneous magnetization

... models for collective magnetism

The Ising model:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i$$

- Simplification of the Heisenberg model: Spins are restricted to one direction and treated classically $S_k \in \{+1, -1\}$
- Ising model on two-dimensional square lattice is the most primitive system that shows a spontaneous magnetization.

Spontaneous magnetization

... the difference between magnetization and spontaneous magnetization

Why the magnetization is always zero:

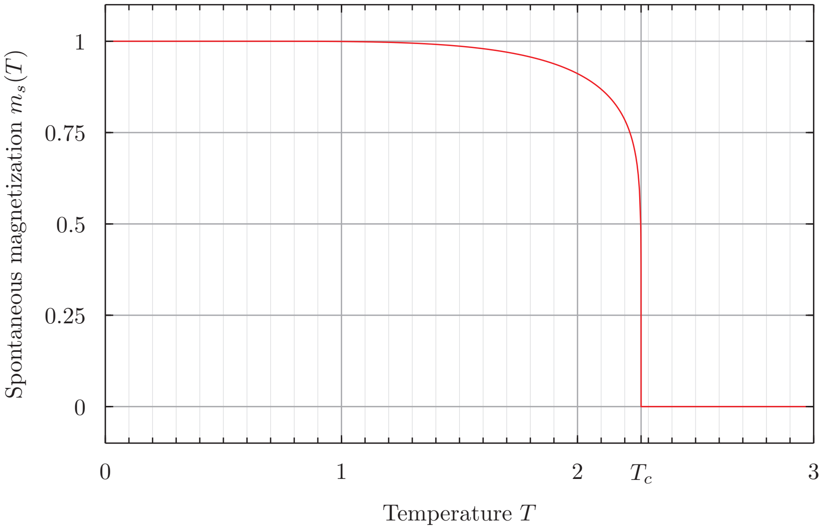
$$M(T,B) = \left\langle \sum_i S_i \right\rangle = \frac{1}{Z} \sum_{\{S_k=\pm 1\}} \sum_i S_i \, \mathrm{e}^{-\beta H}$$

- Notice that H is invariant under $\{S_k\} \to \{-S_k\}$ for $B=0$, but $\sum_i S_i$ changes its sign!
- $\Rightarrow$ For every microstate with magnetization $\sum_i S_i$, there is a microstate with $-\sum_i S_i$ and the same weight in the sum!
- $\Rightarrow$ There can not be any magnetization $M \neq 0$ for $B=0$!

Definition of the spontaneous magnetization:

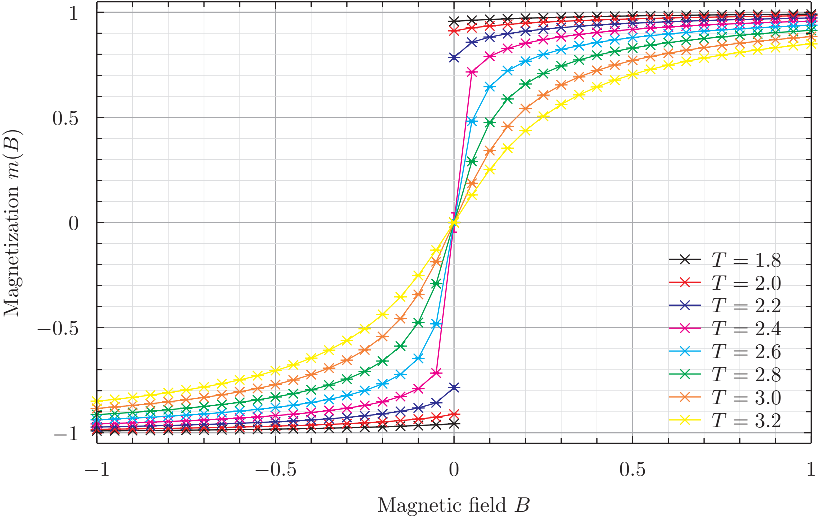
$$M_s(T) \equiv \lim_{B \to 0^+} M(T,B) \neq M(T,0)$$

Spontaneous magnetization
... the Ising model



Spontaneous magnetization

... the Ising model



Spontaneous magnetization

... an example of spontaneous symmetry breaking

Fact:

There are systems with a spontaneous magnetization!

Spontaneous symmetry breaking:

- The state of the system has fewer symmetries than the system's hamiltonian.
- Physical reason for spontaneous symmetry breaking is the breakdown of the ergodic hypothesis: System picks a subspace of its entire phase space and remains there.
- General concept: Ferromagnetism is only one example for spontaneous symmetry breaking.

Contents

Magnons

... excitations of the Heisenberg model

Lets consider a ferromagnetic ($J > 0$) spin-S Heisenberg model with N spins:

$$|\psi\rangle = |S_1^z, S_2^z, \ldots, S_N^z\rangle$$

For $B = 0$ the following is one of the ground states:

$$|\psi_0\rangle = |S, S, \ldots, S\rangle$$

One might think that the following state is an elementary excitation:

$$|\psi_j\rangle = |S, S, \ldots, \underbrace{S-1}_{\text{at } R_j}, \ldots, S\rangle$$

But this is <u>not</u> an eigenstate of the Heisenberg hamiltonian!

Magnons
... excitations of the Heisenberg model

Magnons

1. Construct eigenstate of $H_{\text{heisenberg}}$ as a linear combination of the single spin excitations:

$$\left|\psi_{\vec{q}}\right\rangle = \frac{1}{\sqrt{N}} \sum_j \mathrm{e}^{\mathrm{i}\vec{q}\cdot\vec{R}_j} \left|\psi_j\right\rangle$$

2. Gapless excitation with dispersion relation:

$$H_{\text{heisenberg}} \left|\psi_{\vec{q}}\right\rangle = \left(E_0 + E_{\vec{q}}\right) \left|\psi_{\vec{q}}\right\rangle \quad \text{with} \quad E_{\vec{q}} \propto q^2$$

3. Magnons are bosonic quasiparticles.
4. Every excited Magnon reduces the magnetization by $\hbar$.
5. Low temperature approximation!

Contents

The Mermin-Wagner theorem
... what does it say?

The theorem:

At finite temperatures, the spin-S Heisenberg model with isotropic and finite-range exchange interactions on one- or two-dimensional lattices can be neither ferro- nor antiferromagnetic. [MW66]

... in a more general formulation:

Continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$. [Wiki]

The Mermin-Wagner theorem

... why is it plausible?

Let's look at the special case of a ferromagnetic Heisenberg model with only nearest-neighbour interaction.

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \frac{g\mu_B}{\hbar} B_z \sum_i S_i^z$$

$$\text{with} \quad J > 0 \quad \text{and} \quad B_z \to 0^+$$

The Mermin-Wagner theorem
... why is it plausible?

Ansatz:

The spontaneous magnetization at $T = 0$ will be reduced by the excitation of magnons for $T > 0$.

$$M_s(T) = M_s(0) - \Delta M_s(T)$$

We know that the elementary excitations are bosonic quasiparticles and every magnon reduces the spontaneous magnetization by $\hbar$.

$$\Delta M_s(T) \propto \int_0^\infty \frac{D(E)}{\mathrm{e}^{\frac{E}{k_B T}} - 1} \mathrm{d}E$$

The Mermin-Wagner theorem

... why is it plausible?

Calculate the density of states from the magnon dispersion relation!

$$D(E) \propto \int_{S(E)} \frac{\mathrm{d}s}{\left|\frac{\partial}{\partial k} E(k)\right|}$$

$$\text{with} \quad S(E) \propto k^{d-1} \propto E^{\frac{d-1}{2}} \quad \text{and} \quad \left|\frac{\partial}{\partial k} E(k)\right| \propto \frac{1}{\sqrt{E}}$$

$$\Rightarrow \quad D(E) \propto \frac{E^{\frac{d-1}{2}}}{\sqrt{E}} = E^{\frac{d-2}{2}}$$

The Mermin-Wagner theorem
... why is it plausible?

$$\Delta M_s(T) \propto \int_0^\infty \frac{E^{\frac{d-2}{2}}}{\mathrm{e}^{\frac{E}{k_B T}} - 1} \mathrm{d}E \propto T^{\frac{d}{2}} \int_0^\infty \frac{x^{\frac{d-2}{2}}}{\mathrm{e}^x - 1} \mathrm{d}x$$

The integrand has a singularity at $x = 0$. Does the integral exist?

$$\frac{x^{\frac{d-2}{2}}}{\mathrm{e}^x - 1} \approx \frac{x^{\frac{d-2}{2}}}{x} = x^{\frac{d}{2}-2}$$

The integral only exists for $d > 2$ because:

$$\int_0^\epsilon x^\alpha \mathrm{d}x < \infty \quad \Leftrightarrow \quad \alpha > -1$$

Conclusion:

There is no spontaneous magnetization for $T > 0$ and $d \leq 2$!

Thank you for your attention!

Sources

N. D. Mermin and H. Wagner.
Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic heisenberg models.
Phys. Rev. Lett., 17:1133–1136, Nov 1966.

Roser Valentí.
Advanced solid state theory, lecture notes.
Goethe-Universität Frankfurt am Main, 2011.

Reinhold Kleiner and Frank Schreiber.
Experimentalphysik V, Kondensierte Materie (Festkörperphysik), Ergänzungen zur Vorlesung: Magnetism in two dimensions (Mermin-Wagner theorem).
Universität Tübingen, 2011.

Tim Herfurth.
Exakte Diagonalisierung des Heisenbergmodells: Bestimmung unterer Schranken für die Grundzustandsenergie unendlicher Spinsysteme.
Bachelor's thesis, Goethe-Universität Frankfurt am Main, 2011.

Robert Rüger.
Monte Carlo Methoden in der statistischen Physik und ihre Anwendung zur Simulation von Spinsystemen.
Bachelor's thesis, Goethe-Universität Frankfurt am Main, 2011.

Reminder

... symmetric and antisymmetric states for two spins

$$|\text{triplett}\rangle = \begin{cases} |\uparrow\uparrow\rangle \\ \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \Big) \\ |\downarrow\downarrow\rangle \end{cases}$$

$$|\text{singlett}\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \Big)$$