Topology in Magnetism
- a phenomenological account

Wednesday: vortices
Friday: skyrmions

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Many figures copied from internet
Topology in Magnetism

• 2016 Nobel Prize: Kosterlitz, Thouless and Haldane

• The Kosterlitz-Thouless transition
  – Phase transitions: Broken symmetry, Goldstone mode
  – Mermin-Wagner theorem
  – Kosterlitz-Thouless transition
  – Correlation lengths and neutron scattering

• The Haldane chain
  – Quantum fluctuations suppress order
  – S=1/2 chain: Bethe solution, spinons
  – S=1 chain: Haldane gap, hidden order
  – Inelastic neutron scattering

• Hertz-Millis
The Nobel Prize in Physics 2016

David J. Thouless
Prize share: 1/2

F. Duncan M. Haldane
Prize share: 1/4

J. Michael Kosterlitz
Prize share: 1/4

The Nobel Prize in Physics 2016 was awarded with one half to David J. Thouless, and the other half to F. Duncan M. Haldane and J. Michael Kosterlitz “for theoretical discoveries of topological phase transitions and topological phases of matter”.
Aspen Center for Physics 2000: Workshop on Quantum Magnetism

- David Thouless: Transition without broken symmetry
- My laptop, just broken
ICCMP Brasilia 2009: Workshop on Heisenberg Model (80+1 year anniversary)

- Duncan Haldane
- 4h bus ride with Bethe chatter
The Nobel Prize in Physics 2016

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Topological phase transitions

Topological phases of matter

Illustration: © Johan Jarnestad/The Royal Swedish Academy of Sc
Topology

- In mathematics, **topology** (from the Greek τόπος, place, and λόγος, study) is concerned with the properties of space that are preserved under **continuous** deformations.

- Euler
  - 1736: 7 bridges of Konigsberg
  - 1750: Polyhedra: vertices + faces = edges + 2

\[
\begin{align*}
\text{tetrahedron} & : 4 + 4 = 6 + 2 \\
\text{octahedron} & : 6 + 8 = 12 + 2 \\
\text{cube} & : 8 + 6 = 12 + 2 \\
\text{icosahedron} &
\end{align*}
\]

Proof that Euler was wrong!

But, need long distance and long time!
The hairy ball theorem

• "you can't comb a hairy ball flat without creating a cowlick"

• Topology concern non-local properties!
Topological phase transitions

• Driven by topological defects

• Vortices (for spins rotating on 2D circle)
  – The Kosterlitz Thouless transition in 2D XY model
  – Superfluid films
  – Josephson junction arrays

• Skyrmions (for spins rotating on 3D sphere)
  – Lecture on Friday
Mean field theory of magnetic order

- **GS of a many-body Hamiltonian**
  \[ H = -\sum_{ij} J_{ij} S_i \cdot S_j + g\mu_B S_i \cdot B \]

- **Mean-field approx.**
  \[ \sum J_{ij} S_i \cdot S_j \approx S_i \cdot (\sum J_{ij} < S_j >) \Rightarrow H = g\mu_B \sum_i S_i \cdot B_{eff} \]
  where \( B_{eff} = B + \sum J_{ij} < S_j > / g\mu_B = B + \lambda M \)

- **Solution**
  Eigen states \( H | S^z = m > = E_m | S^z = m > \), \( E_m = g\mu_B m B_{eff} \)
  Magnetization \( M = N < S^z >= \sum_m m e^{-E_m/k_B T} / \sum_m e^{-E_m/k_B T} \)
  \( \Rightarrow B_J \) Brillouin function

- **Self-consistency**
  \( M = M_s B_J (g\mu_B B + \lambda M / k_B T) \)
Order in Ferromagnet

\[ M = M_s B_J (g \mu_B B + \lambda M / k_B T), \]

self-consistency equation

\[ B_J(y) \approx (J+1)y/3J \quad \text{for } y << 1 \]

\begin{align*}
\text{T} &< T_c: \text{solution } M > 0, \quad k_B T_c = 2zJS(S+1)/3 \\
\text{T} &> T_c: \text{solution } M = 0 \\
\text{Susceptibility: } &\chi = \lim_{B \to 0} \mu_0 M/B \\
&\Rightarrow \chi \sim C/(T-T_c) \\
\text{Curie Weiss susceptibility} \\
\text{Diverge at } T_c
\end{align*}

\[ T \text{ near } 0: M(T) \sim M_s e^{-2T_c/T} \]
\[ T \text{ near } T_c: M(T) \sim (T_c - T)^\beta \]
Order in Antiferromagnet

Two sublattices with \(<S_a> = -<S_b>\)

Selfconsistency \(\Rightarrow M = M_s B J (g \mu_B B - \lambda M / k_B T)\)

Same solutions:
- Antiferromagnetic order at \(k_B T_N = 2zJS(S+1)/3\)
- Susceptibility \(\chi \sim 1/(T + T_N)\)

General: \(\chi \sim 1/(T - \theta)\), \(\theta = 0\) Paramagnet
\(\theta > 0\) Ferromagnet
\(\theta < 0\) Antiferromagnet

Generalisation: \(J_{ij} \Rightarrow J_d(q)\) and \(<S_d(q)>\) Fourier
Allow meanfield of incommensurate order and multiple magnetic sites, \(d\), in unit cell

\(\chi_q \sim 1/(T - \theta)\) diverges at \(T_c\)
So always order at finite \(T\)?
No, mean-field neglects fluctuations!

\(\theta = T_c\)
\(\theta = T_N\)
\(\theta = 0\)
Spin waves in ferromagnet

\[ H = -\sum_{\langle r, r' \rangle} J_{rr'} S_r \cdot S_{r'} + \frac{1}{2} \langle S^+_r S^z_{r'} + S^z_r S^+_r \rangle \]

Ordered ground state, all spin up: \( H \ket{g} = E_g \ket{g}, \quad E_g = -z N S^2 J \)

Single spin flip not eigenstate: \( \ket{r} = (2S)^{-\frac{1}{2}} S^{-r} \ket{g}, \quad S^z_r S^z_{r'} \ket{r} = 2S \ket{r'} \)

\[ H \ket{r} = (-z N S^2 J + 2z S J) \ket{r} - 2S J \sum_d \ket{r+d} \]

flipped spin moves to neighbours

Periodic linear combination: \( \ket{k} = N^{-\frac{1}{2}} \sum_r e^{ikr} \ket{r} \)

plane wave

Is eigenstate: \( H \ket{k} = E_g + E_k \ket{k}, \quad E_k = S J \sum_d \left( 1 - e^{ikd} \right) \)

dispersion = \( 2S J \left( 1 - \cos(kd) \right) \) in 1D

Time evolution: \( \ket{k(t)} = e^{iHt} \ket{k} = e^{iE_k t} \ket{k} \)

sliding wave

Dispersion:
relation between time- and space-modulation period

Same result in classical calculation \( \Rightarrow \) precession:
Magnetic order - Against all odds

• Bohr – van Leeuwen theorem: (cf Kenzelmann yesterday)
  – No FM from classical electrons

• $\langle M \rangle = 0$ in equilibrium (cf Canals yesterday)

• Mermin – Wagner theorem:
  – No order at $T>0$ from continuous symmetry in $D \leq 2$

• No order even at $T=0$ in 1D
Bohr – van Leeuwen theorem

• "At any finite temperature, and in all finite applied electrical or magnetical fields, the net magnetization of a collection of electrons in thermal equilibrium vanishes identically."

\[
Z \propto \prod_i d^3r_i d^3p_i \exp \left( -\beta H(r_1, \ldots; p_1, \ldots) \right) \quad H = \frac{1}{2m} \sum_i \left( p_i + eA(r_i) \right)^2 + V(r_1, \ldots)
\]

\[
p_i \rightarrow p_i = p_i + eA(r_i)
\]

Allowed because \( p \) is integrated to infinity

\[
Z \propto \prod_i d^3r_i d^3\tilde{p}_i \exp \left[ -\beta \left( \frac{1}{2m} \sum_i \tilde{p}_i^2 + V \right) \right]
\]

\[
F = -\frac{1}{\beta} \ln Z \quad M = -\frac{\partial F}{\partial B} = 0
\]

https://en.wikipedia.org/wiki/Bohr%E2%80%93van_Leeuwen_theorem
ABSENCE OF FERROMAGNETISM OR ANTIFERROMAGNETISM IN ONE- OR TWO-DIMENSIONAL ISOTROPIC HEISENBERG MODELS*

N. D. Mermin† and H. Wagner‡
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York
(Received 17 October 1966)

It is rigorously proved that at any nonzero temperature, a one- or two-dimensional isotropic spin-$S$ Heisenberg model with finite-range exchange interaction can be neither ferromagnetic nor antiferromagnetic. The method of proof is capable of excluding a variety of types of ordering in one and two dimensions.

- Generalized to:

“Continuous symmetries cannot be spontaneously broken at finite temperature in systems of dimension $d \leq 2$ with sufficiently short-range interactions “
General Mermin Wagner

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

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

\[ A = S^-(-k + K), \quad C = S^+(k) \]

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

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

https://itp.uni-frankfurt.de/~valenti/TALKS_BACHELOR/mermin-wagner.pdf
Specific case of ferromagnet in 2D:

- Magnetization reduced by thermally excited spin waves

- Dispersion: \[ E \sim k^n \quad \Rightarrow \quad k^{d-1} \sim E^{d-1/n} \]

- Volume element in d-dimensional k space:
  \[ k^{d-1}dk = \frac{E^{(d-n)/n}}{dE} \]

- Density of states:
  \[ N(E) \sim E^{(d-n)/n} \quad \text{For } n=2 \text{ and } d=2 \]
  \[ N(E) = \text{constant} \]

\[
\Delta M(T) \sim \int_0^\infty N(E)[1/(e^{E/k_BT} - 1)]dE
\[
\sim T \int_0^\infty [1/(e^x - 1)]dx
\]

- Diverges logarithmically \( \Rightarrow M(T) = M(T=0) - \Delta M(T) \to 0 \) for any \( T>0 \)
- Also works for anti-ferromagnet; Does not diverge for \( d>n \)
So how does the system behave at finite temperature?
Example: 2D Heisenberg anti-ferromagnet

\[ \mathcal{H} = J \sum S_i \cdot S_j \]

Correlations decay exponentially with \( r \)

\[ \langle S_{r'}(t) S_r(t) \rangle \propto e^{-|r-r'|/\xi} \]

Correlation length diverge as \( T \to 0 \)

\[ \xi(T) \propto \exp(J/T) \]
Let's look at 2D XY model: spins rotate only in the plane

- Mermin-Wagner: No ordered symmetry broken state for $T > 0$

- Calculations of correlation function

For high $T$:

$$\langle S_0 S_r \rangle \propto \exp\left(-\frac{r}{\xi}\right)$$

For low $T$ (assuming smooth rotations):

$$\langle S_0 S_r \rangle \propto r^{-\eta}$$

- What happens in between?

$$\langle S(r)S(0) \rangle \approx \begin{cases} e^{-\text{const.} T} & \text{for } d > 2 \\ \left(\frac{r}{L}\right)^{-\eta} & \text{for } d = 2 \\ \exp\left(-\frac{T}{2Ja} r\right) & \text{for } d = 1. \end{cases}$$
Different types of defects
2D XY – spins live in the plane

• How does a defect in almost ordered system look?

“Repairable” smooth

“non-repairable” singular

A vortex changes the phase also far from the defect.

https://abeekman.nl
Topological defects

- The topological charge ($q$) is a winding number.
- Consider rotation of magnetisation along closed loop around core.

![Images of magnetic fields with different winding numbers $q = 0, 1, -1, 2, -2$.](image-url)
Energy of a vortex
Energy of a vortex
Free energy of a vortex
Free energy of a vortex
Energy of a vortex

\[ H = -J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{i,j} \cos(\theta_i - \theta_j) \]

If we assume that the direction of the rotors varies smoothly from site to site, we approximate \( \cos(\theta_i - \theta_j) \) by the first two terms \( 1 - \frac{1}{2}(\theta_i - \theta_j)^2 \) in the Taylor expansion of

\[ H = E_0 + \frac{J}{2} \int d\mathbf{r}(\nabla \theta)^2 \]

\( E_{\text{vor}} - E_0 \) is given by

\[ E_{\text{vor}} - E_0 = \frac{J}{2} \int d\mathbf{r} [\nabla \theta(\mathbf{r})]^2 \]
\[ = \frac{Jn^2}{2} \int_0^{2\pi} \int_0^L r dr \frac{1}{r^2} \]
\[ = \pi n^2 J \ln\left(\frac{L}{a}\right). \]

\[ F = E - TS \]

the entropy from the number of places where we can position the vortex centre, namely on each of the \( L^2 \) plaquette of the square lattice, i.e., \( S = k_B \ln(L^2/a^2) \). Accordingly the free energy is given by

\[ F = E_0 + (\pi J - 2k_B T) \ln(L/a). \]

For \( T < \pi J/2k_B \) the free energy will diverge to plus infinity as \( L \to \infty \). For \( T > \pi J/2k_B \) the system can lower its free energy by producing vortices.

For all paths that don’t encircle the vortex position \( \mathbf{r}_0 \)

\[ \int \nabla \theta(\mathbf{r}) \cdot d\mathbf{l} = 0. \]

For all closed curves encircling the position \( \mathbf{r}_0 \) of the centre of the vortex

\[ \int \nabla \theta(\mathbf{r}) \cdot d\mathbf{l} = 2\pi n. \]

\[ \theta(\mathbf{r}) = \theta(\mathbf{r}) \]

\[ 2\pi n = \int \nabla \theta(\mathbf{r}) \cdot d\mathbf{l} = 2\pi r |\nabla \theta| \]

\[ |\nabla \theta(\mathbf{r})| = n/r \]
Vortex anti-vortex pairs

- Does not destroy algebraic correlations $<S_0 S_r>^\infty$
Vortex anti-vortex pairs
Vortex anti-vortex pairs

• Are created already $T < T_{KT}$,
• But does not destroy algebraic correlations $\langle S_0 S_r \rangle \propto r^{-\eta}$
Unbound vortices create global disorder: $\langle S_R S_{R+r} \rangle \propto \exp(-r/\xi)$

- The Kosterlitz-Thouless transition occurs when vortices bind/unbind
Kosterliz-Thouless

$T = 0$ LRO

vortex-antivortex pair

gas of pairs

$T_{KT}$ unbound vortices
Correlation lengths

Heisenberg
\[ \xi(T) \propto e^{J/T} \]

Kosterlitz-Thouless:
\[ \xi(T) \propto e^{b/\sqrt{t}} \quad t = (T - T_{KT})/T_{KT} \]

Anisotropic Heisenberg cross-over:
\[ \xi(T) \propto e^{b/\sqrt{t}} \quad \text{for } \xi > 100, \]
\[ \xi(T) \propto e^{b/t} \quad \text{for } \xi < 100, \]
Measuring correlations with neutrons

Dynamic structure factor

\[ S^{\alpha\beta}(Q, \omega) = \frac{1}{2\pi} \sum_{RR'} \int dt e^{iQ(R-R') - i\omega t} \langle S^\alpha_R(0) S^\beta_{R'}(t) \rangle \]

Instantaneous equal-time structure factor:

\[ S(Q) = \int d\omega S(Q, \omega) \]

\[ \propto \int_{-\infty}^{\infty} dt \delta(t - t') \langle S^\alpha_{r'}(t) S^\alpha_r(t') \rangle = \langle S^\alpha_{r'}(t) S^\alpha_r(t) \rangle \]

\[ \langle S^\alpha_{r'}(t) S^\alpha_r(t) \rangle \propto e^{-|r - r'|/\xi} \]

\[ S(Q) \propto \frac{1}{1 + Q^2 \xi^2} \]

Width ⇒ Correlation length ξ

Heisenberg system

• Scales as predicted

\[ \xi = \frac{e}{8} \frac{\nu_s}{2\pi \rho_s} \exp \left( \frac{2\pi}{k_B T} \right) \left[ 1 - \frac{1}{2} \frac{k_B T}{2\pi \rho_s} + O \left( \frac{k_B T}{2\pi \rho_s} \right)^2 \right] \]

• No cross-over to Quantum Critical yet

\[ \xi \sim e^{J/T} \]

\[ \xi \sim \text{const.} \]

Figure 4.25. The measured correlation length \( \xi(T) \) for each of the four configurations. The data are compared to the NLSM predictions (Hasenfratz and Niedermayer, 1991, dashed black) and (Hasenfratz, 1999, solid black) and the PQSCHA result (dot-dashed red).

PRL 82, 3152 (1999);
Conclusion:
We can see KT scaling of $\xi$
But in quasi-2D TKT always forestalled by 3D order

$$\xi_{KT} = A e^{b(T_{KT}/(T - T_{KT}))^{1/2}}$$

where $A$ and $b$ are non-universal constants. We get an excellent fit with the parameters $A = 1.58 \pm 0.34 \, \text{Å}$, $b = 1.87 \pm 0.36$ and $T_{KT} = 54.8 \pm 4 \, \text{K}$. Bramwell and size $L = \sqrt{J/J'}$, for which the following relation holds:

$$\frac{T_N - T_{KT}}{T_{KT}} = \frac{b^2}{(\ln L)^2}.$$  \hfill (2)

Solving for $b$ and using the KT expression for $\xi(T_N) = 27.5 \, \text{Å}$ gives $A = 1.37 \, \text{Å}$ and $b = 1.98$. These values are quite close to those obtained from the fit to the KT expression for $\xi(T)$, which shows that the description is consistent.

Correlation lengths

Real materials are quasi-2D:
Interlayer coupling $J' \ll J$

3D order: $T_N \sim J' \xi(T_N)^2 \Rightarrow$

$$\xi(T_N) \sim 100 \text{ if } J' = 10^{-4}J$$

So Kosterlitz-Thouless transition never really reached in magnetic materials!
Topological phase transitions

• Driven by topological defects

• Vortices (for spins rotating on 2D circle)
  – The Kosterlitz Thouless transition in 2D XY model
  – Superfluid films
  – Josephson junction arrays

• Skyrmions (for spins rotating on 3D sphere)
  – Lecture on Friday
What about Duncan? – T=0 and quantum states

Topological phases of matter

• The Haldane S=1 chain

• Quantum Hall states

• Topological Quantum Spin Liquids
AFM spin waves
Spin waves in antiferromagnet

• Up sites (A) and down sites (B) – bipartite lattice

\[ S^\pm = S^x \pm iS^y \]

• Holstein-Primakoff bosonisation

\[
\begin{align*}
S_A^z &= S - a^{\dagger}a \\
S_A^+ &= \sqrt{2S}a^{\dagger}f(S) \\
S_A^- &= \sqrt{2S}f(S)a
\end{align*}
\]

\[
\begin{align*}
S_B^z &= b^{\dagger}b - S \\
S_B^+ &= \sqrt{2S}f(S)b \\
S_B^- &= \sqrt{2S}b^{\dagger}f(S)
\end{align*}
\]

• Linearization

\[ f(S) \approx 1 - e^{iCJ/S} + \cdots \]

\[ S_A \cdot S_B \simeq -S^2 + S(a^{\dagger}a + b^{\dagger}b + a^{\dagger}b^{\dagger} + ab) \quad \text{Hamiltonian still mix A and B, r and r'} \]

• Fourier transformation: decouple from r,r' to q

\[
\begin{align*}
\mathcal{H}^{(2)} &= -\frac{2}{N}JS^2 + zJS\sum_q [a^{\dagger}_aq_q + b^{\dagger}_qb_q + \gamma_q(a^{\dagger}_qb^{\dagger}_q + a_qb_q)] \\
\gamma_q &= \frac{1}{z} \sum_{\delta} e^{iq \cdot \delta}
\end{align*}
\]
\[ \mathcal{H}^{(2)} = -\frac{z}{2} N J S^2 + z J S \sum_{q} [a_q^\dagger a_q + b_q^\dagger b_q + \gamma_q (a_q^\dagger b_q^\dagger + a_q b_q)] \quad \gamma_q = \frac{1}{z} \sum_{\delta} e^{i\mathbf{q} \cdot \mathbf{\delta}} \]

- Bogoliubov trans. to decouple a,b
  \[ \begin{align*}
  a_q^\dagger &= u_q \alpha_q^\dagger - v_q \beta_q \\
  b_q^\dagger &= -v_q \alpha_q + u_q \beta_q^\dagger \\
  a_q &= u_q \alpha_q - v_q \beta_q^\dagger \\
  b_q &= -v_q \alpha_q^\dagger + u_q \beta_q
  \end{align*} \]

- Diagonalise:
  \[ 2\theta_q = \gamma_q \quad u_q = \cosh \theta_q \quad v_q = \sinh \theta_q \]

\[ \mathcal{H} = -\frac{z}{2} N J S (S + \eta) + z J S \sum_{q} \sqrt{1 - \gamma_q^2 (\alpha_q^\dagger \alpha_q + \beta_q^\dagger \beta_q)} \]

Ground state excitations = spin waves

\[ \omega_q = z J S \sqrt{1 - \gamma_q^2} \quad \text{dispersion} \]
AFM spin wave dispersion

\[ \omega_q = z J S \sqrt{1 - \gamma_q^2} \]

\[ \gamma_q = \frac{1}{z} \sum_{\delta} e^{i \mathbf{q} \cdot \delta} \]

Average spin-wave population = zero point fluctuations

\[ \epsilon \equiv \frac{1}{N} \sum_q \langle c_q^\dagger c_q \rangle = \frac{1}{N} \sum_q \left( \frac{1}{(1 - \gamma_q^2)^{1/2}} - 1 \right) \]

\[ \approx 0.078 \ll 1 \text{ in D}=3 \]
\[ \approx 0.197 \text{ in D}=2 \]
\[ \text{Diverges in D}=1 ! \]

Quantum fluctuations destroy order in 1D

reduced moment: 60% left in 2D

\[ m \equiv \frac{1}{N} \sum_r (-1)^r \langle S_r^z \rangle \simeq \frac{1}{2} - \epsilon = 0.303 \]
antiferromagnetic spin chain

$$\mathcal{H} = J \sum s_n^z s_{n+1}^z + \frac{1}{2} (s_n^+ s_{n+1}^- + s_n^- s_{n+1}^+)$$

Ground state (Bethe 1931) – a soup of domain walls
Spinon excitations

Elementary excitations:
- “Spinons”: spin S = ½ domain walls with respect to local AF ‘order’
- Need 2 spinons to form S=1 excitation we can see with neutrons

Energy: \( E(q) = E(k_1) + E(k_2) \)
Momentum: \( q = k_1 + k_2 \)
Spin: \( S = \frac{1}{2} \pm \frac{1}{2} \)

Continuum of scattering \( \Rightarrow \)
The antiferromagnetic spin chain

FM: ordered ground state (in 5T mag. field)
- semiclassical spin-wave excitations

AFM: quantum disordered ground state
- Staggered and singlet correlations
- Spinon excitations

- Algebraic Bethe ansatz for inelastic lineshape
- Beyond Müller-conjecture

Mourigal, Enderle, HMR, Caux
Surprise: 1D S=1 chain has a gap!

- Haldane’s conjecture 1983: “Integer spin chains have a gap”
- No classical order
- Hidden topological order

coupled S=1 model with string order

- See lecture by Kenzelmann
Hertz-Millis

• A quantum system in D dimensions

\[ \uparrow \downarrow \]

• A classical system in D+1 dimensions
Topological phases transition

• Topological defects
• 2D XY model, BKT transition

Topological phases

• The Haldane $S=1$ chain – confirmed by neutron spectroscopy
• Quantum Hall states – theory and experiments
• 2D and 3D topological spin liquids?
  – Found in constructed models
  – Can we find them in real materials?

Friday: Skyrmions

  – Local topological defects
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