Intertwined order

- consider a spin Hamiltonian $H[S_{\alpha i}]$

component ↗ ↑ site

•) magnetic order is signaled by the expectation value $\langle S_{\alpha i}\rangle$

it breaks i) spin-rotation symmetry

ii) time reversal symmetry

) Spin liquids are states without symmetry breaking of local operators

a state somewhat in-between possesses quadrupolar (or higher multipolar) order

Here, one considers expectation values of the type

$$K_{jl,\mu\nu} = \langle S_{j\mu} S_{l\nu}\rangle - \frac{\delta_{\mu\nu}}{3}\langle \vec{S}_j \cdot \vec{S}_l\rangle$$

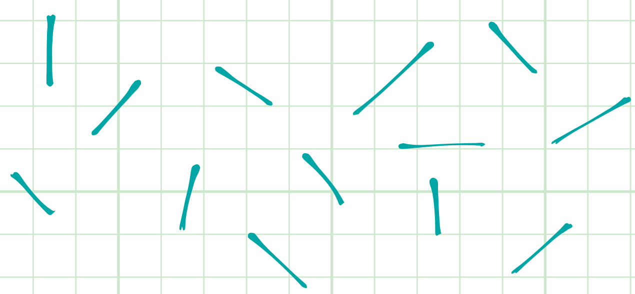
H. Chen + P. M. Levy PRL (1971)

A.F. Andreev + A. Grishchuk JETP (1984)

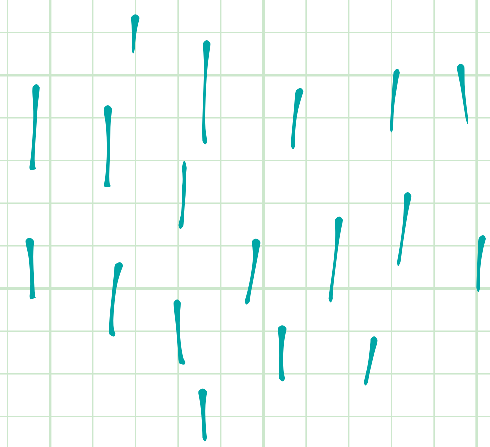
can we have states with $K_{jl,\mu\nu} \neq 0$ but $\langle S_{j\mu}\rangle = 0$ **spin-nematic**

$\boxed{\text{nematic order, a brief detour}}$

rod-shaped molecules



$T > T_{nem}$



$T < T_{nem}$

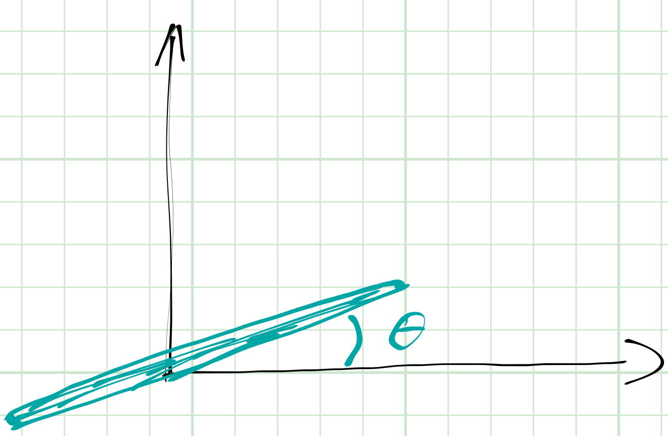
(νῆμα = thread)

order parameter: it cannot be the unit vector $\vec{n}$ pointing along the axis of the molecule (the director)

$\vec{n}$; $-\vec{n}$ are not distinguishable

$\Downarrow$

$\theta \to \theta + \pi$



not $\langle \cos\theta \rangle$

but $\langle \cos^2\theta \rangle - \frac{1}{d}$

more precisely

dimension of vector $\vec{n}$

$$Q_{\alpha\beta} = \left\langle n_\alpha n_\beta - \frac{1}{d}\,\delta_{\alpha\beta} \right\rangle \; ; \; \vec{n}^{\,2} = 1$$

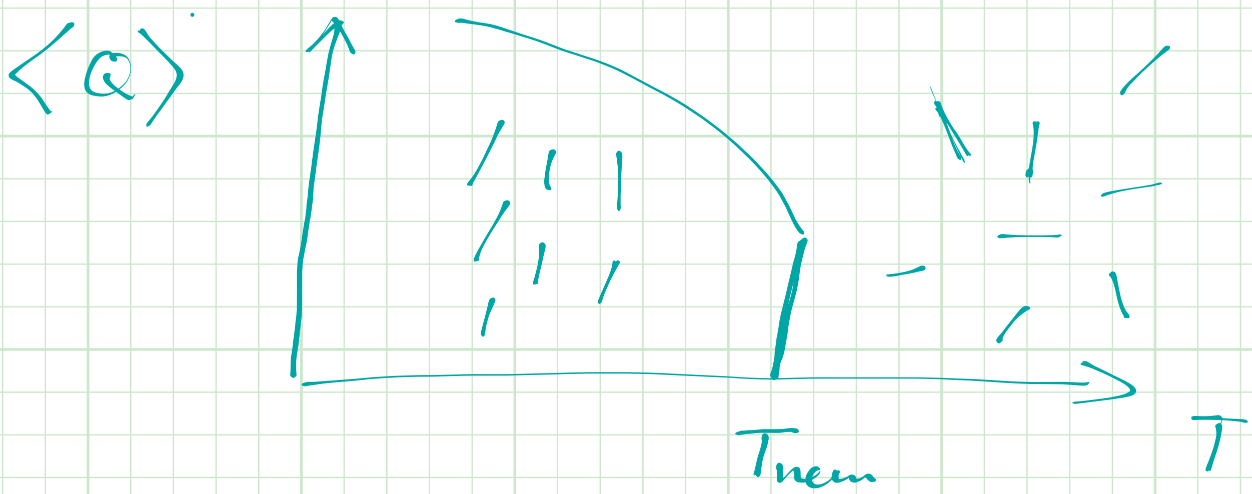
quadrupolar order

$\mathrm{Tr}\,Q = 0$

theory of phase transitions:

$$f[Q] = f_0 + \frac{a}{2}\,\mathrm{tr}(Q^2) + \underline{\underline{\frac{b}{3}\,\mathrm{tr}(Q^3)}}$$
$$+ \frac{c}{4}\,\mathrm{tr}(Q^4) + \frac{c'}{4}\left(\mathrm{tr}\,Q^2\right)^2$$

cubic invariant ($\Rightarrow$ 1st order transition)



note: if the director is confined to $d=2$ (even for a nominally three-dimensional system)

$$Q_{\alpha\beta} = \begin{pmatrix} Q_1 & Q_2 \\ Q_2 & Q_1 \end{pmatrix} \Rightarrow \mathrm{tr}\,Q^3 = 0$$

$\Rightarrow$ two-dimensional directors yield second order phase transitions back to spins ... (now we almost know why this is a spin nematic)

$$K_{jl,\mu\nu} = \langle S_{j\mu} S_{l\nu} \rangle - \frac{\delta_{\mu\nu}}{3} \langle \vec{S}_j \cdot \vec{S}_l \rangle$$

classification w.r.t. chirality

$$P_{jl,\lambda} \equiv \varepsilon_{\lambda\mu\nu} K_{jl,\mu\nu}$$
$$= \langle (\vec{S}_j \times \vec{S}_l)_\lambda \rangle$$ spin chirality

$$\boxed{Q_{jl,\mu\nu} = \frac{1}{2} \left(K_{jl,\mu\nu} + K_{jl,\nu\mu} \right)}$$ spin nematic

$\langle Q \rangle$:) breaks rotation invariance in spin space

:) does not break TRI (Q doesn't change sign under TRS)

:) it may also break transl. symmetry

example $NiGa_2S_4$

(Heisenberg spins on a triangular lattice ($S=1$) Y. Nakatsuji, Science 2005)

$$H = H_0 + H_b = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j \right)^2$$

$\vec{S}$: Spin 1 operator

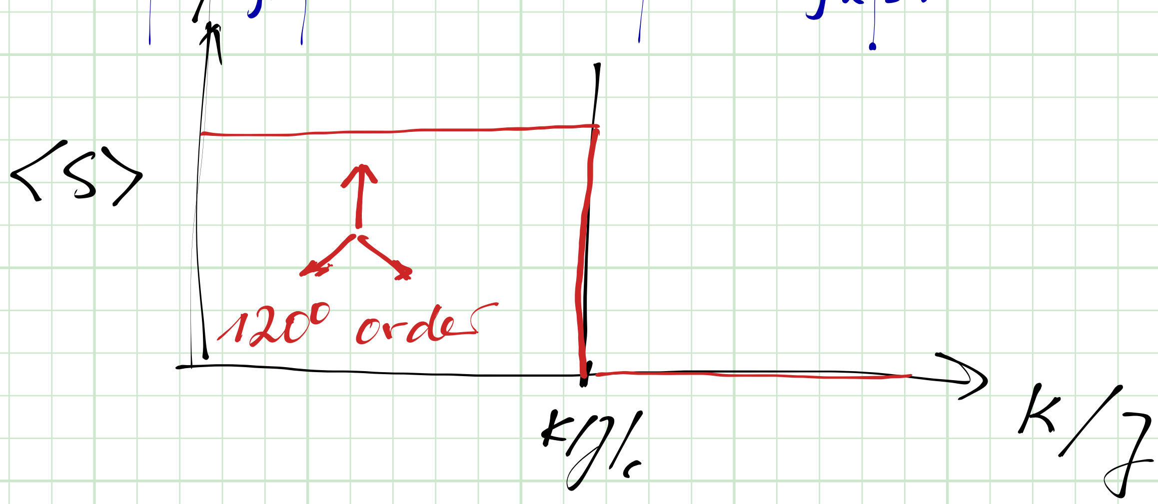
$$\Uparrow$$

$$Q_{ii\alpha\beta}\, Q_{jj\alpha\beta}$$

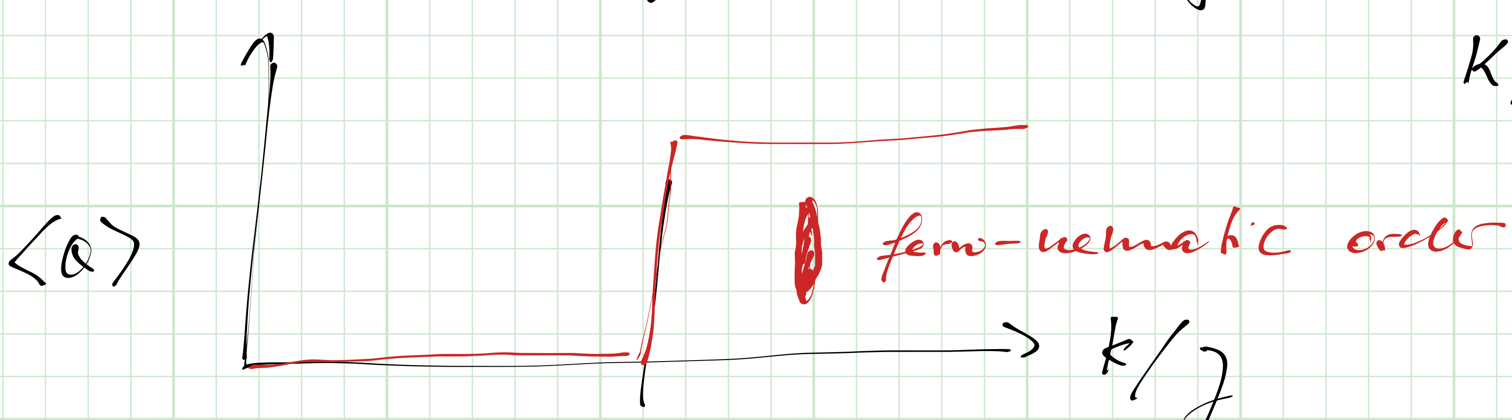
the easiest approach is mean field

$$\vec{S}_i \cdot \vec{S}_j \simeq \langle \vec{S}_i \rangle \cdot \vec{S}_j + \vec{S}_i \langle \vec{S}_j \rangle - \langle \vec{S}_i \rangle \langle \vec{S}_j \rangle$$

$$Q_{i\alpha\beta}\, Q_{j\alpha\beta} \simeq Q_{i\alpha\beta} \langle Q_{j\alpha\beta} \rangle + \langle Q_{i\alpha\beta} \rangle Q_{j\alpha\beta} - \langle Q_{i\alpha\beta} \rangle \langle Q_{j\alpha\beta} \rangle$$



$K/J|_c = 1.143$



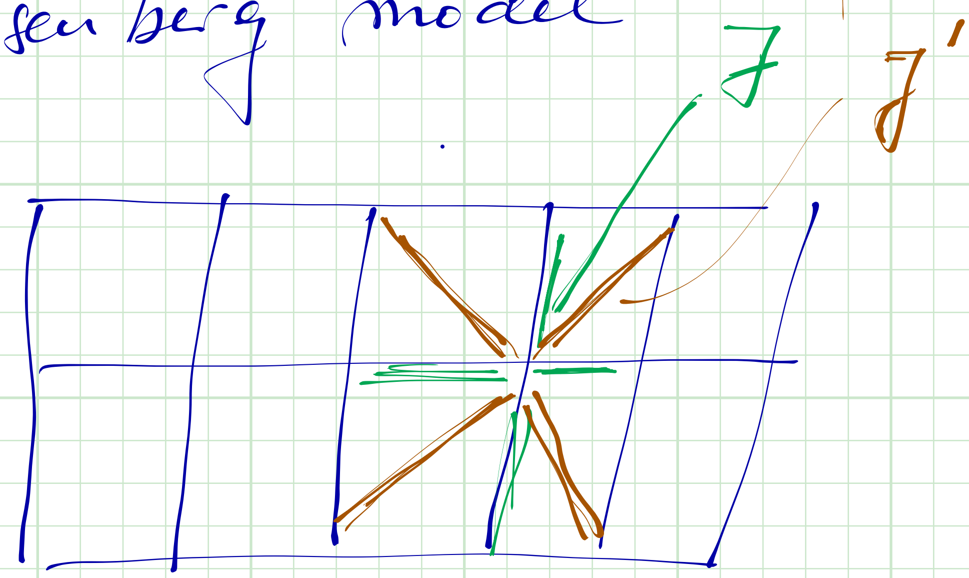
$K/J|_c$

numerics suggests at least strong nematic fluct. at finite T

Can one induce nematicity via fluctuations?

Are there spin systems with nematicity in real space (not spin space).

$J_1 - J_2$ Heisenberg model

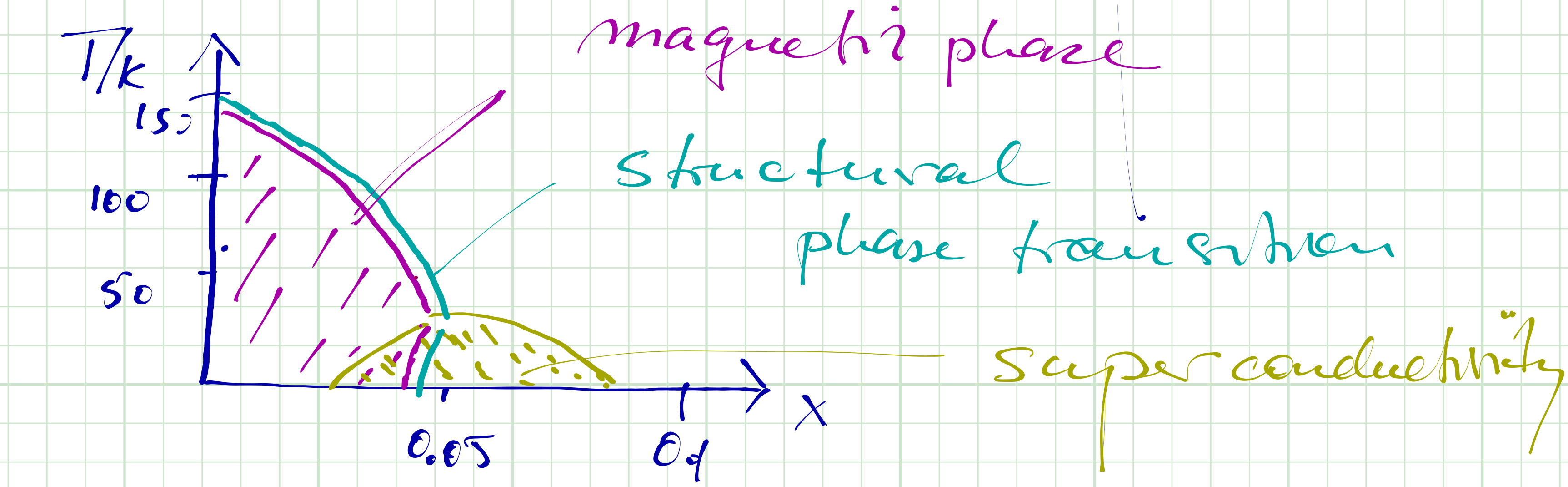


P. Chandra, A. Larkin, P. Coleman ('89)

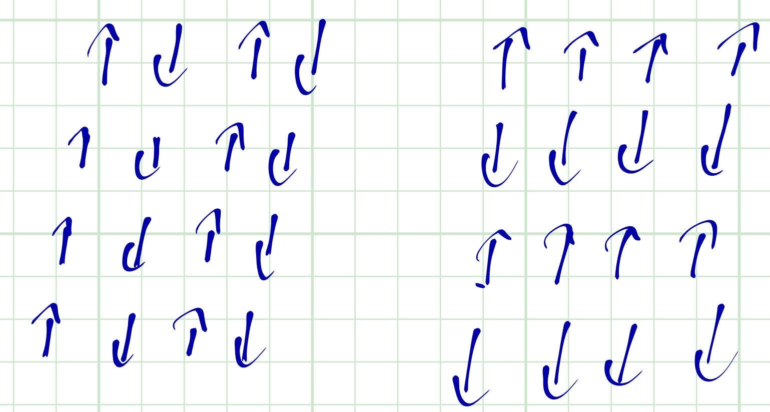
We will not solve this specific Heisenberg model, but rather consider a correspond. long wave-length model.

Before we do this, let us summarize some experimental facts of the magnetic state in the iron-based superconductors.

Phase diagram $Ba(Fe_{1-x}Co_x)_2As_2$



the magnetism:



$\vec{Q}_x = (\pi, 0)$ $\qquad$ $\vec{Q}_y = (0, \pi)$

magnetization

$$\vec{S}(\vec{r}) = \underline{\vec{m}_x(\vec{r})}\, e^{i\vec{Q}_x\cdot\vec{r}} + \underline{\vec{m}_y(\vec{r})}\, e^{i\vec{Q}_y\cdot\vec{r}}$$

two three-component order-parameters!

effective action: (no gradients for the moment)

$$S = r_0\left(\vec{m}_x^{\,2} + \vec{m}_y^{\,2}\right) + \frac{u}{2}\left(\vec{m}_x^{\,2} + \vec{m}_y^{\,2}\right)^2$$

$$- \frac{g}{2}\left(\vec{m}_x^{\,2} - \vec{m}_y^{\,2}\right)^2 + v\left(\vec{m}_x \cdot \vec{m}_y\right)^2$$

microscopic calc. yields for most cases

$g > 0 \quad , \quad |v| \ll |g|$

to make progress we will analyze the above action in the limit of large N where N is the # of components of $\vec{m}_i$

another detour: large - N

$$S = \frac{1}{2}\int_{x,\tau}\left(r_0 \vec{\phi}^2 + (\nabla\vec{\phi})^2 + \frac{u}{2N}\vec{\phi}^{2\,2}\right) + S_{dyn}$$

$$S_{dyn} = \frac{\gamma}{2} T \int_x \sum_n{}' |\omega_n|^\alpha \, \vec{\phi}(x,\omega_n)\,\vec{\phi}(x,-\omega_n)$$

$$\vec{\phi} = (\phi_1, \dots, \phi_N)$$

Hubbard - Stratonovich transformation

$$\int_{-i\infty}^{i\infty} \mathcal{D}\lambda \; e^{\frac{N}{4u}\int \lambda^2 - \frac{1}{2}\int \lambda \vec{\phi}^2} \sim e^{-\frac{N}{4u}\int_x (\vec{\phi}^2)^2}$$

$$\Rightarrow S[\phi,\lambda] = S_{dyn} - \int \frac{N}{4u}\lambda^2 + \frac{1}{2}\int\left((\nabla\vec{\phi})^2 + (r+\lambda)\vec{\phi}^2\right)$$

now we can integrate out $\vec{\phi}$

$$\Rightarrow \quad S(\lambda) = N\left(\frac{1}{2}\,\mathrm{tr}\log \mathcal{G}^{-1}(\lambda) - \frac{1}{4u}\int \lambda^2\right)$$

$$\mathcal{G}^{-1}(x,x',\omega_n) = \gamma|\omega_n|^{\alpha} + \left(r - \nabla_x^2 + \lambda(x)\right)\delta(x-x')$$

Saddle point w.r.t. λ

$$\lambda(x) = uT\sum_n \mathcal{G}(x,x,i\omega_n)$$

generalization with long range order: $\langle\vec{\phi}\rangle = (\sigma, 0, 0)$

$$\lambda = u\int_{q,\omega} \frac{1}{\underbrace{r+\lambda}_{r} + q^2 + \gamma|\omega|^{2/z}} + \frac{\sigma^2}{N}$$

$$h = \sigma\left(r_0 + \lambda\right) \qquad \left(q^2 + \gamma|\omega|^2 \to q^2\right)$$

$$\Rightarrow \quad r = r_0 + u\int_q \frac{1}{q^2 + r} + \sigma^2/\cancel{N}$$

$$r\sigma = h$$

transition $\quad r=0 \quad \Rightarrow \quad r_0^c = -u\int \frac{1}{q^2}$

$(d>2)$

$r=0$ in the ordered state (Goldstone modes)

$$r = r_0 - r^c + u\int_q \left(\frac{1}{q^2+r} - \frac{1}{q^2}\right)$$

$$= r_0 - r_0^c - u\, r \underbrace{\int_q \frac{1}{q^2(r+q^2)}}_{r^{\frac{d}{2}-2}}$$

$d>4$ last term negligible

$\xi^{-2} = r \sim r_0 - r^c$

$d<4$ l.h.s. is negligible

$\xi^{2} \sim (r_0 - r_0^c)^{2/(d-2)} \sim (r_0 - r_0^c)^{2\nu}$

correlation length critical exponent $\boxed{\nu = \frac{1}{d-2}}$

O.k. now we know how to do a large-N calculation

$$S = r_0 \left(\vec{m}_x^2 + \vec{m}_y^2\right) + \frac{u}{2}\left(\vec{m}_x^2 + \vec{m}_y^2\right)^2$$

$$- \frac{g}{2}\left(\vec{m}_x^2 - \vec{m}_y^2\right)^2$$

Hubbard-Stratonovich transformation

$$S = \int \chi_q \left(\vec{m}_x^2 + \vec{m}_y^2\right) + N\int\left(\frac{\phi^2}{2g} - \frac{\lambda^2}{2u}\right)$$

$$+ \int \gamma\left(\vec{m}_x^2 + \vec{m}_y^2\right) + \int \phi\left(\vec{m}_x^2 - \vec{m}_y^2\right)$$

integrating out:

$$S_{eff} = N \int \left(\frac{\phi^2}{2g} - \frac{\lambda^2}{2u}\right) + \frac{1}{2}\ln\left((\chi_q^{-1} + \lambda)^2 - \phi^2\right)$$

Saddle point:

$$\frac{\lambda}{u} = \int \frac{r_0 + \lambda + q^2}{(r_0 + \lambda + q^2)^2 - \phi^2}$$

$$\frac{\phi}{g} = \int \frac{\phi}{(r_0 + \lambda + q^2)^2 - \phi^2}$$

equation of state for ϕ

if $\phi \neq 0 \Rightarrow \langle \vec{m}_x^2 - \vec{m}_y^2 \rangle = 0$

(even though $\langle \vec{m}_i \rangle = 0$)

let's add a conjugate field to $\vec{m}_x^2 - \vec{m}_y^2$

$\phi \to \phi + h_n$

$$\phi = g \int \frac{\phi + h_n}{(\chi^{-1})^2 - (\phi + h_n)^2}$$

$$\chi_{nem} = \frac{\partial \phi}{\partial h} = g\, \chi_{nem} \int_q \chi^2 + g \int_q \chi^2$$

$$\boxed{\chi_{nem} = \frac{g \int_q \chi^2}{1 - g \int_q \chi^2}}$$

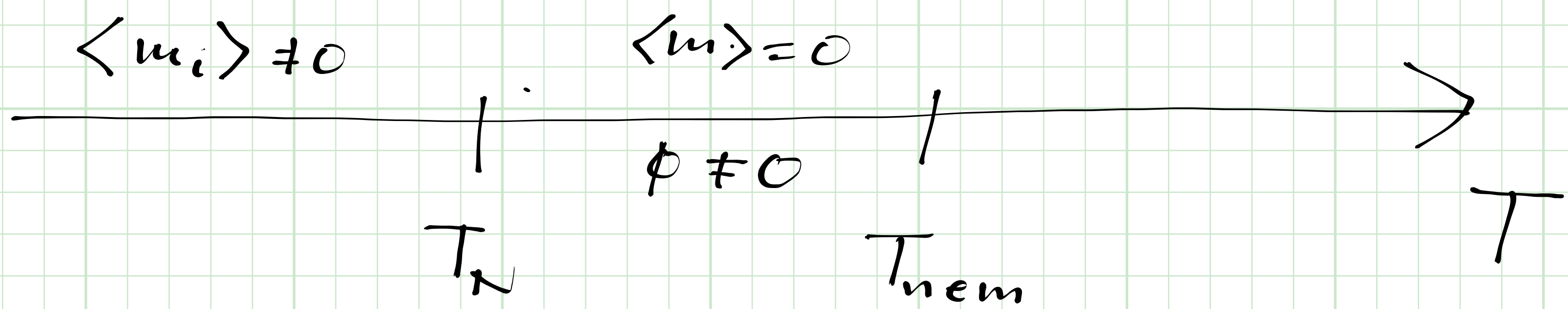
nematic susceptibility

$$\chi(q) = \frac{1}{q^2 + \xi^{-2}} \Rightarrow \int \frac{d^d q}{(2\pi)^d} \frac{1}{(q^2 + \xi^{-2})^2} \sim \xi^{4-1}$$

as we approach a magnetic transition ξ grows

for $d < 4$ $\qquad g\,\xi^{4-d}$ will $\to 1$

at a <u>finite</u> distance to the magnetic transition

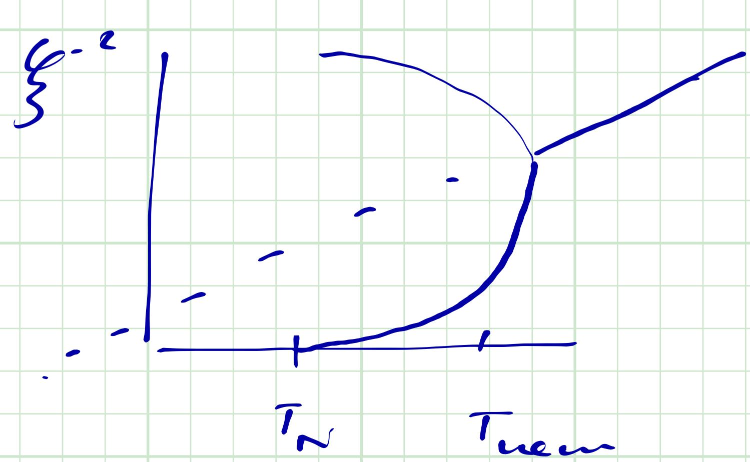


phase with anisotropic fluctuations $\qquad \langle m_x^2 \rangle \neq \langle m_y^2 \rangle$

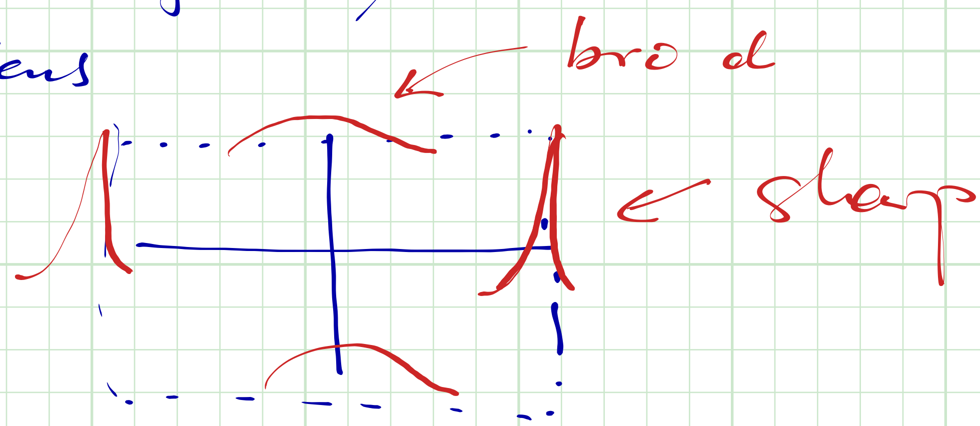
one can also analyze the magnetic susceptibility

$$\chi = \frac{r_0 + \lambda + q^2}{(\underbrace{r_0 + \lambda}_{r} + q^2)^2 - \phi^2}$$

$$\xi_\pm^{-2} = r \pm \phi$$



one length hardens and one length softens



→ we have a nematic interaction with $\langle \vec{m}_x^2 - \vec{m}_y^2 \rangle \neq 0$ $\langle \vec{m}_x \rangle = 0$

·) orientational order in real space

:) full spin-rotation invariance

:) full time reversal symmetry

$$Q_{\alpha\beta} = \begin{pmatrix} \phi & 0 \\ 0 & -\phi \end{pmatrix}$$

as orientational order along axes

→ Ising nematic

$(\mathrm{tr}\, Q^3 = 0)$

Coupling to the lattice

$$S_{el} = \frac{1}{2}\int c_0 (\varepsilon_{xx} - \varepsilon_{yy})^2 + \dots$$

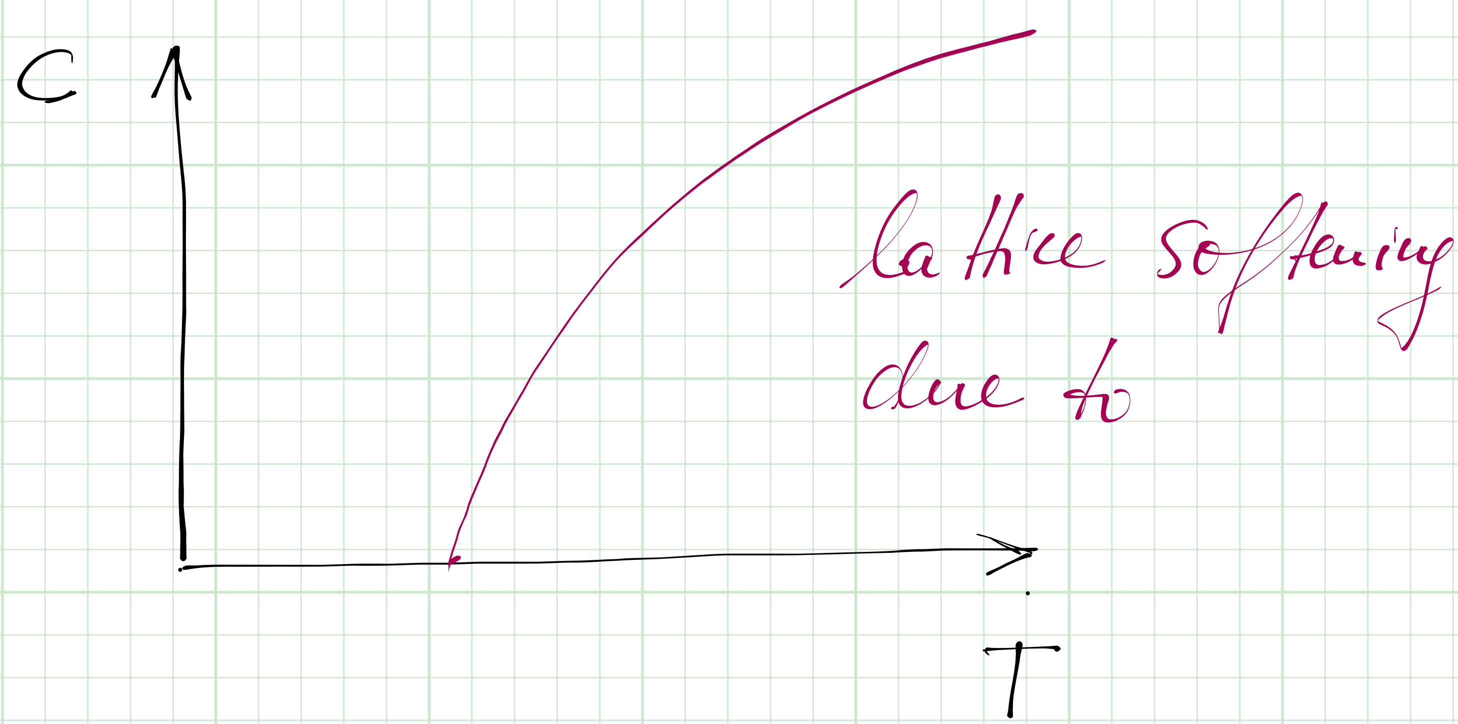
$$- \lambda \, \phi \, (\varepsilon_{xx} - \varepsilon_{yy}) + S_{magnetic}$$

elastic constant $C_0 = C_{11}^0 - C_{22}^0$

renormalization of the elastic constant

$$C^{-1} = C_0^{-1} + \frac{\lambda^2}{C_0} \chi_{nem}$$

C vanishes when χ_{nem} diverges



dynamics $\longrightarrow$ Raman scattering

length scales $\longrightarrow$ phonon softening

Is the nematic order the only allowed one?

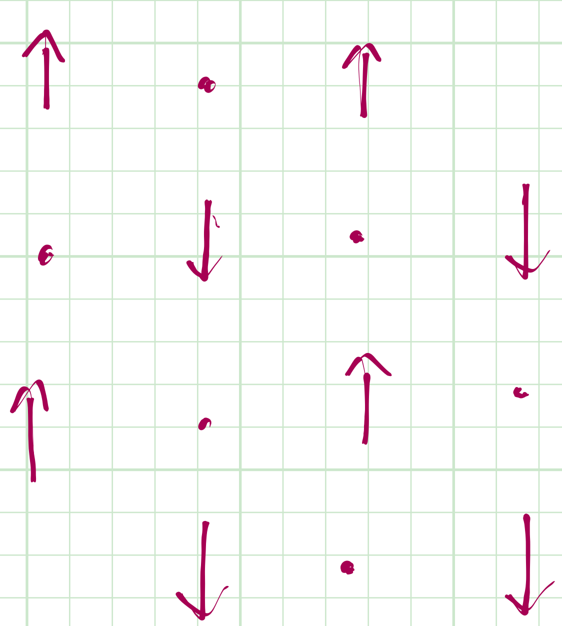
$$S = r_0\left(\vec{m}_x^{\,2} + \vec{m}_y^{\,2}\right) + \frac{u}{2}\left(\vec{m}_x^{\,2} + \vec{m}_y^{\,2}\right)^2 - \frac{g}{2}\left(\vec{m}_x^{\,2} - \vec{m}_y^{\,2}\right)^2 + 2v\left(\vec{m}_x \cdot \vec{m}_y\right)^2$$

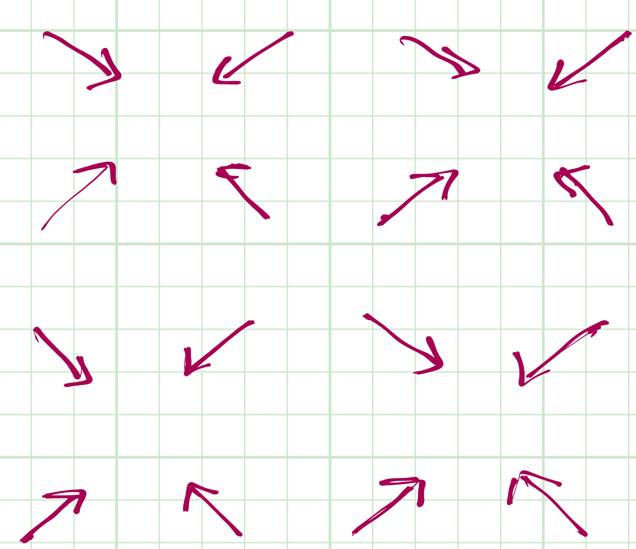
we discussed $\langle \varphi \rangle = \langle \vec{m}_x^{\,2} - \vec{m}_y^{\,2} \rangle$

but, for $g < \max(0, -v)$ this is no longer the classical g.s.

instead $|\vec{m}_x| = |\vec{m}_y|$

$v < 0 : \vec{m}_x \parallel \vec{m}_y$, $v > 0$ $\vec{m}_x \perp \vec{m}_y$





$\varphi = \langle \vec{m}_x \cdot \vec{m}_y \rangle$ $\vec{\varphi} = \vec{m}_1 \times \vec{m}_2$

Underlying symmetry principle

$$f = f + a(T) \sum_{\mu=1}^{n_{irr}} \eta_\mu^2$$

O. P. transforms according to an irreducible representation Γ with dimension $n_{irr} > 1$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

Composite order parameter

$$\varphi = \sum_{\mu\nu}{}' \tau_{\mu\nu}\, \eta_\mu \eta_\nu$$

$$\Gamma \otimes \Gamma = \underset{\overset{\parallel}{A_1}}{\Gamma_1} \oplus \underbrace{\Gamma_2 \oplus \dots \Gamma_n}_{\text{non trivial bilinear forms}}$$

$\Rightarrow$ $\langle \varphi \rangle \neq 0$ breaks a new symmetry

The group: $C_{4v}' = C_{4v} \otimes \{t_0, t_x, t_y, t_{x+y}\}$

our order parameter $(\vec{m}_x, \vec{m}_y)$ transforms as E_5

$$E_5 \otimes E_5 = A_1 \oplus B_1 \oplus B_2' \oplus A_2'$$

our nematic state

$\varphi = \vec{m}_1 \cdot \vec{m}_2$

CDW

$\varphi = \vec{m}_1 \times \vec{m}_2$

chiral order