Collective Effects

in

Equilibrium and Nonequilibrium Physics

Website: http://cncs.bnu.edu.cn/mccross/Course/

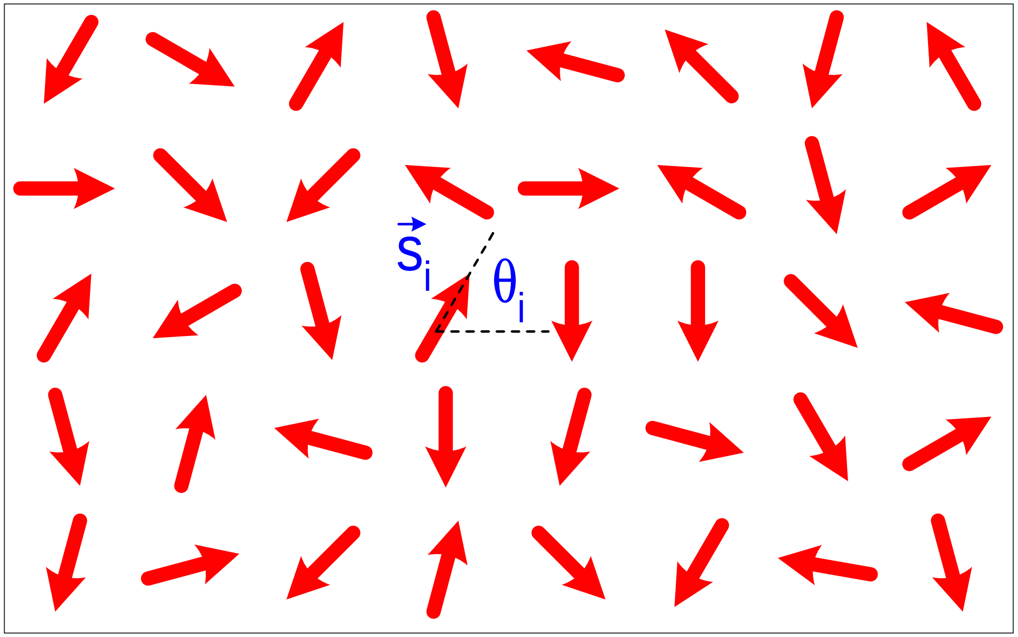
Caltech Mirror: http://haides.caltech.edu/BNU/

Today's Lecture

Magnets with continuous symmetry (XY model)

- Landau free energy and the Mexican hat
- Angle/phase variables
- Goldstone's theorem
- Generalized rigidity
- Spin wave excitations and the Mermin-Wagner theorem
- Topological defects
- Kosterlitz-Thouless transition

XY Model



d-dimensional lattice of N "spins" $\mathbf{s}_i$ with $|\mathbf{s}_i| = 1$ free to rotate in a plane

Hamiltonian

$$H = -\frac{1}{2} J \sum_{\substack{i \\ nn\ \delta}} \mathbf{s}_i \cdot \mathbf{s}_{i+\delta}$$

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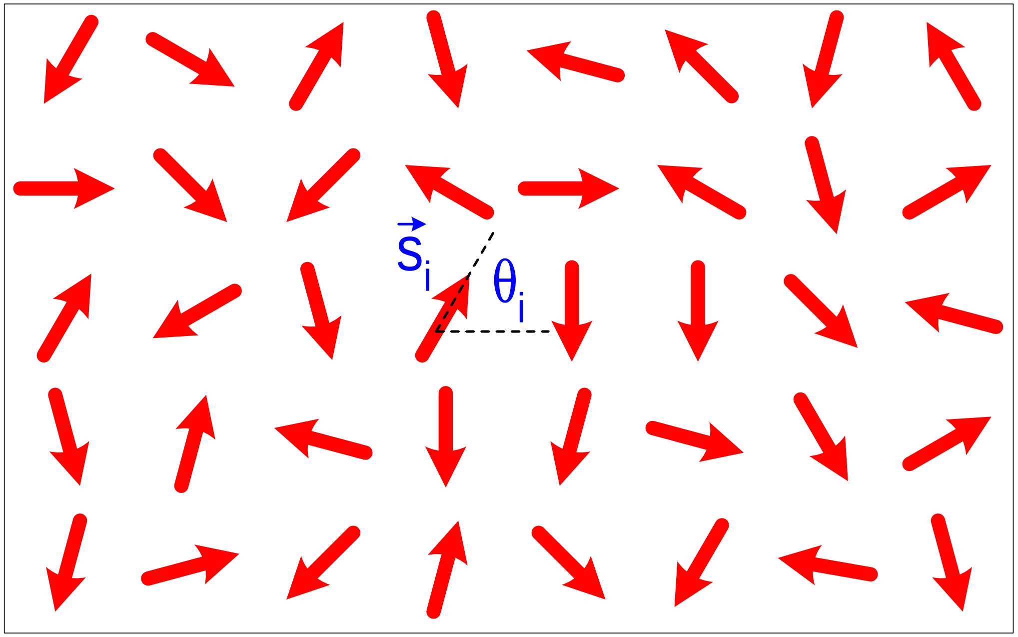

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Mean Field Theory

We could go through mean field theory is before.

I will leave you to show that for free XY spins with $H = -\sum_i \mathbf{s}_i \cdot \mathbf{b}$ the mean spin is given by

$$\langle \mathbf{s}_i \rangle = L_{XY}(\beta b)$$

with the function L_{XY} defined in terms of Bessel functions

$$L_{XY}(x) = \frac{I_1(x)}{I_0(x)} \simeq \frac{x}{2} - \frac{x^3}{16} + \cdots$$

and that there is a phase transition to an ordered phase, $\langle \mathbf{s}_i \rangle = \mathbf{s}$ with nonzero $|\mathbf{s}|$, below a transition temperature T_c given by $k_B T_c = dJ$.

Landau Free Energy

Near T_c we expand the free energy gained from a nonzero **s** as a Taylor expansion

$$\delta f = f(\mathbf{s}, T) - f_o(T) \simeq \alpha(T)\mathbf{s}\cdot\mathbf{s} + \tfrac{1}{2}\beta(T)(\mathbf{s}\cdot\mathbf{s})^2 + \gamma(T)\vec{\nabla}\mathbf{s}\cdot\vec{\nabla}\mathbf{s}$$

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or expanding α, β, γ around their values at T_c

$$\delta f = a(T - T_c)\mathbf{s}\cdot\mathbf{s} + \frac{1}{2}b(\mathbf{s}\cdot\mathbf{s})^2 + \gamma\vec{\nabla}\mathbf{s}\cdot\vec{\nabla}\mathbf{s}$$

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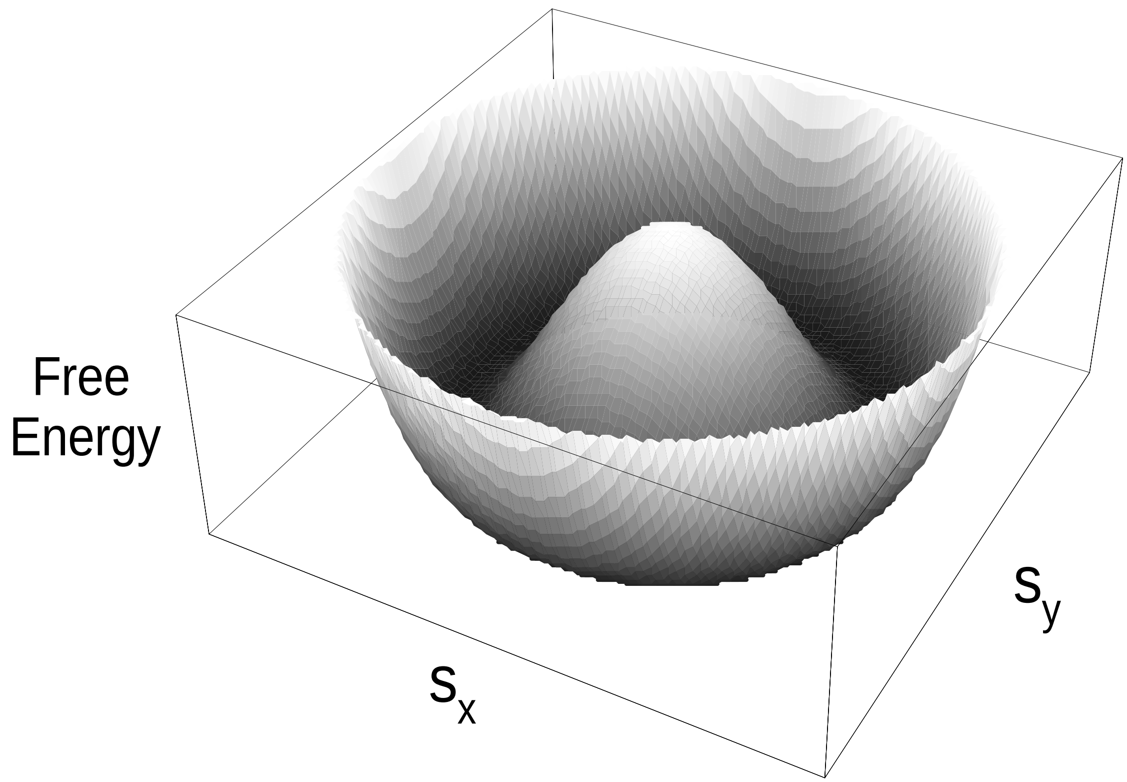
Note that the gradient term is a separate dot product of the $\vec{\nabla}$ and $\mathbf{s}$ vectors

$$\vec{\nabla}\mathbf{s}\cdot\vec{\nabla}\mathbf{s} = \sum_{i,\alpha}\nabla_i s_\alpha \nabla_i s_\alpha$$

“Mexican Hat” Free Energy

$$\delta f = a(T - T_c)\mathbf{s}\cdot\mathbf{s} + \tfrac{1}{2}b(\mathbf{s}\cdot\mathbf{s})^2$$



Rotation of s everywhere through any angle Θ leads to an equivalent state (same free energy, etc.)

Angle remains a thermodynamic variable far below T_c

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The orientation of the order parameter Θ remains a new thermodynamic variable for any temperature in the ordered phase

Goldstones Theorem

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For any continuous symmetry that is broken there is a low frequency collective mode, with a frequency that goes to zero as the wave number of the mode goes to zero

Developed in the context of particle physics where the “low frequency mode” becomes “zero mass boson”. The search for the “Higgs Boson” coming from the supposed breaking of the electro-weak gauge symmetry is one of the great challenges in current experiments at the supercolliders.

Phase Transition with an "Angle" Symmetry

- Easy plane ferromagnets and antiferromagnets
- Superfluidity: Θ is the phase of the Bose condensed wave function
- Superconductivity: Θ is the phase of the electron pair wave function
- Nematic liquid crystals in thin films or electric field: Θ is the orientation of the long molecules in the plane

And to some degree:

- Solids: Θ is the phase of the density wave $\rho \propto e^{i(\mathbf{q}\cdot\mathbf{r}+\Theta)}$ giving the translational position of the atoms
- Smectic liquid crystal: Θ gives the translation of the planes of atoms
- Rayleigh-Bénard convection: Θ gives the translation of the convection rolls

Generalized Rigidity

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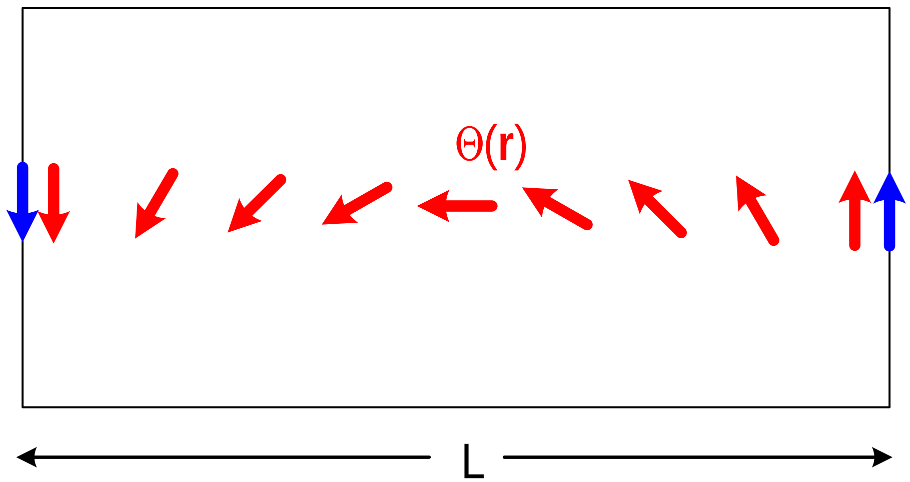
There is a new long range rigidity or stiffness in the system:



Boundary dependent free energy scales as L^{-1} rather than $e^{-L/\xi}$ as in the absence of broken symmetry.

We may use this result to *rigorously define* the stiffness constant K.

This rigidity coming from broken symmetry is of course vital in the world around us:

- Elasticity of solids: shear modulus
- Superfluid and superconducting: superfluid density
- …

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$$\delta\Theta(\mathbf{r}) = \sum_{\mathbf{q}} \delta\Theta_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \qquad (\delta\Theta_{-\mathbf{q}} = \delta\Theta^*_{\mathbf{q}})$$

so that

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- energy of spin wave distortion at wave vector $\mathbf{q}$ proportional to q^2
- quadratic effective Hamiltonian: a “Gaussian model”: $P(\delta\Theta_{\mathbf{q}}) \propto e^{-\beta\Omega K q^2 |\delta\Theta_{\mathbf{q}}|^2/2}$

Mermin-Wagner-Hohenberg Theorem

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Illustrative calculation: assume that long range order exists with order parameter s_0, and look for corrections to this coming from the thermal excitation of the Goldstone modes.

$d = 2$ Illustrative Calculation

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Now lets correct the mean spin for these fluctuations

$$\langle s\rangle = s_0\langle\cos\Theta\rangle \simeq s_0\left(1 - \tfrac{1}{2}\langle\delta\Theta^2\rangle\right)$$

with

$$\langle\delta\Theta(\mathbf{r})^2\rangle = \left\langle \sum_{\mathbf{q}} \delta\Theta_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{q}'} \delta\Theta_{\mathbf{q}'} e^{i\mathbf{q}'\cdot\mathbf{r}} \right\rangle = \sum_{\mathbf{q}} \langle|\delta\Theta_{\mathbf{q}}|^2\rangle$$

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For rigorous proofs see

- Mermin and Wagner: Phys. Rev. Lett. 17, 1133 (1966)
- Hohenberg: Phys. Rev. 158, 383 (1967)

Correlation Function

$$C(|\mathbf{r}-\mathbf{r}'|) = \langle \cos[\Theta(\mathbf{r}) - \Theta(\mathbf{r}')]\rangle = \langle \exp[i(\Theta(\mathbf{r}) - \Theta(\mathbf{r}')\rangle$$

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A general result says for a Gaussian model (i.e., a model with a quadratic effective Hamiltonian such as given by our free energy)

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The result only depends on $\mathbf{r}-\mathbf{r}'$ by the translational invariance, and so we may take $\mathbf{r}' = 0$ for convenience.

Then introducing the Fourier mode representation

$$\begin{aligned}
\langle [\Theta(\mathbf{r}) - \Theta(\mathbf{0})]^2 \rangle &= \sum_{\mathbf{q}\mathbf{q}'} \langle \delta\Theta_{\mathbf{q}} \delta\Theta_{\mathbf{q}'} \rangle (e^{i\mathbf{q}\cdot\mathbf{r}} - 1)(e^{i\mathbf{q}'\cdot\mathbf{r}} - 1) \\
&= \sum_{\mathbf{q}} \langle |\delta\Theta_{\mathbf{q}}|^2 \rangle 2(1 - \cos \mathbf{q}\cdot\mathbf{r})
\end{aligned}$$

We can roughly see how this comes as follows. Introduce the modes

$$C(r) = \left\langle \exp\left[i \sum_{\mathbf{q}} \delta\Theta_{\mathbf{q}} (e^{i\mathbf{q}\cdot\mathbf{r}} - 1) \right] \right\rangle$$

Now expand the exponential, and use the fact that averages of odd powers of $\delta\Theta_{\mathbf{q}}$ are zero

$$\begin{aligned} C(r) &= \mathrm{Re}[1 - \tfrac{1}{2} \sum_{\mathbf{q}\mathbf{q}'} \langle \delta\Theta_{\mathbf{q}} \delta\Theta_{\mathbf{q}'} \rangle (e^{i\mathbf{q}\cdot\mathbf{r}} - 1)](e^{i\mathbf{q}'\cdot\mathbf{r}} - 1)] + \cdots] \\ &= 1 - \sum_{\mathbf{q}} \langle |\delta\Theta_{\mathbf{q}}|^2 \rangle (1 - \cos \mathbf{q}\cdot\mathbf{r}) + \cdots \\ &= \exp\left[- \sum_{\mathbf{q}} \langle |\delta\Theta_{\mathbf{q}}|^2 \rangle (1 - \cos \mathbf{q}\cdot\mathbf{r}) \right] \end{aligned}$$

(it can be shown that the higher order terms work for the last expression)

$$C(\mathbf{r}) = \exp[-\sum_{\mathbf{q}} \langle |\delta\Theta_{\mathbf{q}}|^2 \rangle (1 - \cos \mathbf{q} \cdot \mathbf{r})]$$

The sum appearing in the exponential is almost the same one we did before, since for large $\mathbf{q} \cdot \mathbf{r}$ the $\cos(\mathbf{q} \cdot \mathbf{r})$ term oscillates rapidly and may be replaced by its average value of zero. However for small $q < r^{-1}$ the $(1 - \cos \mathbf{q} \cdot \mathbf{r})$ factor becomes proportional to q^2, and the logarithmic divergence is cutoff:

$$\sum_{\mathbf{q}} \langle |\delta\Theta_{\mathbf{q}}|^2 \rangle (1 - \cos \mathbf{q} \cdot \mathbf{r}) \simeq \frac{k_B T}{2\pi K} \int_{r^{-1}}^{q_c} \frac{dq}{q} = \frac{k_B T}{2\pi K} \ln q_c r$$

Note that inaccuracies in our evaluation of the integral can be absorbed into the definition of the constant q_c.

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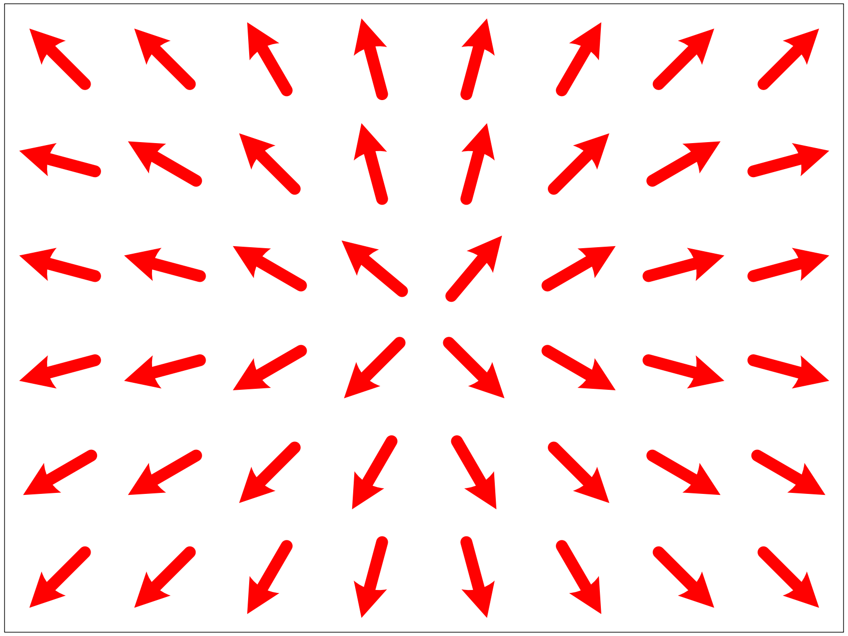
We get the important result of *power law* decay of correlations with an exponent that depends on temperature

$$C(r) \propto r^{-\eta} \qquad \text{with} \qquad \eta(T) = \frac{k_B T}{2\pi K}$$

Topological Defects



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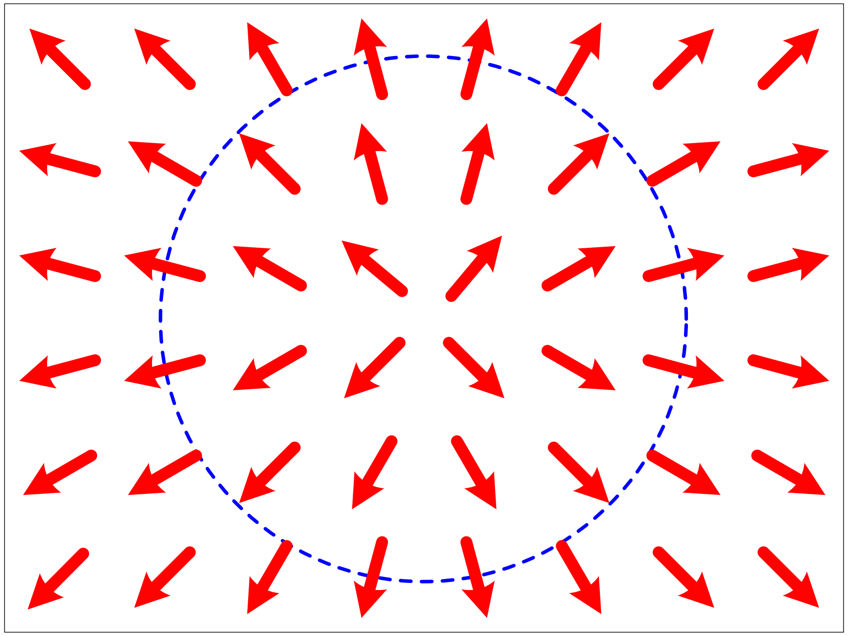

Topological invariant (winding number)

$$\frac{1}{2\pi}\oint \nabla\Theta \cdot \mathbf{dl} = 1$$

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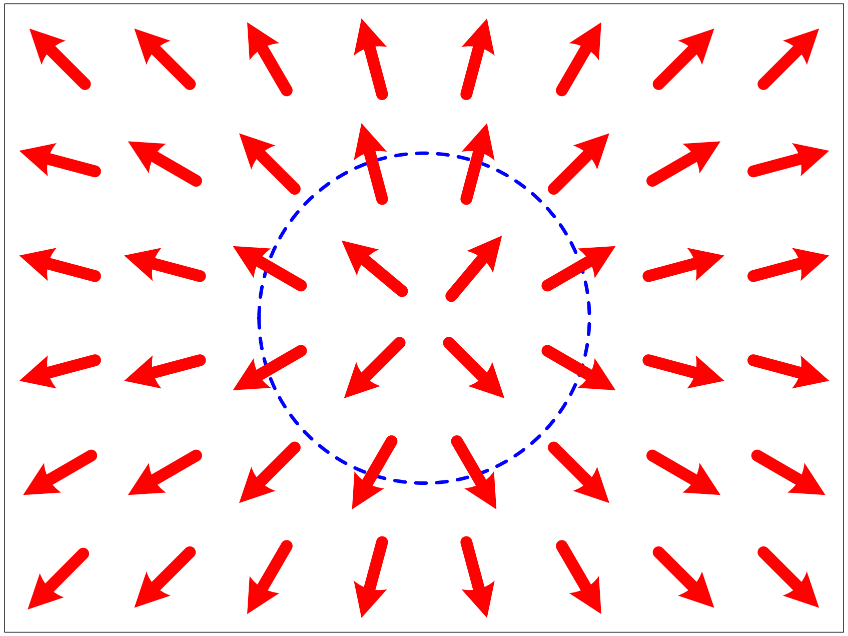

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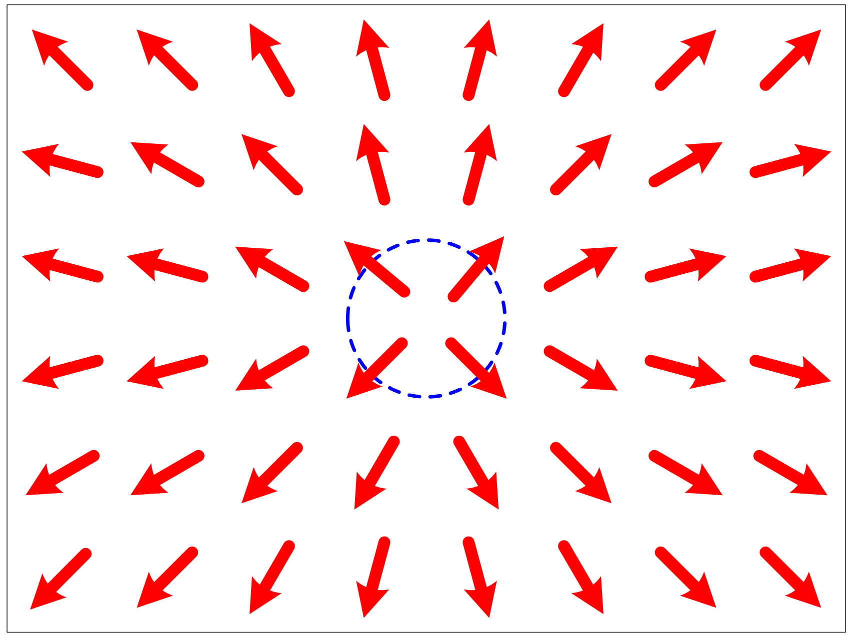

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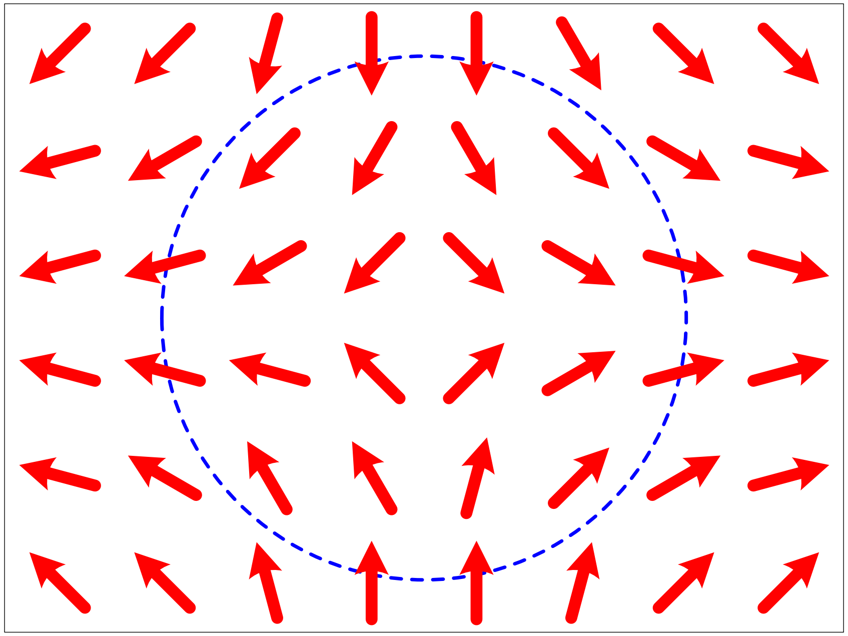

Topological invariant (winding number)

$$\frac{1}{2\pi}\oint \nabla\Theta \cdot \mathbf{dl} = -1$$

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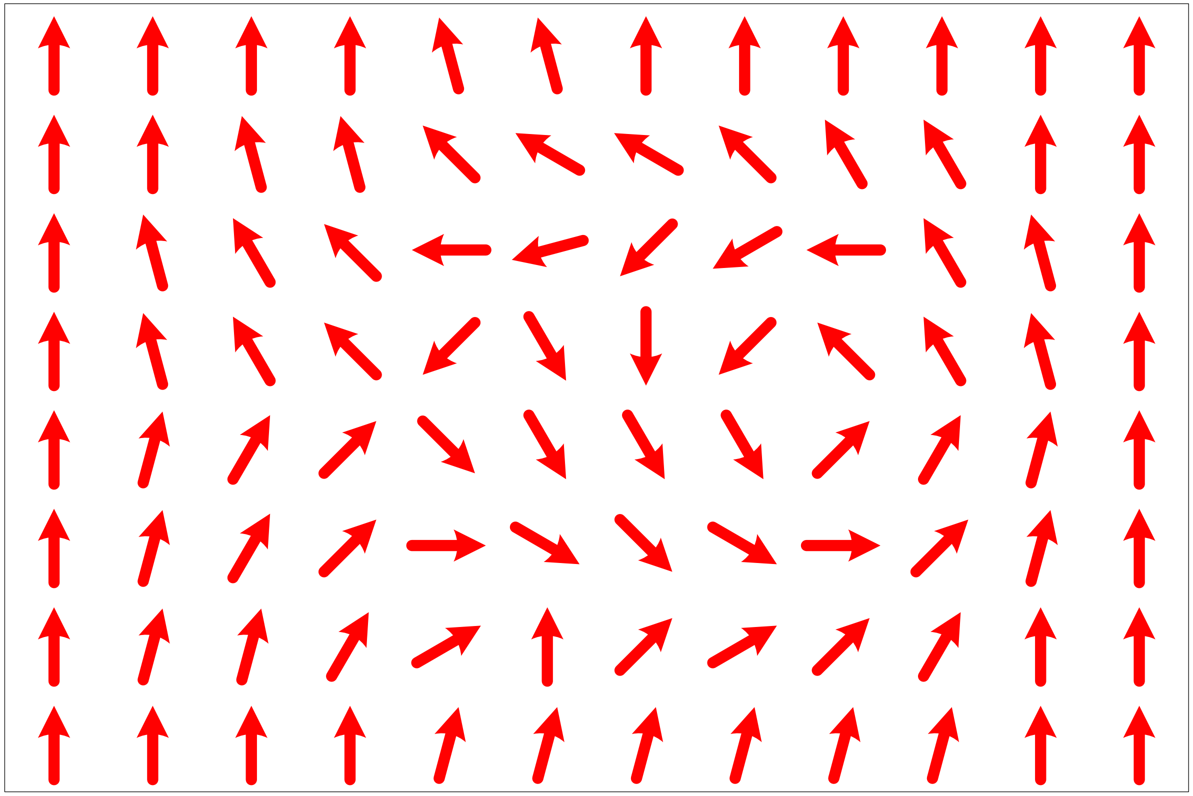

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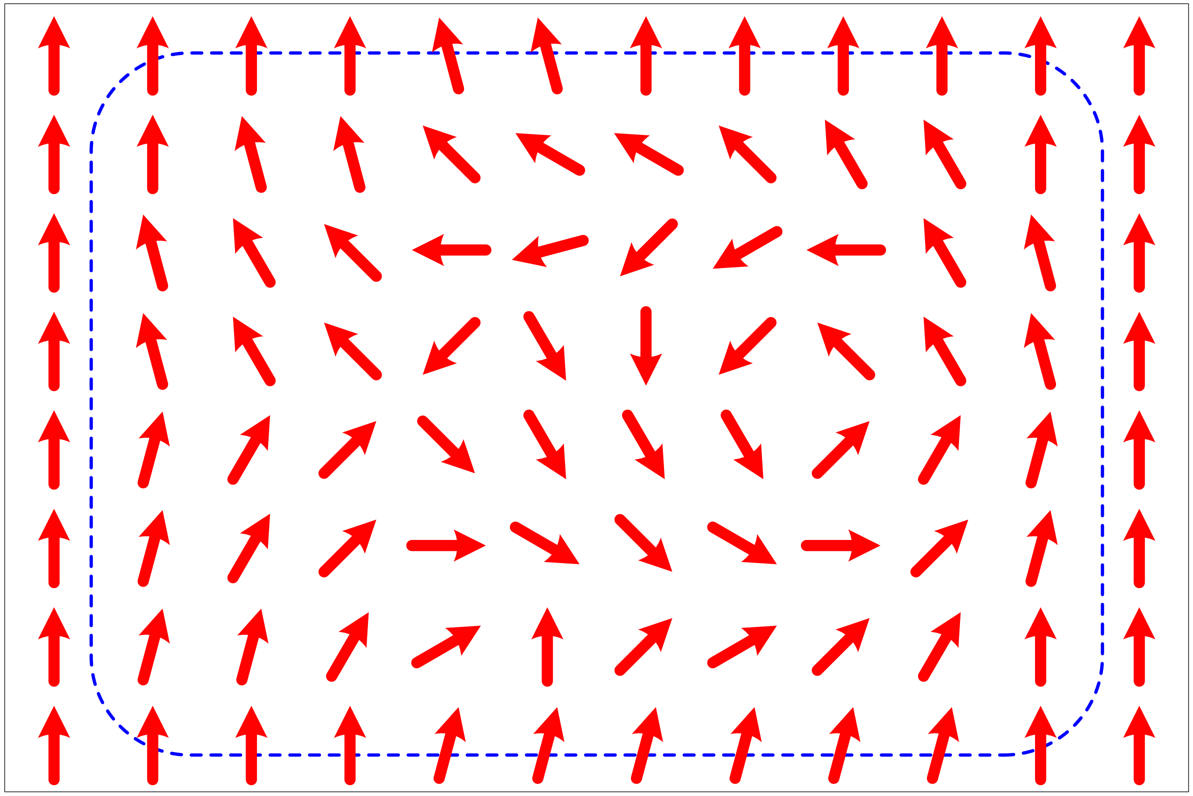
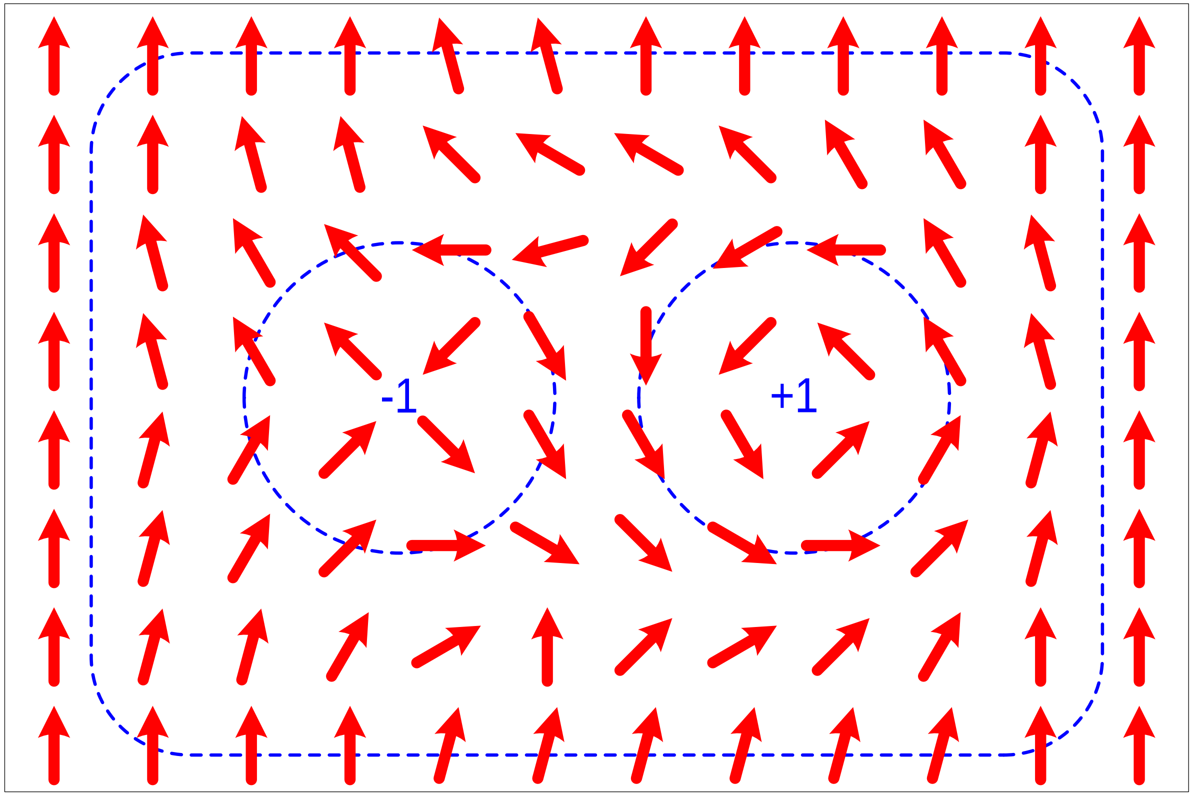


Plus-minus pair gives winding number 0

$$\frac{1}{2\pi}\oint \nabla\Theta \cdot \mathbf{dl} = 0$$

Topological Defects



Plus-minus pair gives winding number 0

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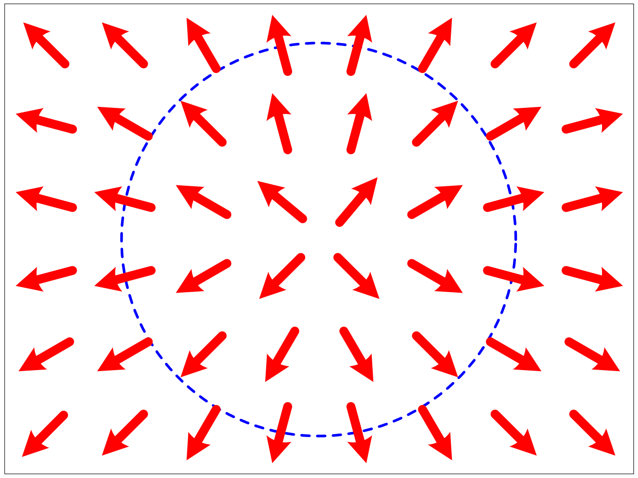
Importance of Topological Defects

- Random arrangement of defects (of both signs) eliminates long range order and gives exponential decay of correlations
- May eliminate the generalized rigidity
  - ◇ Dislocations in crystals
  - ◇ Vortices in superfluids and superconductors
- Provide a mechanism for dynamics in an ordered state
- Dominate dynamics in quenches from disordered initial conditions (coarsening, cf. cosmic strings, the Kibble mechanism)
- May be important in phase transition (e.g., $2d$ XY model)

Vortex Energetics in 2d



Energy of a vortex

$$E = \tfrac{1}{2}K \int d^2x (\nabla\Theta)^2 = \tfrac{1}{2}K \int 2\pi r \, dr \, r^{-2}$$

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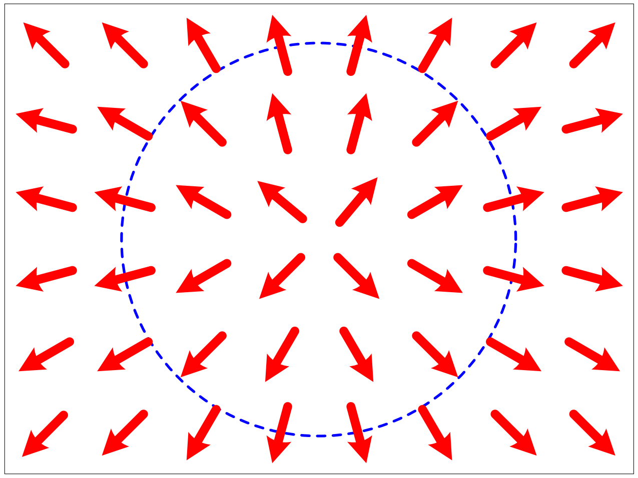

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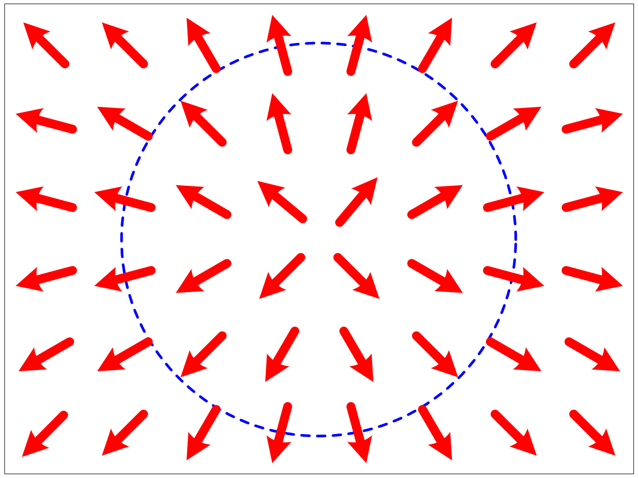

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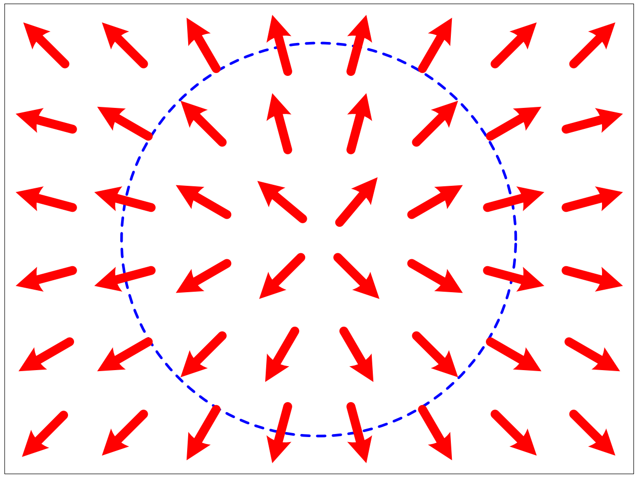

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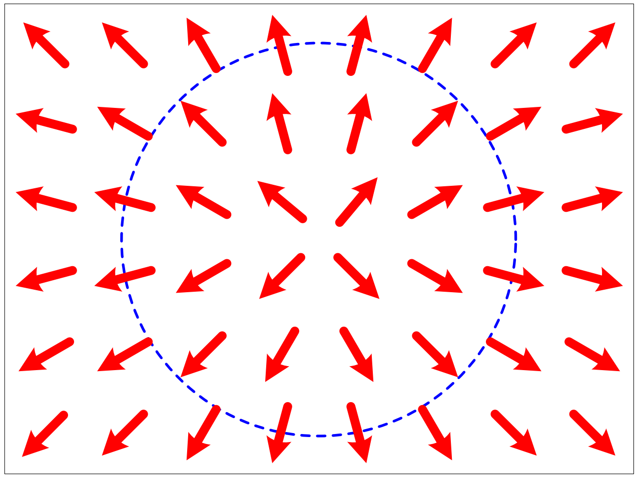

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Free energy of a vortex

$$F = (\pi K - 2k_B T) \ln(L/\xi) + c'' < 0 \quad \text{for } T > \pi K/2k_B$$

Kosterlitz-Thouless Transition - 2d XY Model

- At low temperatures there is a phase with a nonzero spin stiffness constant K but no long range order: correlations decay as a power law that depends on temperature

$$C(r) \propto r^{-\eta} \qquad \text{with} \qquad \eta(T) = \frac{k_B T}{2\pi K(T)}$$

- In the low temperature phase there are bound pairs of plus-minus vortices, but no free vortices
- At the Kosterlitz-Thouless temperature T_{KT} given by $k_B T_{KT} = \pi K/2$ there is a "vortex unbinding" transition leading to free vortices
- For $T > T_{KT}$ there is exponential decay of correlations
- At $T = T_{KT}$ the stiffness constant K jumps discontinuously to zero
- The ratio $K(T_{KT})/k_B T_{KT} = 2/\pi$ and is universal

Dynamics

Have not yet specified the dynamics.

Different dynamics is appropriate for different physical systems, depending on what other thermodynamic variables there are, and how the order parameter couples to them.

Some examples follow:

Thin Film Nematic

Θ describes the orientation of long molecules in the plane, and relaxes to minimize the free energy.

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Most easily expressed in complex notation $(s_x, s_y) \Rightarrow S = |S|e^{i\Theta}$. Free energy becomes

$$F = \int d^d x \left[a(T - T_c)|S|^2 + \tfrac{1}{2} b|S|^4 + \gamma |\nabla S|^2 \right]$$

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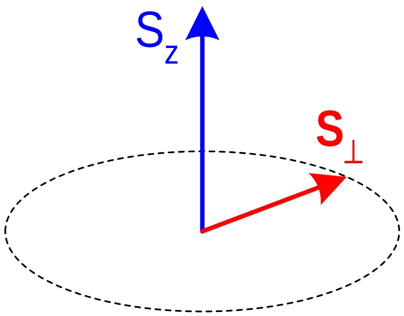
Vortex dynamics may also be important.

Easy Plane Magnet



Spins can point in any direction, but anisotropy favors alignment in XY plane.

The XY and Z components of the spin have different properties:

$$S_z = \Omega^{-1} \sum_{i \text{ in } \Omega} \langle s_{iz} \rangle \qquad \text{is a } \textit{conserved quantity}$$

$$\mathbf{S}_\perp = \Omega^{-1} \sum_{i \text{ in } \Omega} \langle \mathbf{s}_{i\perp} \rangle \qquad \text{is the XY } \textit{order parameter}$$

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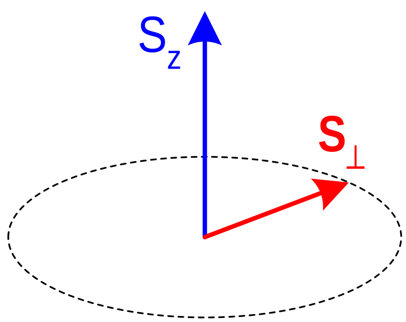

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S_z and Θ are canonically conjugate variables in the Hamiltonian equations

$$\dot{S}_z = -\frac{\delta F}{\delta \Theta}, \qquad \dot{\Theta} = \frac{\delta F}{\delta S_z}$$

where the free energy (away from T_c)

$$F = \int d^d x \left[\frac{1}{2} K (\nabla \Theta)^2 + \frac{S_z^2}{2\chi} - S_z b_z \right]$$

plays the role of the effective Hamiltonian (b_z is μB_z with B_z the external field in the z direction, χ is the z-spin susceptibility, and I've chosen the simple case of $\mathbf{B}_\perp = 0$)

$$F = \int d^d x \, [\tfrac{1}{2} K (\nabla \Theta)^2 + \tfrac{1}{2} S_z^2/\chi - S_z b_z]$$

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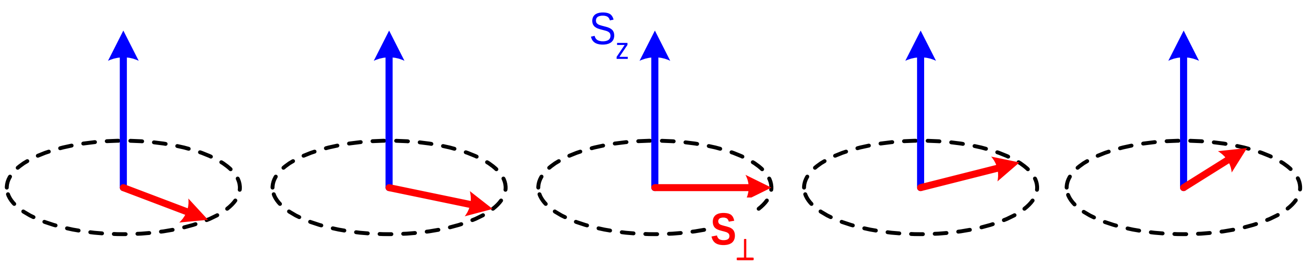

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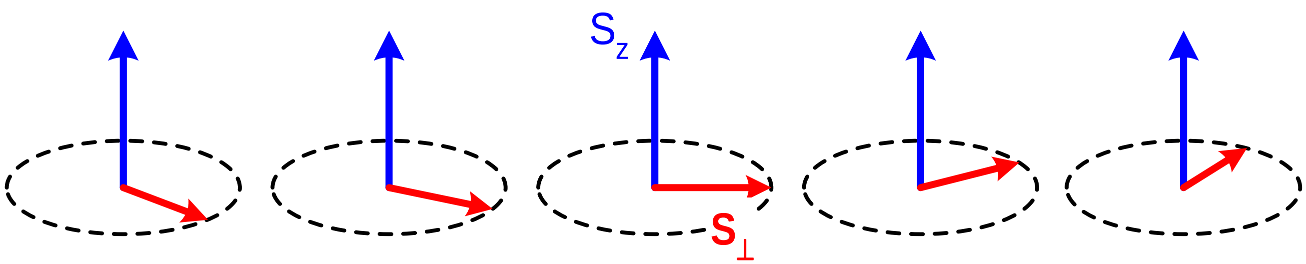

For $b_z = 0$ and small deviations $\delta\Theta$ from the uniform state

$$\delta \dot{S}_z = K \nabla^2 \delta\Theta$$

$$\delta \dot{\Theta} = \chi^{-1} \delta S_z$$

leading to propagating spin waves $\propto e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}$ with the dispersion relation $\omega = cq$ and the propagation speed $c = \sqrt{K/\chi}$

Next Lecture

Superfluids and superconductors

- What are superfluidity and superconductivity?
- Description in terms of a macroscopic phase
- Josephson effect
- Supercurrents that flow for ever
- Four sounds