1. Orbital models
2. Charge order, SDW and multiferroicity

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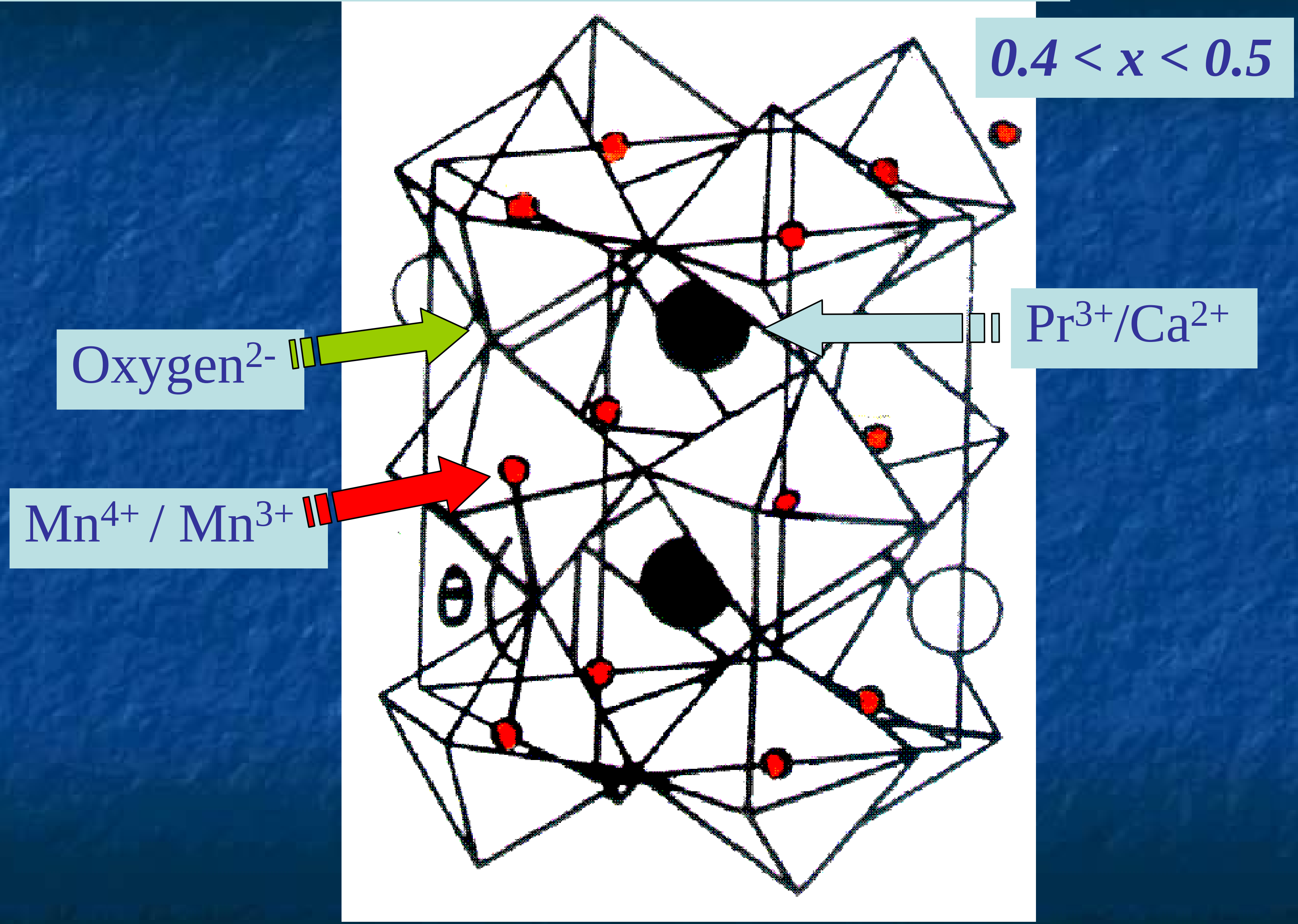
Santa Barbara 9/11/2007

1.

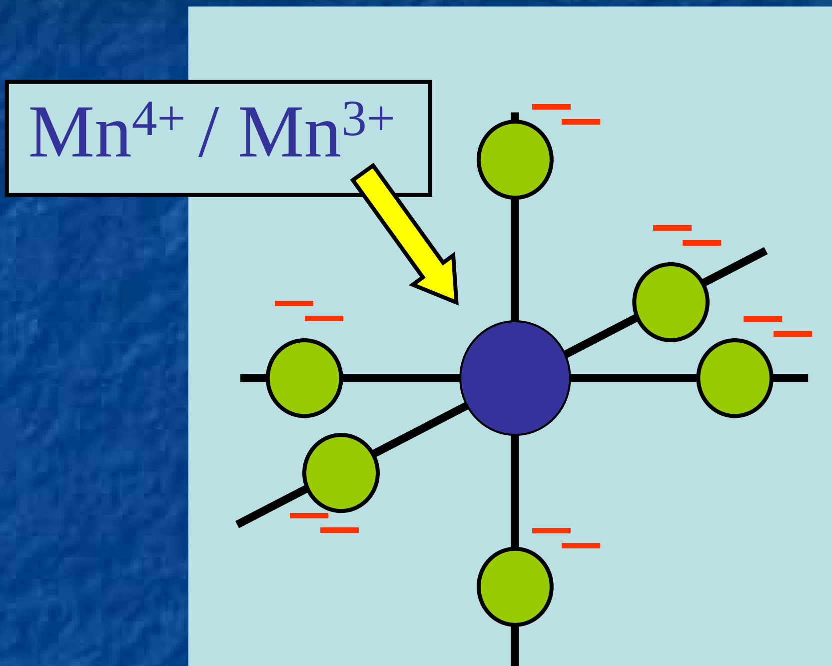
Order and disorder in orbital compass models

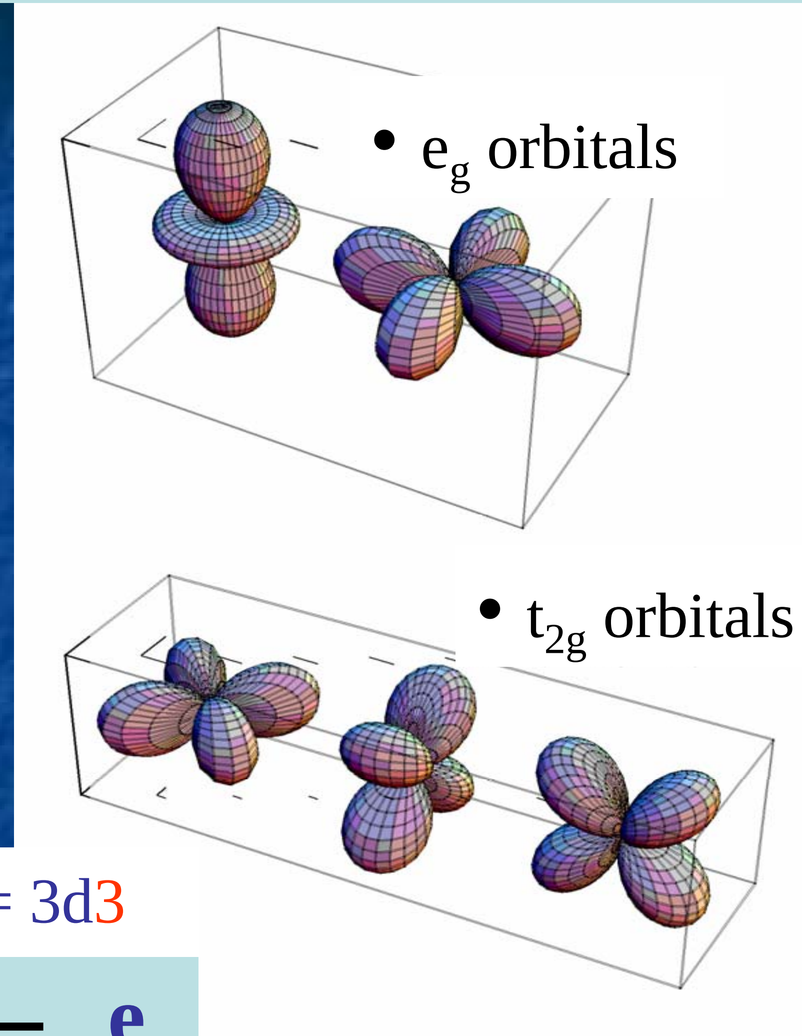
Perovskite crystal structure of $Pr_{1-x}Ca_xMnO_3$



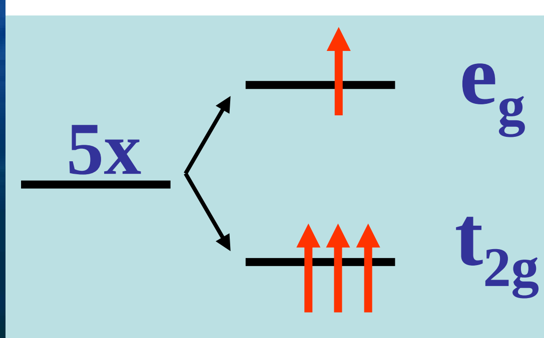
Local considerations

Cubic Crystal field splitting

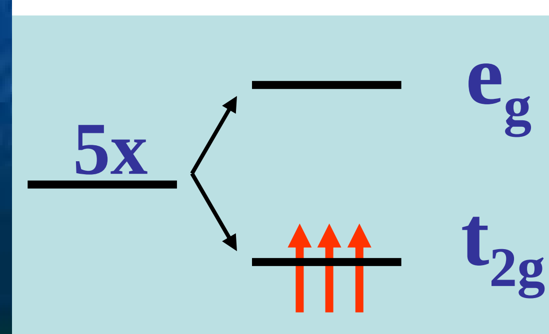




Mn (3+) = 3d4

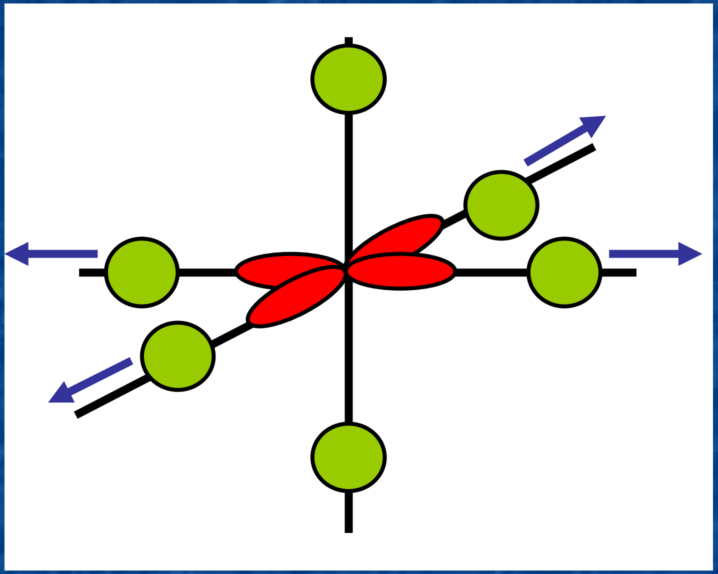


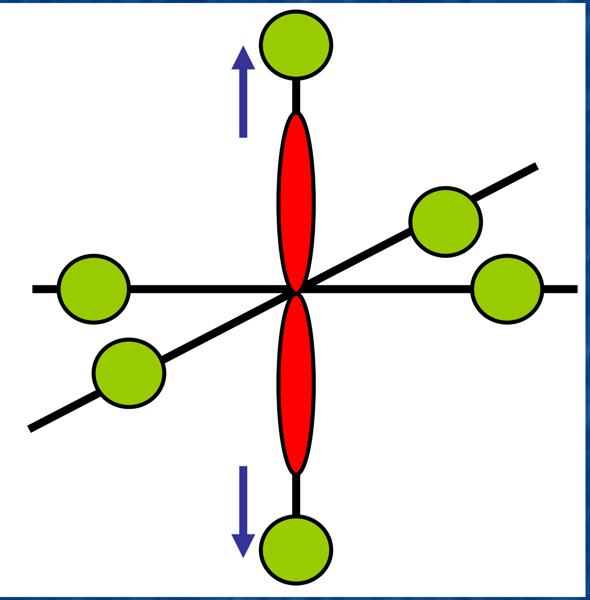
Mn (4+) = 3d3

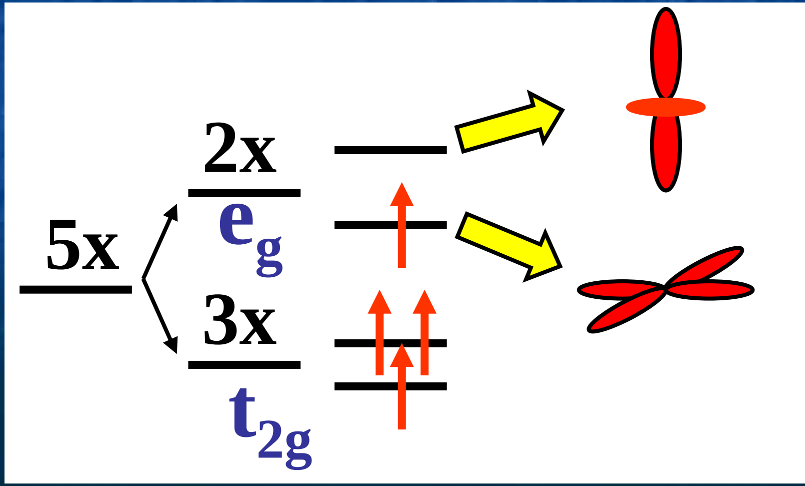


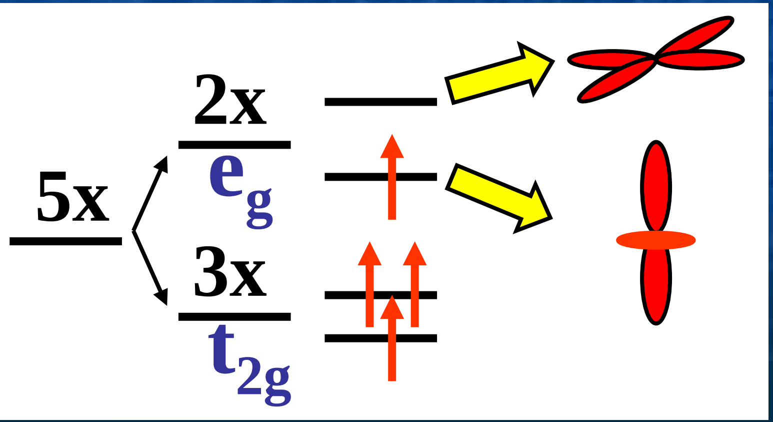
Lifting of degeneracy: lattice

Crystal field splitting of e_g levels → Jahn-Teller distortion





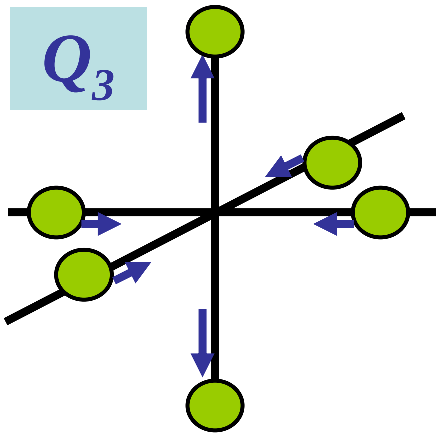


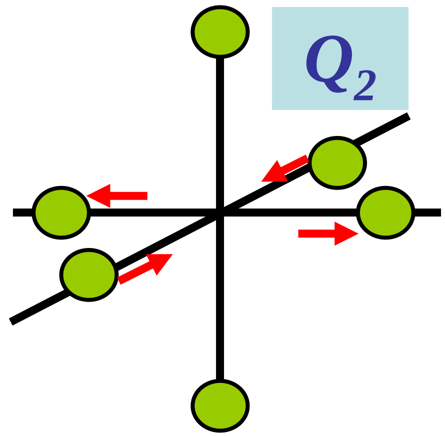


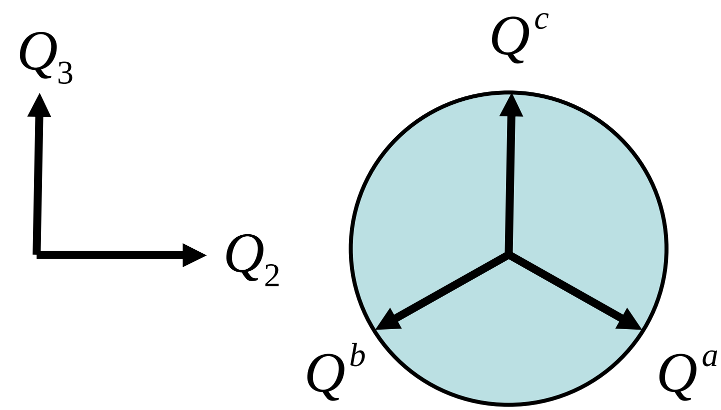
Local e_g Jahn-Teller distortions

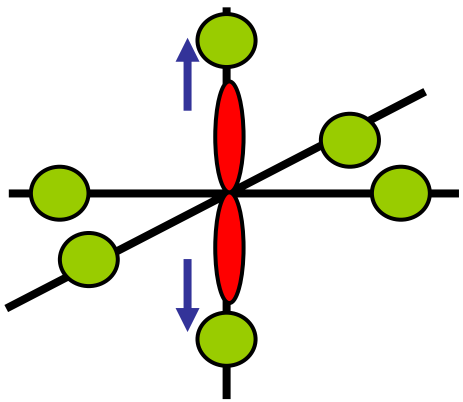
$$\vec{Q} = \begin{bmatrix} Q_2 \\ Q_3 \end{bmatrix} = Q \begin{bmatrix} \sin\varphi \\ \cos\varphi \end{bmatrix}$$

$$|Q_2|^2 + |Q_3|^2 = |\vec{Q}|^2 = const$$

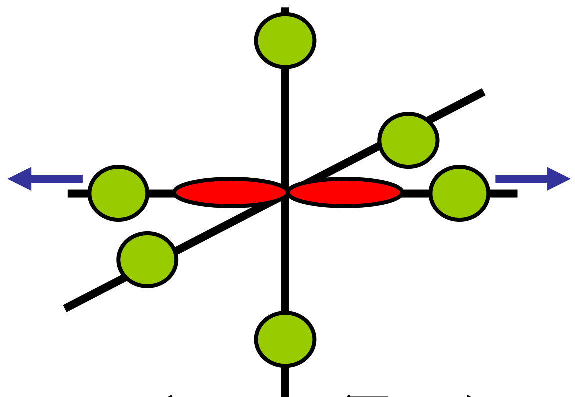




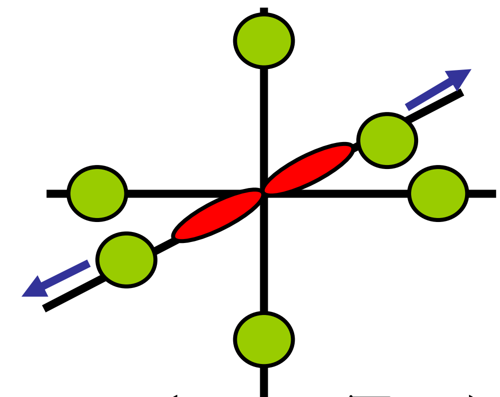




$$Q^c = Q_3$$



$$Q^b = \left(Q_3 + \sqrt{3}Q_2\right)/2$$



$$Q^a = \left(Q_3 - \sqrt{3}Q_2\right)/2$$

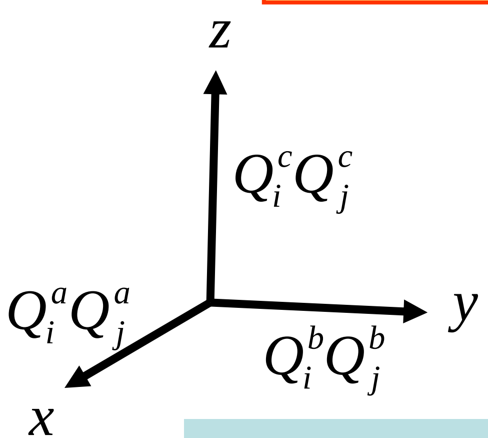
Interaction between Jahn-Teller centers

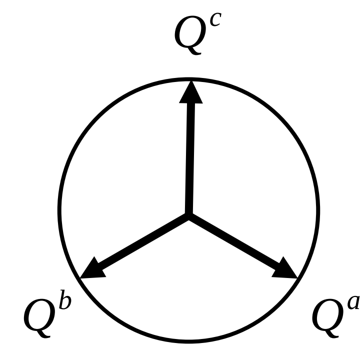
Ordering?

$$H_{JT} = \sum_i Q_i^a Q_{i+x}^a + Q_i^b Q_{i+y}^b + Q_i^c Q_{i+z}^c$$
$$= \tfrac{1}{2} \sum_{i,\alpha} (Q_i^\alpha - Q_{i+\alpha}^\alpha)^2 + const$$

120º model: a,b,c

vectors on unit disk





Hints for disorder:

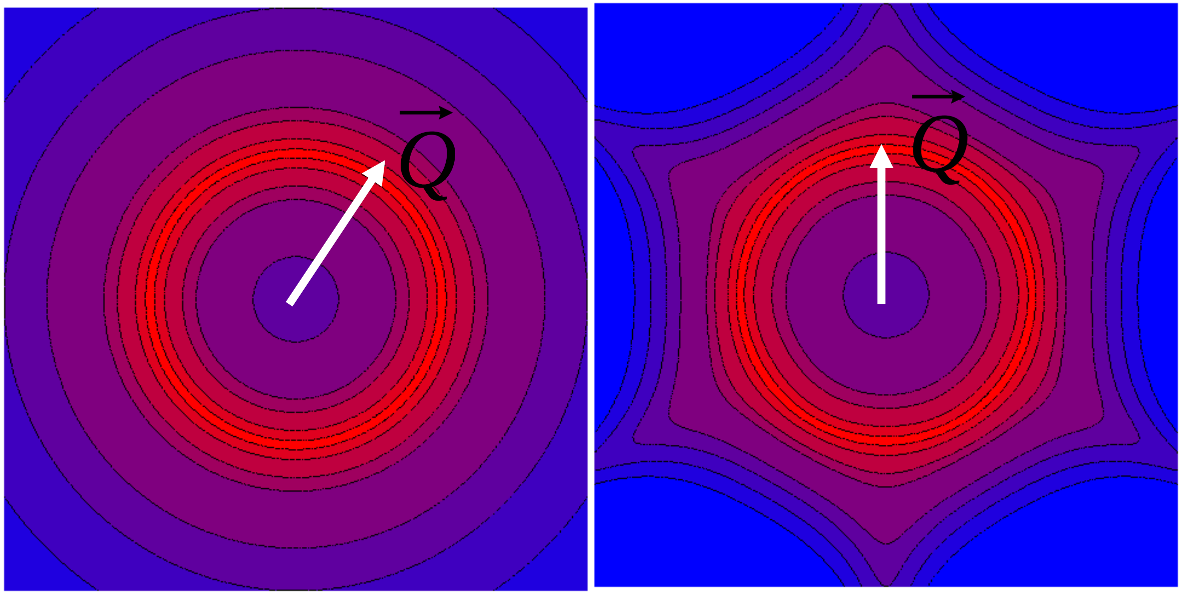
-- infinite degeneracy: any constant field is a groundstate

-- in 120º model Gaussian fluctuations are two dimensional

Nussinov, Biskup, Chayes, JvdB,
Europhys. Lett. 67, 990 (2004)

Order by disorder: contour plot of free energy (AI)

$$\vec{Q} = \begin{bmatrix} Q_2 \\ Q_3 \end{bmatrix} = Q \begin{bmatrix} \sin\varphi \\ \cos\varphi \end{bmatrix}$$



Rotational invariant system

120º model

-- excited states break rotational invariance

-- symmetry breaking + ordering at finite T because of finite T

Nussinov, Biskup, Chayes, JvdB, Europhys. Lett. 67, 990 (2004)

Orbital only part of Kugel-Khomskii Hamiltonian:

$$H_{ORB} = \sum_i Q_i^a Q_{i+x}^a + Q_i^b Q_{i+y}^b + Q_i^c Q_{i+z}^c$$

super-exchange of fermions in e_g orbitals on cubic lattice

$$Q^c = T^z$$
$$Q^b = \left(T^z + \sqrt{3}T^x\right)/2$$
$$Q^a = \left(T^z - \sqrt{3}T^x\right)/2$$

$$\left[T^\alpha, T^\beta\right] = \varepsilon_{\alpha\beta\gamma} T^\gamma$$

"spin" 1/2 operators

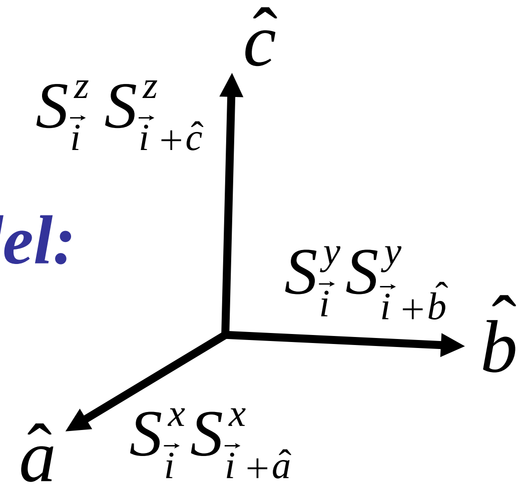
quantum *order from disorder*

JvdB, Mack, Horsch, Oles, Phys. Rev. B. 59, 6795 (1999)

Ken Kubo, JPSJ 71 1308 (2002)

Related orbital model

90º compass model:



$$H^{3D}_{compass} = \sum_{\vec{i}} S^x_{\vec{i}} S^x_{\vec{i}+\hat{a}} + S^y_{\vec{i}} S^y_{\vec{i}+\hat{b}} + S^z_{\vec{i}} S^z_{\vec{i}+\hat{c}}$$

$$H^{2D}_{compass} = \sum_{\vec{i}} S^x_{\vec{i}} S^x_{\vec{i}+\hat{a}} + S^y_{\vec{i}} S^y_{\vec{i}+\hat{b}}$$

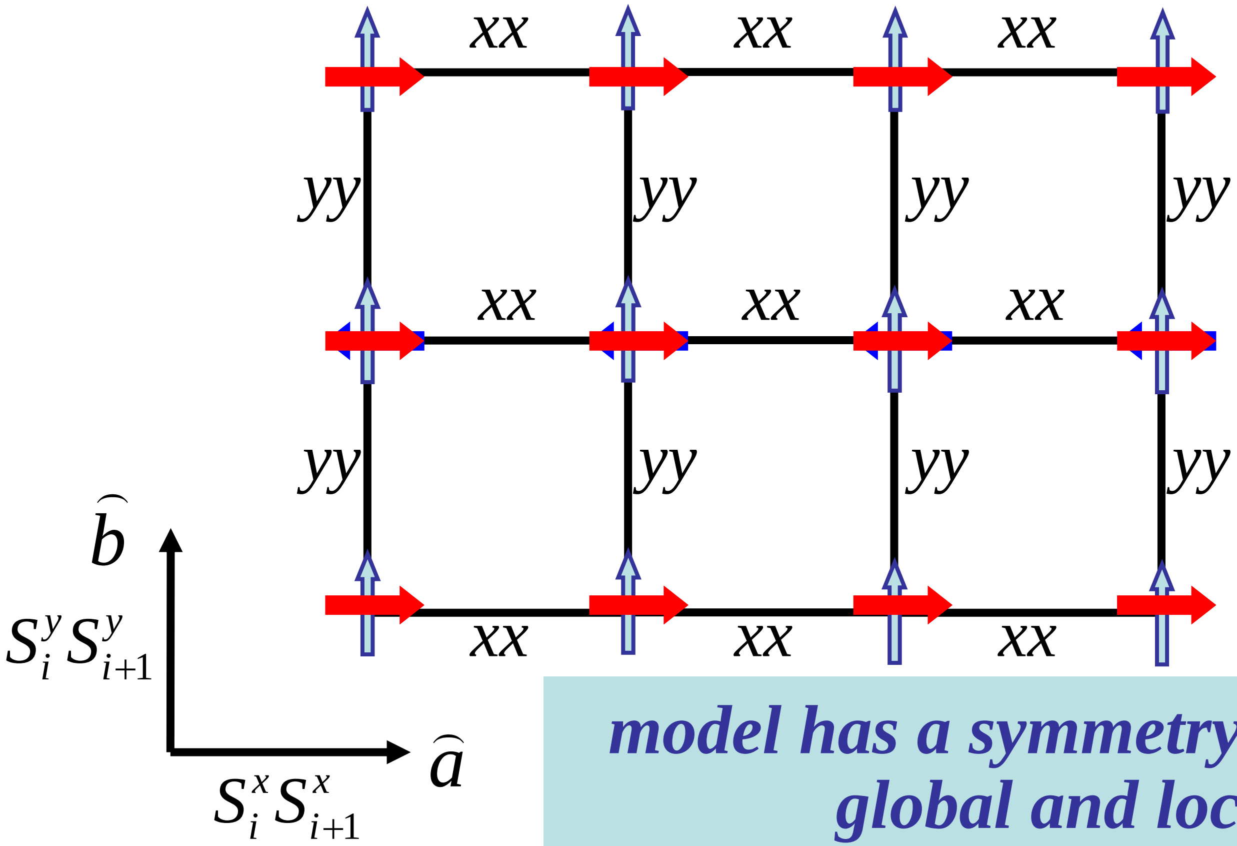
Kugel-Khomskii, Sov. Phys. JETP 37725 (1973)
Nussinov, Biskup, Chayes, JvdB, Europhys. Lett. 67, 990 (2004)
JvdB, NJP 6, 201 (2004)
Mishra, Ma, Zhang, PRL 93, 207201 (2004)

Mishra, Ma, Zhang, PRL 93, 207201 (2004)
Nussinov, Fradkin, PRB 71, 195120 (2005)
Doucot, Feigel'man,PRB 71 024505 (2005)
Dorier, Becca, Mila, PRB 72, 024448 (2005)
Tanaka, Ishihara PRL, 98 256402 (2007)

Groundstate degeneracy of classical/quantum compass model

$$H^{2D}_{compass} = -\sum_{\vec{i}} S^x_{\vec{i}} S^x_{\vec{i}+\hat{a}} + S^y_{\vec{i}} S^y_{\vec{i}+\hat{b}}$$

on a N by N lattice



$\sim 2^N$ degeneracy

model has a symmetry that is in between global and local (gauge)

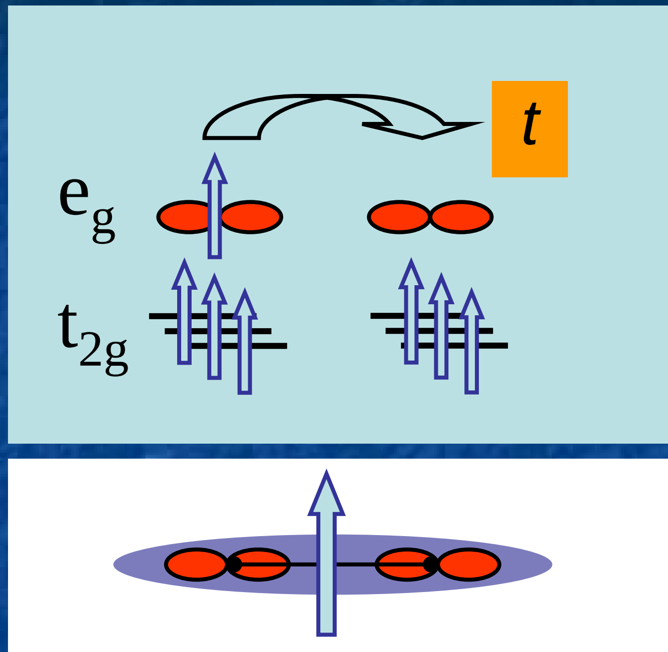
and nematic order parameter

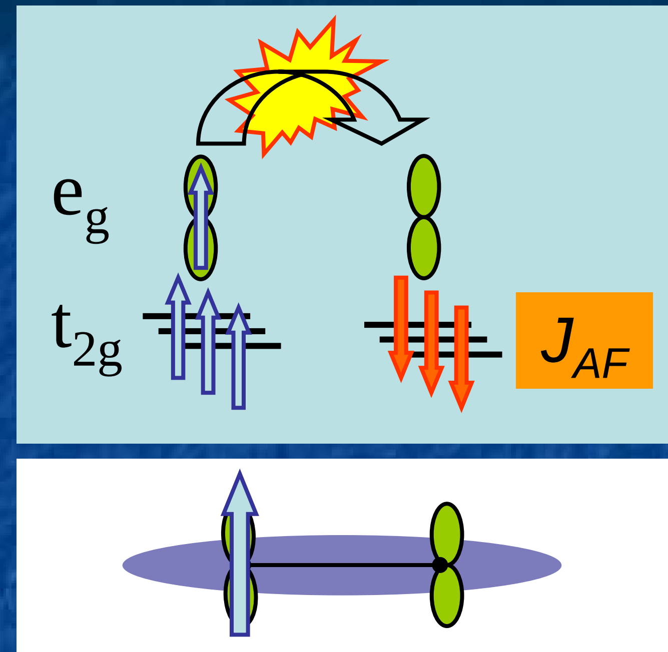
Zohar Nussinov and JvdB

2.

Multiferroicity by
Charge and orbital order
Dislocated Spin Density Waves

Mn-Mn dimer: Interplay orbital, spin and charge



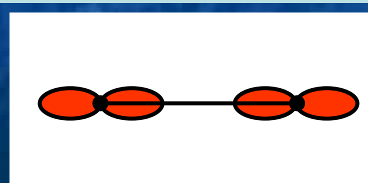


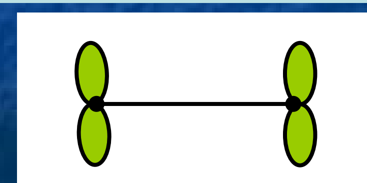
Bond center

Site center

Ferro

Antiferro





Formally: DDEX model

JvdB, Khomskii, PRL 82, 1016 (1999)

DDEX model

$$H_{DDEX} = \Sigma_{<ij>} t_{ij} \Gamma_{ij}^{\alpha\beta} c_{i\alpha}^{+} c_{j\beta} + J \Sigma_{<ij>} \vec{S}_i \cdot \vec{S}_j ,$$

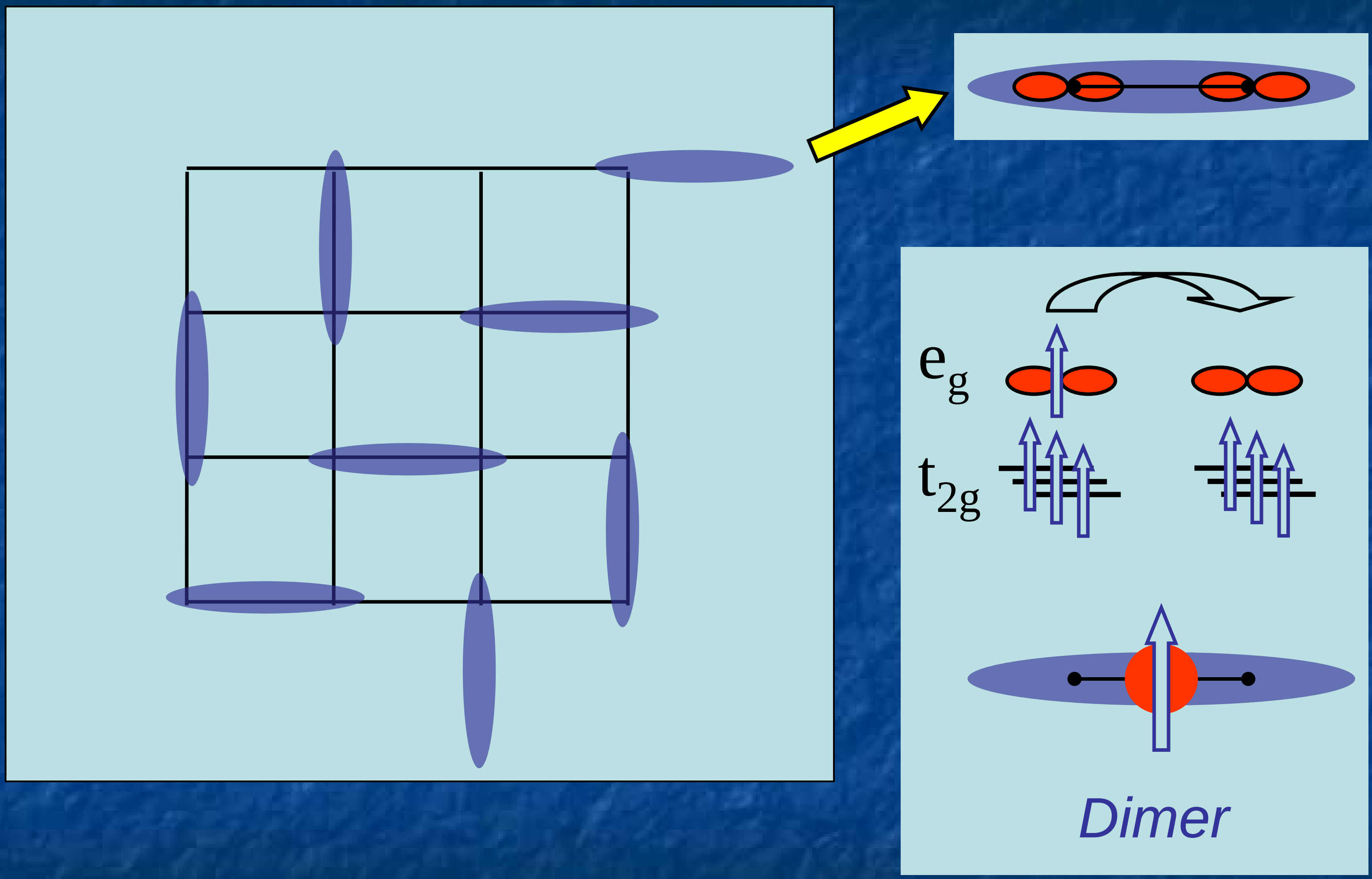
$$\Gamma_{\langle ij \rangle // z}^{z^2, z^2} = 1, \Gamma_{\langle ij \rangle // x}^{z^2, z^2} = \tfrac{1}{4}$$

$$\Gamma_{\langle ij \rangle // x}^{x^2-y^2, x^2-y^2} = \tfrac{3}{4}.$$

$$J \vec{S}_i \cdot \vec{S}_j = J \cos \theta_{ij}$$

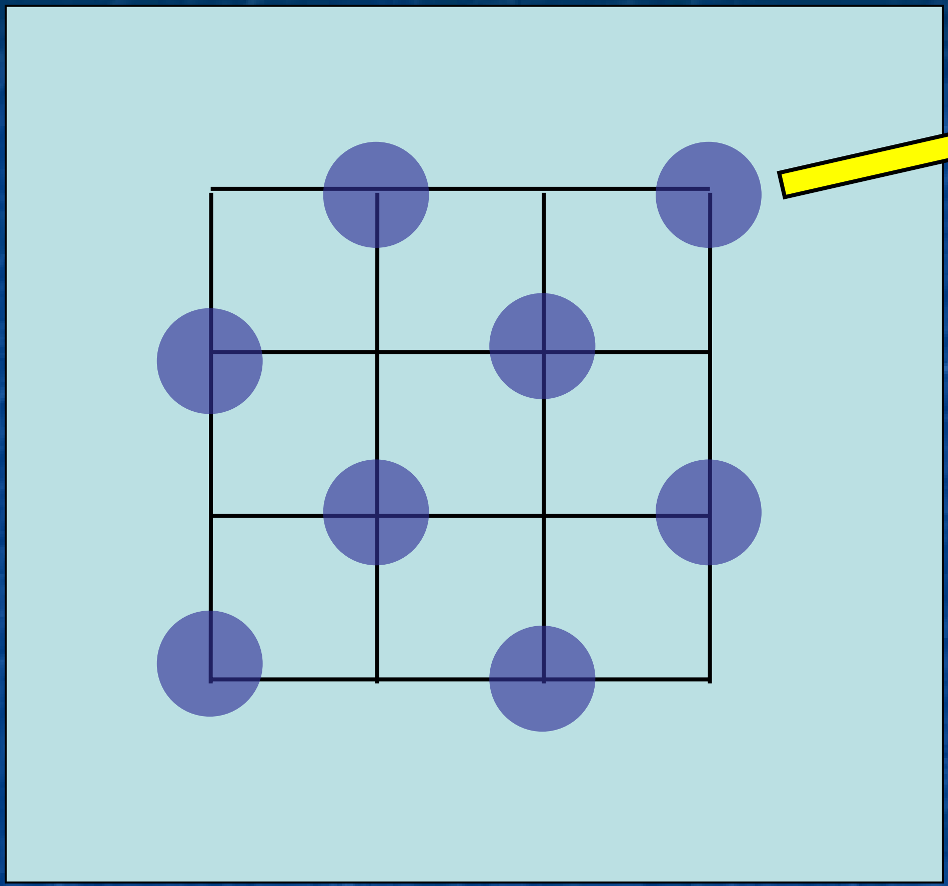
$$t_{ij} = t \cos \theta_{ij} / 2$$

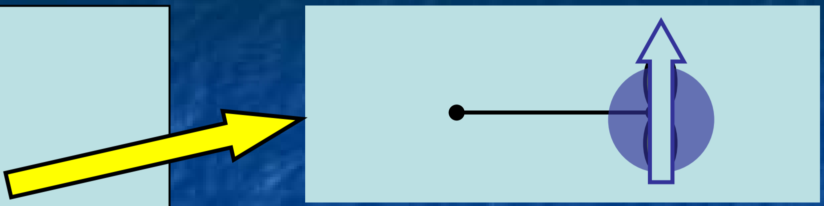
Near x=0.4 : Bond-centered charge ordering



A.Daoud-Aladine et al., PRL 89 97205 (2002)

Near x=0.5: Site-centered charge ordering





E.O. Wollan and W.C. Koeler, Phys. Rev. 100, 545 (1955)

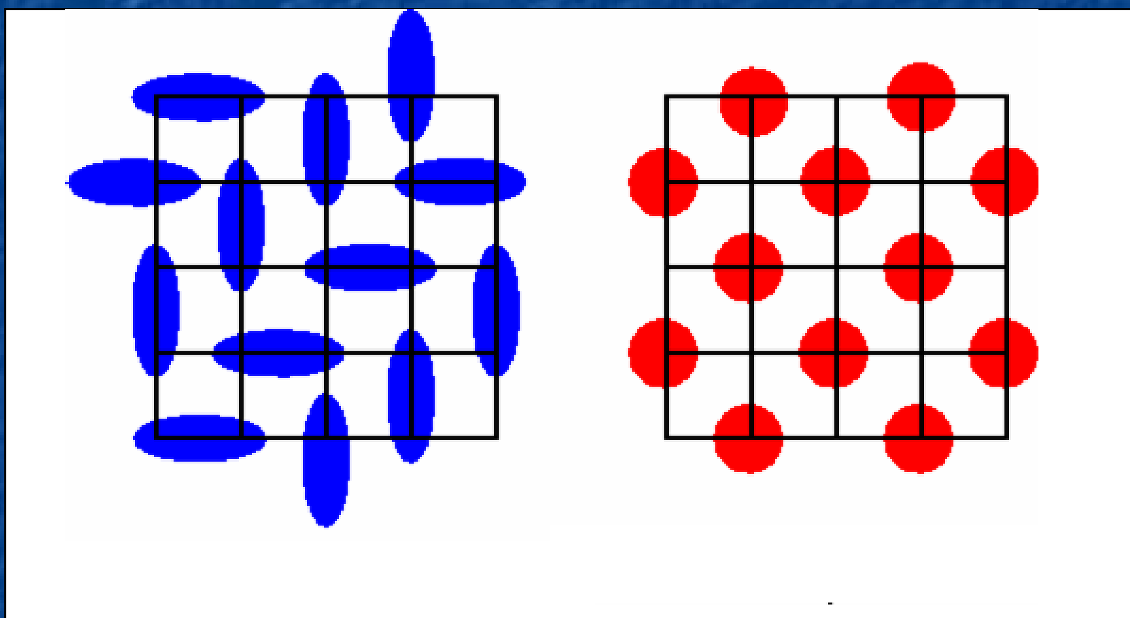
Ferroelectric?

x=0.4

Bond centered CO

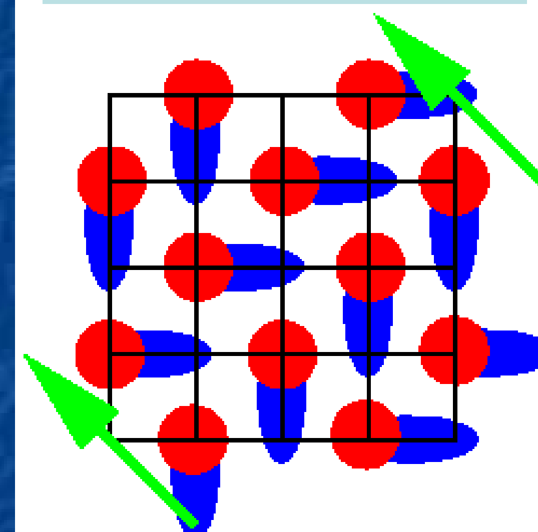
x=0.5

Site centered CO



0.4 < x < 0.5

intermediate



Ferro-electric groundstate

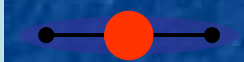
It is allowed by symmetry: Can happen → Will happen

Continous transition from

Site centered CO

to

Bond centered CO



"In between" centered CO

Breaking of inversion symmetry in the intermediate phase

→ *Ferro-electricity* *Magnetism*

Dima Efremov, JvdB, Daniel Khomskii, Nature Mat. (2004)

Magneto-electric coupling: Ginzburg-Landau

Electric polarization $\vec{P}(\vec{r})$

Magnetization $\vec{M}(\vec{r})$

couple these two orderparameters

Free energy must be invariant for:

time reversal

$$t \rightarrow -t$$

$$\vec{M} \rightarrow -\vec{M}$$

$$\vec{P} \rightarrow \vec{P}$$

spatial inversion

$$\vec{r} \rightarrow -\vec{r}$$

$$\vec{P} \rightarrow -\vec{P}$$

$$\vec{M} \rightarrow \vec{M}$$

$$\vec{\nabla} \rightarrow -\vec{\nabla}$$

Magneto-electric coupling: Ginzburg-Landau

To build an invariant we need

$$\vec{P},\ \vec{\nabla},\ \vec{M},\ \vec{M}$$

$$F_{ME}(\vec{r}) = \vec{P} \cdot \left[\gamma\, \vec{\nabla}(\vec{M}^2) + \gamma' \left(\vec{M}(\vec{\nabla} \cdot \vec{M}) - (\vec{M} \cdot \vec{\nabla})\vec{M} \right) + \ldots \right]$$

We are interested in ferroelectrics: uniform electric polarization so that

$$\vec{P}(\vec{r}) = \vec{p}_0$$

which implies that:

$$\int_V d\vec{r}^{\,3}\, \vec{P} \cdot \vec{\nabla}(\vec{M}^2) = \vec{p}_0 \cdot \int_V d\vec{r}^{\,3}\, \vec{\nabla}(\vec{M}^2) \propto \vec{M}^2 \Big|_{surface}$$

However

$$F_{ME}(\vec{r}) = \vec{P} \cdot \left[\gamma \, \vec{\nabla}(\vec{M}^2) \right]$$

becomes active if SDW dislocated

$$M = M_0 \cos(q_m x + \phi)$$

magnetization is shifted with respect to the lattice (but inversion invariant)

Betouras, Giovannetti, JvdB, PRL 98, 257601 (2007)

Minimize Free Energy

$$F_{ME}(\vec{r}) = \vec{P} \cdot \left[\gamma \vec{\nabla}(\vec{M}^2)\right]$$

$$F_E(\vec{r}) = \frac{\vec{P}(\vec{r})^2}{2\chi_E(\vec{r})}$$

$$M = M_0 \cos(q_m x + \phi)$$

$$\chi_E^{-1} = e_0 + e_1 \cos(qx)$$

with Ansatz for polarization

$$P = p_0 + p_1 \cos(qx)$$

gives finite p_0 and p_1

only when $q_m = q/2$

$$p_0 = \frac{-\gamma q_m M_0^2}{2} \frac{e_1}{2e_0^2 - e_1^2} \sin 2\phi$$

$$p_1 = -2e_0 p_0 / e_1$$

because

$$\int_V d\vec{r}^{\,3} \vec{P}(\vec{r}) \cdot \vec{\nabla}(\vec{M}^2) \propto V$$

polarization and magnetization TOGETHER break inversion invariance

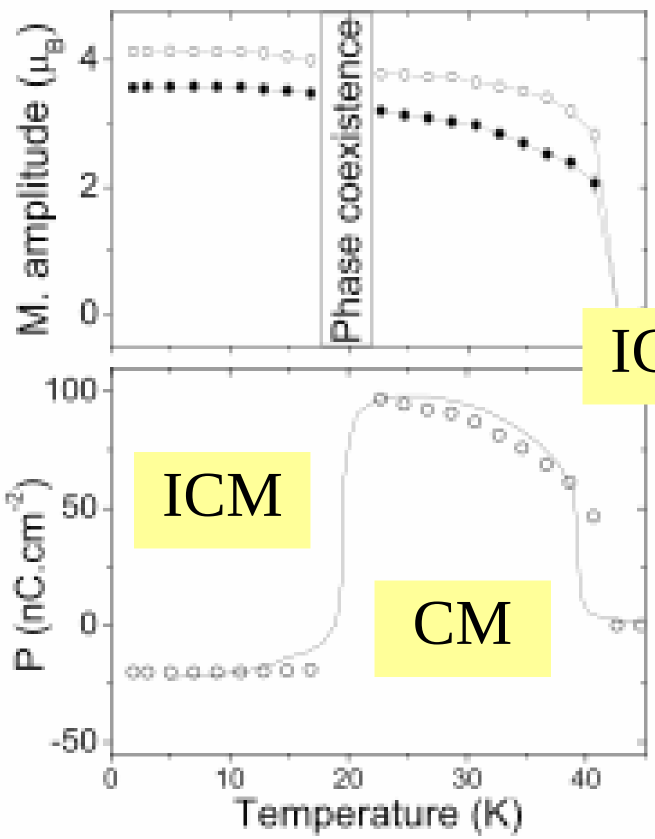
so, in order to have FE induced by magnetization....

IS IT SUFFICIENT TO HAVE

commensurate acentric magnetic order

YMn_2O_5

CM:
commensurate



ICM:
incommensurate
magnetic ordering

ICM and CM state have the same symmetry!

Chapon, Radaelli, Blake, Park, Cheong
Phys. Rev. Lett. **96**, 097601 (2006)

in orbital models:

interesting order (by disorder, nematic, topological?)

multiferroicity:

by in between bond and site center charge ordering

by dislocated spin density waves

suggesting:

multiferroic behavior in other dislocated SDW systems, for instance the charge transfer TCNQ salts