SOLITONIC PHASE IN MANGANITES.

cond-mat/0505093

Topological explanation of inhomogeneities in Manganites near x=0.5

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OUTLINE

- **INTRODUCTION TO MANGANITES.**
- **UNIFORM PHASES.**
- **INHOMOGENEOUS PHASES.**

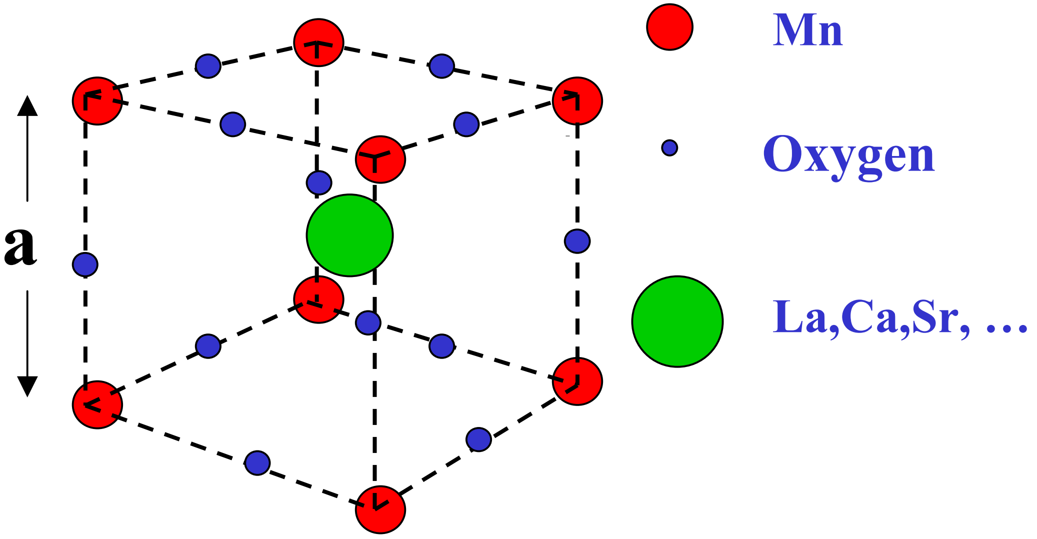
SOLITONIC PHASE IN MANGANITES

$T_{1-x}D_xMnO_3$

T: (La) trivalent

D: (Ca, Sr …) divalent

x: hole concentration.



Ideal cubic perovskite structure.

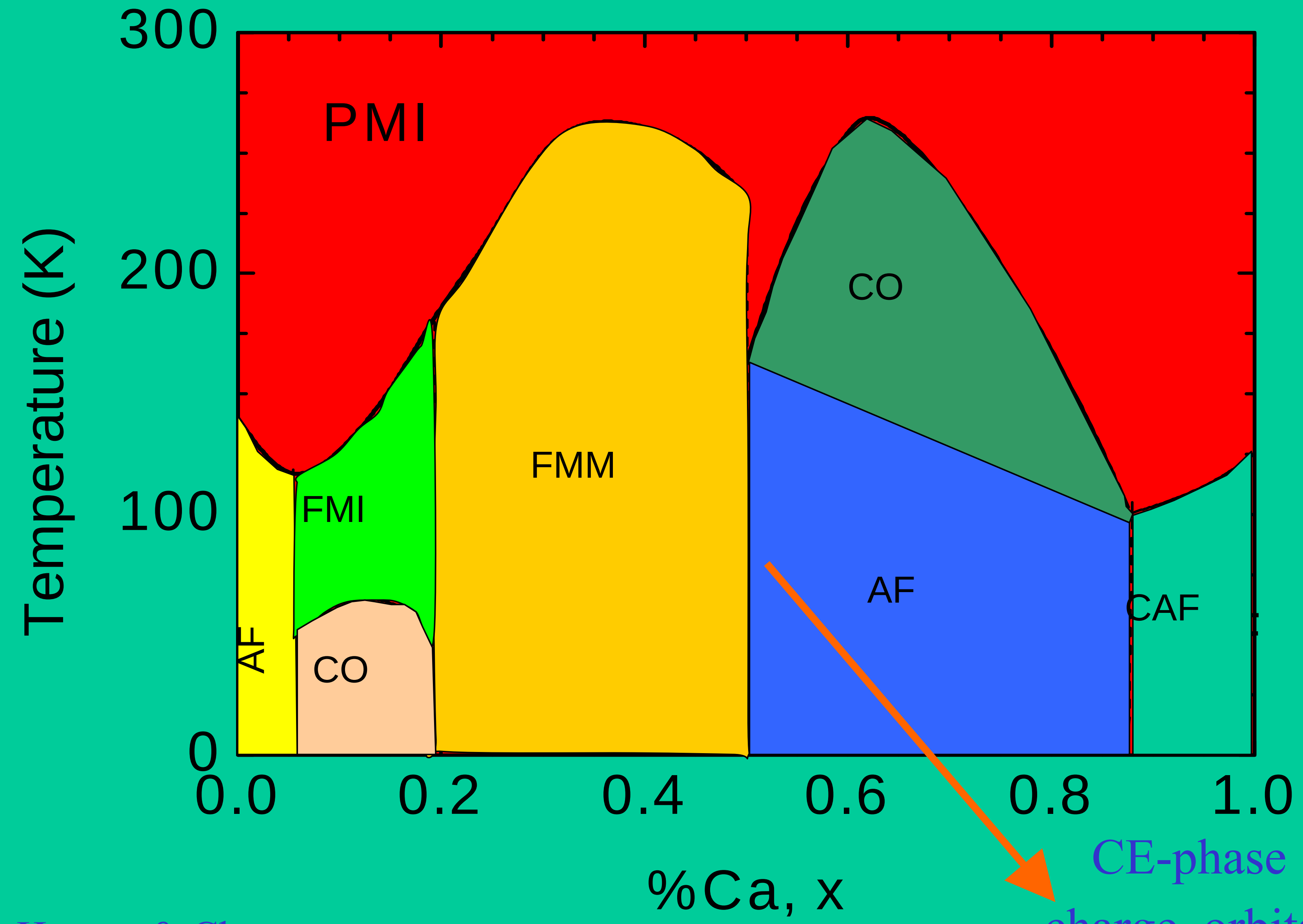
This structure is distorted by

Cation size mismatch. Jahn Teller effects.

La	$5d^1\ 6s^2$	3+
Ca	$4s^2$	2+
Mn	$3d^5 4s^2$	3+
O	$2s^2\ 2p^4$	2-

Electric active orbitals Mn . x holes in the Mn d-orbitals

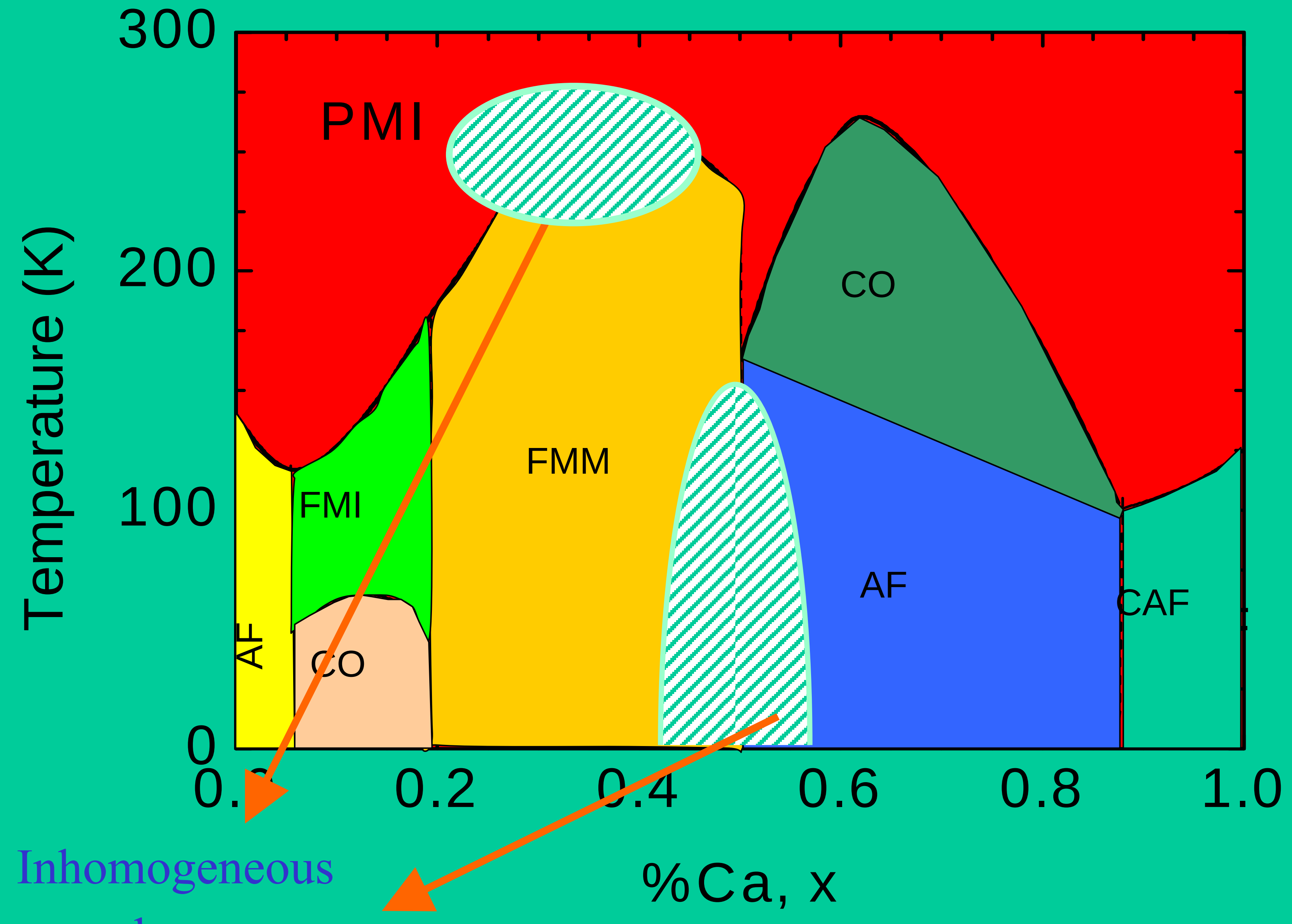
SIMPLIFIED PHASE DIAGRAM.



CE-phase
charge, orbital
and spin order.

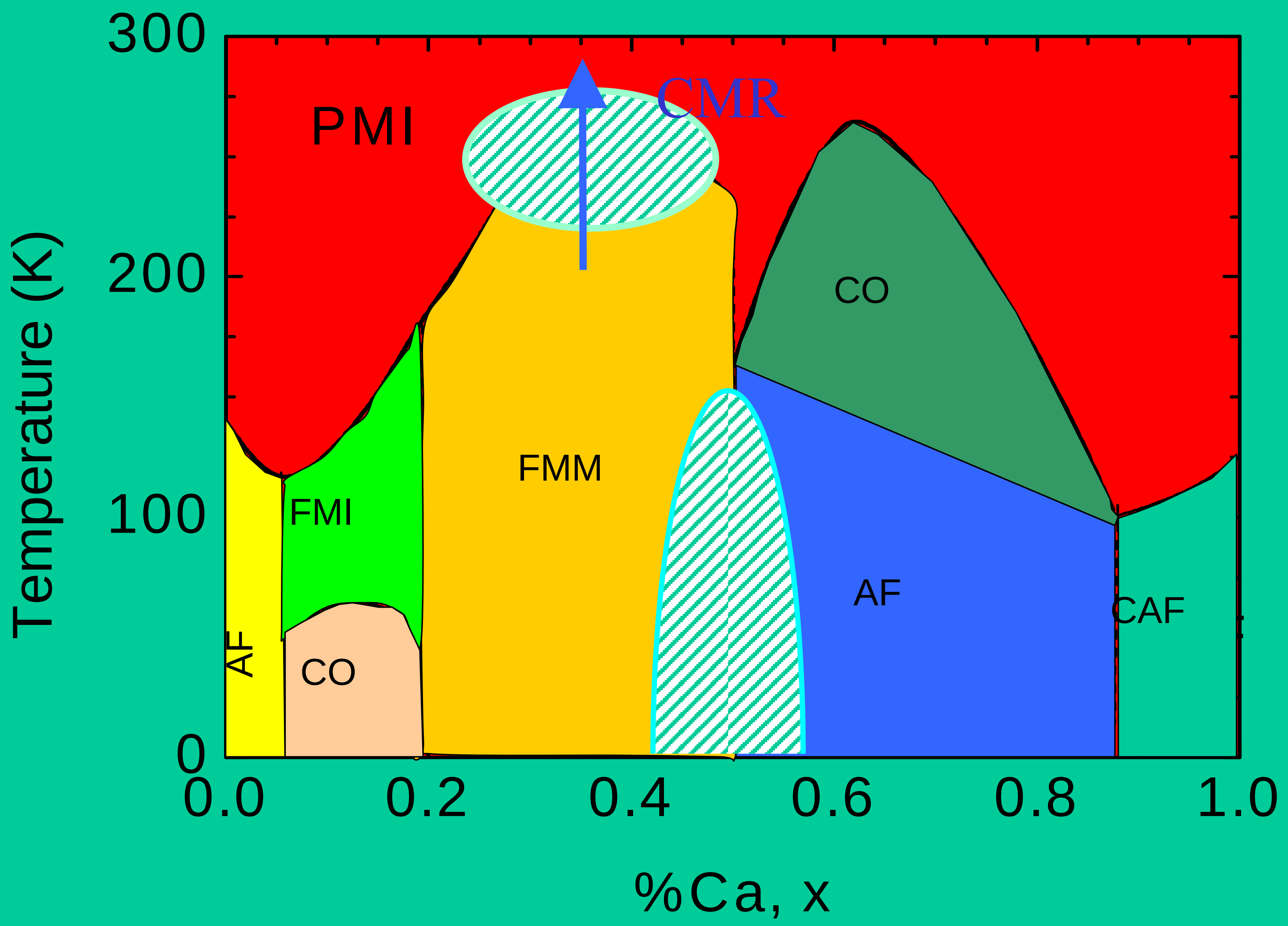
Hwang & Cheong

SIMPLIFIED PHASE DIAGRAM.

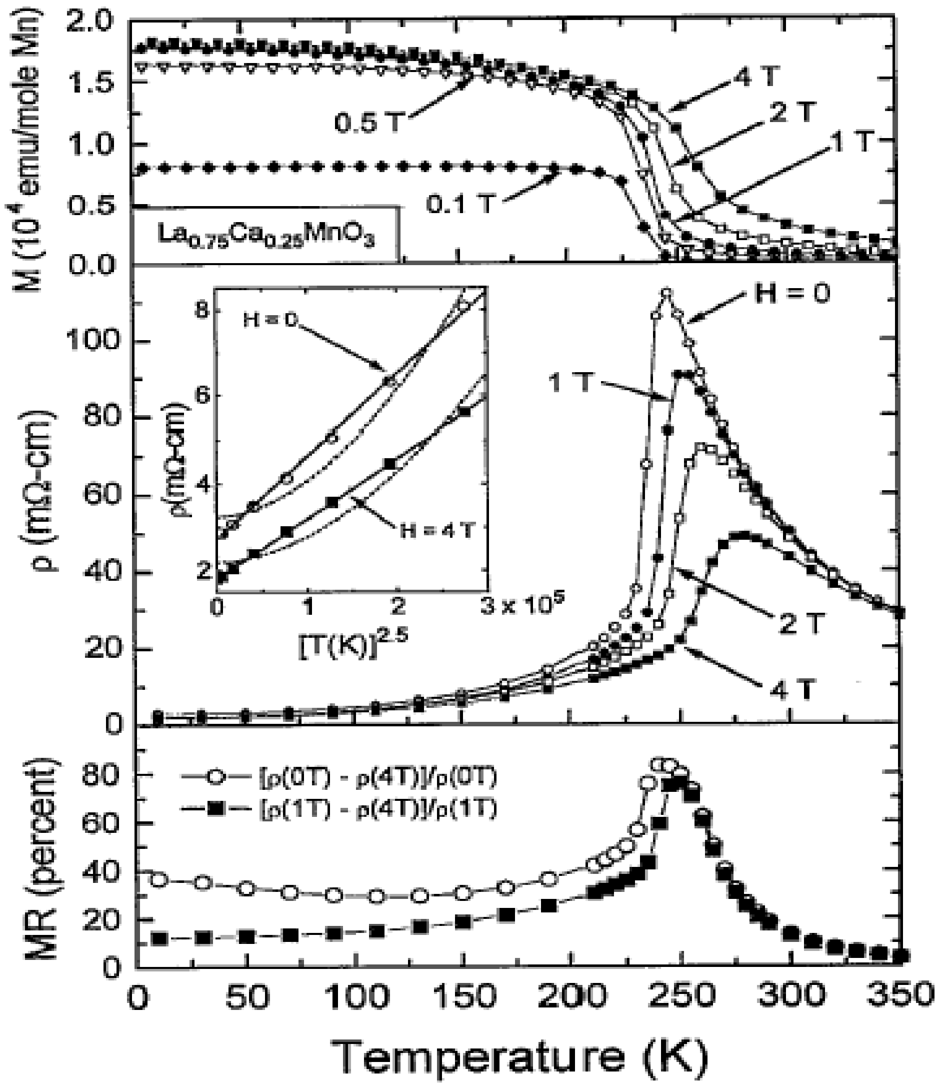


Inhomogeneous phases.

COLOSSAL MAGNETORESISTANCE



Colossal Magneto Resistance



$La_{0.75}Ca_{0.25}MnO_3$

P.Schiffer et al. PRL ('95)

Many Questions.

For explaining CMR we need a metal-insulator transition coupled to a ferromagnetic paramagnetic transition.

- **Nature of the insulating (homogeneous) phases. Charge Ordered phase, Polaronic phase...**

Inhomogeneities seems to be crucial to the understanding of CMR.

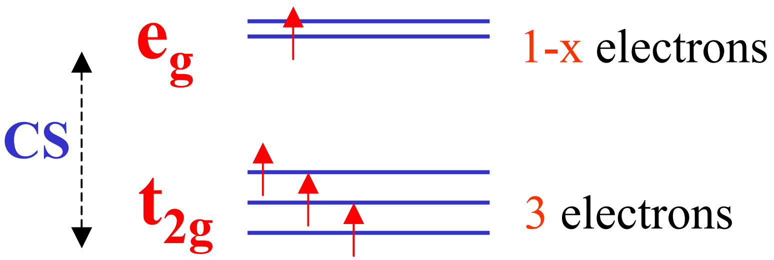
- **Origen of the inhomogeneous phases and phase coexistence.**

HOMOGENEOUS PHASES. INGREDIENTS.

- Kinetic Energy (two Mn d-orbitals)

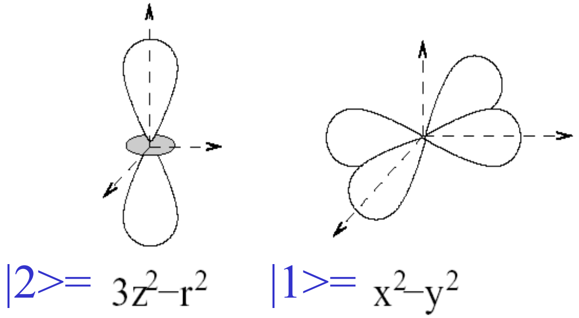
KINETIC ENERGY $La_{1-x}Ca_xMnO_3$

Active orbitals Mn d (5 plus spin) 4-x electrons per Mn atom



1-x electrons

3 electrons



Hund's Coupling

A density of holes, x, moving in these orbitals. The hopping is through the oxygen, and depends on the orbital type and on the hopping direction.

In the z-direction

$t_{22}=4/3\ t$

$t_{12}=t_{11}=0.$

In the xy-plane

$t_{22}=t/3$

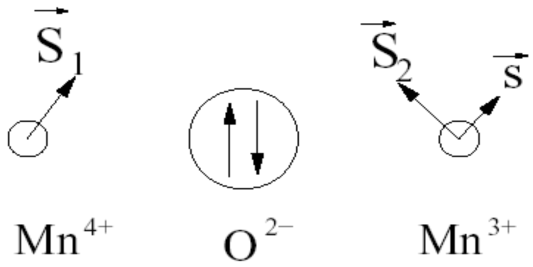
$t_{12}^x=+t/(3)^{1/3}$ $t_{12}^y= -t/(3)^{1/3}$
$t_{11}=t$

INGREDIENTS.

- Kinetic Energy (two d-orbitals)
- Hunds coupling. (Double Exchange)

Hund's coupling. Double Exchange Mechanism.

(Zener, DeGennes, Anderson, '50)



- •Holes moving around.
- •Strong Hund's coupling. $\vec{\sigma}\cdot\vec{S}$
- •Tunneling conserves spin.

$$J_H \to \infty$$

$$H_{KE} + H_{Hund} = -\sum f_{i,j}\, t_{aa'} C^{+}_{ia} C_{ja'}$$

$$f_{i,j} = \cos\frac{\theta_{ij}}{2}\, e^{i\phi_{ij}}$$

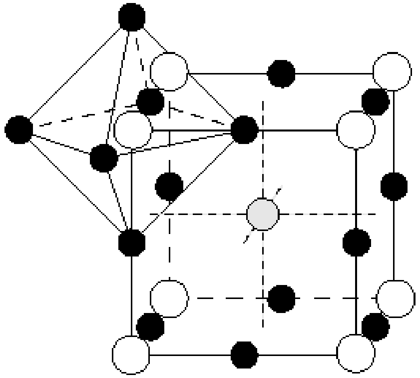
Long range ferromagnetic interaction mediated by the carriers.

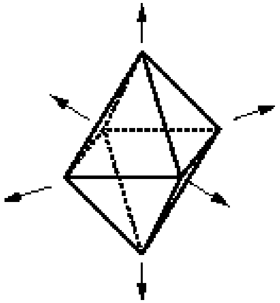
INGREDIENTS.

- Kinetic Energy (two d-orbitals)
- Hunds coupling. (Double Exchange)
- Electron phonon coupling

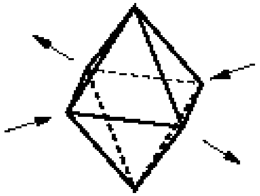
Electron Phonon Coupling.

The active **Jahn-Teller** modes of the oxygen octahedra, couples with the e_g orbitals.

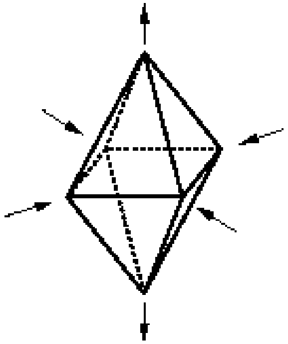




Q_1



Q_2



Q_3

$$H_{el-ph} = \lambda \sum_i \left(Q_{1i}\rho_i + Q_{2i}\tau_{xi} + Q_{3i}\tau_{zi} \right)$$

$$H_{elastic} = \frac{1}{2} \sum_i (\beta Q_{1i}^2 + Q_{2i}^2 + Q_{3i}^2)$$

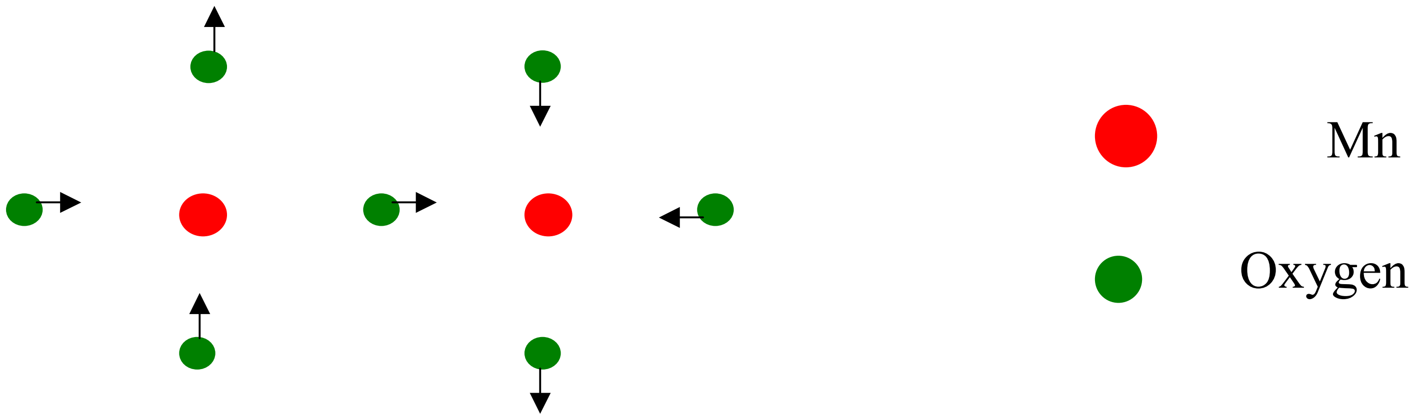
$$\tau_{xi} = C_{i1}^{+}C_{i2} + C_{i2}^{+}C_{i1}$$

$$\tau_{zi} = C_{i1}^{+}C_{i1} - C_{i2}^{+}C_{i2}$$

τ are the orbital pseudospin densities.

Cooperative Jahn-Teller effect

Cooporative. Distortions are inhomogeneous, and produce long range interactions.



INGREDIENTS.

- Kinetic Energy (two d-orbitals)
- Hunds coupling. (Double Exchange)
- Electron phonon coupling
- Superexchange interaction between Mn's

$$J_{AF} \sum_{<i,j>} \vec{S}_i \vec{S}_j$$

HAMILTONIAN

$$H_{KE} + H_{Hund} = -\sum f_{i,j}\, t_{aa'} C^{+}_{ia} C_{ja'}$$

$$H_{el-ph} = \lambda \sum_{i} \left(Q_{1i}\rho_i + Q_{2i}\tau_{xi} + Q_{3i}\tau_{zi} \right)$$

$$H_{elastic} = \frac{1}{2} \sum_{i} (\beta Q_{1i}^{2} + Q_{2i}^{2} + Q_{3i}^{2})$$

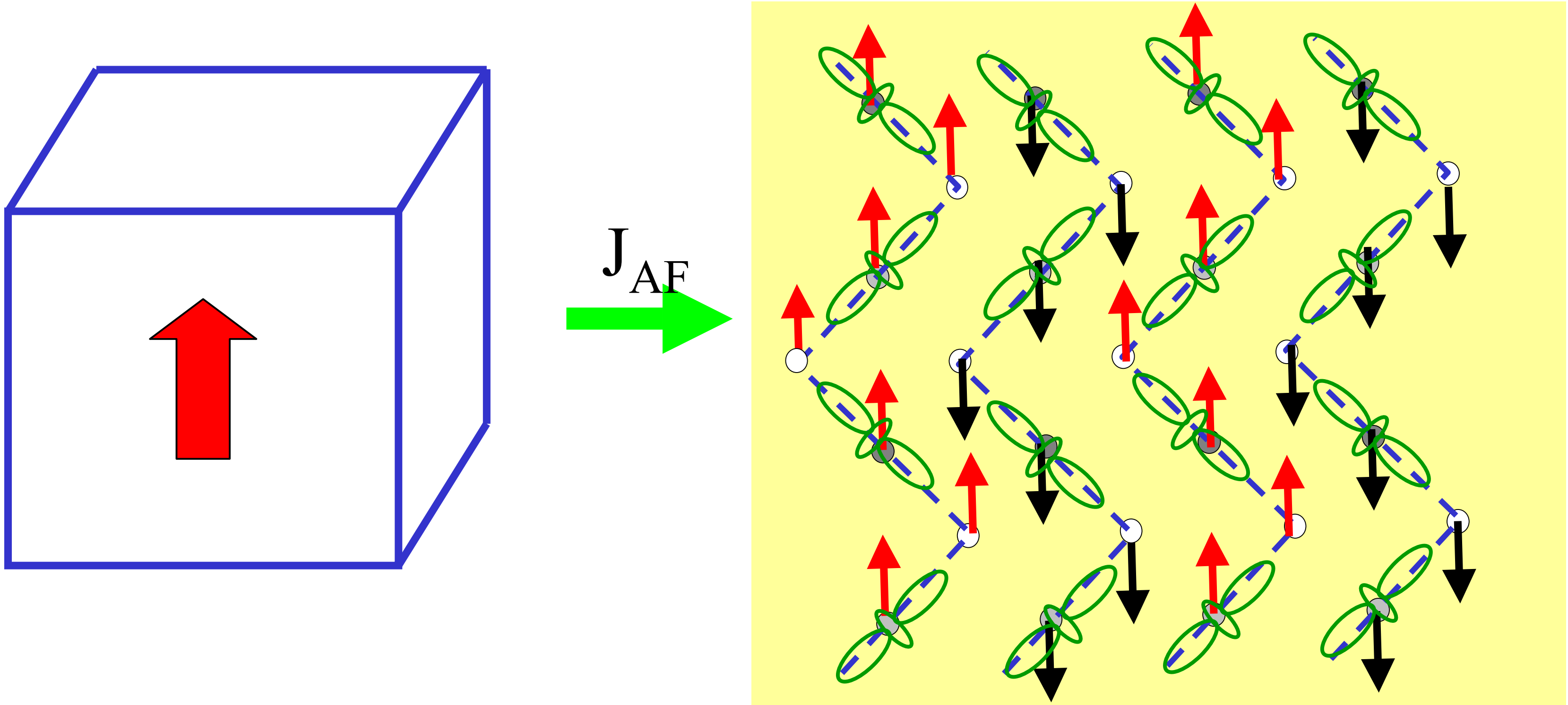
$$H_{AF} = J_{AF} \sum_{<i,j>} \vec{S}_i \vec{S}_j$$

J_{AF}, x, λ, T

In manganites the energies involved in these interactions are comparable so different ground state can have very similar energies.

- **Ferromagnetic metallic phase**
- **AF Mott insulator**
- **Stripe phases**
- **Ferromagnetic charge ordered phases**
- **Phase separation…**

Low temperature phases. (x=0.5)



Ferromagnetic Metallic

CE-OO

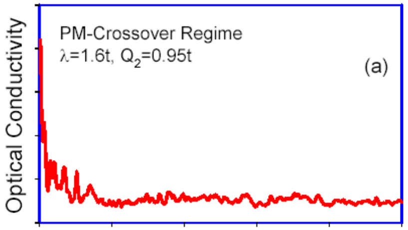
$\lambda \neq 0$, CO

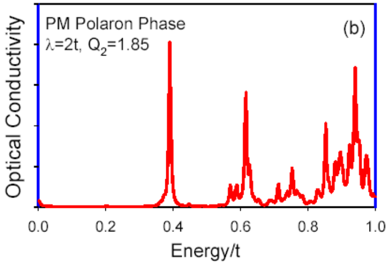
Solovyev,
Dagotto,
Khomskii,
Millis....

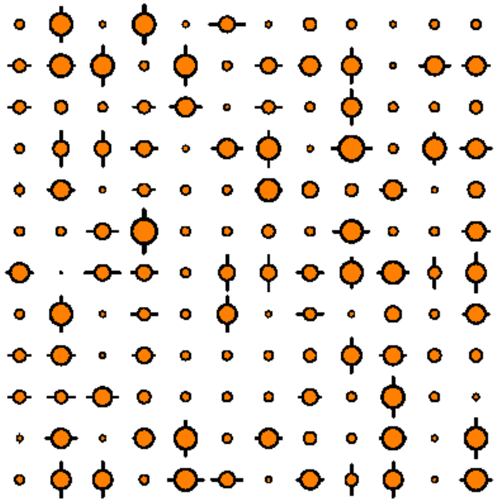
x=2/3, 3/5   LB, PRL’04

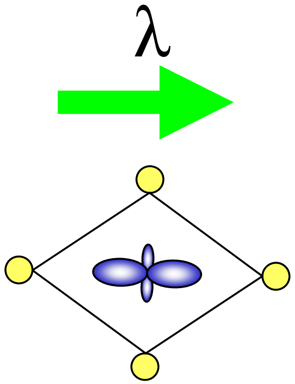
Melting of the CE phase.

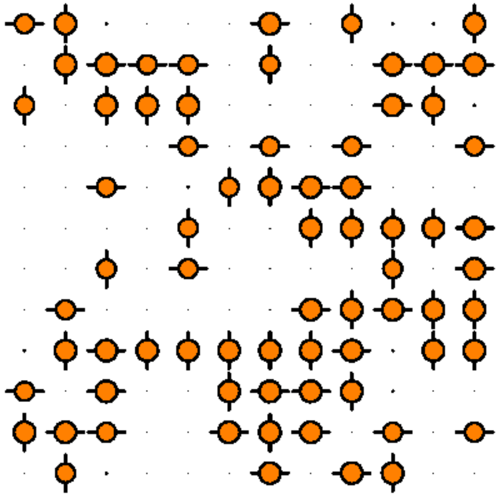
LB, PRB’05

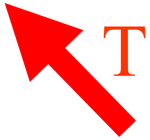


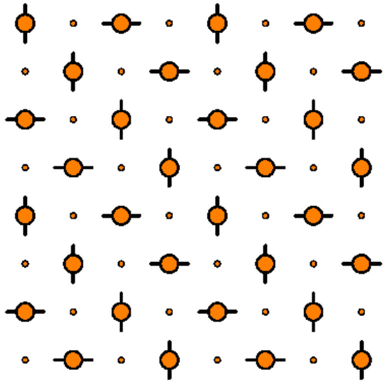


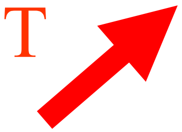








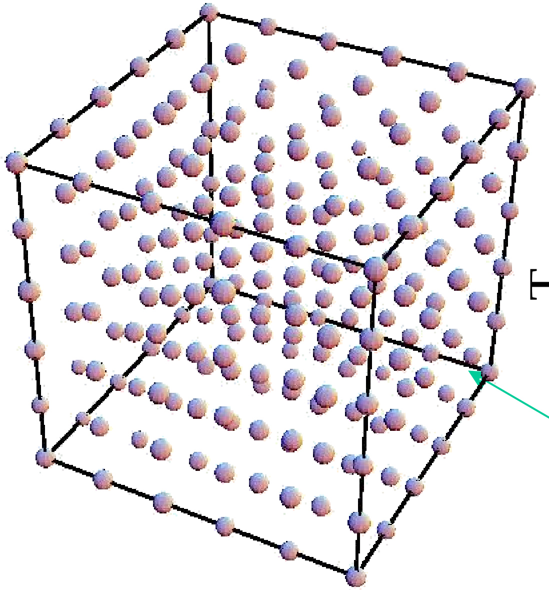




Weak charge modulation.
Octahedra disorder phase.
Metallic Phase.

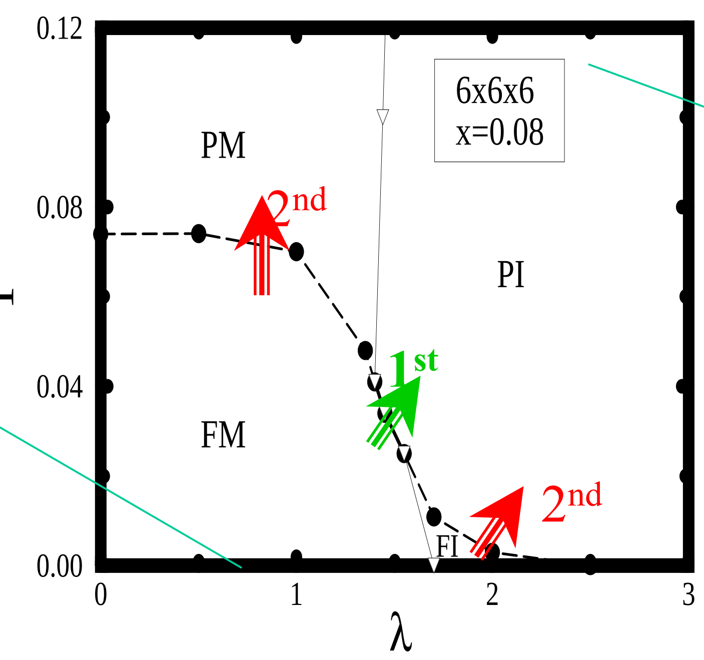
Strong charge modulation.
Disorder Polaronic
Insulator Phase.

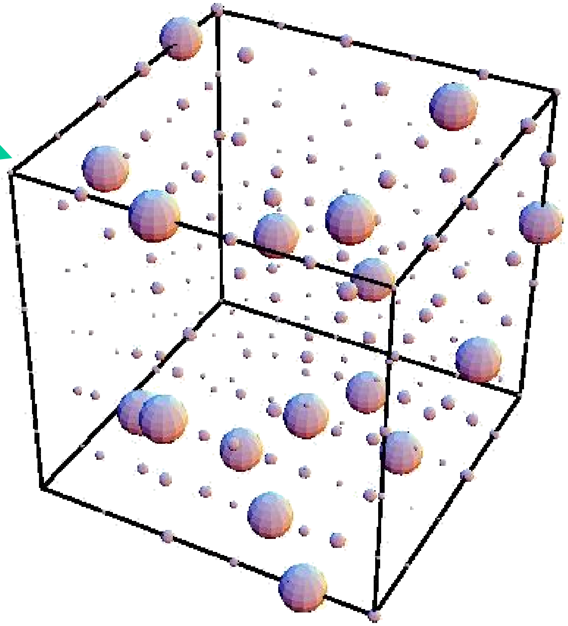
Metal-Insulator transition increasing Temperature.



NO POLARONS, 17 electrons

Ferromagnetic.





17 POLARONS

Paramagnetic.

Vergés, Martín-Mayor and LB, PRL '02

Many Questions.

- Nature of the insulating (homogeneous) phases. Charge Ordered phase, Polaronic phase... ✓

- Origen of the inhomogeneous phases and phase coexistence.

Inhomogeneous phases and Phase Coexistence

Inhomogeneities seems to be crucial to the understanding of CMR

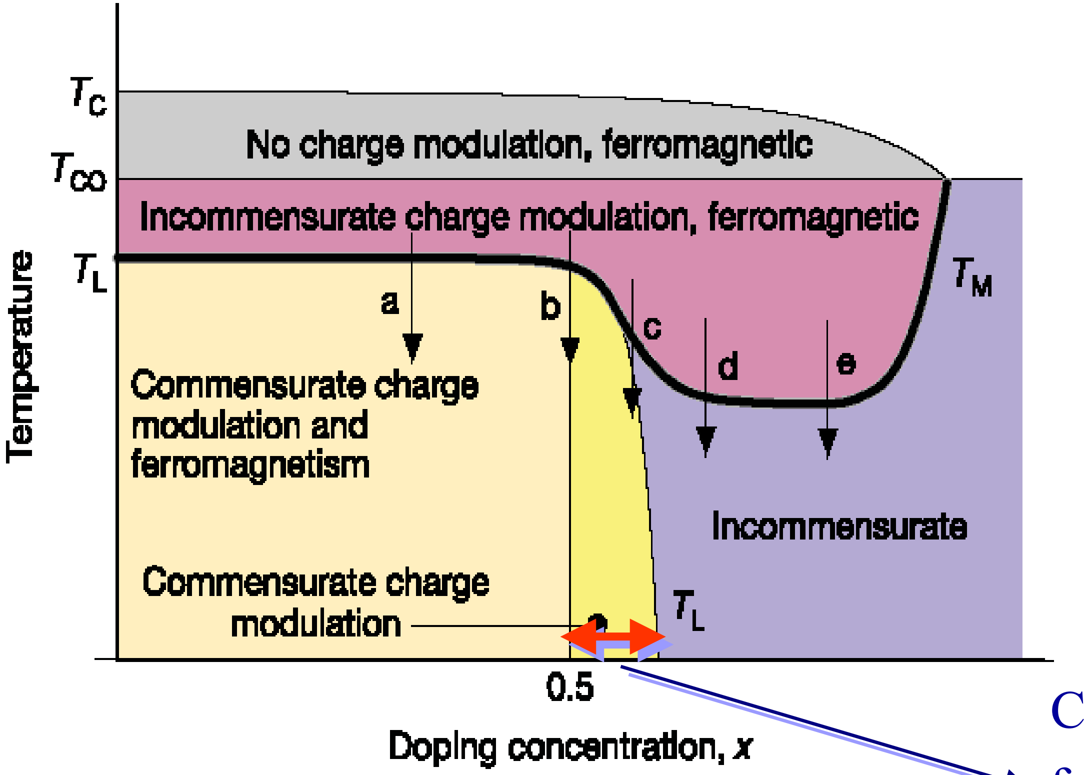
1. **Ginzburg-Landau phenomenological theory**
2. **Strain induces kinetic phenomenon**
3. **Phase competition in the presence of quenched disorder**

Inhomogeneous phases and Phase Coexistence

Ginzburg-Landau phenomenological theory.

Inhomogeneities as result of coupling between order parameters.

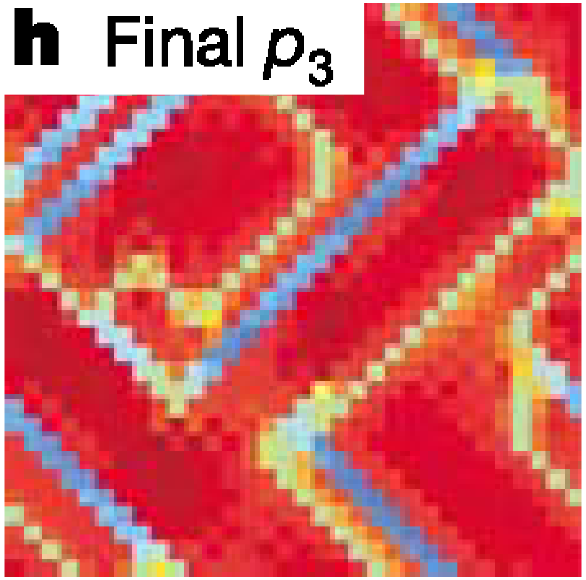
Coexistence of FM and CO. *Milward et al. Nature 2005.*



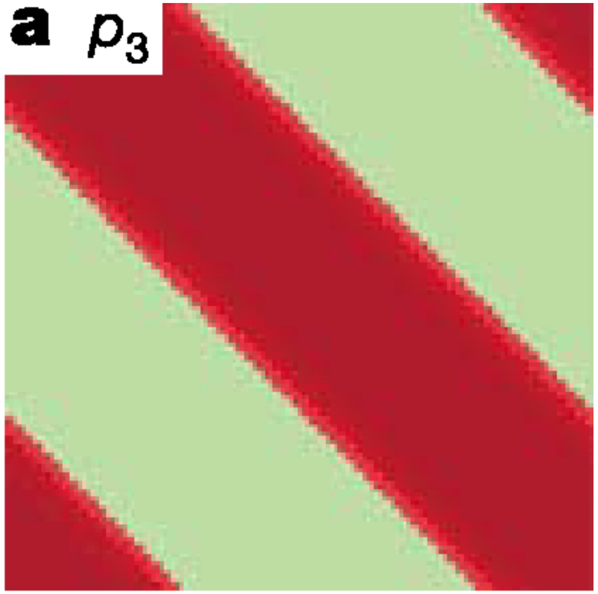
Critical hole density for lock in transition.

Inhomogeneous phases and Phase Coexistence

Strain induces kinetic phenomenon. Coupling between short and long range strains produces inhomogeneities in the nanometer and micrometer scales. *Ahn et al. Nature 2004.*



32x32



64x64

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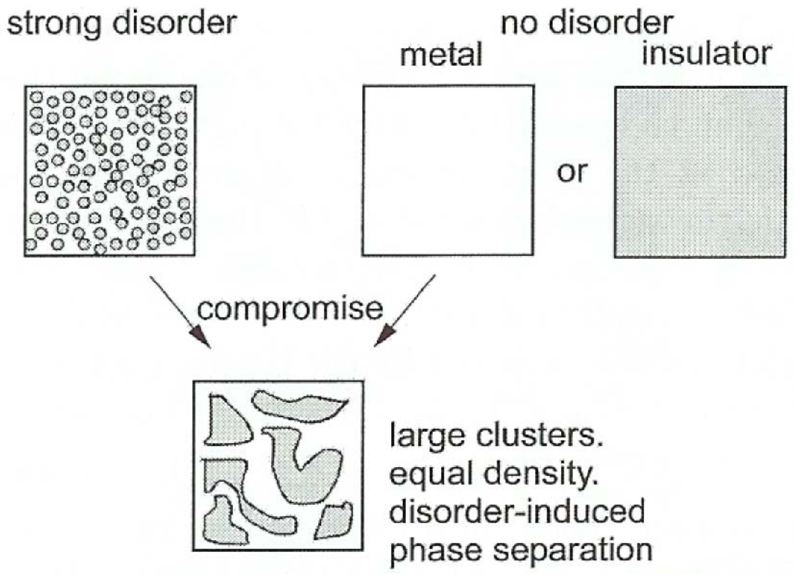
Inhomogeneous phases and Phase Coexistence

Near a first order phase transition the presence of quenched disorder can produce phase coexistence.



At zero disorder, no interfaces exist. Al large disorder, small size cluster are formed. At weak disorder, the compromise between the two tendencies leads to large clusters. *Dagotto, Moreo PRL, 2000.*

Inhomogeneous phases and Phase Coexistence

- Ginzburg-Landau phenomenological theory.
- Strain induces kinetic phenomenon.
- Phase competition in the presence of quenched disorder.

The first proposal is phenomenological and the last two are based in oversimplified models.

Strong topological concepts confirmed by realistic microscopic models.

INHOMOGENEOUS PHASES NEAR HALF FILLING COULD BE A SOLITONIC PHASE

Main Result.

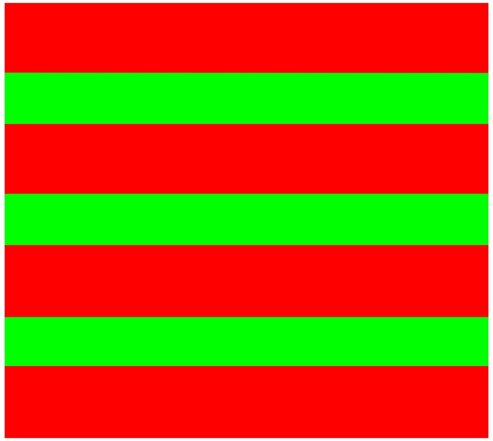
Manganites at half doping present orbital order that
support topological defects in the orbital sector:

Solitons.

Topological Charge ⇔ Electric Charge.

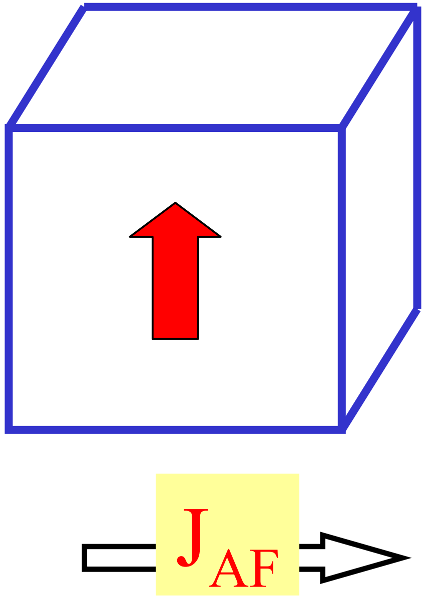
Charged solitons are the relevant charge excitations and charge added to the system creates an

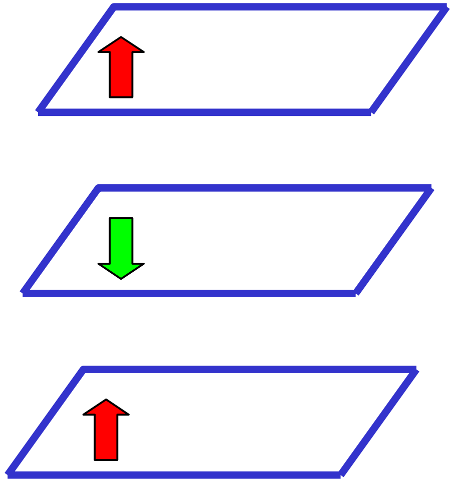
incommensurate array of solitons.

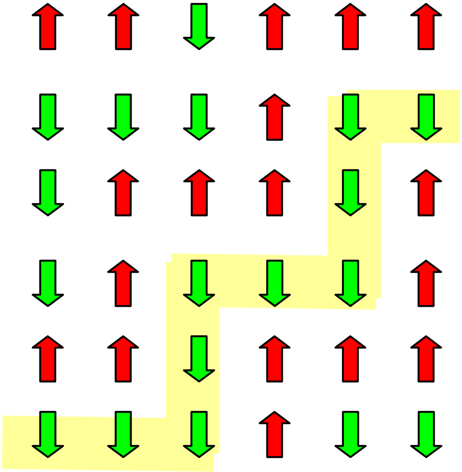


Inhomogeneous phases
in manganites near half doping.

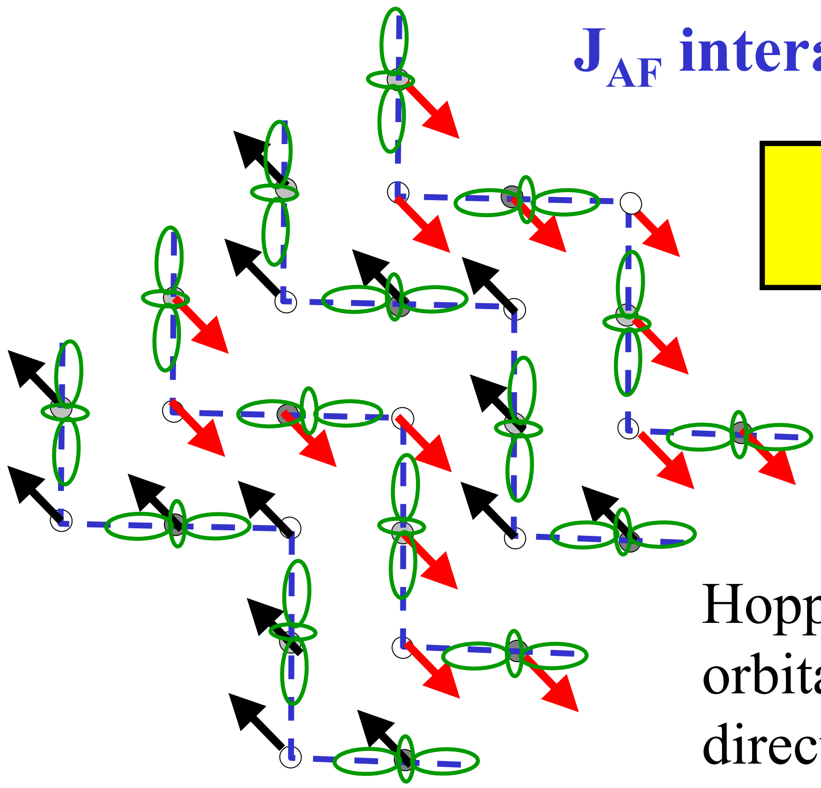
Ground state x=1/2 $R_{1-x}A_xMnO_3$







CE-Phase.



J_{AF} interaction favors FM chains coupled AF.

Why zigzag chains?

Hopping amplitude between $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ e_g orbital changes sign when is along the x or the y direction.

$$\cdots C - B_x - C - B_y - C - B_x \cdots$$

$$\cdots - d_{x^2-y^2} - d_{3x^2-r^2} - d_{x^2-y^2} - d_{3y^2-r^2} - d_{x^2-y^2} - d_{3x^2-r^2} - \cdots$$

With this orbital order the system opens a gap at the Fermi energy and minimize the kinetic energy. Band insulator.

ISOSPIN LENGUAGE.

$d_{x^2-y^2} \rightarrow |\uparrow>$

$d_{3z^2-r^2} \rightarrow |\downarrow>$

$\cdots$- $d_{x^2-y^2}$ - $d_{3x^2-r^2}$ - $d_{x^2-y^2}$ - $d_{3y^2-r^2}$ - $d_{x^2-y^2}$ - $d_{3x^2-r^2}$ - $\cdots$

Orbital order along the chain: $\boxed{\tau_x(i) = A\cos\left(\frac{\pi}{2} i + \phi\right)}$ $\phi = 0, \frac{\pi}{2}, \pi, 3\frac{\pi}{2}$

(i position along the chain.)

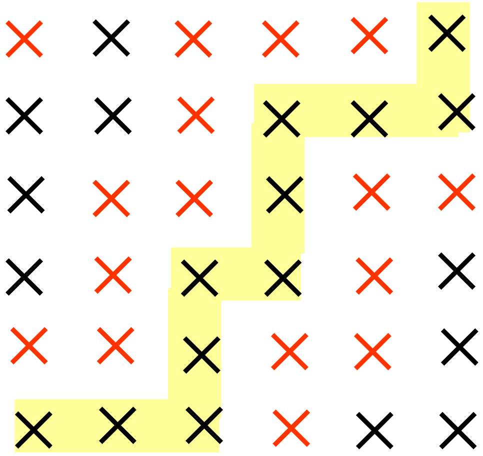
Associated with this degeneracy we expect SOLITONS, where the phase changes slowly from 0 to ±π/2. Topological charge ±1/2.

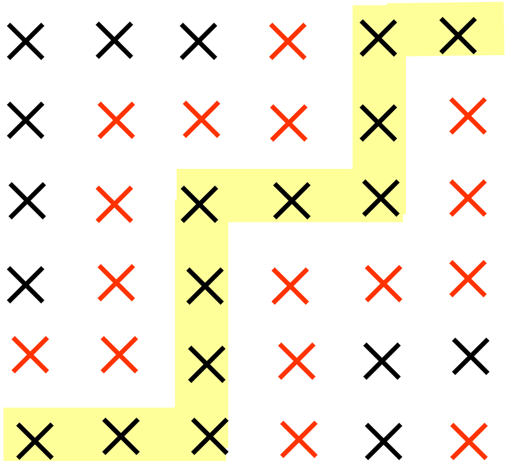
Topological charge ⇔to electric charge.

For a modulation $\tau_x(i) = A\cos\left(\frac{\pi}{2}i+\phi\right)$, π/2 is k_F and is related to the hole concentration, x, trough π/2= πx, except in the region inside the soliton.

Assuming ϕ changes slowly , the pseudospin modulation can be written as $A\cos(\pi xi+\nabla\phi i+\phi_0)$ and the local charge inside the soliton is $\pi(x+\nabla\phi/\pi)$. By integrating between 0 and ± π/2, we obtain the total **charge of the soliton ±1/2.**

How to create solitons in the CE phase





$\cdots$-C-B$_y$-C-C-B$_y$-C-B$_x$-C$\cdots$

$\cdots$ C-B$_x$-C-B$_y$-B$_y$-C-B$_x$-C-B$_y$$\cdots$

The phase changes in ±π/2 when going from -∞ to +∞.

Soliton +1/2.

Antisoliton -1/2

Introduce the defect and solve microscopic model…

Introduce the defect and solve microscopic model…

HAMILTONIAN

$$H_{KE} + H_{Hund} = -\sum f_{i,j}\, t_{aa'} C^{+}_{ia} C_{ja'}$$

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$$H_{elastic} = \frac{1}{2} \sum_{i} (\beta Q_{1i}^2 + Q_{2i}^2 + Q_{3i}^2)$$

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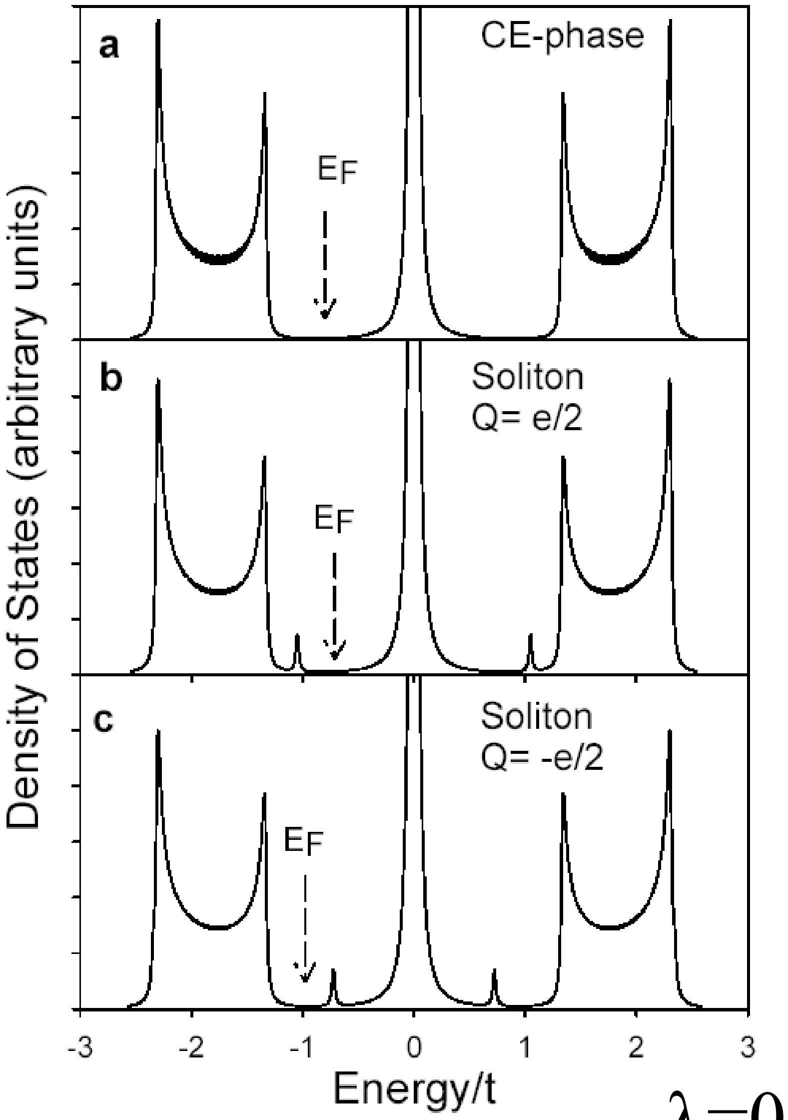
Density of States.

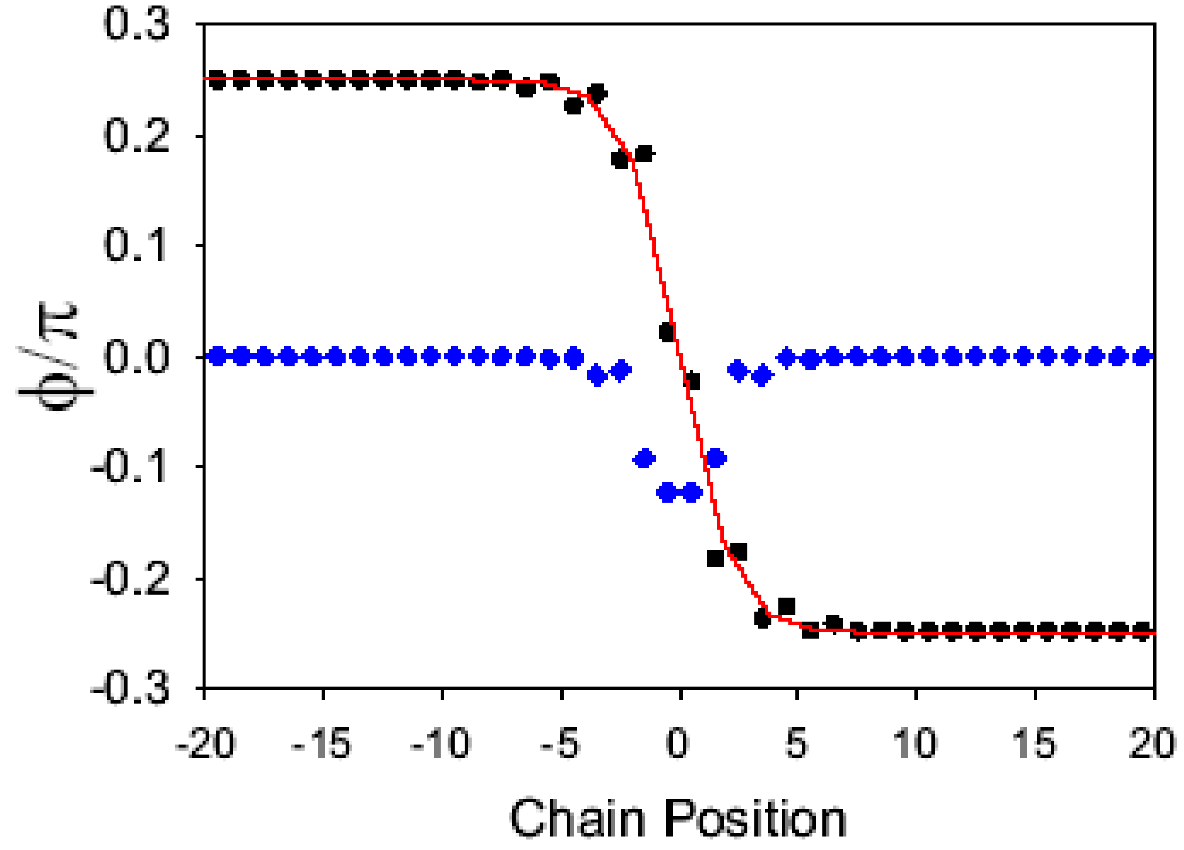


$\lambda=0$

Localized states in the gap. Half of the spectral weight from VB other CB. Occupying/emptying these states we add ±1/2 electron to the system.

Similar results for finite electron-phonon coupling.

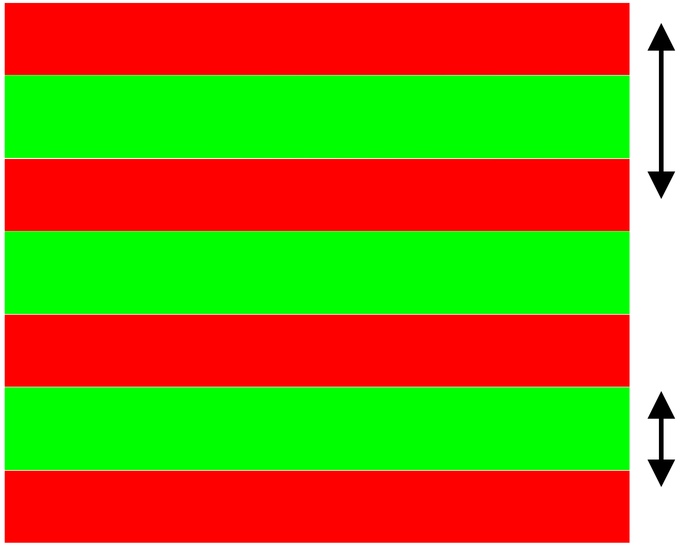
Soliton shape



$$\phi(i) = \frac{\pi}{2}\tanh\left(-\frac{i}{i_0}\right) \qquad \text{with} \quad i_0 = 2.25$$

Incommensurate Solitonic Phase

Added charge forms an array of half charged solitons separated by 1/2|x-0.5| ions along the chains, and produces a continuous orbital, charge and spin modulation of wavevector $q=(1-x)a$. (Incomensurate phase).



1/2|x-0.5|

Soliton thickness~10

PHASE DIAGRAM. J_{AF}=0.1t

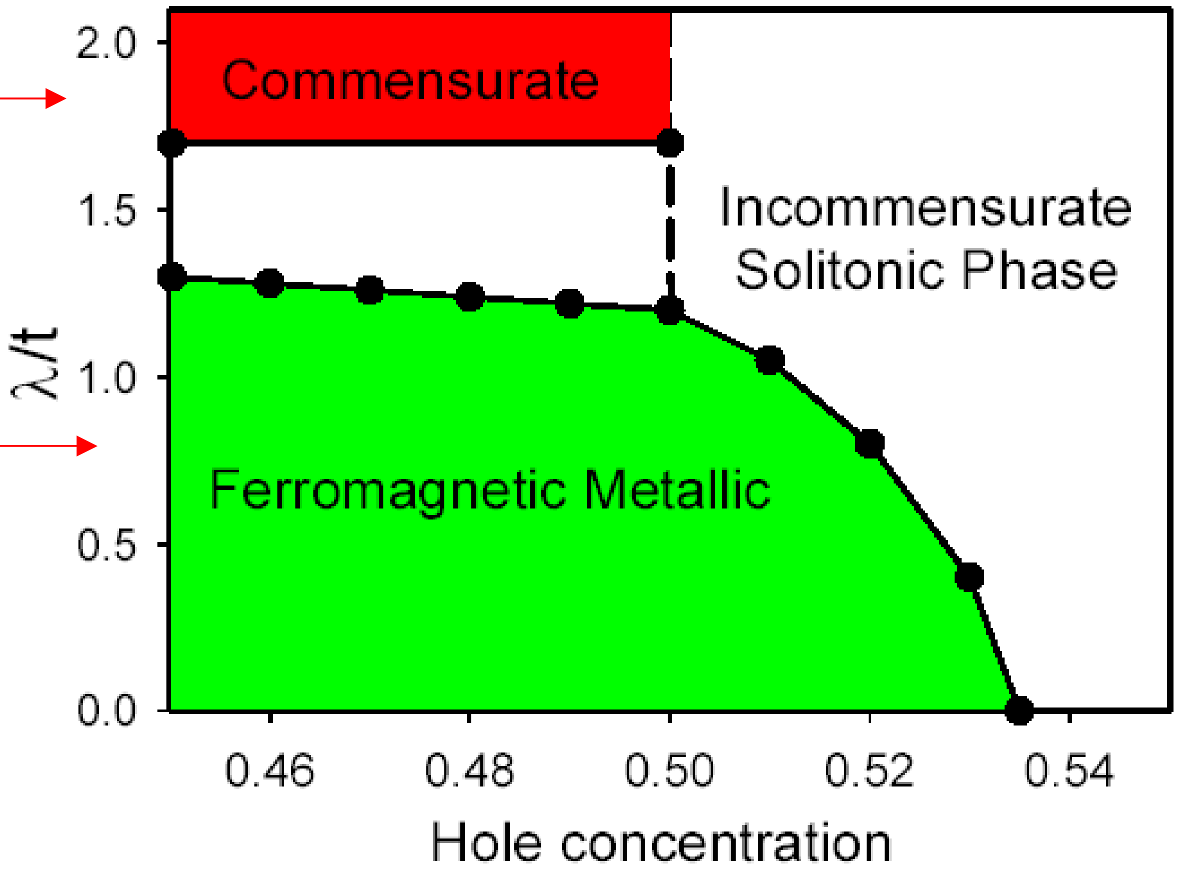
λ=1.8, Δq=0.6

$PrCaMnO_3$

LaCaMnO3

λ=1, Δq=0.14

$LaSrMnO_3$



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Topological Charge ⇔ Electric Charge.

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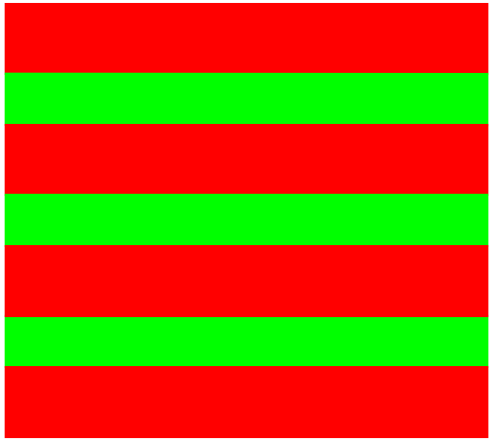

Inhomogeneous phases
in manganites near half doping.