The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

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School and Workshop on Highly Frustrated Magnets and Strongly Correlated Systems: From Non-Perturbative Approaches to Experiments

30 July - 17 August, 2007

Quadrupolar and Nematic Order

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Budapest

August 6th, 2007
HFM school, ICTP

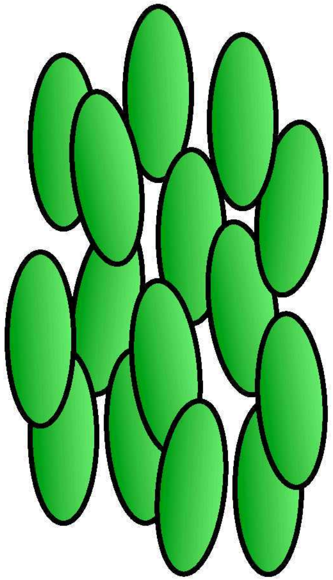
Outline

(1) Nematic phases in classical spin models

(2) Quadrupolar phases in quantum spin model

(3) Nematic phases in quantum spin model

Nematic liquid crystals



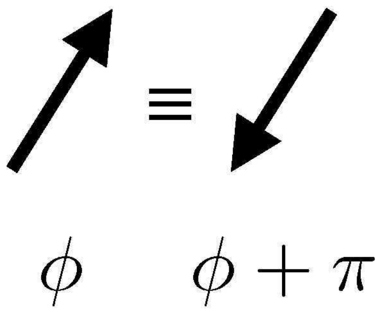
Rod like molecules that are free to move, but like to line up in the same direction

$\mathbf{n}(\mathbf{r})$

no positional order (liquid)

long range orientational order: O(3) symmetry broken,characterized by the director $\mathbf{n}(\mathbf{r})$

Spin quadrupol/nematic order parameter



$$\begin{aligned}
\exp 2i\phi &= \cos 2\phi + i \sin 2\phi \\
&= \cos^2\phi - \sin^2\phi + i\, 2\sin\phi\cos\phi \\
&= S_x^2 - S_y^2 + i\, 2S_xS_y \\
&= Q_{x^2-y^2} + i\, Q_{xy}
\end{aligned}$$

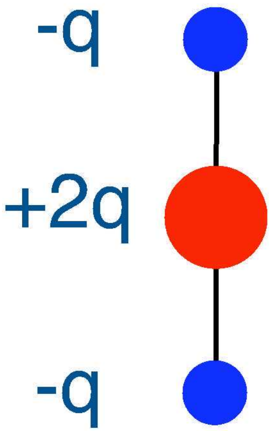
traceless rank 2 tensor-operator

$$\hat{\mathbf{Q}}_i = \begin{pmatrix} \hat{Q}_i^{x^2-y^2} \\ \hat{Q}_i^{3z^2-r^2} \\ \hat{Q}_i^{xy} \\ \hat{Q}_i^{yz} \\ \hat{Q}_i^{xz} \end{pmatrix} = \begin{pmatrix} (S_i^x)^2 - (S_i^y)^2 \\ \frac{1}{\sqrt{3}}\left[2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2\right] \\ S_i^xS_i^y + S_i^yS_i^x \\ S_i^yS_i^z + S_i^zS_i^y \\ S_i^xS_i^z + S_i^zS_i^x \end{pmatrix}$$

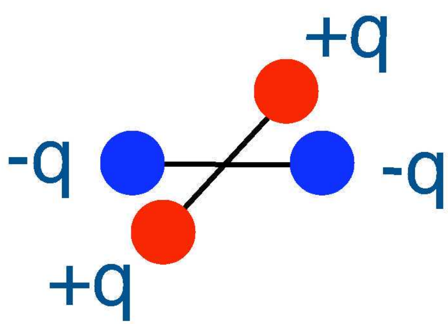
$$Q^{\alpha\beta} = S^\alpha S^\beta + S^\beta S^\alpha - \frac{2}{3}(\mathbf{S}\cdot\mathbf{S})\delta_{\alpha\beta}$$

Comparison to electric quadrupoles

$$\hat{\mathbf{Q}}_i = \begin{pmatrix} \hat{Q}_i^{x^2-y^2} \\ \hat{Q}_i^{3z^2-r^2} \\ \hat{Q}_i^{xy} \\ \hat{Q}_i^{yz} \\ \hat{Q}_i^{xz} \end{pmatrix} = \begin{pmatrix} (S_i^x)^2 - (S_i^y)^2 \\ \frac{1}{\sqrt{3}}\left[2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2\right] \\ S_i^x S_i^y + S_i^y S_i^x \\ S_i^y S_i^z + S_i^z S_i^y \\ S_i^x S_i^z + S_i^z S_i^x \end{pmatrix}$$



$$V(\mathbf{r}) \propto \frac{3z^2 - r^2}{r^5}$$

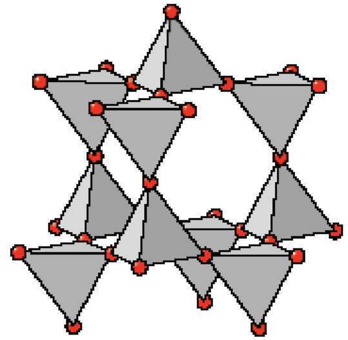


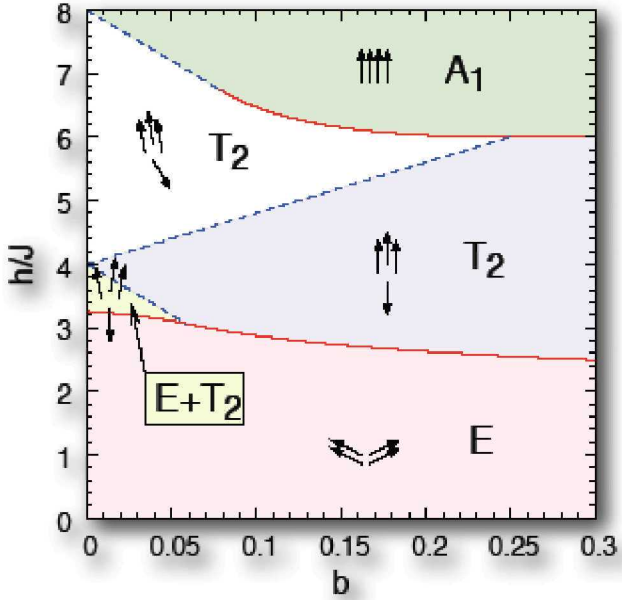
$$V(\mathbf{r}) \propto \frac{x^2 - y^2}{r^5}$$

Nemattic phase with classical spins

pyrochlor lattice,
Heisenberg model with biqadratic exchange
(favors collinearity)

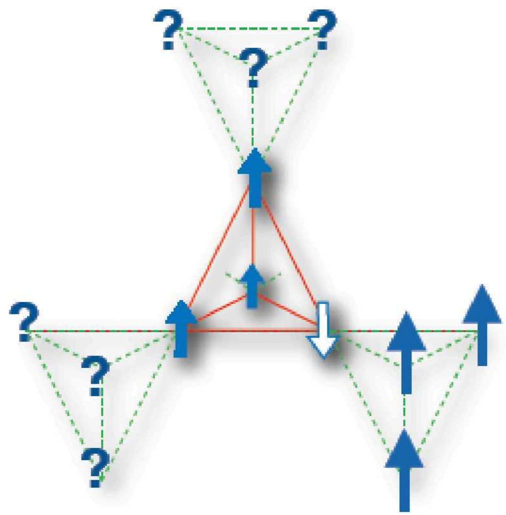
$$\mathcal{H} = \sum_{\langle i,j \rangle} J\left[\mathbf{S}_i\mathbf{S}_j - b(\mathbf{S}_i\mathbf{S}_j)^2\right] - \mathbf{h}\sum_i \mathbf{S}_i$$





Spin configurations for a single tetrahedron

Corner shared tetrahedra - ground state degeneracy



Finite temperature phase diagram

2:2 spin arrangement for each tetrahedron

macroscopic (ice) degeneracy

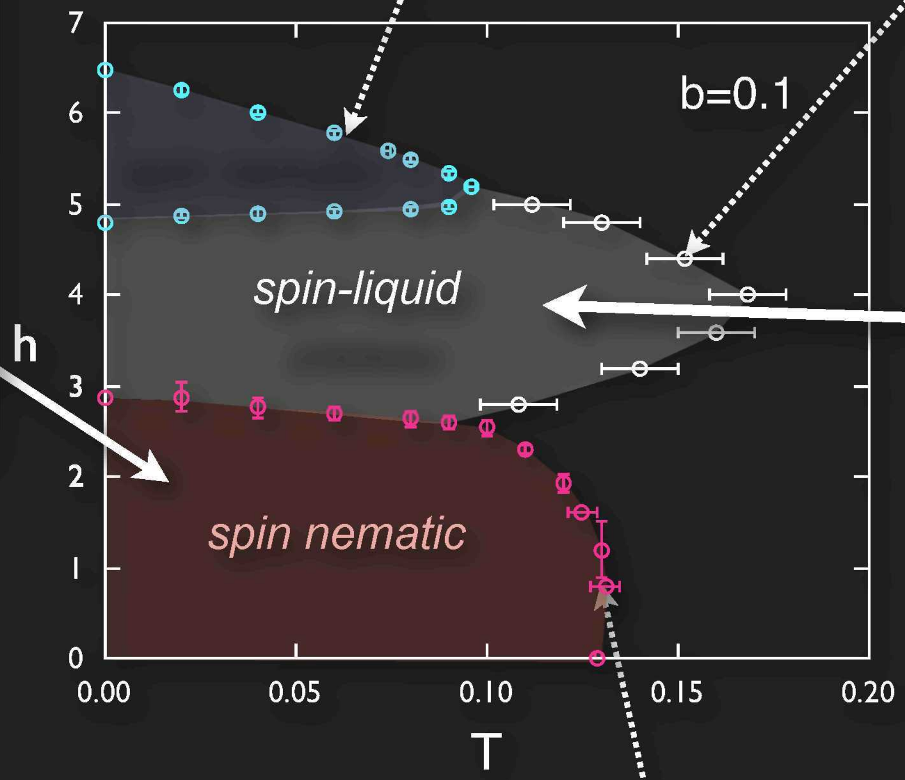
spin nematic order

power law decay of spin correlations

phase transition

T* (crossover)

wide peak in specific heat, but no symmetry breaking

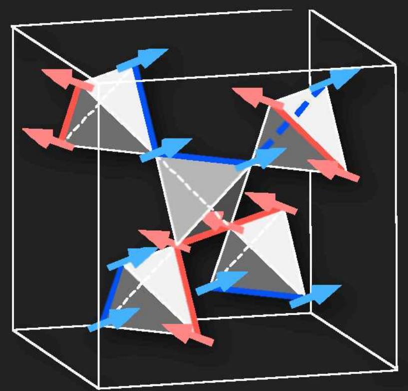


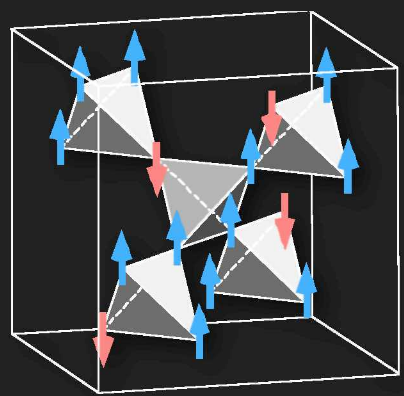
phase transition

3 up : 1 down spin for each tetrahedron

macroscopic degeneracy

magnetization plateau





Motome, Shannon, Penc, unpublished

How about quantum spins ?

Can a quantum spin be without a magnetic moment?

Wave-function of an S=1/2 spin pointing in direction $\hat{\mathbf{\Omega}} = \begin{pmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{pmatrix}$

that is $\langle\hat{\Omega}|S^\alpha|\hat{\Omega}\rangle = S\,\hat{\Omega}_\alpha$ and $\langle\hat{\Omega}|\hat{\Omega}\rangle = 1$:

$$|\hat{\Omega}\rangle = |\vartheta,\varphi\rangle = \cos\frac{\theta}{2}e^{-i\varphi/2}\,|\uparrow\rangle + \sin\frac{\theta}{2}e^{i\varphi/2}\,|\downarrow\rangle$$

2 complex amplitudes

overall phase

4 - 1 -1 = 2 free parameters, corresponding to two spherical angles

normalization

$$(\hat{\Omega}\cdot\mathbf{S})|\hat{\Omega}\rangle = S|\hat{\Omega}\rangle$$

spin coherent state

And how about S=1 ?

Wave-function of an S=1 spin pointing in direction $\hat{\Omega} = \begin{pmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{pmatrix}$

6 - 1 -1 = 4 free parameters,
2 corresponding to two spherical angles, 2 are left

$$|\vartheta,\varphi\rangle = \frac{1+\cos\vartheta}{2}e^{-i\varphi}|1\rangle + \frac{\sin\vartheta}{\sqrt{2}}|0\rangle + \frac{1-\cos\vartheta}{2}e^{i\varphi}|\bar{1}\rangle$$

ϑ	$\vert\vartheta,\varphi=0\rangle$
0	$\vert 1\rangle$
$\pi/3$	$\frac{3}{4}\vert 1\rangle + \frac{\sqrt{6}}{4}\vert 0\rangle + \frac{1}{4}\vert\bar{1}\rangle$
$\pi/2$	$\frac{1}{2}\vert 1\rangle + \frac{1}{2}\vert\bar{1}\rangle$
π	$\vert\bar{1}\rangle$

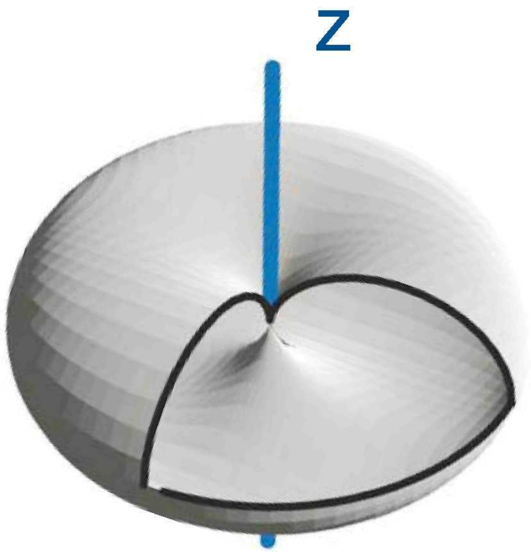
The $|0\rangle$ state is not a spin coherent state (we can't get it by rotating $|1\rangle$)

So where is the spin pointing to in the $|0\rangle$ spin state?

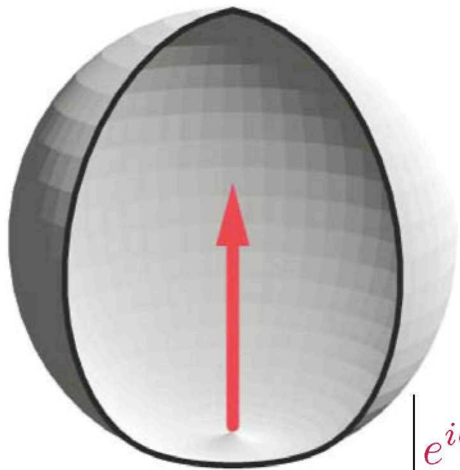
Where does the spin point in the $|S^z\!=\!0\rangle$ state?

$$\hat{\mathbf{1}} = 3\int \frac{\sin\vartheta d\vartheta d\varphi}{4\pi}|\vartheta,\varphi\rangle\langle\vartheta,\varphi| = \frac{2S+1}{4\pi}\int d\hat{\mathbf{\Omega}}|\hat{\mathbf{\Omega}}\rangle\langle\hat{\mathbf{\Omega}}|$$

$$|\vartheta,\varphi\rangle = \frac{1+\cos\vartheta}{2}e^{-i\varphi}|1\rangle + \frac{\sin\vartheta}{\sqrt{2}}|0\rangle + \frac{1-\cos\vartheta}{2}e^{i\varphi}|\bar{1}\rangle$$



$$\left|\frac{\sin\vartheta}{\sqrt{2}}\right|^2$$



$$\left|e^{i\varphi}\frac{1+\cos\vartheta}{2}\right|^2$$

$$|0\rangle = \frac{3}{4\pi}\int d\hat{\mathbf{\Omega}}|\hat{\mathbf{\Omega}}\rangle\frac{\sin\vartheta}{\sqrt{2}}$$

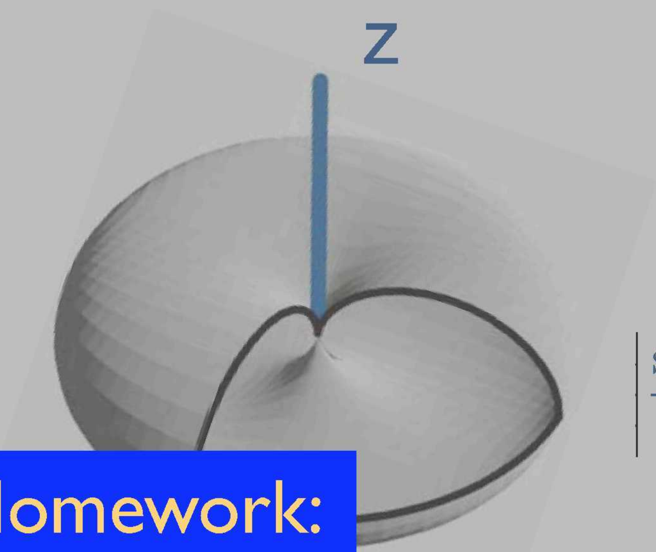
$$|1\rangle = \frac{3}{4\pi}\int d\hat{\mathbf{\Omega}}|\hat{\mathbf{\Omega}}\rangle e^{i\varphi}\frac{1+\cos\vartheta}{2}$$

Where does the spin point in the $|S^z=0\rangle$ state?

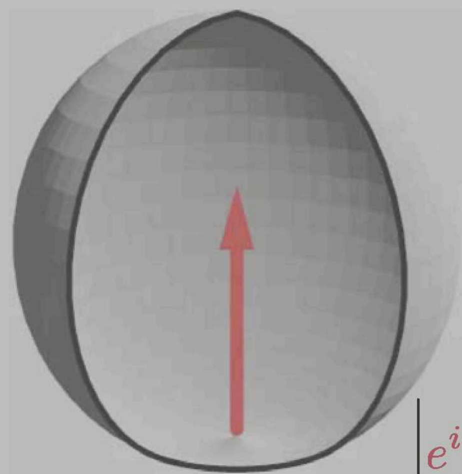
Homework:

$$\hat{\mathbf{1}} = 3\int \frac{\sin\vartheta d\vartheta d\varphi}{4\pi}|\vartheta,\varphi\rangle\langle\vartheta,\varphi| = \frac{2S+1}{4\pi}\int d\hat{\mathbf{\Omega}}|\hat{\mathbf{\Omega}}\rangle\langle\hat{\mathbf{\Omega}}|$$

$$|\vartheta,\varphi\rangle = \frac{1+\cos\vartheta}{2}e^{-i\varphi}|1\rangle + \frac{\sin\vartheta}{\sqrt{2}}|0\rangle + \frac{1-\cos\vartheta}{2}e^{i\varphi}|\bar{1}\rangle$$



$$\left|\frac{\sin\vartheta}{\sqrt{2}}\right|^2$$



$$\left|e^{i\varphi}\frac{1+\cos\vartheta}{2}\right|^2$$

Homework:

$$|0\rangle = \frac{3}{4\pi}\int d\hat{\mathbf{\Omega}}|\hat{\mathbf{\Omega}}\rangle\frac{\sin\vartheta}{\sqrt{2}} \qquad |1\rangle = \frac{3}{4\pi}\int d\hat{\mathbf{\Omega}}|\hat{\mathbf{\Omega}}\rangle e^{i\varphi}\frac{1+\cos\vartheta}{2}$$

Time reversal & quadrupoles

Finite magnetic moment means that the time reversal symmetry is broken.

Time reversal operation for S=1/2:

$$|\uparrow\rangle \longrightarrow |\downarrow\rangle$$
$$|\downarrow\rangle \longrightarrow -|\uparrow\rangle$$

and complex conjugation

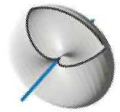
Time reversal operation for S=1:

$$|1\rangle \longrightarrow |\bar{1}\rangle$$
$$|0\rangle \longrightarrow -|0\rangle$$
$$|\bar{1}\rangle \longrightarrow |1\rangle$$

and complex conjugation

Time reversal invariant basis for S=1:

$$|x\rangle = \frac{i}{\sqrt{2}}\left(|1\rangle - |\bar{1}\rangle\right)$$



$$|y\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + |\bar{1}\rangle\right)$$

$$|z\rangle = -i|0\rangle$$

Competing spin and quadrupolar ordering

$$\mathcal{H} = J \sum_{i,j} \left[\cos\vartheta \mathbf{S}_i \mathbf{S}_j + \sin\vartheta \left(\mathbf{S}_i \mathbf{S}_j \right)^2 \right] - h \sum_i S_i^z$$

bilinear-biquadratic Heisenberg model for S=1 spins.

$$\hat{\mathbf{Q}}_i \hat{\mathbf{Q}}_j = 2 \left(\hat{\mathbf{S}}_i \hat{\mathbf{S}}_j \right)^2 + \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j - 8/3$$

Competing spin and quadrupolar ordering

$$\mathcal{H} = J \sum_{i,j} \left[\cos\vartheta \mathbf{S}_i \mathbf{S}_j + \sin\vartheta \left(\mathbf{S}_i \mathbf{S}_j \right)^2 \right] - h \sum_i S_i^z$$

bilinear-biquadratic Heisenberg model for S=1 spins.

Homework: show that for S=1

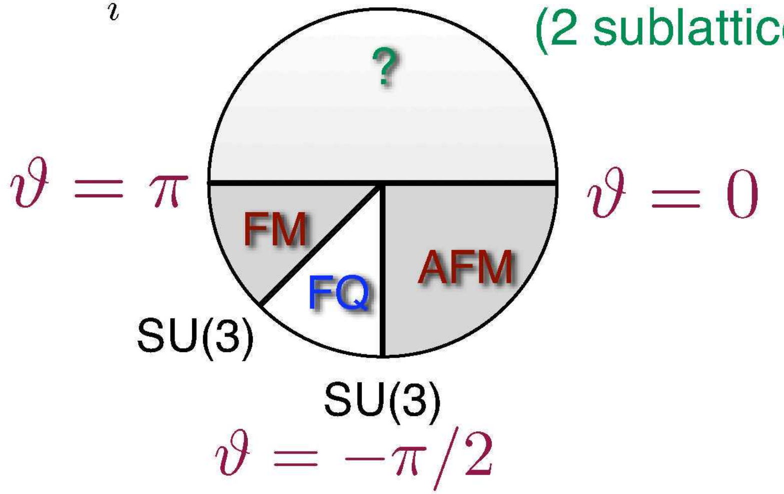
$$\hat{\mathbf{Q}}_i \hat{\mathbf{Q}}_j = 2 \left(\hat{\mathbf{S}}_i \hat{\mathbf{S}}_j \right)^2 + \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j - 8/3$$

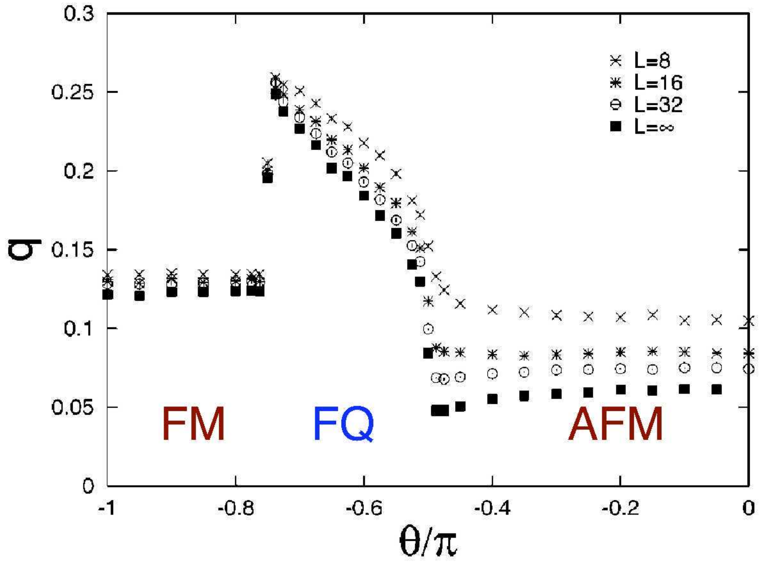
Square and cubic lattice, S=1

$$\mathcal{H} = J \sum_{i,j} \left[\cos\vartheta \mathbf{S}_i \mathbf{S}_j + \sin\vartheta \left(\mathbf{S}_i \mathbf{S}_j\right)^2 \right] - h \sum_i S_i^z$$

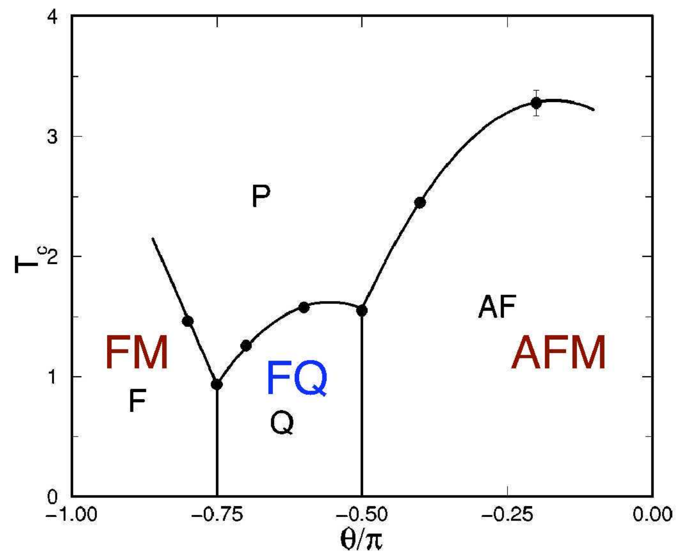
QMC sign problem;
quadrupoles are frustrated
(2 sublattices vs. 3 states)

Quantum Monte-Carlo:
K. Harada and N. Kawashima,
Phys. Rev. B **65**, 052403 (2002)





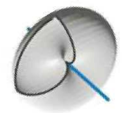
square lattice



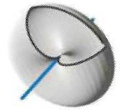
cubic lattice

Mean field treatment of quadrupol states

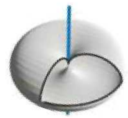
basis: 3 time reversal invariant states



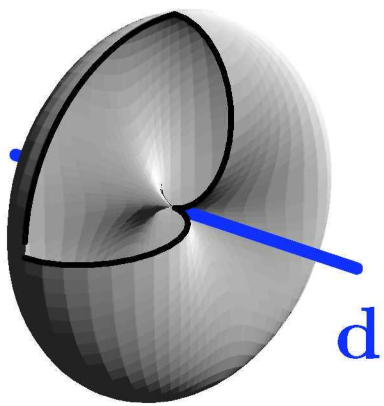
$$|x\rangle = \frac{i}{\sqrt{2}}(|1\rangle - |\bar{1}\rangle)$$



$$|y\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |\bar{1}\rangle)$$



$$|z\rangle = -i|0\rangle$$



$$\mathbf{d} = (d_x, d_y, d_z)$$

$$|\mathbf{d}\rangle = \sum_{\xi=x,y,z} d_\xi |\xi\rangle$$

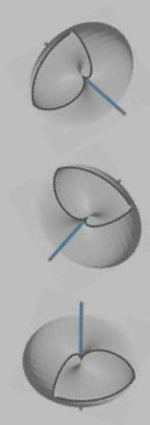
$$\langle \hat{\mathbf{Q}}_i \cdot \hat{\mathbf{Q}}_j \rangle = 2(\mathbf{d}_i \cdot \mathbf{d}_j)^2 - \frac{2}{3}$$

max., if $\mathbf{d}_i \parallel \mathbf{d}_j$

min., ha $\mathbf{d}_i \perp \mathbf{d}_j$

Mean field treatment of quadrupol states

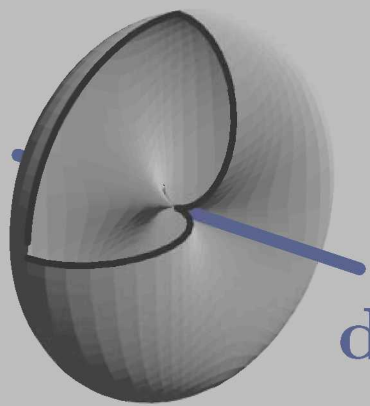
basis: 3 time reversal invariant states



$$|x\rangle = \frac{i}{\sqrt{2}}(|1\rangle - |\bar{1}\rangle)$$

$$|y\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |\bar{1}\rangle)$$

$$|z\rangle = -i|0\rangle$$



$$\mathbf{d} = (d_x, d_y, d_z)$$

$$|\mathbf{d}\rangle = \sum_{\xi=x,y,z} d_\xi |\xi\rangle$$

Homework: show that for the $\Psi = |d_i\rangle|d_j\rangle$ site factorized variational wave function:

$$\langle \hat{\mathbf{Q}}_i \cdot \hat{\mathbf{Q}}_j \rangle = 2(\mathbf{d}_i \cdot \mathbf{d}_j)^2 - \frac{2}{3}$$

max., if $\mathbf{d}_i \parallel \mathbf{d}_j$

min., ha $\mathbf{d}_i \perp \mathbf{d}_j$

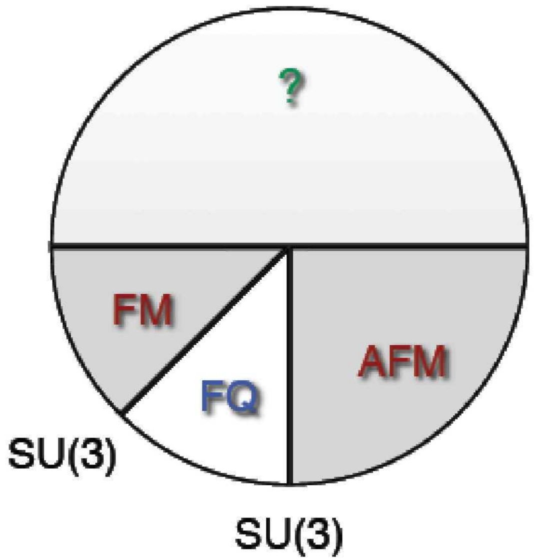
Mean field treatment of quadrupol states

$$\langle \hat{\mathbf{Q}}_i \cdot \hat{\mathbf{Q}}_j \rangle = 2(\mathbf{d}_i \cdot \mathbf{d}_j)^2 - \frac{2}{3}$$

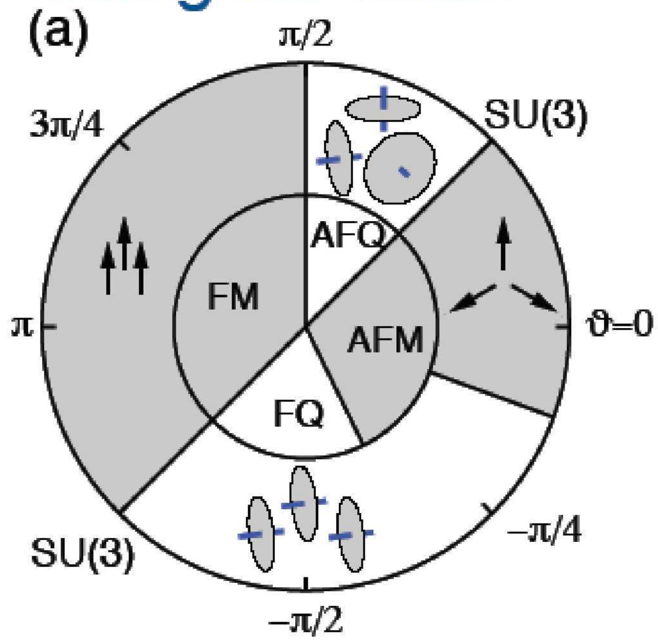
max., if $\mathbf{d_i} \parallel \mathbf{d_j}$

min., ha $\mathbf{d_i} \perp \mathbf{d_j}$

square lattice



triangular lattice

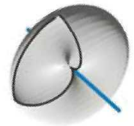


Tsunetsugu & Arikawa, J. Phys. Soc. Jpn. 75, 083701 (2006)

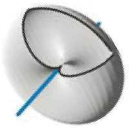
Läuchli, Mila & Penc, Phys. Rev. Lett. 97, 087205 (2006)

Bhattacharjee, Shenoy &Senthil ,Phys. Rev. B 74, 092406 (2006).

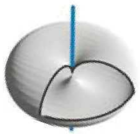
SU(3) flavour-wave theory



$$|x\rangle = \frac{i}{\sqrt{2}}(|1\rangle - |\bar{1}\rangle)$$



$$|y\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |\bar{1}\rangle)$$



$$|z\rangle = -i|0\rangle$$

Starting from these states, we introduce the corresponding Schwinger bosons

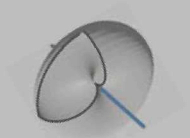
Spin operators:

$$S^x(j) = ia_z^\dagger(j)a_y(j) - ia_y^\dagger(j)a_z(j)$$

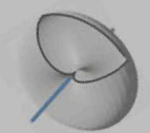
$$S^y(j) = ia_x^\dagger(j)a_z(j) - ia_z^\dagger(j)a_x(j)$$

$$S^z(j) = ia_y^\dagger(j)a_x(j) - ia_x^\dagger(j)a_y(j)$$

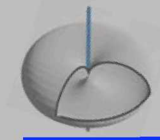
SU(3) flavour-wave theory



$$|x\rangle = \frac{i}{\sqrt{2}}\left(|1\rangle - |\bar{1}\rangle\right)$$



$$|y\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + |\bar{1}\rangle\right)$$



$$|z\rangle = -i|0\rangle$$

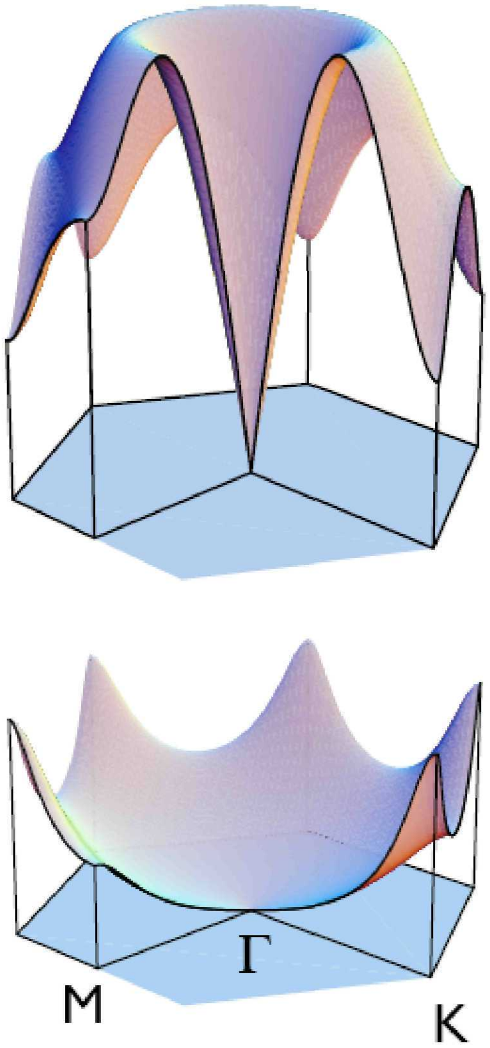
Starting from these states, we introduce the corresponding Schwinger bosons

Homework: derive the expressions below

Spin operators:

$$\begin{aligned} S^x(j) &= i a_z^\dagger(j) a_y(j) - i a_y^\dagger(j) a_z(j) \\ S^y(j) &= i a_x^\dagger(j) a_z(j) - i a_z^\dagger(j) a_x(j) \\ S^z(j) &= i a_y^\dagger(j) a_x(j) - i a_x^\dagger(j) a_y(j) \end{aligned}$$

SU(3) flavour-waves in ferroquadrupolar phase



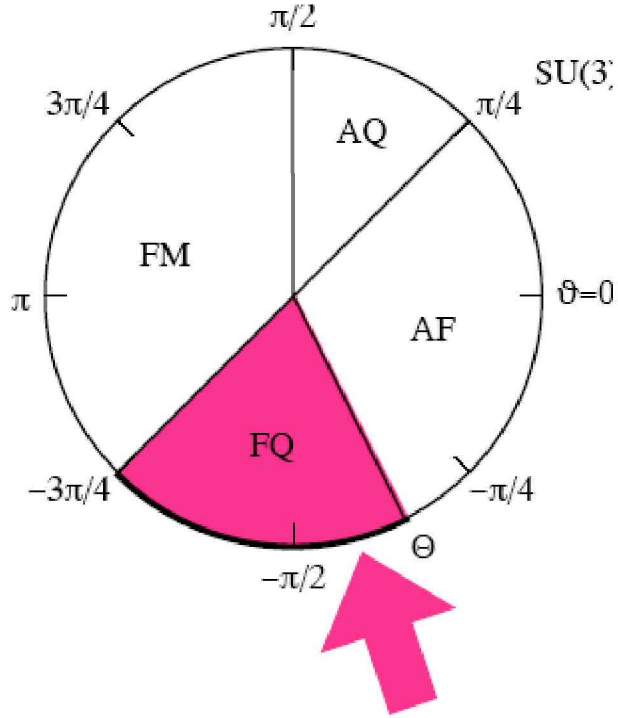
b=-2.5

dispersion

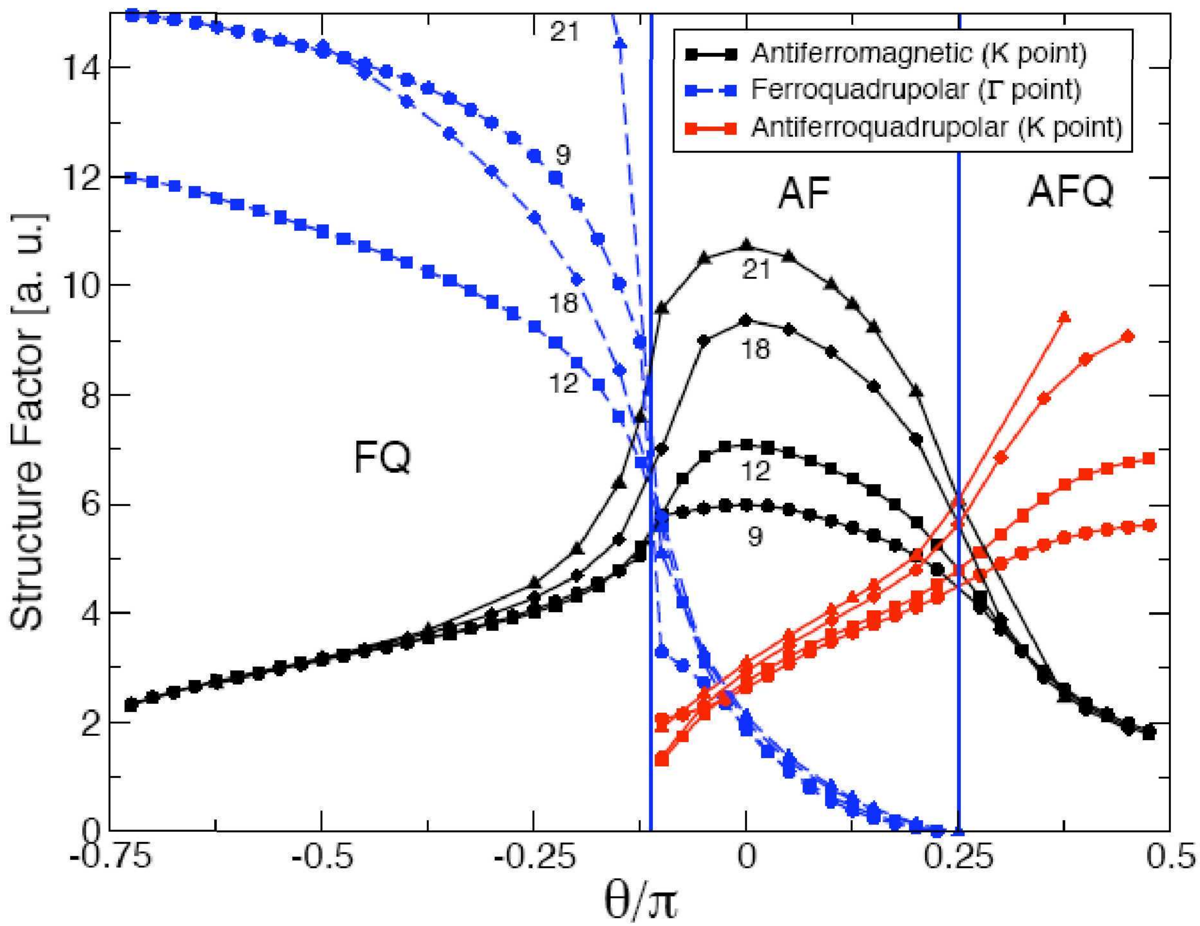
$\omega(q)$

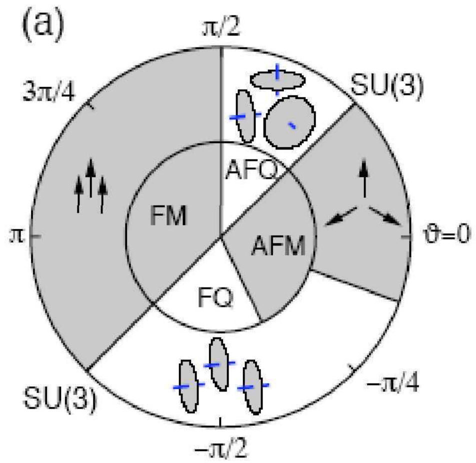
$S(q)$

non-diverging
spin-structure factor



ED of the triangular lattice

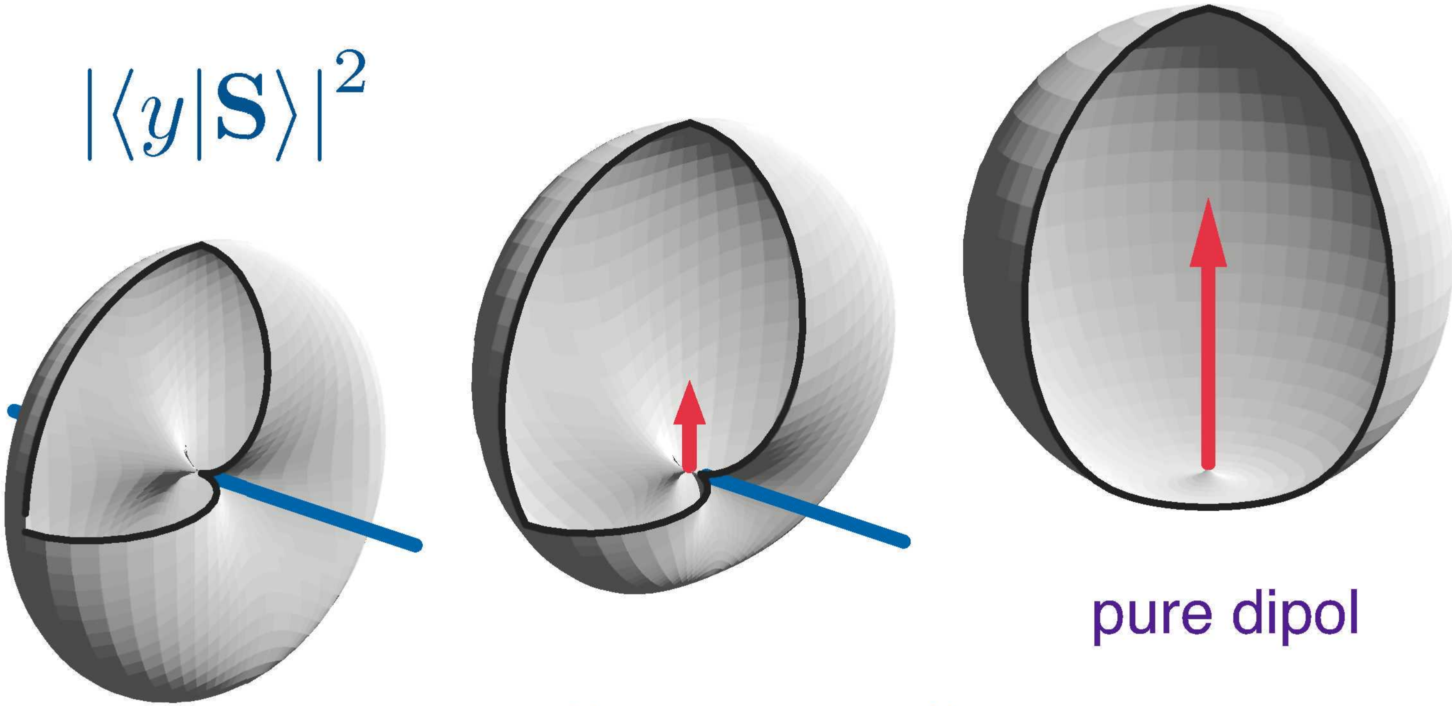




Deformation of a quadrupol in magnetic field

$|\langle 1|\mathbf{S}\rangle|^2$

$|\langle y|\mathbf{S}\rangle|^2$



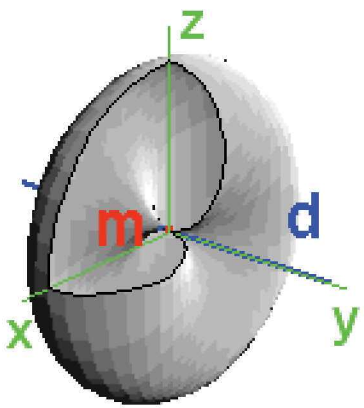
pure dipol

pure quadrupol

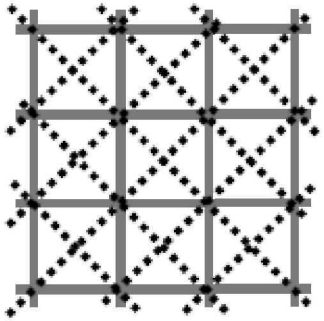
$$\cos\frac{\mu}{2}|y\rangle - i\sin\frac{\mu}{2}|x\rangle$$

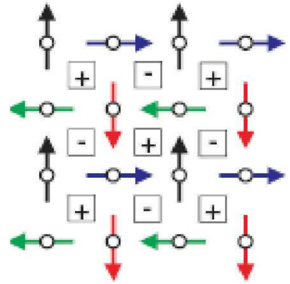
$$\langle S^z\rangle = \sin\mu$$

Deformation of a quadrupol in magnetic field - movie



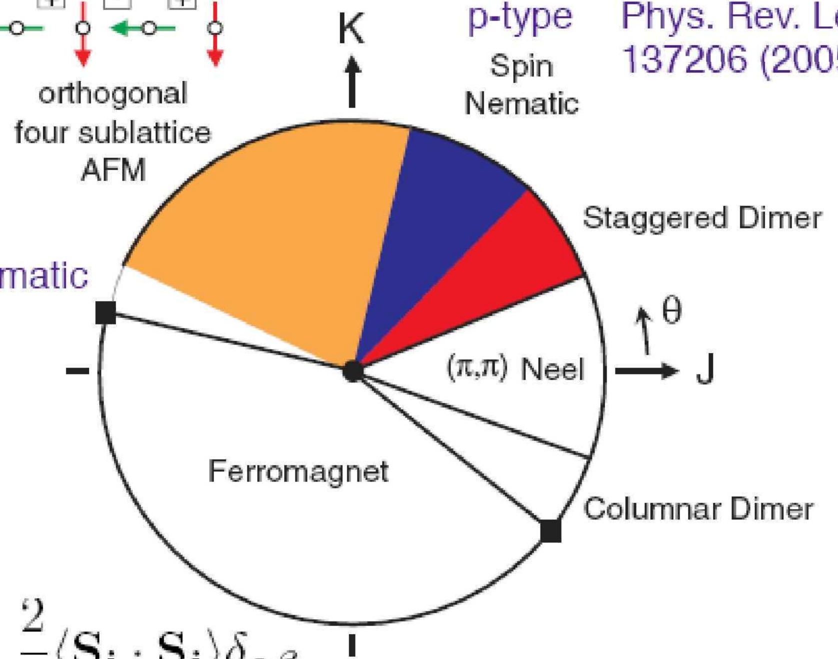
J1-J2 model with ring exchange K





$$V_{i,j} = \mathbf{S}_i \times \mathbf{S}_j$$

A. Lauchli et al.,
Phys. Rev. Lett. **95**, 137206 (2005)



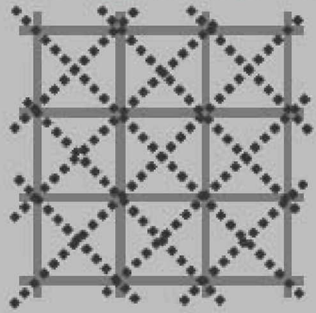
p-type spin nematic

N. Shannon et al.
Phys. Rev. Lett. **96**, 027213 (2006

$$Q_{i,j}^{\alpha\beta} = S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha - \frac{2}{3}\langle \mathbf{S_i} \cdot \mathbf{S_j} \rangle \delta_{\alpha\beta}$$

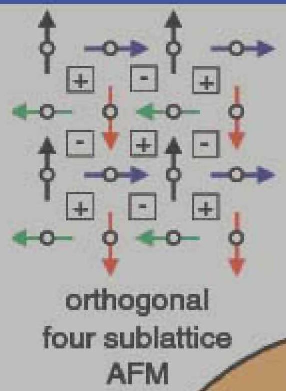
Ne

J1-J2 model with ri

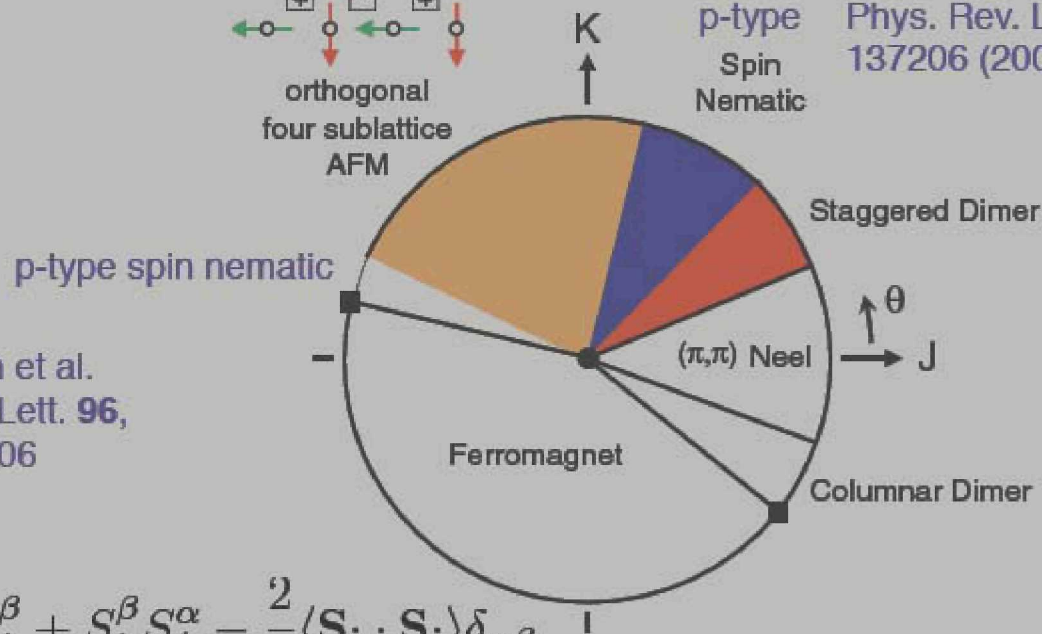


Homework: In analogy with the n-type (quadrupole) nematics, find the states that span the p-type nematic order.

$$V_{i,j} = \mathbf{S}_i \times \mathbf{S}_j$$



A. Lauchli et al., Phys. Rev. Lett. **95**, 137206 (2005)



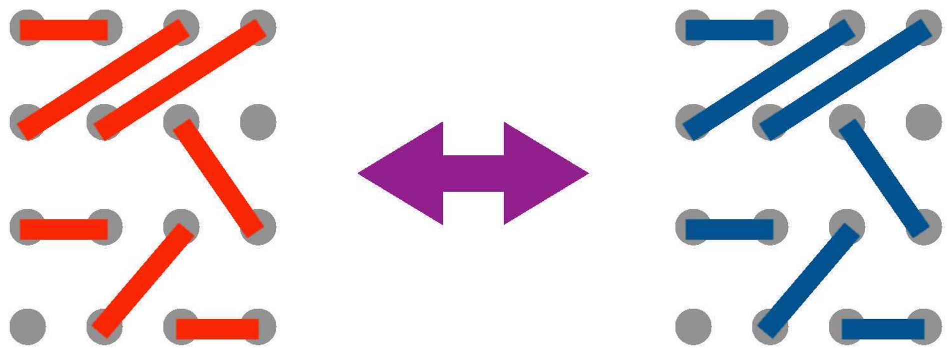
N. Shannon et al. Phys. Rev. Lett. **96**, 027213 (2006

$$Q_{i,j}^{\alpha\beta} = S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha - \frac{2}{3}\langle \mathbf{S_i} \cdot \mathbf{S_j} \rangle \delta_{\alpha\beta}$$

Quantum-entanglement, S=1/2

lattice made out of S=1/2 spins: the $|0\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$

and $|s\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$ singlet-bond states are both entangled



RVB spin-liquid

spin nematic

Mean field theory ?

Excitations

Additional homework

Calculate the energies of the S=1 bilinear-biquadratic model on a 2-site bond and on a 3-site triangle.

Show that the sum of the quadrupol- and spin-exchange permutes the two S=1 spins (up to a constant), i.e.

$$\hat{\mathbf{Q}}_i \hat{\mathbf{Q}}_j + \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j = -2\mathcal{P}_{i,j} - \frac{2}{3}$$

The End