

Nonlinear (topological) excitations in 2D spin systems with high spin ($s \geq 1$)

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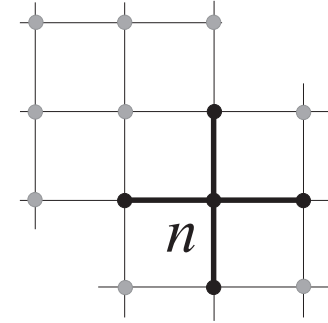
Outline

- Quantum model of 2D spin systems with high spin ($s \geq 1$)
 - Bilinear Hamiltonian
 - Mean field approximation. Ordered states
 - Motion equations for large-scale fluctuations
- Classical model as Hamiltonian hierarchy on coadjoint orbits of Lie group
 - Effective Hamiltonians
 - Geometry and topology of orbits
 - An example of topological excitations

Spin system in question

Consider a planar atomic lattice.

Each atom has a spin $s \geq 1$ (high spin).



Each atom is assigned to three **spin operators**:

$$\{\hat{S}_n^1, \hat{S}_n^2, \hat{S}_n^3\} = \hat{\mathbf{S}}_n, \quad [\hat{S}_n^a, \hat{S}_m^b] = i\epsilon_{abc}\hat{S}_n^c\delta_{nm},$$

where $a, b, c \in \{1, 2, 3\}$, and δ_{nm} is the Kronecker symbol.

$\{\hat{S}_n^a\}$ are Hermitian operators.

Quantum model

The **quantum model** is described by a **generalized Heisenberg Hamiltonian**:

- as $s = 1$ with **biquadratic exchange**

$$\hat{\mathcal{H}} = - \sum_{n,\delta} \left(J(\hat{\mathbf{S}}_n, \hat{\mathbf{S}}_{n+\delta}) + K(\hat{\mathbf{S}}_n, \hat{\mathbf{S}}_{n+\delta})^2 \right),$$

δ runs over the nearest-neighbour sites;

- as $s = 3/2$ with **bicubic exchange**

$$\hat{\mathcal{H}} = - \sum_{n,\delta} \left(J(\hat{\mathbf{S}}_n, \hat{\mathbf{S}}_{n+\delta}) + K(\hat{\mathbf{S}}_n, \hat{\mathbf{S}}_{n+\delta})^2 + L(\hat{\mathbf{S}}_n, \hat{\mathbf{S}}_{n+\delta})^3 \right);$$

- spin s with $2s$ -th power of exchange interaction.

Space of representation ($s=1$)

The spin operators $\{\hat{S}_n^a\}$ are naturally considered over $(2s + 1)$ -dimensional space of irreducible representation of group $SU(2)$. *In the case $s=1$, the space is 3-dimensional, canonical basis: $\{|+1\rangle, |-1\rangle, |0\rangle\}$.*

The operators $\{\hat{S}_n^a\}$ generate an associative matrix algebra over the space of representation.

*In the case $s=1$, in addition to $\{\hat{S}_n^a\} \in \text{Mat}_{3 \times 3}$ we introduce **quadrupole operators**: $\{\hat{Q}_n^{12}, \hat{Q}_n^{13}, \hat{Q}_n^{23}, \hat{Q}_n^{[2,2]}, \hat{Q}_n^{[2,0]}\}$ as tensor operators of weight 2,*

$$\hat{Q}_n^{ab} = \hat{S}_n^a \hat{S}_n^b + \hat{S}_n^b \hat{S}_n^a, \quad a \neq b, \quad \hat{Q}_n^{[2,2]} = (\hat{S}_n^1)^2 - (\hat{S}_n^2)^2,$$

$$\hat{Q}_n^{[2,0]} = \sqrt{3}((\hat{S}_n^3)^2 - \frac{2}{3}).$$

Space of representation ($s=3/2$)

In the case $s=3/2$, the space of representation is 4-dim, canonical basis: $\{ |+\frac{3}{2}\rangle, |+\frac{1}{2}\rangle, |-\frac{1}{2}\rangle, |-\frac{3}{2}\rangle \}$.

We complete the associative algebra of $\{\hat{S}_n^a\} \in \text{Mat}_{4 \times 4}$ by tensor operators of weight 2 — **quadrupole operators**:

$$\hat{Q}_n^{ab} = \frac{\sqrt{5}}{2\sqrt{3}} \left(\hat{S}_n^a \hat{S}_n^b + \hat{S}_n^b \hat{S}_n^a \right), \quad a, b \in \{1, 2, 3\}, \quad a \neq b$$

$$\hat{Q}_n^{[2,2]} = \frac{\sqrt{5}}{2\sqrt{3}} \left((\hat{S}_n^1)^2 - (\hat{S}_n^2)^2 \right), \quad \hat{Q}_n^{[2,0]} = \frac{\sqrt{5}}{2} \left((\hat{S}_n^3)^2 - \frac{5}{4} \right),$$

and of weight 3 — **sextupole operators**:

$$\hat{T}_n^{ab} = \frac{1}{\sqrt{6}} \left((\hat{S}_n^a)^2 \hat{S}_n^b + \hat{S}_n^b (\hat{S}_n^a)^2 + \hat{S}_n^a \hat{S}_n^b \hat{S}_n^a - (\hat{S}_n^b)^3 \right), \quad \hat{T}_n^{a3} = (\hat{Q}_n^{a2} \hat{S}_n^3 + \hat{S}_n^3 \hat{Q}_n^{a2}),$$

$$\hat{T}_n^{3a} = \frac{1}{\sqrt{10}} \left(\hat{Q}_n^{a3} \hat{S}_n^3 + \hat{S}_n^3 \hat{Q}_n^{a3} + \sqrt{3} (\hat{Q}_n^{[2,0]} \hat{S}_n^a + \hat{S}_n^a \hat{Q}_n^{[2,0]}) \right), \quad a, b \in \{1, 2\}, \quad a \neq b,$$

$$\hat{T}_n^{[3,0]} = \frac{1}{12} \left(41 \hat{S}_n^3 - 20 (\hat{S}_n^3)^3 \right).$$

Bilinear Hamiltonian

In terms of tensor operators (together $\{\hat{P}_n^a\}$) over the space of representation we obtain **bilinear Hamiltonians**:
(N is the overall number of sites in the lattice)

$$\hat{\mathcal{H}}^{\text{spin } 1} = -\left(J - \frac{1}{2}K\right) \sum_{n,\delta} \sum_b \hat{S}_n^b \hat{S}_{n+\delta}^b - \frac{1}{2}K \sum_{n,\delta} \sum_\alpha \hat{Q}_n^\alpha \hat{Q}_{n+\delta}^\alpha - \frac{4}{3}KN;$$

$$\begin{aligned} \hat{\mathcal{H}}^{\text{spin } 3/2} = & -\left(J - \frac{1}{2}K + \frac{587}{80}L\right) \sum_{n,\delta} \sum_b S_n^b S_{n+\delta}^b - \frac{75}{32}(4K - L)N - \\ & - \frac{6}{5}(K - 2L) \sum_{n,\delta} \sum_\alpha Q_n^\alpha Q_{n+\delta}^\alpha - \frac{9}{10}L \sum_{n,\delta} \sum_\beta T_n^\beta T_{n+\delta}^\beta. \end{aligned}$$

Remark. The operators $\{\hat{P}_n^a\}_{a=1}^8$ form an orthogonal basis in $\mathfrak{su}(3)$.

The operators $\{\hat{P}_n^a\}_{a=1}^{15}$ form an orthogonal basis in $\mathfrak{su}(4)$.

Mean field Hamiltonian

We introduce a vector field: $\{\mu_a(\mathbf{x}_n)\}_{a=1}^8 = \{\langle \hat{S}_n^1 \rangle, \langle \hat{S}_n^2 \rangle, \langle \hat{S}_n^3 \rangle, \langle \hat{Q}_n^{12} \rangle, \langle \hat{Q}_n^{13} \rangle, \langle \hat{Q}_n^{23} \rangle, \langle \hat{Q}_n^{[2,2]} \rangle, \langle \hat{Q}_n^{[2,0]} \rangle\}$ called a **mean field**.

Here $\langle \cdot \rangle$ denotes a **quasiaverage** (which means a quantum-mechanical and thermodynamical average after a spontaneous breaking of symmetry).

*In the case $s=1$, a **mean field Hamiltonian**:*

$$\begin{aligned} \hat{\mathcal{H}}_{MF}^{spin\ 1} = & -(J - \frac{1}{2}K)z \sum_n \sum_{a=1}^3 \hat{P}_n^a \mu_a(x_n) - \\ & - \frac{1}{2}Kz \sum_n \sum_{a=4}^8 \hat{P}_n^a \mu_a(x_n) - \frac{4}{3}KzN, \end{aligned}$$

z is a number of the nearest-neighbour sites.

Order parameters

The mean field Hamiltonian is $SU(2)$ -invariant.
By action of $SU(2)$ it can be reduced to the diagonal form:

$$\hat{\mathcal{H}}_{\text{MF}}^{\text{spin } 1} = -z \sum_n \left((J - \frac{1}{2}K) \hat{S}_n^3 \mu_3(x_n) + \frac{1}{2}K \hat{Q}_n^{[2,0]} \mu_8(x_n) \right) - \frac{4}{3}KzN.$$

In the case of thermodynamical equilibrium and unlimited lattice, μ_3 and μ_8 are constants. We call them **order parameters**.

μ_3 describes a normalized **magnetization** (a ratio of z -projection of magnetic moment to a saturation magnetization)

μ_8 is a normalized **projection of quadrupole moment**.

Self-consistent equations (SCEq)

A mean field exists if self-consistent relations are held:

(\hat{h}_{MF} is a one-site Hamiltonian: $\hat{h}_{\text{MF}} = \hat{\mathcal{H}}_{\text{MF}}/N$)

$$\mu_3 = \langle \hat{S}^3 \rangle_{\text{MF}} = \frac{\text{Tr} \hat{S}^3 e^{-\frac{\hat{h}_{\text{MF}}}{kT}}}{\text{Tr} e^{-\frac{\hat{h}_{\text{MF}}}{kT}}}, \quad \mu_8 = \langle \hat{Q}^{[2,0]} \rangle_{\text{MF}} = \frac{\text{Tr} \hat{Q}^{[2,0]} e^{-\frac{\hat{h}_{\text{MF}}}{kT}}}{\text{Tr} e^{-\frac{\hat{h}_{\text{MF}}}{kT}}}.$$

In the case $s=1$, **self-consistent equations are**

$$\mu_3 = \frac{2 \sinh \frac{(J-K/2)\mu_3}{kT}}{\exp \left\{ -\frac{\sqrt{3} K \mu_8}{2kT} \right\} + 2 \cosh \frac{(J-K/2)\mu_3}{kT}},$$

$$\mu_8 = \frac{2}{\sqrt{3}} \frac{\cosh \frac{(J-K/2)\mu_3}{kT} - \exp \left\{ -\frac{\sqrt{3} K \mu_8}{2kT} \right\}}{\exp \left\{ -\frac{\sqrt{3} K \mu_8}{2kT} \right\} + 2 \sinh \frac{(J-K/2)\mu_3}{kT}}.$$

This is a kind of
Weiss equation

Motion equations

Motion equations in the quantum model are

$$i\hbar \frac{d\hat{P}_n^a}{dt} = [\hat{P}_n^a, \hat{\mathcal{H}}]. \quad (1)$$

Suppose we take the quasiaverage as explained above (**mean field average**) of (1), and take a **large-scale limit** with zero correlations between fluctuations, then the equations (1) transform into

$$\frac{\partial \mu_a}{\partial t} = \frac{Jz}{\hbar} C_{abc} \mu_b (\mu_{c,xx} + \mu_{c,yy}), \quad (2)$$

where C_{abc} are structure constants for the Lie algebra of operators $\{\hat{P}_n^a\}$: $[\hat{P}_n^a, \hat{P}_m^b] = iC_{abc} \hat{P}_n^c \delta_{nm}$.

Remark. The equations (2) are a **generalization of Landau-Lifshits equation** to the case of vector field $\{\mu_a\}$.

Classical model

The generalized Landau-Lifshits equation (2) can be interpreted as a **Hamiltonian hierarchy on a coadjoint orbit of a Lie group**:

$SU(3)$ in the case $s = 1$,

$SU(4)$ in the case $s = 3/2$,

$SU(2s+1)$ in the case of spin s .

That is why we use the method of Hamiltonian systems on coadjoint orbits of Lie groups (**orbital method**) to investigate a **generalized Landau-Lifshits equation, which is a classical model** for the system in question.

The matrices $\{\hat{P}^a\}$ serve as a basis in the Lie algebra $\mathfrak{su}(2s+1)$. The components of mean field $\{\mu_a\}$ serve as coordinates in the dual space to $\mathfrak{su}(2s+1)$.

Motion equations on orbit

By the orbital method we obtain **Hamiltonian equations on coadjoint orbits** of the Lie group $SU(2s+1)$.

Depending on an orbit we have **different equations implied by different ways of the mean field averaging**. For example, if we neglect correlations between fluctuations of the quantum fields $\{\hat{P}_n^a\}$ we come to Hamiltonian equations on the maximal degenerate orbit.

In the case $s = 1$:

$$\frac{\partial \mu_a}{\partial t} = \frac{1}{3h_0} C_{abc} \mu_b (\mu_{c,xx} + \mu_{c,yy}), \quad h_0 = (\mu_8^0(T))^2, \quad (3)$$

the parameter h_0 depends on initial conditions, which generally depend on a temperature T .

Effective Hamiltonians

Each orbit has a Hamiltonian. We call the Hamiltonians on all orbits of $SU(2s+1)$ **effective Hamiltonians** of the model. Equations determining orbits serve as **constraints**.

*In the case $s = 1$, we deal with the group $SU(3)$, which has **two types of orbits**: degenerate and generic. Thus, we propose **two effective Hamiltonians**.*

$$\mathcal{H}_{\text{eff},1} = \frac{1}{6h_0} \int \sum_{a=1}^8 \left((\mu_{a,x})^2 + (\mu_{a,y})^2 \right) dx dy,$$

$$d_{abc} \mu_b \mu_c + \sqrt{h_0/3} \mu_a - \frac{2h_0}{3} = 0, \quad \text{for a degenerate orbit}$$

where $d_{abc} = \frac{1}{4} \text{Tr}(\hat{P}_a \hat{P}_b \hat{P}_c + \hat{P}_b \hat{P}_a \hat{P}_c)$ is a symmetric tensor.

Remark. The Hamiltonian $\mathcal{H}_{\text{eff},1}$ gives rise to the generalized Landau-Lifshits equation (3), which coincides with (2).

Effective Hamiltonians

Another Hamiltonian is

$$\mathcal{H}_{\text{eff},2} = \frac{1}{8(h_0^3 - 3f_0^2)} \sum_{a=1}^8 \left(h_0^2 (\nabla \mu_a)^2 + 3h_0 (\nabla \xi_a)^2 - 6f_0 \langle \nabla \mu_a, \nabla \xi_a \rangle \right),$$

$$d_{abc} \mu_b \xi_c - h_0 \mu_a - \frac{2}{3} f_0 = 0, \quad \text{for a generic orbit}$$

ξ_a is a quadratic form in $\{\mu_a\}$: $\xi_a = d_{abc} \mu_b \mu_c$.

The parameters h_0, f_0 depend on initial conditions, and generally depend on a temperature T .

Remark. One can quantize $\mathcal{H}_{\text{eff},1}$ -, and $\mathcal{H}_{\text{eff},2}$ -models. Such effective models are called **σ -models** in quantum field theory. Evidently, they describe slow fluctuations. One can take into account quick fluctuations by means of a renormalization group connected to the coefficients

$$\frac{1}{8(h_0^3(T) - 3f_0^2(T))} \text{ and } \frac{1}{6h_0(T)}.$$

Geometry of orbits

Effective Hamiltonians have a geometrical nature.

For an **orbit** is a homogeneous space that admits a **Kählerian structure**, we use a complex parameterization (by means of *generalized stereographic projection*) and reduce effective Hamiltonians to the form:

$$\mathcal{H}_{\text{eff}} = \int \sum_{\alpha, \beta} h_{\alpha\bar{\beta}} \left(\frac{\partial w_\alpha}{\partial z} \frac{\partial w_\beta}{\partial \bar{z}} + \frac{\partial w_\alpha}{\partial \bar{z}} \frac{\partial w_\beta}{\partial z} \right) dz d\bar{z},$$

$h_{\alpha\bar{\beta}}$ are components of a Kählerian metrics on an orbit;
 $\{w_\alpha\}$ are complex parameters on an orbit.

Remark. *The geometric form of an effective Hamiltonian does not depend on an orbit. A density of Hamiltonian is defined by a Kählerian metrics.*

Generalized stereographic projection

$$\begin{aligned}
 \mu_1 &= \frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2\sqrt{2}} \cdot \frac{w_2 + w_3 + \bar{w}_2 + \bar{w}_3}{1 + |w_2|^2 + |w_3|^2} - \frac{\mu_3^0}{\sqrt{2}} \frac{(1 - w_1)(\bar{w}_3 - \bar{w}_1\bar{w}_2) + (1 - \bar{w}_1)(w_3 - w_1w_2)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_2 &= \frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2i\sqrt{2}} \cdot \frac{w_3 - w_2 - \bar{w}_3 + \bar{w}_2}{1 + |w_2|^2 + |w_3|^2} + \frac{i\mu_3^0}{\sqrt{2}} \frac{(1 + w_1)(\bar{w}_3 - \bar{w}_1\bar{w}_2) - (1 + \bar{w}_1)(w_3 - w_1w_2)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_3 &= -\frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2} \cdot \frac{|w_2|^2 - |w_3|^2}{1 + |w_2|^2 + |w_3|^2} + \frac{\mu_3^0(1 - |w_1|^2)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_4 &= \frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2i} \cdot \frac{\bar{w}_2w_3 - w_2\bar{w}_3}{1 + |w_2|^2 + |w_3|^2} + \frac{i\mu_3^0(w_1 - \bar{w}_1)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_5 &= \frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2i\sqrt{2}} \cdot \frac{w_2 + w_3 - \bar{w}_2 - \bar{w}_3}{1 + |w_2|^2 + |w_3|^2} + \frac{i\mu_3^0}{\sqrt{2}} \frac{(1 - \bar{w}_1)(w_3 - w_1w_2) - (1 - w_1)(\bar{w}_3 - \bar{w}_1\bar{w}_2)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_6 &= \frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2\sqrt{2}} \cdot \frac{w_3 - w_2 + \bar{w}_3 - \bar{w}_2}{1 + |w_2|^2 + |w_3|^2} - \frac{\mu_3^0}{\sqrt{2}} \frac{(1 + w_1)(\bar{w}_3 - \bar{w}_1\bar{w}_2) + (1 + \bar{w}_1)(w_3 - w_1w_2)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_7 &= \frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2} \cdot \frac{\bar{w}_2w_3 + w_2\bar{w}_3}{1 + |w_2|^2 + |w_3|^2} - \frac{\mu_3^0(w_1 + \bar{w}_1)}{1 + |w_1|^2 + |w_3 - w_1w_2|^2} \\
 \mu_8 &= -\frac{\mu_3^0 - \sqrt{3}\mu_8^0}{2\sqrt{3}} \cdot \frac{2 - |w_2|^2 - |w_3|^2}{1 + |w_2|^2 + |w_3|^2} + \frac{\mu_3^0}{\sqrt{3}} \cdot \frac{1 + |w_1|^2 - 2|w_3 - w_1w_2|^2}{1 + |w_1|^2 + |w_3 - w_1w_2|^2}.
 \end{aligned}$$

Topology of orbits

A coadjoint orbit $SU(3)$ is parameterized by $\{w_1, w_2, w_3\}$.
Kählerian potentials are

$$\Phi = \mu_3^0 \Phi_1 + \frac{\sqrt{3}\mu_8^0 - \mu_3^0}{2} \Phi_2,$$

$$\Phi_1 = \ln(1 + |w_1|^2 + |w_3 - w_1 w_2|^2), \quad \Phi_2 = \ln(1 + |w_2|^2 + |w_3|^2).$$

On a generic orbit $\dim H^2 = 2$ (H^2 is a cohomology class).

On a degenerate orbit: $\mu_3^0 = 0, w_1 = 0$ or $\mu_3^0 = \sqrt{3}\mu_8^0, w_2 = 0$,
evidently, $\dim H^2 = 1$.

Density of the effective Hamiltonians

$$h_{\alpha, \bar{\beta}} = \frac{\partial^2 \Phi_1}{\partial w_\alpha \partial \bar{w}_\beta} + \frac{\partial^2 \Phi_2}{\partial w_\alpha \partial \bar{w}_\beta} + \frac{2\omega_{\alpha\bar{\beta}}}{e^{\Phi_1} e^{\Phi_2}},$$

$$\omega_{2\bar{2}} = |w_1|^2, \quad \omega_{2\bar{3}} = \bar{\omega}_{3\bar{2}} = -w_1, \quad \omega_{2\bar{2}} = 1.$$

Topological charge

Introduce a **topological charge of a mean field configuration** on a Kählerian manifold by

$$Q = \frac{1}{4\pi} \int \sum_{\alpha, \beta} i h_{\alpha\bar{\beta}} \left(\frac{\partial w_\alpha}{\partial z} \frac{\partial w_\beta}{\partial \bar{z}} - \frac{\partial w_\alpha}{\partial \bar{z}} \frac{\partial w_\beta}{\partial z} \right) dz \wedge d\bar{z}.$$

The expressions for Q and \mathcal{H}_{eff} differ only in the sign.

Remark. Compare with $\mathcal{H}_{\text{eff}} = \int \sum_{\alpha, \beta} h_{\alpha\bar{\beta}} \left(\frac{\partial w_\alpha}{\partial z} \frac{\partial w_\beta}{\partial \bar{z}} + \frac{\partial w_\alpha}{\partial \bar{z}} \frac{\partial w_\beta}{\partial z} \right) dz d\bar{z}$.

Evidently,

$$\mathcal{H}_{\text{eff}} \geq 4\pi |Q|.$$

A **minimum of \mathcal{H}_{eff}** is realized if the equality holds, that takes place if $\{w_\alpha\}$ **are holomorphic or antiholomorphic.**

Large-scale topological excitations

Example. Consider a planar magnet with spin 1, and the effective $\mathcal{H}_{\text{eff},1}$ -model. This corresponds to a degenerate orbit of $SU(3)$.

Assign $\mu_3^0 = 0$, $\mu_8^0 = -\frac{2}{\sqrt{3}}$ (an equilibrium nematic state).

Take a mean field configuration with the holomorphic functions ($Q = 2$):

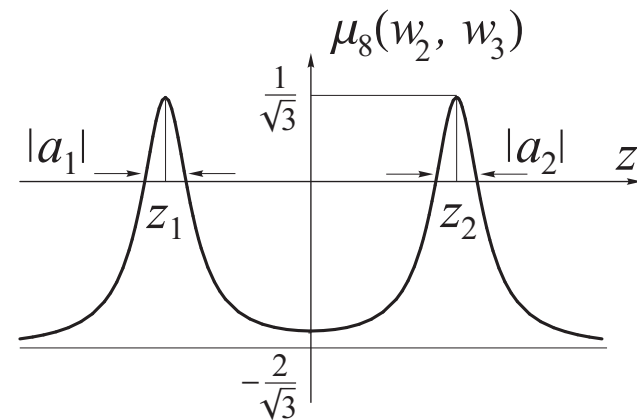
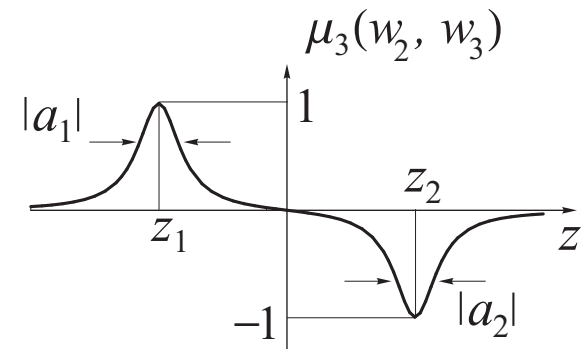
$$w_2(z) = \frac{a_1}{z - z_1}, \quad w_3(z) = \frac{a_2}{z - z_2},$$

$$a_1, z_1, a_2, z_2 \in \mathbb{C}.$$

This is a kind of Belavin-Polyakov soliton.

$\mathcal{H}_{\text{eff},1}$ does not depend on a_1, z_1, a_2, z_2 .

Thus, the excitation can infinitely enlarge without energy input, that causes destruction of the nematic order.



Results

- The example shows that **in a 2D magnet an ordered state is easily destroyed at any temperature $T > 0$** (that agrees with Mermin-Wagner theorem).
Moreover, **we propose a mechanism of destruction of ordered states in 2D magnets.** That is, we suggest that an order exists, but any excitation easily destroys it.
- The well-known fact: an order exists in 3D magnets.
How does it disappear in 2D?
A prospect: to construct a quasi2D theory that considers a planar magnet with a fixed thickness, and takes into account anisotropic effects (demagnetization in normal direction).

The end