2022.6.01 Lecture 8

10:25 – 11:55

Lecture on

Magnetic Properties of Materials

磁性 (Magnetism)

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Review

- Spin Hamiltonian and quantum entanglement
  - Hubbard Hamiltonian
  - Superexchange interaction
  - RKKY interaction
  - Double exchange interaction

Ch. 5 Theory of Magnetic insulators

- Molecular field approximation

Outline

- Molecular field approximation
- Phenomenology of phase transition GL theory
    - Free energy
    - Spontaneous Symmetry Breaking
- Critical Exponent
- Theoretical models of magnetic materials
    - XY model
    - Ising model
- Antiferromagnetic Heisenberg model

Molecular-field approximation on ferromagnetic Heisenberg model

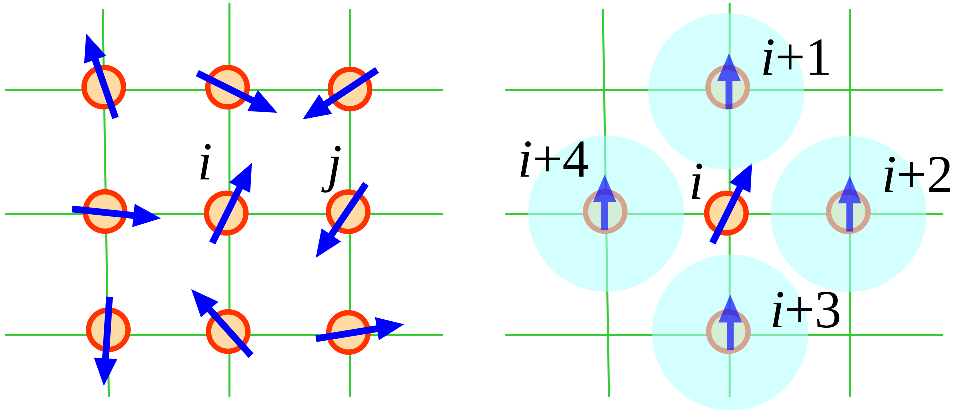
Ferromagnetic (J >0) Heisenberg model:

$$\mathscr{H} = -2J\sum_{\langle i,j\rangle}\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \mu\sum_i \boldsymbol{B}\cdot\boldsymbol{S}_i$$

nearest neighbor

Mean field (molecular-field) approximation:

Replace the neighboring spins with averaged one



$$\mathscr{H}_{\text{eff}}(i) = -2J\sum_{\delta}\langle\boldsymbol{S}_{i+\delta}\rangle\cdot\boldsymbol{S}_i - \mu\boldsymbol{B}\cdot\boldsymbol{S}_i = -\mu\boldsymbol{B}_{\text{eff}}\cdot\boldsymbol{S}_i$$

The averaged spins work as an effective field:

$$\mu\boldsymbol{B}_{\text{eff}} = 2J\sum_{\delta}\langle\boldsymbol{S}_{i+\delta}\rangle + \mu\boldsymbol{B}$$

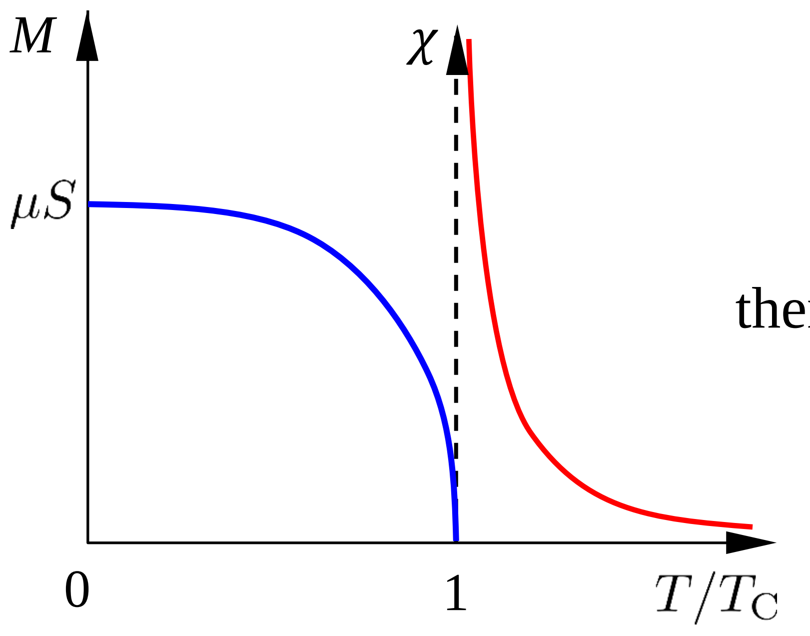
Remember paramagnetic representation of magnetization:

$$M = g_J\mu_{\text{B}}JB_J\left(\frac{g_J\mu_{\text{B}}JB}{k_{\text{B}}T}\right)$$

Replacement: $g_J\mu_{\text{B}} \to \mu,\ J \to S,\ B_J \to B_S \quad B \to B_{\text{eff}}$

then $$M = \mu SB_S\left[\frac{\mu S}{k_{\text{B}}T}\left(B + \frac{2\alpha_z J}{\mu^2}M\right)\right]$$

Curie-Weiss law



Brillouin function is expanded as

$$B_S(x) = \frac{S+1}{3S}x - \frac{1}{90}\frac{[(S+1)^2+S^2](S+1)}{S^3}x^3 + \cdots$$

then $$\left(1 - \frac{2\alpha_z J}{\mu^2}\chi_0\right) M + \frac{1}{90}[(S+1)^2+S^2]\frac{1}{(k_B T)^3}\left(\frac{2\alpha_z J}{\mu^2}\right)^2 M^3 = \chi_0 B$$

where $$\chi_0 = \frac{\mu^2 S(S+1)}{3k_B T}$$: the Curie law

The first order term drops at $k_B T_C = \dfrac{2}{3}S(S+1)\alpha_z J$

which gives the Curie temperature and the Curie-Weiss law

$$\chi = \chi_0 \left(1 - \frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1} = \mu^2 \frac{S(S+1)}{3k_B(T-T_C)}$$

$T < T_C$

There exists non-zero solution for M, which has lower energy than M =0.

Solving the above we get

$$M = \mu\sqrt{\frac{10}{3}\frac{S(S+1)}{\sqrt{(S+1)^2+S^2}}}\sqrt{1-\frac{T}{T_C}}$$

$T \ll T_C$

$$x \gg 1 \qquad B_S(x) \sim 1 - \frac{1}{S}\exp\left(-\frac{x}{S}\right)$$

$$M = \mu\left[S - \exp\left(-\frac{3}{S+1}\frac{T_C}{T}\right)\right]$$

Ginzburg-Landau Theory(1)

The Curie-Weiss law $$\chi \propto \frac{1}{1-(T_C/T)} = 1 + \frac{T_C}{T} + \left(\frac{T_C}{T}\right)^2 + \left(\frac{T_C}{T}\right)^3 + \cdots$$

involves that the establishment of spontaneous magnetization is the result of a cooperative phenomenon.

Phenomenology: discuss the physical properties that do not depend on details of models.

The Ginzburg-Landau theory was developed for phenomenology of superconductivity.

Consider a symmetry of the Heisenberg model at *B* =0. $$\mathscr{H} = -2J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

A symmetry operation: $\forall i \;\; \boldsymbol{S}_i \to -\boldsymbol{S}_i$

$\mathscr{H}$: unchanged

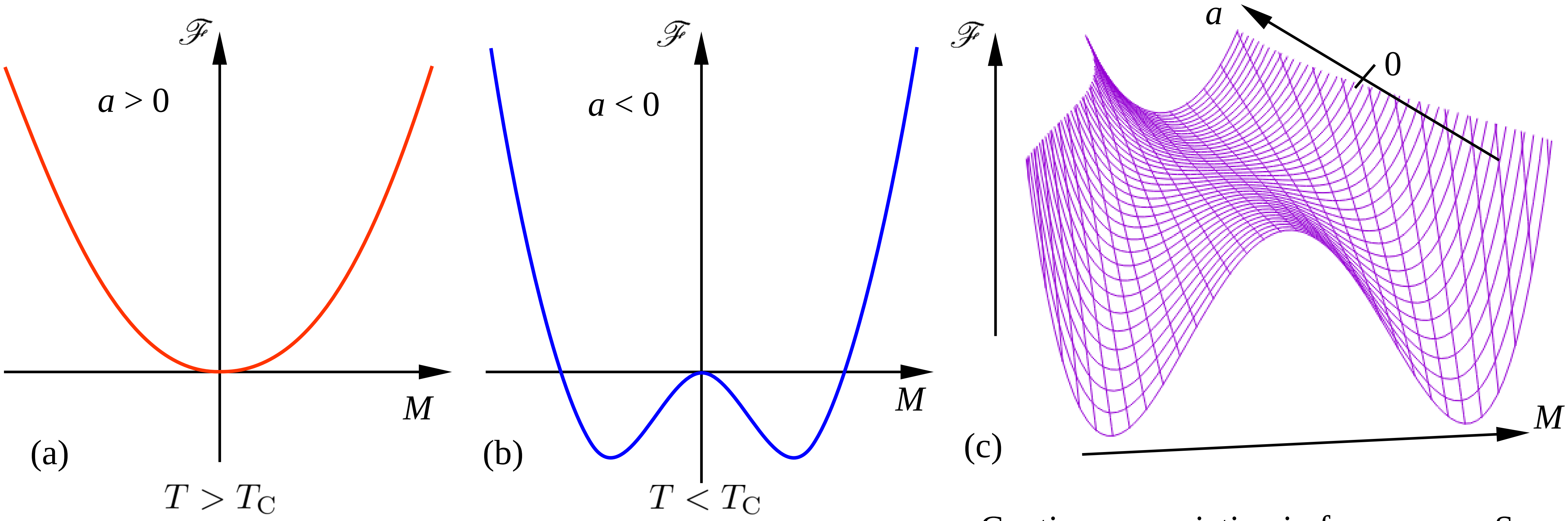
Free energy $\mathscr{F}$: unchanged

On the other hand $\boldsymbol{M} = \langle \boldsymbol{S}_i \rangle \to \langle -\boldsymbol{S}_i \rangle = -\boldsymbol{M}$ hence $\mathscr{F}(M) = \mathscr{F}(-M)$

Expansion to the series of power should be $\mathscr{F}(M) = \mathscr{F}_0 + aM^2 + bM^4$

To obtain stable (minimum) points $$\frac{\partial \mathscr{F}}{\partial M} = 0 = 2aM + 4bM^3 = 2M(2bM^2 + a)$$

Ginzburg-Landau Theory (2)



Continuous variation in free energy: Second order phase transition

$$\mathscr{F}(M) = \mathscr{F}_0 + aM^2 + bM^4$$

$$a = k(T_C - T)/T_C$$

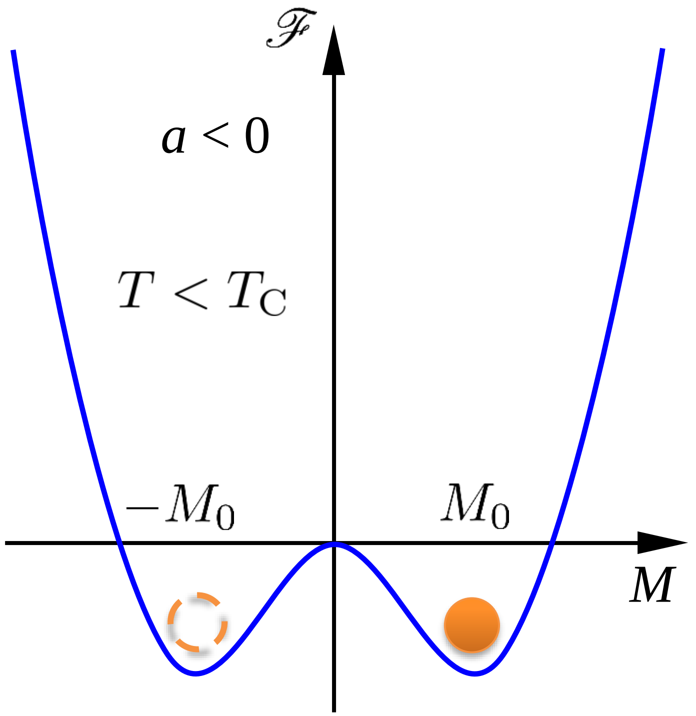
T : relevant parameter

$$\frac{\partial \mathscr{F}}{\partial M} = 0 = 2aM + 4bM^3 = 2M(2bM^2 + a)$$

Magnetic equation of state

$$M_0 = \sqrt{-\frac{a}{2b}} = \sqrt{\frac{k(T_C - T)}{2bT_C}}$$

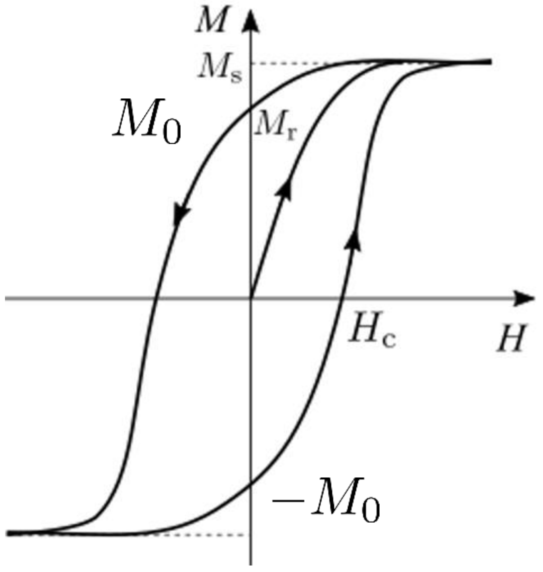
Spontaneous Symmetry Breaking



Spontaneous Symmetry Breaking

Spontaneous magnetization

$$M_0 = \sqrt{-\frac{a}{2b}} = \sqrt{\frac{k(T_C - T)}{2bT_C}}$$



MH curve

The symmetry of the system (Hamiltonian) is kept unchanged.

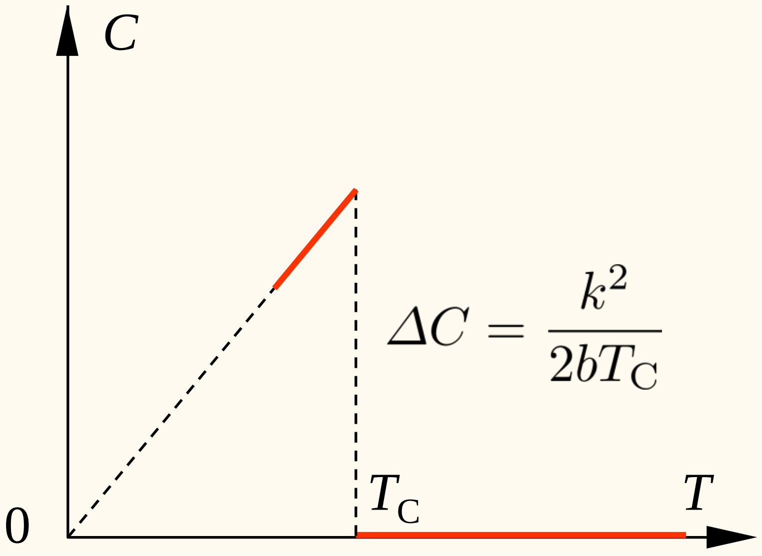
However the symmetry of the state is broken.

One of the central concepts in physics.

Phase transition, mass appearance, big bang, $\cdots$

Associated with appearance of Nambu-Goldstone mode

Critical exponent



In the presence of spontaneous magnetization, the free energy around the stable point is

$$\mathscr{F}(T) = \mathscr{F}_0 + aM_0^2 + bM_0^4 = \mathscr{F}_0 - \frac{a^2}{4b} = \mathscr{F}_0 - \frac{k^2(T_C - T)^2}{4bT_C^2}$$

Then the specific heat is obtained by

$$C = -T\frac{\partial^2 \mathscr{F}}{\partial T^2} = \frac{k^2 T}{2bT_C^2} \qquad T < T_C$$

$$\mathscr{F}(T) = \mathscr{F}_0 \qquad \therefore C = 0 \qquad T > T_C$$

$$\Delta C = \frac{k^2}{2bT_C}$$

Small B $\quad \mathscr{F}(M) = \mathscr{F}_0 + aM^2 + bM^4 - BM \qquad \dfrac{\partial \mathscr{F}}{\partial M} = 0 = 2aM + 4bM^3 - B$

$M^3 \propto B$ at the critical point

$$M \propto \begin{cases} B^{1/\delta} & (T = T_C), \\ (T_C - T)^{\beta} & (T < T_C), \end{cases} \qquad \chi \propto \begin{cases} (T - T_C)^{-\gamma} & (T > T_C), \\ (T_C - T)^{-\gamma'} & (T < T_C), \end{cases} \qquad C \propto \begin{cases} (T - T_C)^{-\alpha} & (T > T_C), \\ (T_C - T)^{-\alpha'} & (T < T_C). \end{cases}$$

Physical quantity that appears at the critical point $\quad A \propto (x - x_c)^{\nu} \quad$ Shift of a relevant parameter from the critical point

ν : Critical Exponent

Critical Exponent and Universality Class

Universality Class: Classification of the systems by symmetry, range of interaction, etc.
Each system which belongs to a universality class has the same set of critical exponents.

In the case of mean field approximation:

Critical exponent	α	β	γ	δ
Mean field approximation	0	1/2	1	3

One of the key features in analyzing phase transitions.

class	dimension	Symmetry	α	β	γ	δ	ν	η
3-state Potts	2	S_3	$\frac{1}{3}$	$\frac{1}{9}$	$\frac{13}{9}$	14	$\frac{5}{6}$	$\frac{4}{15}$
Ashkin-Teller (4-state Potts)	2	S_4	$\frac{2}{3}$	$\frac{1}{12}$	$\frac{7}{6}$	15	$\frac{2}{3}$	$\frac{1}{4}$
Ordinary percolation	1	1	1	0	1	∞	1	1
	2	1	$-\frac{2}{3}$	$\frac{5}{36}$	$\frac{43}{18}$	$\frac{91}{5}$	$\frac{4}{3}$	$\frac{5}{24}$
	3	1	−0.625(3)	0.4181(8)	1.793(3)	5.29(6)	0.87619(12)	0.46(8) or 0.59(9)
	4	1	−0.756(40)	0.657(9)	1.422(16)	3.9 or 3.198(6)	0.689(10)	−0.0944(28)
	5	1	≈ −0.85	0.830(10)	1.185(5)	3.0	0.569(5)	−0.075(20) or −0.0565
	6^+	1	−1	1	1	2	$\frac{1}{2}$	0
Directed percolation	1	1	0.159464(6)	0.276486(8)	2.277730(5)	0.159464(6)	1.096854(4)	0.313686(8)
	2	1	0.451	0.536(3)	1.60	0.451	0.733(8)	0.230
	3	1	0.73	0.813(9)	1.25	0.73	0.584(5)	0.12
	4^+	1	−1	1	1	2	$\frac{1}{2}$	0
Conserved directed percolation (Manna, or "local linear interface")	1	1		0.28(1)		0.14(1)	1.11(2)[1]	0.34(2)[1]
	2	1		0.64(1)	1.59(3)	0.50(5)	1.29(8)	0.29(5)
	3	1		0.84(2)	1.23(4)	0.90(3)	1.12(8)	0.16(5)
	4^+	1		1	1	1	1	0
Protected percolation	2	1		5/41[2]	86/41[2]			
	3	1		0.28871(15)[2]	1.3066(19)[2]			
Ising	2	$\mathbb{Z}_2$	0	$\frac{1}{8}$	$\frac{7}{4}$	15	1	$\frac{1}{4}$
	3	$\mathbb{Z}_2$	0.11008(1)	0.326419(3)	1.237075(10)	4.78984(1)	0.629971(4)	0.036298(2)
XY	3	$O(2)$	-0.01526(30)	0.34869(7)	1.3179(2)	4.77937(25)	0.67175(10)	0.038176(44)
Heisenberg	3	$O(3)$	−0.12(1)	0.366(2)	1.395(5)		0.707(3)	0.035(2)
Mean field	all	any	0	$\frac{1}{2}$	1	3	$\frac{1}{2}$	0
Molecular beam epitaxy[3]								
Gaussian free field								

Wikipedia

Models of magnetic systems (spin systems)

XY model: Spins are confined in a two-dimensional plane. $\boldsymbol{S}_i = (S_i^x, S_i^y)$

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j)$$

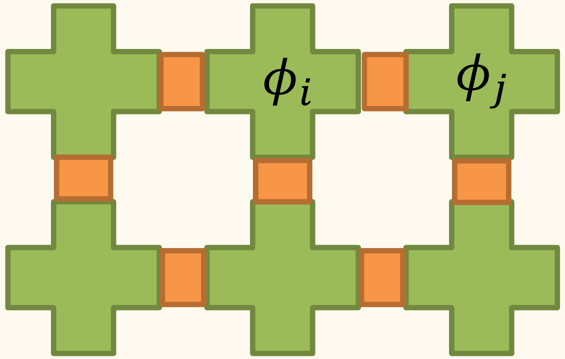
ϕ_i : Angle of each spin

Two-dimensional XY model: No long range order (Mermin-Wagner theorem)

Berezinskii-Kosterlitz-Thouless (BKT) transition

Quasi long range order (power decay)

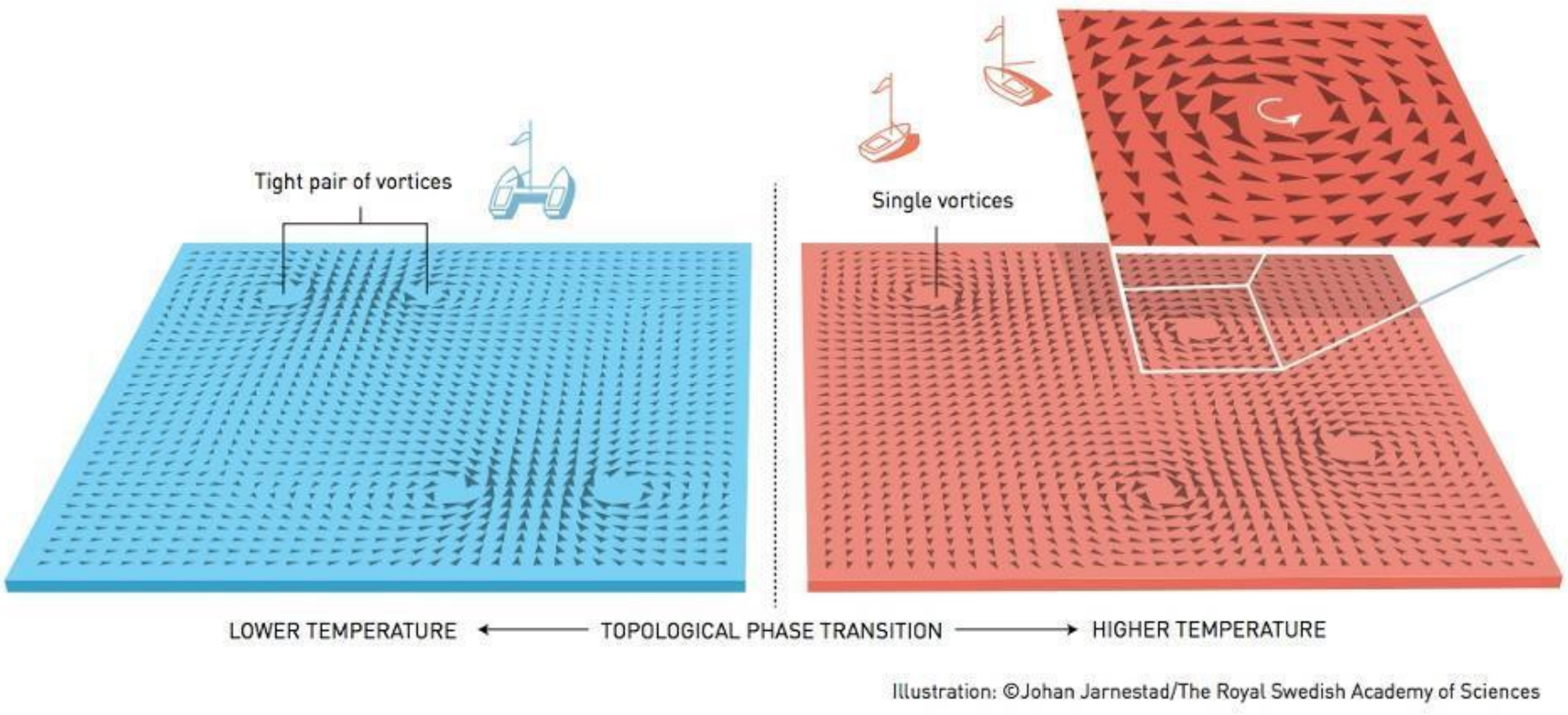
Realization of XY model: Josephson array



Josephson energy

$$E_{\mathrm{J}} = -E_0 \cos(\phi_i - \phi_j)$$

Berezinskii-Kosterlitz-Thouless Transition

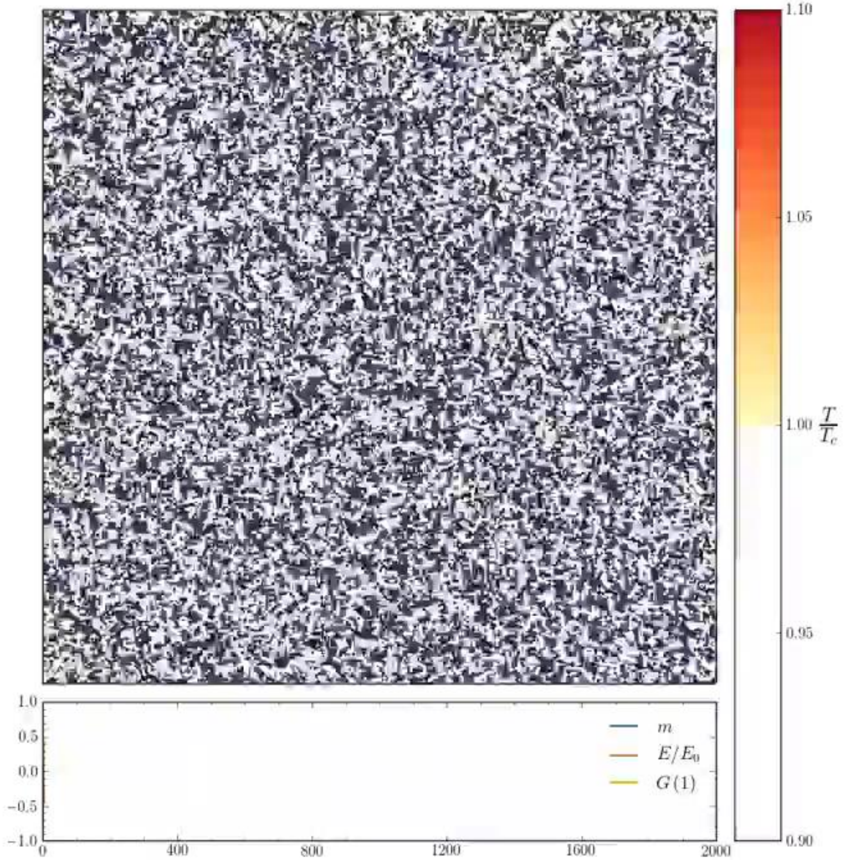


Ising model

Directions of spins are limited to *z*

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

Solution: 1d Ising, 2d Onsager



Model (Universality class)	α	β	γ	δ
2D Ising	0	1/8	7/4	15
3D Ising	0.115	0.324	1.239	4.82
3D XY	−0.01	0.34	1.32	4.9
3D Heisenberg	−0.11	0.36	1.39	4.9
Mean field approximation	0	1/2	1	3

https://www.youtube.com/watch?v=kjwKgpQ-l1s

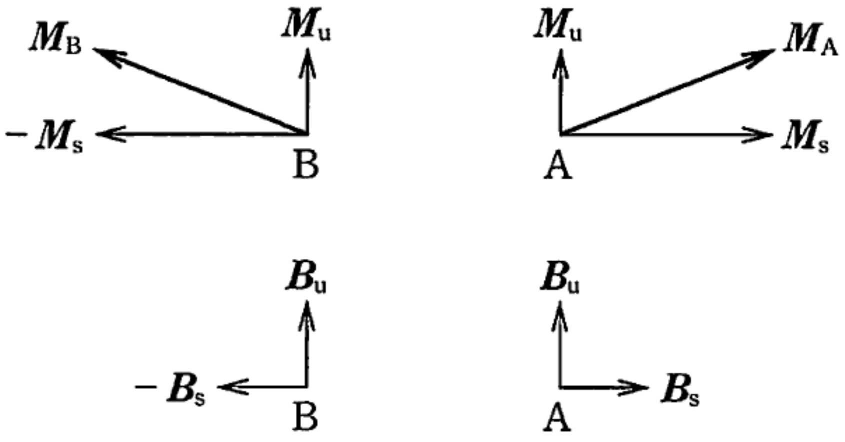
Antiferromagnetic Heisenberg model: Néel order and lattice partitioning

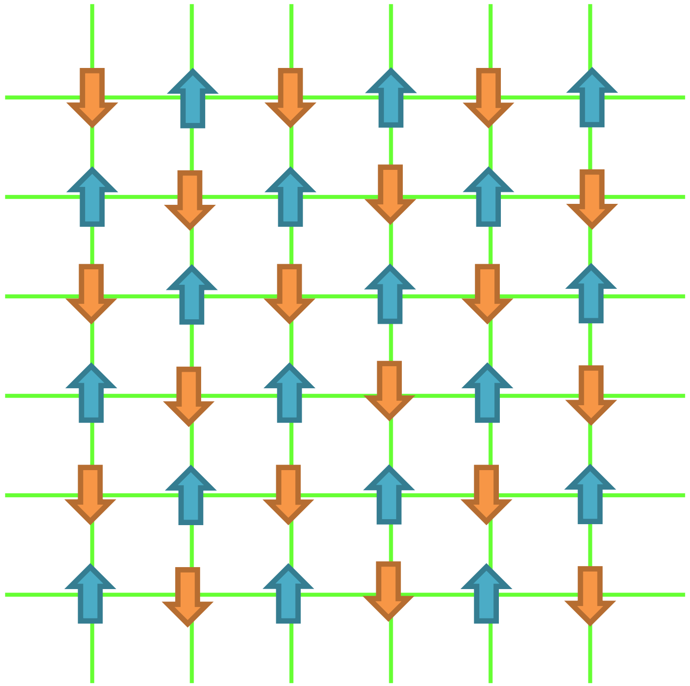
Antiferromagnetic
Heisenberg Hamiltonian

$$\mathscr{H} = -2J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \mu \sum_i \boldsymbol{B} \cdot \boldsymbol{S}_i$$

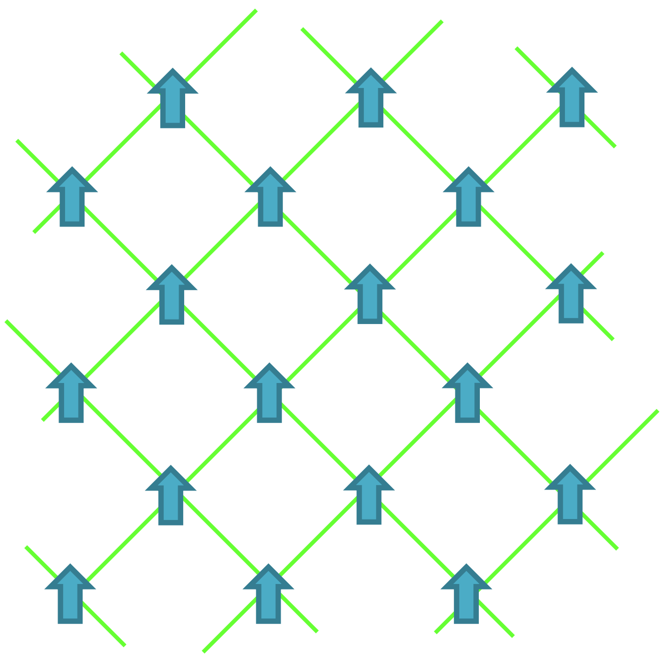
$J < 0$

$$\boldsymbol{B}_{\mathrm{A}} = \boldsymbol{B}_{\mathrm{u}} + \boldsymbol{B}_{\mathrm{s}}$$
$$\boldsymbol{B}_{\mathrm{B}} = \boldsymbol{B}_{\mathrm{u}} - \boldsymbol{B}_{\mathrm{s}}$$

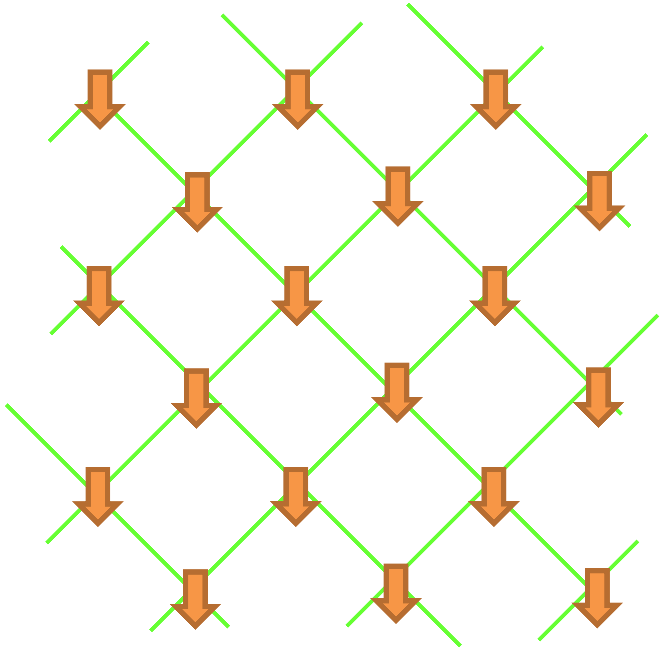




Néel order in 2D square lattice



Partial Lattice A



Partial Lattice B

Antiferromagnetic Heisenberg model(2)

Molecular-field effective Hamiltonian

$$\mathscr{H}_{\mathrm{eff}}(i) = -2J\sum_{\delta}\langle \boldsymbol{S}_{i+\delta}\rangle\cdot\boldsymbol{S}_i - \mu\boldsymbol{B}_{\mathrm{A}}\cdot\boldsymbol{S}_i \quad (i\in\mathrm{A})$$

$$\mathscr{H}_{\mathrm{eff}}(j) = -2J\sum_{\delta}\langle \boldsymbol{S}_{j+\delta}\rangle\cdot\boldsymbol{S}_j - \mu\boldsymbol{B}_{\mathrm{B}}\cdot\boldsymbol{S}_j \quad (j\in\mathrm{B})$$

Averaged moments

$$\begin{cases} \boldsymbol{M}_{\mathrm{A}} = \mu\langle\boldsymbol{S}_i\rangle = \boldsymbol{M}_{\mathrm{u}} + \boldsymbol{M}_{\mathrm{s}} \\ \boldsymbol{M}_{\mathrm{B}} = \mu\langle\boldsymbol{S}_j\rangle = \boldsymbol{M}_{\mathrm{u}} - \boldsymbol{M}_{\mathrm{s}} \end{cases}$$

Vector Brillouin function

$$\vec{B}_S(\boldsymbol{x}) = B_S(x)\frac{\boldsymbol{x}}{x}$$

Self-consistent equation

$$\boldsymbol{M}_{\mathrm{u}} + \boldsymbol{M}_{\mathrm{s}} = \mu S\vec{B}_S\left\{\frac{\mu S}{k_{\mathrm{B}}T}\left[\boldsymbol{B}_{\mathrm{u}} + \boldsymbol{B}_{\mathrm{s}} + \frac{2\alpha_z J}{\mu^2}(\boldsymbol{M}_{\mathrm{u}} - \boldsymbol{M}_{\mathrm{s}})\right]\right\}$$

Uniform susceptibility

$$\chi_{\mathrm{u}} = \lim_{B_{\mathrm{u}}\to 0}\frac{M_{\mathrm{u}}}{B_{\mathrm{u}}} = \chi_0\left(1 - \frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1}$$

Alternative susceptibility

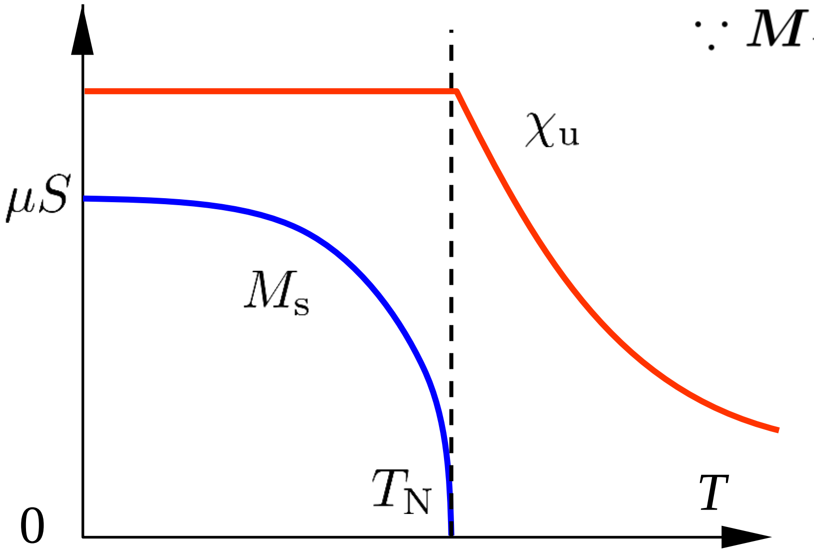
$$\chi_{\mathrm{s}} = \lim_{B_{\mathrm{s}}\to 0}\frac{M_{\mathrm{s}}}{B_{\mathrm{s}}} = \chi_0\left(1 + \frac{2\alpha_z J}{\mu^2}\chi_0\right)^{-1}$$

Antiferromagnetic Heisenberg model

Around stable points

$$\boldsymbol{M}_{\rm u} + \boldsymbol{M}_{\rm s} = \mu S \left[\vec{B}_S \left(\frac{\mu S}{k_{\rm B} T} \frac{-2\alpha_z J}{\mu^2} \boldsymbol{M}_{\rm s} \right) + \frac{d}{dM_{\rm s}} B_S \left(\frac{\mu S}{k_{\rm B} T} \frac{-2\alpha_z J}{\mu^2} \boldsymbol{M}_{\rm s} \right) \left(-\boldsymbol{M}_{\rm u} - \frac{\mu^2}{2\alpha_z J} \boldsymbol{B}_{\rm u} \right) \right]$$

$$\because \boldsymbol{M}_{\rm u} \perp \boldsymbol{M}_{\rm s}$$



Self-consistent equation for M_S

$$M_{\rm s} = \mu S B_S \left(\frac{\mu S}{k_{\rm B} T} \frac{-2\alpha_z J}{\mu^2} M_{\rm s} \right)$$

$$1 = \mu S \frac{d}{dM_{\rm s}} B_S \left(\frac{\mu S}{k_{\rm B} T} \frac{-2\alpha_z J}{\mu^2} M_{\rm s} \right)$$

$$\boldsymbol{M}_{\rm u} = -\boldsymbol{M}_{\rm u} - \frac{\mu^2}{2\alpha_z J} \boldsymbol{B}_{\rm u}$$

$$\chi_{\rm u} = \lim_{B_{\rm u} \to 0} \frac{M_{\rm u}}{B_{\rm u}} = -\frac{\mu^2}{-4\alpha_z J}$$

Summary

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