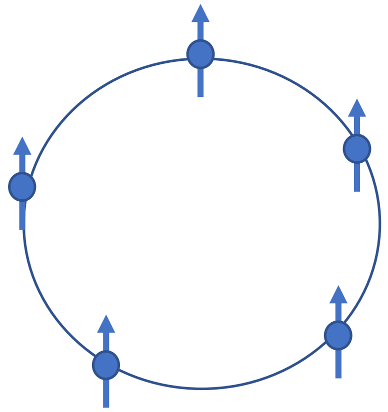
Lecture 24

12.04.2018

Landau mean-field theory

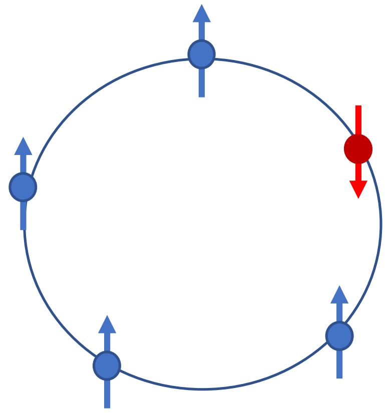
1D Ising model: No phase transition



At any nonzero temperature, it is energetically favorable to create defects (kinks) due to thermal fluctuations

Change in energy for flipping a spin (kink in the ordered state)

$$U_0 = -NJ\ (order), \qquad U_1 = -(N-2)J + 2J\ (with\ a\ kink) \rightarrow \Delta U = 4J$$



Change in entropy for flipping a spin anywhere in the 1D chain (N sites)

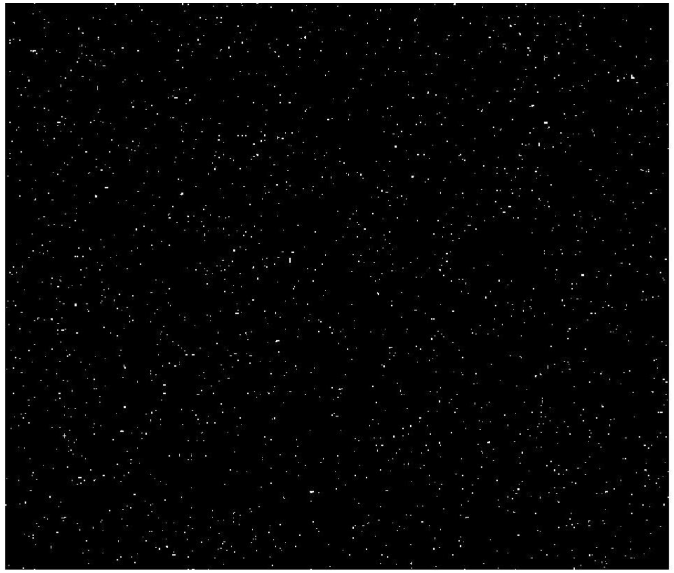
$$\Delta S = k \log N$$

The spin flipping due to thermal fluctuations is favored when it lowers the **Helmholtz free energy**

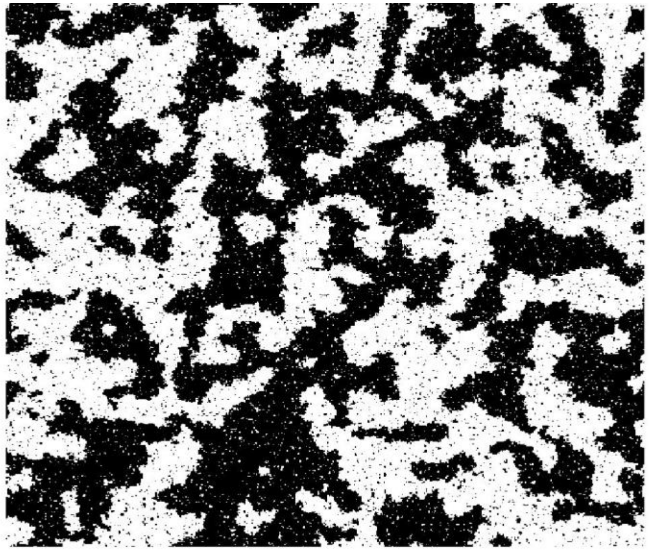
$$\Delta F = \Delta U - T\Delta S < 0 \rightarrow J - kT \log N < 0$$

At any $\mathrm{T} > 0$, spins are disordered and there is no net magnetization.

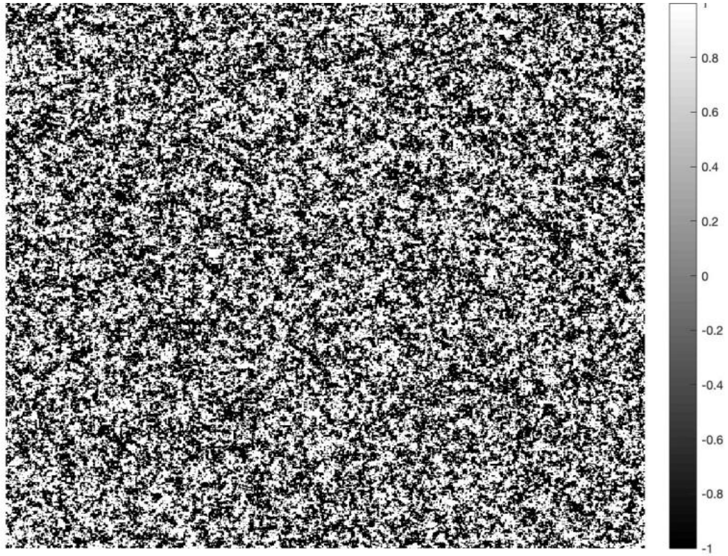
Ising model does capture phase transitions in $d > 1$



$T < T_C$



$T \lesssim T_C$



$T > T_C$

Critical phase transition occurs at a unique point in the $B - T$ diagram: $(B_c = 0, T_c)$

Q: How do we *theoretically* predict this critical point and the behavior near it?

A: Mean-field approximation, Landau field theory, renormalization group techniques

Landau field theory

- Critical phase transitions are characterized by universal properties, i.e. specific details of the systems tend not to matter

- Based on determining key elements that capture the universality class
  - Symmetry
  - Intrinsic dimension of the order parameter
  - Range of interactions

- Landau's free energy is typically a phenomenological Helmholtz free energy as the function of the order parameter and its gradients.

Landau field theory: Ising universality class at $B = 0$

- The local magnetization $m(\vec{r}, T)$ is a continuous variable of space $\vec{r}$ and temperature T
- Coarse-grained Helmholtz free energy functional is integral over space of the free energy density per unit volume

$$\mathcal{F}[m, T] = \int d^d\vec{r}\, f\big(m(\vec{r}, T)\big)$$

- The free energy density has a *local term* and *non-local term*

$$f\big(m(\vec{r}, T)\big) = f_{loc}\big(m(\vec{r}, T)\big) + f_{non-loc}(\nabla \mathrm{m})$$

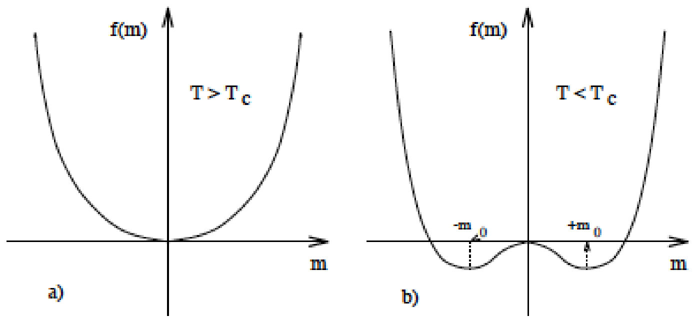
By symmetry it has to be invariant under spin inversion, $m \to -m$. This is a discrete symmetry

- *Local free energy density below T_c has the universal form of the double-well potential*

$$f_{loc}(m(T)) = f_0(T) + \frac{\epsilon(T)}{2} m^2 + \frac{u(T)}{4} m^4$$

With the important parameter related to the deviation from the critical point

$$\epsilon(T) \sim (T - T_c)$$



$\epsilon > 0$ $\epsilon < 0$

Landau field theory: Ising universality class

- Helmholtz free energy functional has a *local term* and *non-local term*

$$\mathcal{F}[m,T] = \int d^d\vec{r}\{f_{loc}(m(\vec{r},T)) + f_{non-loc}(\nabla \mathrm{m})\}$$

Has to be invariant under spin inversion, $m \rightarrow -m$

- *Non-local free energy density quantifies the energy cost for spatial variations of the magnetization*

  In the simplest form, it is determined by different powers of the gradient field, $\nabla \mathrm{m}$: the lowest power that is symmetric under spin inversion *is* $(\nabla m)^2$

$$f_{non-loc}(\nabla m) = \frac{1}{2}(\nabla m)^2$$

  It corresponds to the energy associated to an interface between regions with opposite magnetization, also known as domain wall

Gibbs free energy and equilibrium condition

- Helmholtz free energy functional has a *local term* and *non-local term*

$$\mathcal{F}[m,T] = \int d^d\vec{r}\left\{f_{loc}\left(m(\vec{r},T)\right) + f_{non-loc}(\mathbf{\nabla}\mathrm{m})\right\}$$

Has to be invariant under spin inversion, $m \rightarrow -m$

$$\mathcal{F}[m,T] = F_0(T) + \int d^d\vec{r}\left\{\frac{\epsilon}{2}m^2 + \frac{u}{4}m^4 + \frac{1}{2}|\nabla m|^2\right\}$$

- At nonzero applied field, the equilibrium condition is given by minimum of the Gibbs free energy

$$\mathcal{G}[B,T] = \mathcal{F}[m,T] - \int d^d\vec{r}\, m(\vec{r},T)\cdot B(\vec{r})$$

Equilibrium condition: $\boldsymbol{\delta\mathcal{G} = 0}$

Equilibrium condition

- Gibbs free energy functional

$$\mathcal{G}[B,T] = \int d^d\vec{r} \left\{ \frac{1}{2}|\nabla m|^2 + \frac{\epsilon}{2}m^2 + \frac{u}{4}m^4 - m \cdot B \right\}$$

Equilibrium condition: $\boldsymbol{\delta\mathcal{G} = 0}$

Variational of $\mathcal{G}$

$$\delta\mathcal{G} = \int d^d\vec{r}\{-\nabla^2 m + \epsilon m + u m^3 - B\}\delta m = 0$$

Integral is zero for arbitrary variations in magnetization, hence

$$-\nabla^2 m(\vec{r}) + \epsilon m(\vec{r}) + u m^3(\vec{r}) = B(\vec{r})$$

Susceptibility

Spatially dependent susceptibility measures the response in magnetization at a position r due to an applied magnetic field at another position r'

$$\chi(r, r') = \frac{\partial m(r)}{\partial B(r')}$$

- Equilibrium condition provides an equation for susceptibility

$$-\nabla^2 m(r) + \epsilon m(r) + u m^3(r) = B(r) \rightarrow$$

$$[-\nabla^2 + \epsilon + 3um^2]\chi(r, r') = \delta(r - r')$$

  - *Solution can be found using the Fourier transform*

$$\chi(r - r') = \int \frac{d^d q}{(2\pi)^d} \hat{\chi}(q) e^{-iq\cdot(r - r')}$$

Susceptibility

- Equilibrium condition provides an equation for susceptibility

  - $[-\nabla^2 + \epsilon + 3um^2(r)]\chi(r, r') = \delta(r - r')$ *(1)*

$$\chi(r - r') = \int \frac{d^d q}{(2\pi)^d} \hat{\chi}(q) e^{-iq\cdot(r-r')}$$

Eq. (1) contains the magnetization $\mathrm{m(r)}$ which can depend on position. Hence the equation is in general more difficult to solve for any T. However, we can solve at temperatures above the critical one when $\mathrm{m} = 0$ and the equation is linear.

- $T > T_c \rightarrow m = 0$: $[-\nabla^2 + \epsilon]\chi(r, r') = \delta(r - r')$

And in the Fourier space given by $[q^2 + \epsilon]\hat{\chi}(q) = 1$ *with the solution*

$$\hat{\chi}(q) = \frac{1}{q^2 + \epsilon}$$

Susceptibility and critical exponent

- Equilibrium condition provides an equation for susceoptibility

$$[-\nabla^2 + \epsilon + 3um^2]\chi(r, r') = \delta(r - r')$$

$T > T_c \rightarrow m = 0$: $\hat{\chi}(q) = \frac{1}{q^2+\epsilon}$

$$\chi(r - r') = \int \frac{d^3q}{(2\pi)^3} \frac{1}{q^2 + \epsilon} e^{-iq\cdot(r-r')}$$

$$\chi(r - r') = \frac{1}{(2\pi)^2}\int_0^\infty dq \frac{q^2}{q^2+\epsilon}\int_{-1}^1 dz\, e^{-iq|r-r'|z} = \frac{1}{2\pi^2|r-r'|}\int_0^\infty dq \frac{q}{q^2+\epsilon}\sin(q|r-r'|)$$

Susceptibility depends on the two points separations as

$$\chi(r - r') = \frac{1}{4\pi|r - r'|} e^{-\frac{|r-r'|}{\xi}},$$

Where the correlation lengthscale is $\xi(T) = \frac{1}{\sqrt{\epsilon}} \sim (T - T_c)^{-\nu}$, $\nu_{MF} = \frac{1}{2}$

For distances less than the correlation length, the susceptibility decays as $1/r$, while for longer distances is falls off exponentially. This means that the effects of the applied field on the magnetization is mostly local and on distances smaller that the correlation length. This picture holds true far above from the critical point. But it is not valid below and near the critical temperature where we notice that $\xi(T)$ diverges, i.e. becomes very large and of the same order as a the system size. Then the applied field at a given point affects the magnetization everywhere in the system no matter how far away.

Spin-spin correlation function and susceptibility

Correlation function measure the «spin coherence» between the magnetization field at two separate locations

$$C(r,r') = \langle (m(r) - m_0)(m(r') - m_0) \rangle = \langle m(r)m(r') \rangle - \langle m \rangle^2$$

From the linear response, the correlation and the susceptibility are related by

$$C(r,r') = kT\,\chi(r - r')$$

Partition function for a spin lattice $Z = \sum_{\{\sigma\}} e^{-\beta H(\{\sigma\},B)}$

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i \sigma_j e^{-\beta H(\{\sigma\},B)} = \frac{1}{Z\beta^2} \frac{\partial^2 Z}{\partial B_i \partial B_j} \rightarrow C_{ij} = \frac{1}{Z\beta^2} \frac{\partial^2 Z}{\partial B_i \partial B_j} - \frac{1}{\beta^2} \frac{1}{Z^2} \frac{\partial Z}{\partial B_i} \frac{\partial Z}{\partial B_j}$$

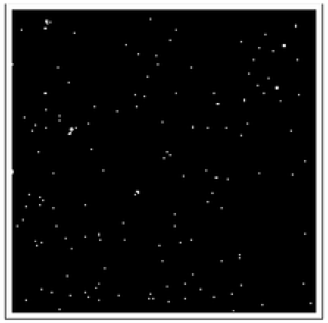
$$\chi_{ij} = \frac{\partial \langle s_i \rangle}{\partial B_j} = \frac{1}{\beta} \frac{\partial}{\partial B_j} \left(\frac{1}{Z} \frac{\partial Z}{\partial B_i} \right) = \frac{1}{Z\beta} \frac{\partial^2 Z}{\partial B_i \partial B_j} - \frac{1}{\beta} \frac{1}{Z^2} \frac{\partial Z}{\partial B_i} \frac{\partial Z}{\partial B_j} = \beta C_{ij} \rightarrow C_{ij} = kT\chi_{ij}$$

Spin-spin correlation function and susceptibility

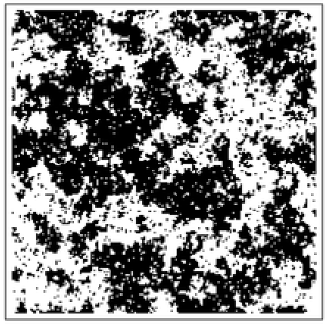
$$C(\boldsymbol{r},\boldsymbol{r}') = \ kT\,\chi(\boldsymbol{r}-\boldsymbol{r}')$$

$$C(\boldsymbol{r}-\boldsymbol{r}') = \frac{kT}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}e^{-\frac{|\boldsymbol{r}-\boldsymbol{r}'|}{\xi}}, in\ 3D$$

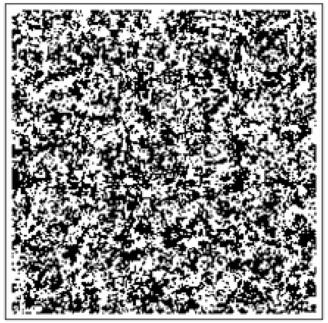
- Correlation length $\xi \sim (T-T_c)^{-\nu}$ is diverging at the critical point
- Clusters of similar magnetization have fractal size distribution and complex spatial shapes with fractal boundaries



$T < T_c$



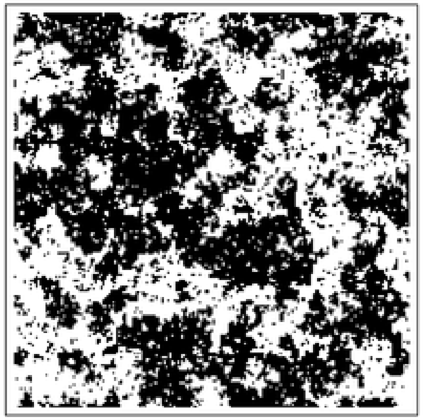
$T \sim T_c$



$T > T_c$

Relation between critical exponents

$$C_{3D}(\boldsymbol{r}-\boldsymbol{r}') = \frac{kT}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}e^{-\frac{|\boldsymbol{r}-\boldsymbol{r}'|}{\xi}}, \xi \sim (T-T_c)^{-\nu}$$



$T \sim T_c$

$$\left.\begin{array}{c}\chi_0(T) = \int_0^\infty dr \frac{1}{4\pi r}e^{-\frac{r}{\xi}} = \hat{\chi}(\boldsymbol{q}=0) = \frac{1}{\epsilon} = \xi^2 \sim (T-T_c)^{-2\nu} \\ \chi_0(T) \sim (T-T_c)^{-\gamma}\end{array}\right\} \rightarrow \gamma = 2\nu$$

$$C_d(\boldsymbol{r}-\boldsymbol{r}') \sim \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^{d-2+\eta}}e^{-\frac{|\boldsymbol{r}-\boldsymbol{r}'|}{\xi}}, \qquad \xi \sim (T-T_c)^{-\nu}, \qquad \eta^{(MF)} = 0$$

Ginzburg-Landau criterion for the mean-field approximation

Relative magnitude of fluctuations is sufficiently small compared to the average

$$\frac{\left|\int_V d^d\boldsymbol{r}' \int_V d^d\boldsymbol{r}\, C_d(\boldsymbol{r}-\boldsymbol{r}')\right|}{\left|\int_V d^d\boldsymbol{r}\, m(\boldsymbol{r})\right|^2} < 1$$

This criterion determines the **upper critical dimension $\boldsymbol{d_c}$** above which mean-field is exact

$$\frac{\left|\int_V d^d\boldsymbol{r}' \int_V d^d\boldsymbol{r}\, C_d(\boldsymbol{r}-\boldsymbol{r}')\right|}{\left|\int_V d^d\boldsymbol{r}\, m(\boldsymbol{r})\right|^2} < 1 \rightarrow \frac{\xi^d \chi_0(T)}{\xi^{2d}(T)\cdot m_0^2(T)} < 1 \quad \left(V \sim \xi^d\right)$$

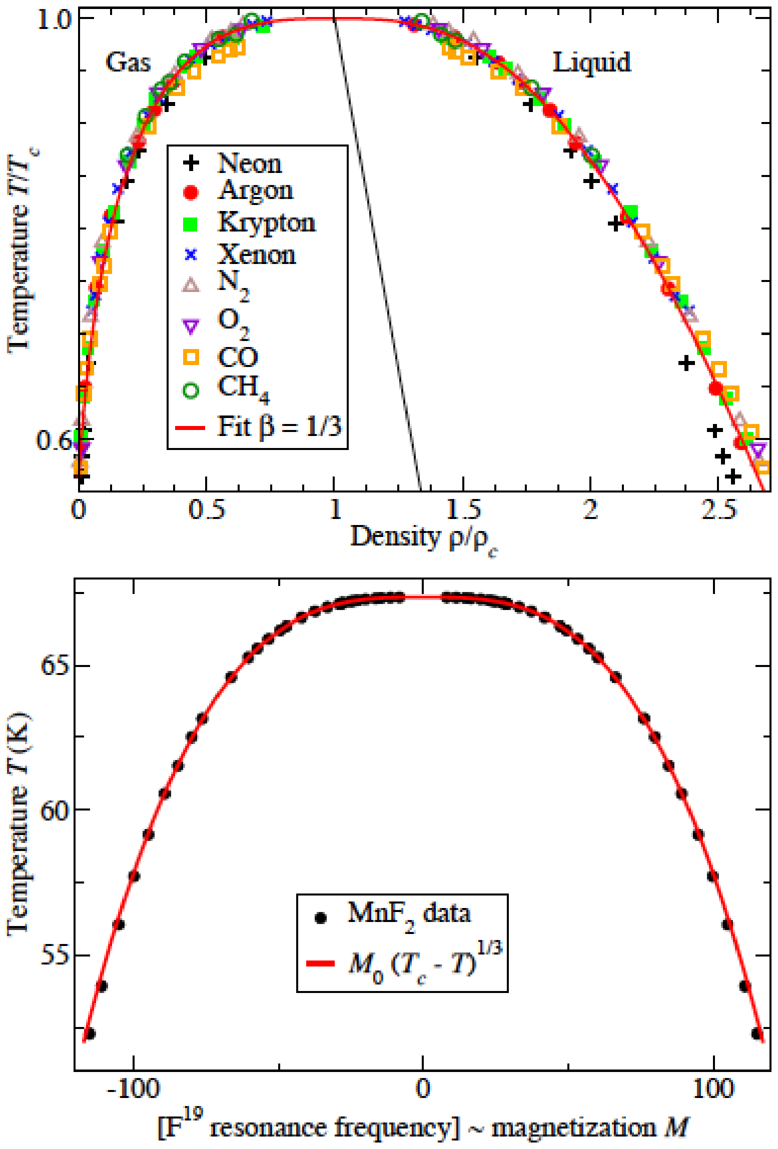
$$\frac{\xi^2}{\xi^d(T)\cdot m_0^2(T)} < 1 \rightarrow \xi^{-d+2}(T) m_0^{-2}(T) < 1, \qquad \xi^{MF} \sim (T_c - T)^{-\frac{1}{2}}, \qquad m_0^{(MF)} \sim (T_c - T)^{\frac{1}{2}}$$

$$(T_c - T)^{\frac{1}{2}(d-2)-1} < 1 \rightarrow (T_c - T)^{\frac{d-4}{2}} < 1 \rightarrow d \geq 4 \rightarrow d_c = 4$$

Ising Universality Beyond the mean field

- Real fluids and magnetics have have similar scaling behavior and this behavior is captured by the mean-field approximations (van-der-Waals and Weiss model). However the values of the scaling exponents in the mean-field approximation are not accurate.

- How can we predict the critical point and the scaling exponents beyond MF?



$$m \sim (T_c - T)^{\beta}$$

Fig. 12.6 Universality. (a) Universality at the liquid–gas critical point. The liquid–gas coexistence lines ($\rho(T)/\rho_c$ versus T/T_c) for a variety of atoms and small molecules, near their critical points (T_c, ρ_c) [54]. The curve is a fit to the argon data, $\rho/\rho_c = 1+s(1-T/T_c) \pm \rho_0(1-T/T_c)^{\beta}$ with $s = 0.75$, $\rho_0 = 1.75$, and $\beta = 1/3$ [54]. (b) Universality: ferromagnetic–paramagnetic critical point. Magnetization versus temperature for a uniaxial antiferromagnet MnF_2 [56]. We have shown both branches $\pm M(T)$ and swapped the axes so as to make the analogy with the liquid–gas critical point (above) apparent. Notice that both the magnet and the liquid–gas critical point have order parameters that vary as $(1 - T/T_c)^{\beta}$ with $\beta \approx 1/3$. (The liquid–gas coexistence curves are tilted; the two theory curves would align if we defined an effective magnetization for the liquid–gas critical point $\rho_{\mathrm{eff}} = \rho - 0.75\rho_c(1-T/T_c)$ (thin midline, above). This is not an accident; both are in the same universality class, along with the three-dimensional Ising model, with the current estimate for $\beta = 0.325 \pm 0.005$ [148, chapter 28].

J. Sethna, **Statistical Mechanics:** Entropy, Order Parameters, and Complexity (Oxford, 2006)

Spontaneous symmetry breaking

Ising model has a discrete symmetry of the order parameter, i.e. Hamiltonian is invariant under spin inversion $s \to -s$. The paramagnetic (disordered) state is symmetric under spin inversion since $m = 0$. The ferromagnetic phase is the ordered state that breaks the spin inversion symmetry of the order parameter, $m \neq 0$.

1D Ising model has no spontaneous symmetry breaking at any finite temperature.

For any $d > 1$, Ising model predicts a spontaneous symmetry breaking at a critical temperature associated to the ferro-paramagnetic phase transition.

! Symmetry breaking is typically accompanied by a phase transition, but no always.

Phase transitions without breaking any symmetry:

- Liquid-gas phase transition
- Kosterlitz-Thouless phase transition
- Glass transition, etc

Mermin-Wagner theorem: Continuous symmetry breaking

Theorem (Mermin-Wagner). Low dimensional systems, i.e. $d \leq 2$, with a continuous symmetry and *short-range interactions* cannot be in an ordered state at any finite temperature. This means that the continuous symmetry cannot be broken in $d \leq 2$. Thermal fluctuations are very strong in low dimensions and they destroy any potential ordering.

- $\langle s \rangle = 0$ average of the order parameter is symmetric (disordered state)
- $\langle s \rangle \neq 0$ average of the order parameter breaks the symmetry (ordered state)

Example of continuous symmetry: rotation, translation

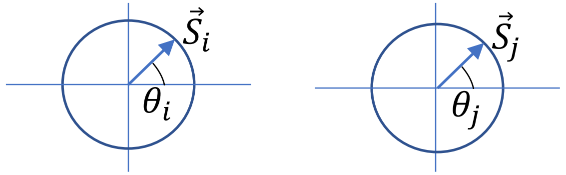
The degree of order is characterized by the shape of the correlation function, i.e. $C(r) \sim r^{-\eta} e^{-\frac{r}{\xi(T)}}$

- $C(r) \sim r^{-\eta}$ long-range correlations, diverging correlation length (ordered macrostate state)
- $C(r) \sim e^{-r/\xi}$ short range correlations within a domian of the size of the correlation length (disordered macrostate state)

Magnets with no continuous symmetry breaking: XY model

Hamiltonian for a system of N-spins $H_N = -J\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j$, $\vec{S} = (\cos(\theta), \sin(\theta))$. It can also be written equivalently

$$H = -J\sum_{\langle i,j\rangle}\cos(\theta_i - \theta_j)$$



This Hamiltonian is rotationally invariant. When the mean magnetization $\langle\vec{S}\rangle$ is also zero, we say the state is also rotationally invariant. In the ground state, however, the system picks the same orientation for all spins and mean magnetization $\langle\vec{S}\rangle$ is non-zero, hence this state breaks the rotational invariance. There are infinitely many ground states since the spins can point in any direction in the plane.

No symmetry breaking in 2D (Mermin-Wagner theorem): $\langle\vec{S}(r)\rangle = 0$ at any finite T

However the correlation function have two very different behaviors

- $kT > J$, the spin-spin correlation function $C(r) = \langle\vec{S}(0)\cdot\vec{S}(r)\rangle$ decays exponentially

  $C(r) \sim e^{-\frac{r}{\xi}}$, (disordered state)

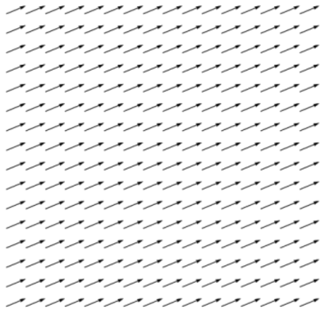
- $kT < J$: $H \sim E_0 + \frac{J}{2}\int dr\,|\nabla\theta|^2$. The correlation function decays a power law $C(r) \sim r^{-\eta(T)}$, (quasi-ordered state). It would correspond to a diverging correlation length ξ.

Kosterlitz-Thouless phase transition (2D)

In 2D, the correlation function decays a power law $C(r - r') \sim r^{-\eta(T)}$, which would correspond to a diverging correlation length ξ. However there is no symmetry breaking. This is consistent with Mermin-Wagner theorem. It does not prevent the system to undergo a topological phase transition, known as the Kosterlitz-Thouless transition.

Continuum approximation in the low T limit: $H = E_0 + \frac{J}{2}\int d\,\vec{r}\,|\nabla\theta|^2$

Equilibrium condition: $\frac{\delta H}{\delta\theta} = 0 \rightarrow \nabla^2\theta = 0$



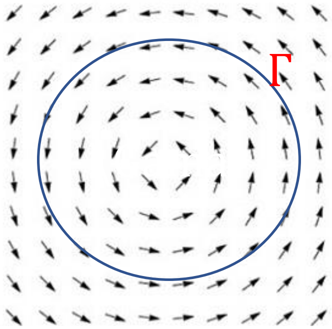
<u>Uniform solution: ground state</u> $\theta(r) = \theta_0$

<u>Singular solution: vortex solution</u>

Any contour integral around the singular vortex is nonzero and given by the winding number

$\oint_\Gamma \mathrm{d}s \cdot \nabla\theta = 2\pi n,\ n = \pm 1$ is winding number (vortex charge)

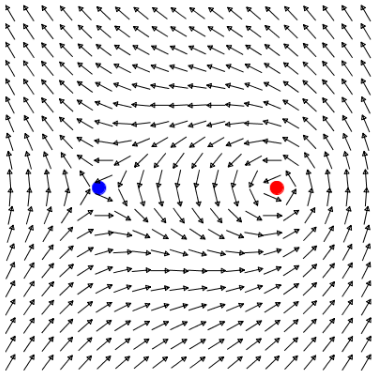
$$|\nabla\theta| = \frac{1}{r}$$



Energy of a single vortex $E = +\frac{J}{2}\int d\,\vec{r}\,|\nabla\theta|^2 = \pi J \ln\left(\frac{L^2}{l}\right)$

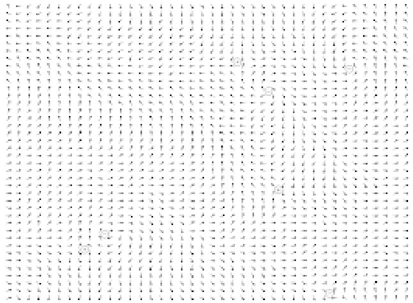
Kosterlitz-Thouless phase transition

In 2D, the correlation function decays a power law $C(r-r') \sim r^{-\eta(T)}$, which would correspond to a diverging correlation length ξ. However there is no symmetry breaking. This is consistent with Mermin-Wagner theorem. It does not prevent the system to undergo a topological phase transition, known as the Kosterlitz-Thouless transition.



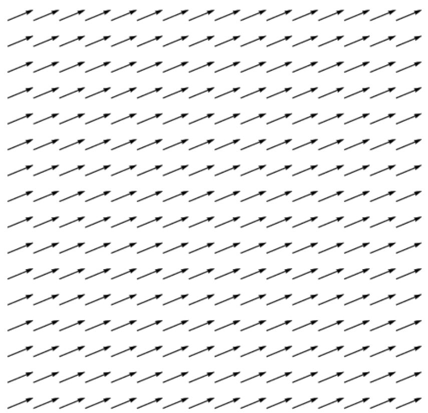
- Below $T < T_{KT}$: there are vortex-anti-vortex pairs (vortex dipoles) such that long-range order is maintained

- At $T \sim T_{KT}$: unbinding of vortex dipoles into free vortices



- Above $T > T_{KT}$: proliferation of free vortices and no long-range order

Kosterlitz-Thouless temperature

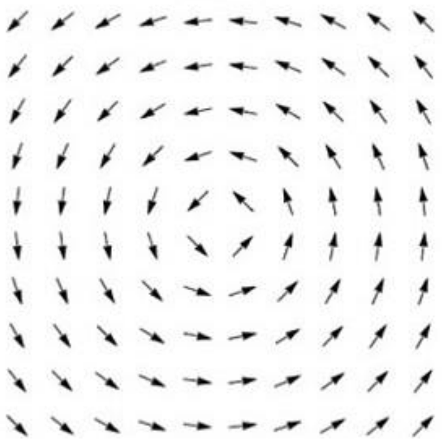


Energy of single vortex $E = \pi J \ln\left(\frac{L}{l}\right)$

Entropy of a vortex $S = k \ln\left(\frac{L^2}{l}\right)$

Change in free energy due to a single vortex

$$\Delta F = (\pi J - 2kT) \ln\left(\frac{L^2}{l}\right)$$



Becomes negative for $T > T_{KT} = \frac{J}{2k}$, meaning that states with free vortices will be energetically favored at temperatures than the Kosterlitz Thouless critical temperature T_{KT}