

- MANGANITES

- DOUBLE EXCHANGE MODEL

No T-dependent M-I transition.

- LATTICE –SPIN MECHANISM

T-dependent M-I transition.

- CONCLUSIONS

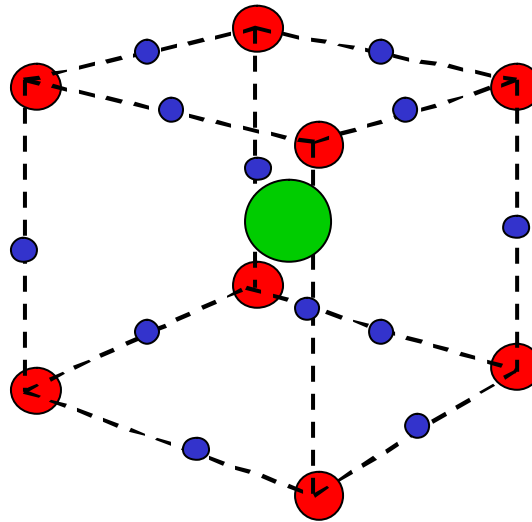


La: trivalent

D: (La, Sr ...) divalent

x: hole concentration.

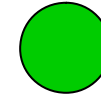
a



Mn



Oxygen



La, Ca, Sr, ...

**Ideal cubic
perovskite structure.**

• **This structure is distorted ($x \neq 0$)**

Cation size mismatch.

Jahn Teller effects.

• **Electric active orbitals Mn.**

La $5d^1 6s^2$ **3+**

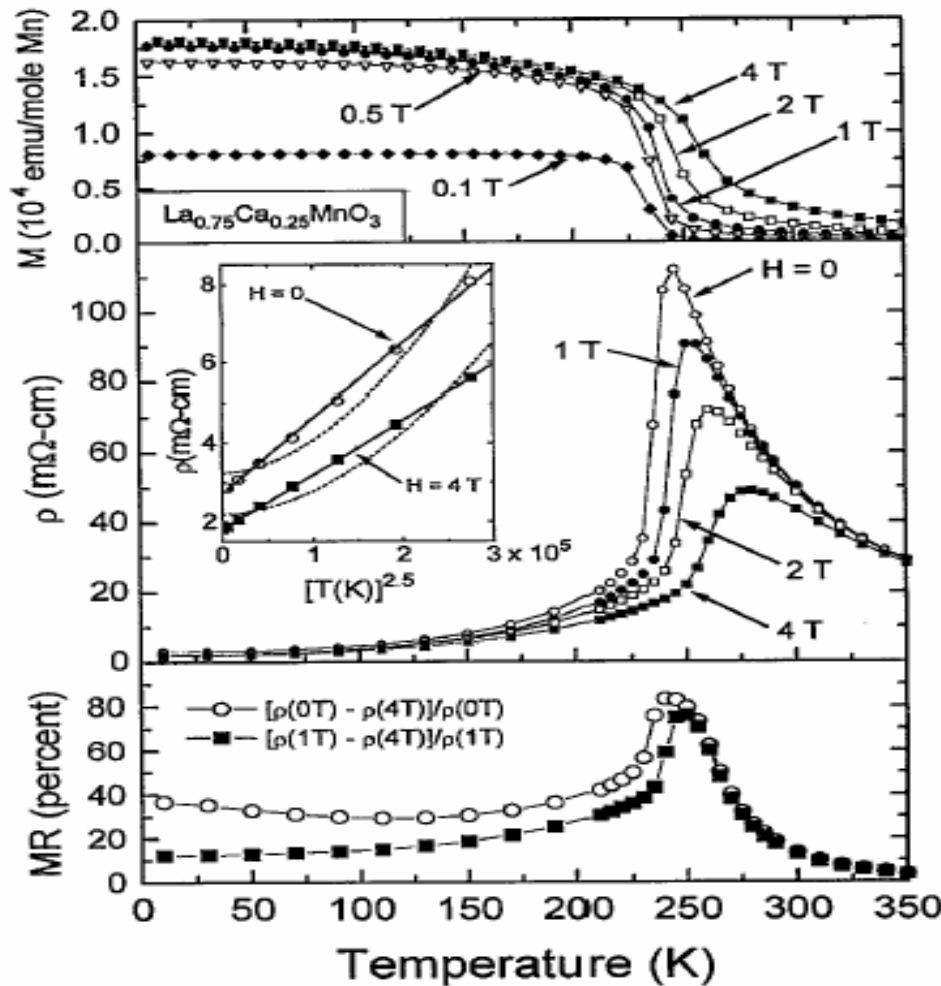
Ca $4s^2$ **2+**

Mn $3d^5 4s^2$ **3+**

O $2s^2 2p^4$ **2-**



Colossal Magneto Resistance

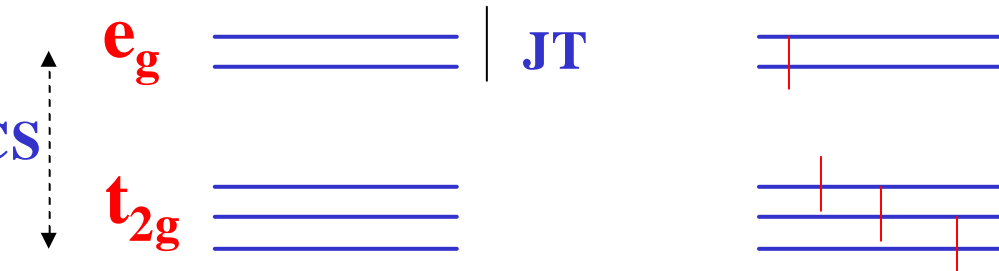


P.Schiffer et al. PRL ('95)

PARENT COMPOUND



? Active orbitals **Mn d** (5 plus spin)



Hund's Coupling

$$S=2$$

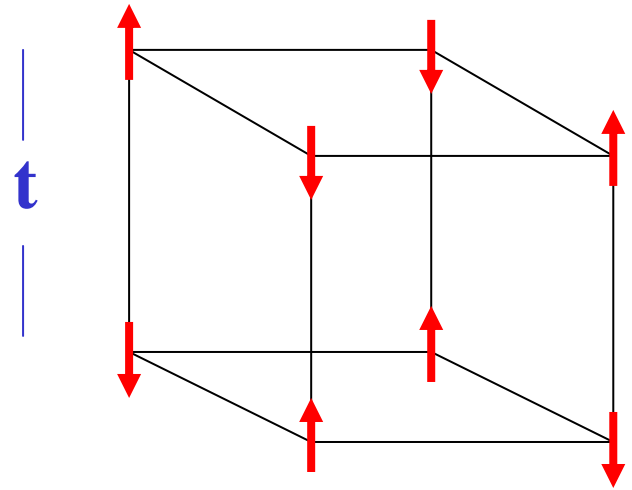
? Bands are fully occupied.

INSULATOR.

? Superexchange interaction between Mn.

ANTIFERROMAGNETIC.

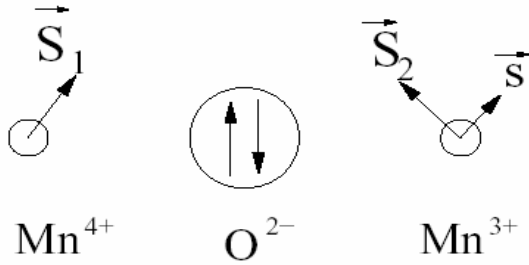
Hopping t





x holes per Mn

Double Exchange Mechanism. (Zener, DeGennes, Anderson, '50)



$$t \rightarrow t \cos \frac{\mathbf{q}_{ij}}{2} e^{i\mathbf{f}_{ij}/2}$$

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

E_K is minimum when mobility is maximum.



Mn spins want to be parallel.

METALLIC AND FERROMAGNETIC

0.1 < x < 0.4

t >> J_{AF}

T increases:

Ferromagnetic ? Paramagnetic.

Reduction BW.

Metal ? Insulator*.

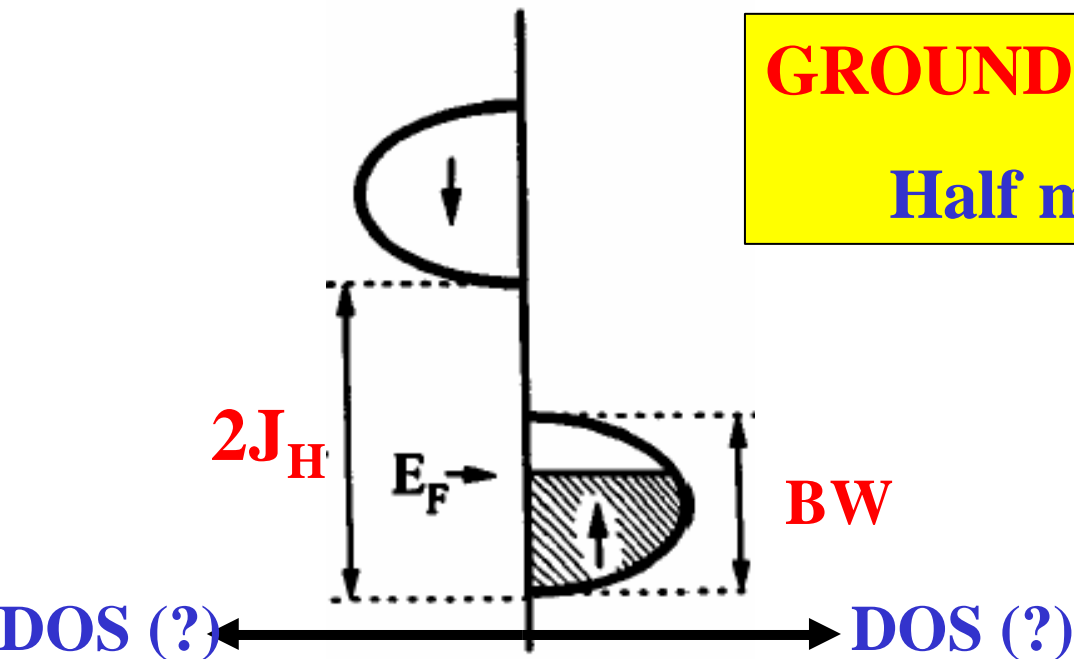
*Anderson localization
e-e interaction
e-phonon coupling.

-DOUBLE EXCHANGE HAMILTONIAN-

$$\hat{H} = -t \sum C_{is}^+ C_{js} - \frac{J_H}{S} \sum C_{is}^+ \vec{s}_{ss'} C_{is'} \vec{S}_i$$

- t : hopping amplitude.
- C_{is}
- J_H : Hund's coupling.
- \vec{S}_i : ion spin at site i . $|\vec{S}|=S$

- J_H very large. \vec{s}_i parallel to \vec{S}_i (S : classical)
- Electrons can lower their energy by hopping from site to site.
- \vec{S}_i ferromagnetically coupled.



GROUND STATE:

Half metallic ferromagnetic.

Spin flip $\sim 2J_H$

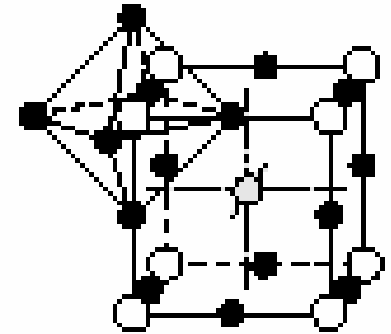
Insulating phase: POLARONIC PHASE.

Millis et al, Roder et al.

- Mean field.
- Half -filling
- Classical phonons.

WE STUDY A DE MODEL COUPLED WITH CLASSICAL COOPERATIVE PHONONS. (breathing modes of the oxygen octahedra)

- Monte Carlo Simulations. Include Fluctuations.
- Variable doping range.

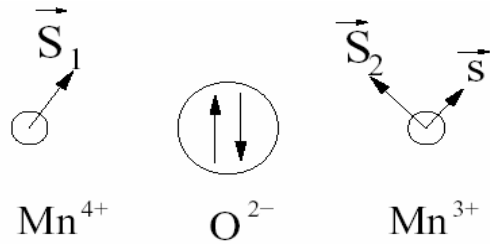


CONCLUSIONS

- For a finite range of doping and el-phonon coupling constant, a first order **M-I** phase transition, that coincides with a **F-P** transition occurs.
- The insulating phase is due to the self-trapping of every carrier within an oxygen octahedron distortion. (**POLARON**)

DOUBLE EXCHANGE MODEL.

$J_H?$ 8

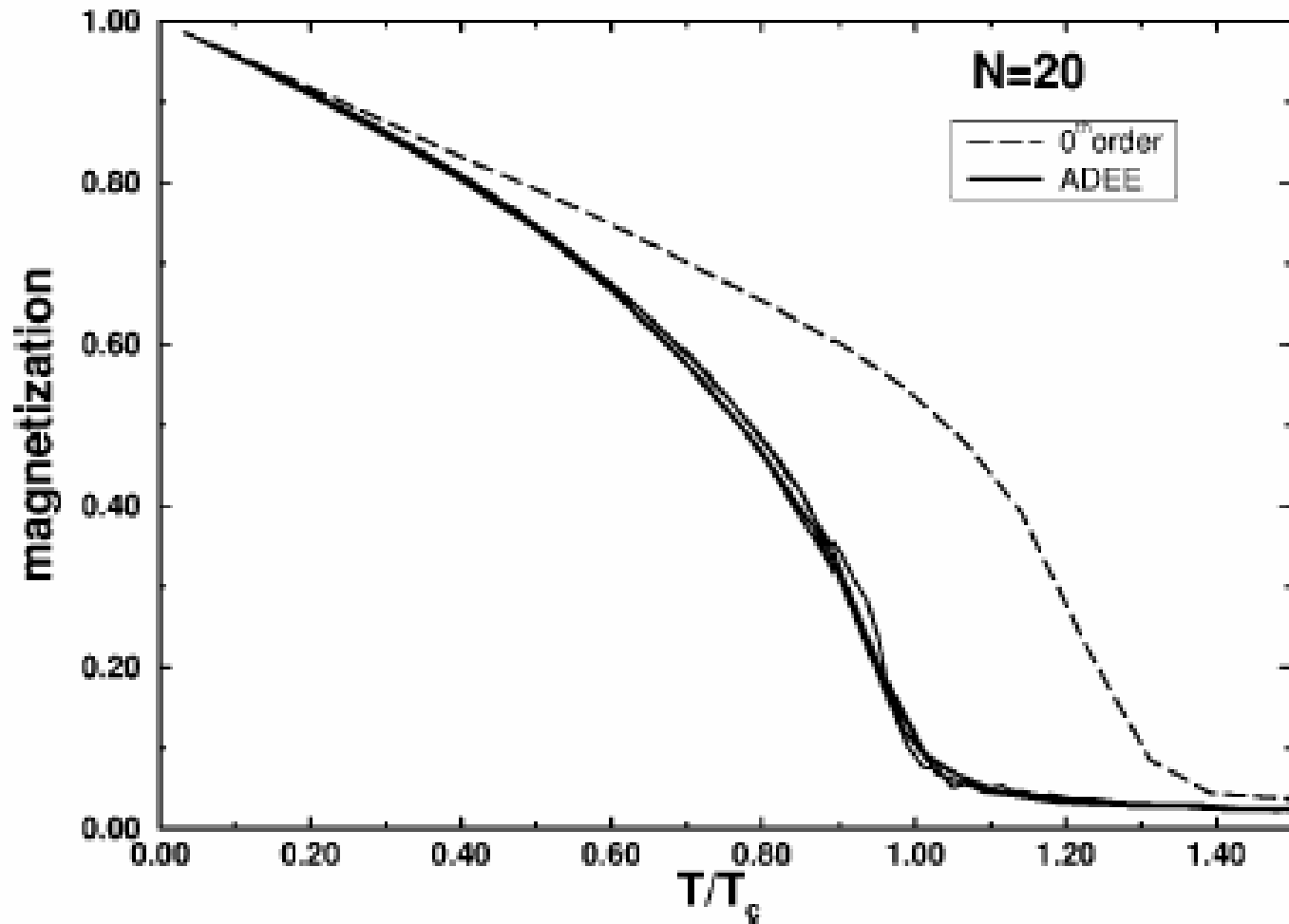


$$\hat{H} = -t \sum \cos \frac{q_{ij}}{2} e^{if_{ij}/2} C_i^+ C_j$$

T_i and f_i : Polar coordinates of S_i C_i : creates an electron at site i , with spin parallel to the core spin.

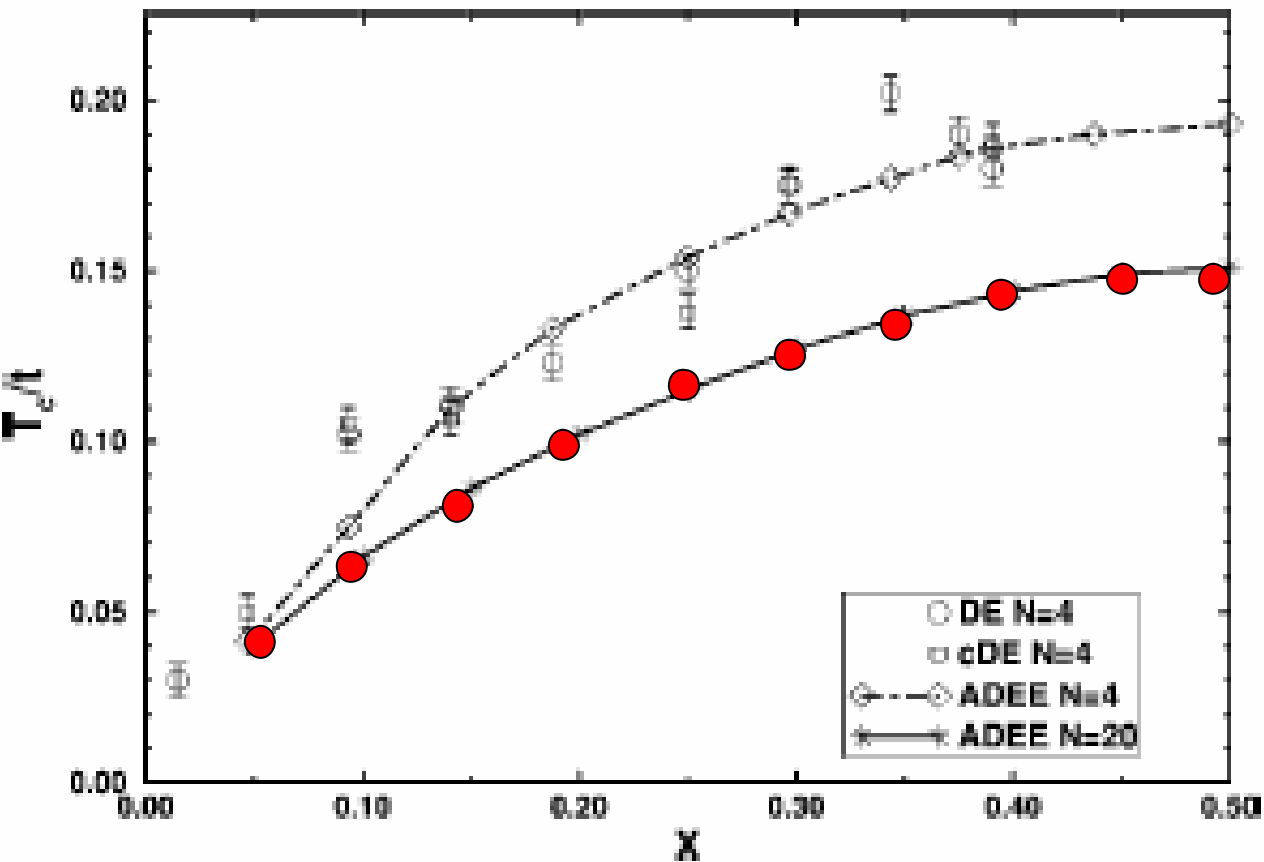
MONTE CARLO SIMULATIONS.

- S_i classical variables.
 - **INTERNAL ENERGY**: KE of electrons. It is obtained by diagonalizing the Hamiltonian.
 - Lattice sizes 6x6x6. (Higher sizes by perturbation theory).
 - Electrons at $T=0$.
 - Kubo formula for electron conductance
- **MAGNETIZATION.**
 - **RESISTANCE.**
 - **DOS.**
 - **BAND-WIDTH**
 -



M.J. Calderón and L. Brey PRB '98

CRITICAL TEMPERATURE VS CARRIER CONCENTRATION IN DE MODEL



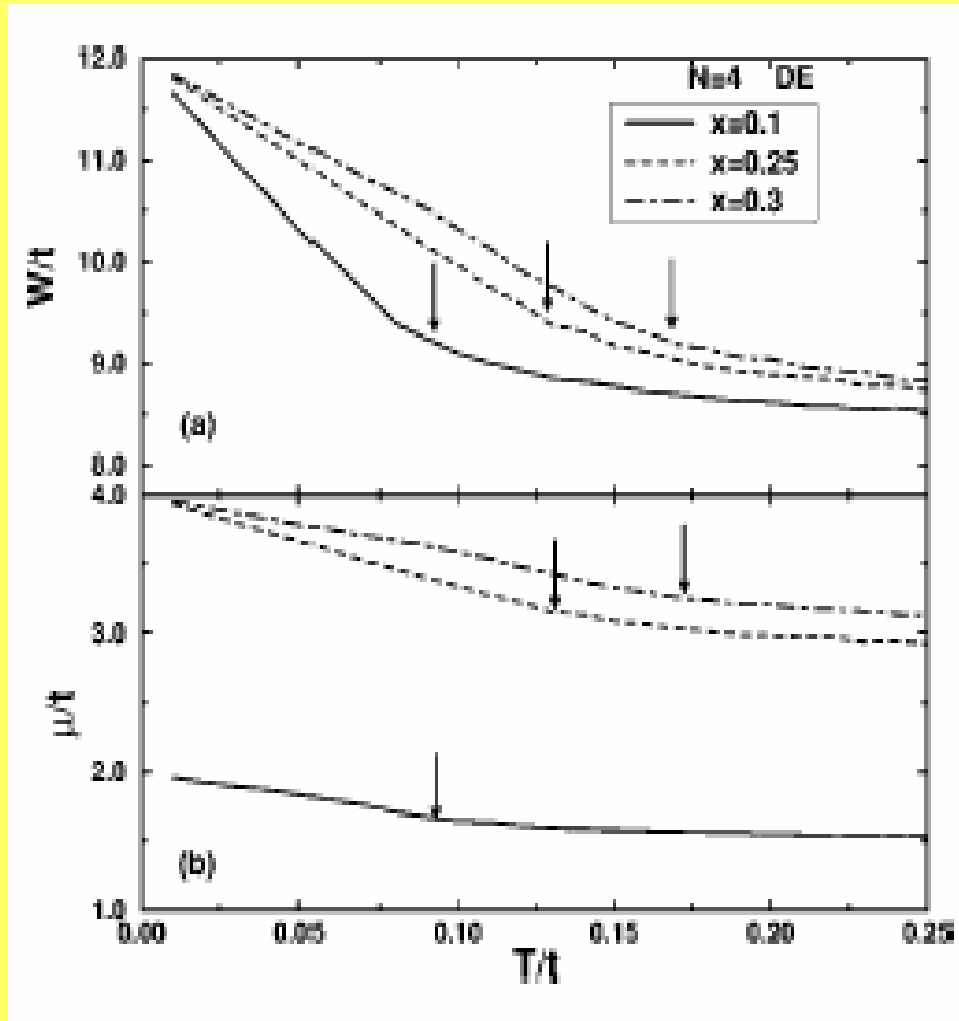
BW~1-4eV

x~0.2

Tc~150-600K

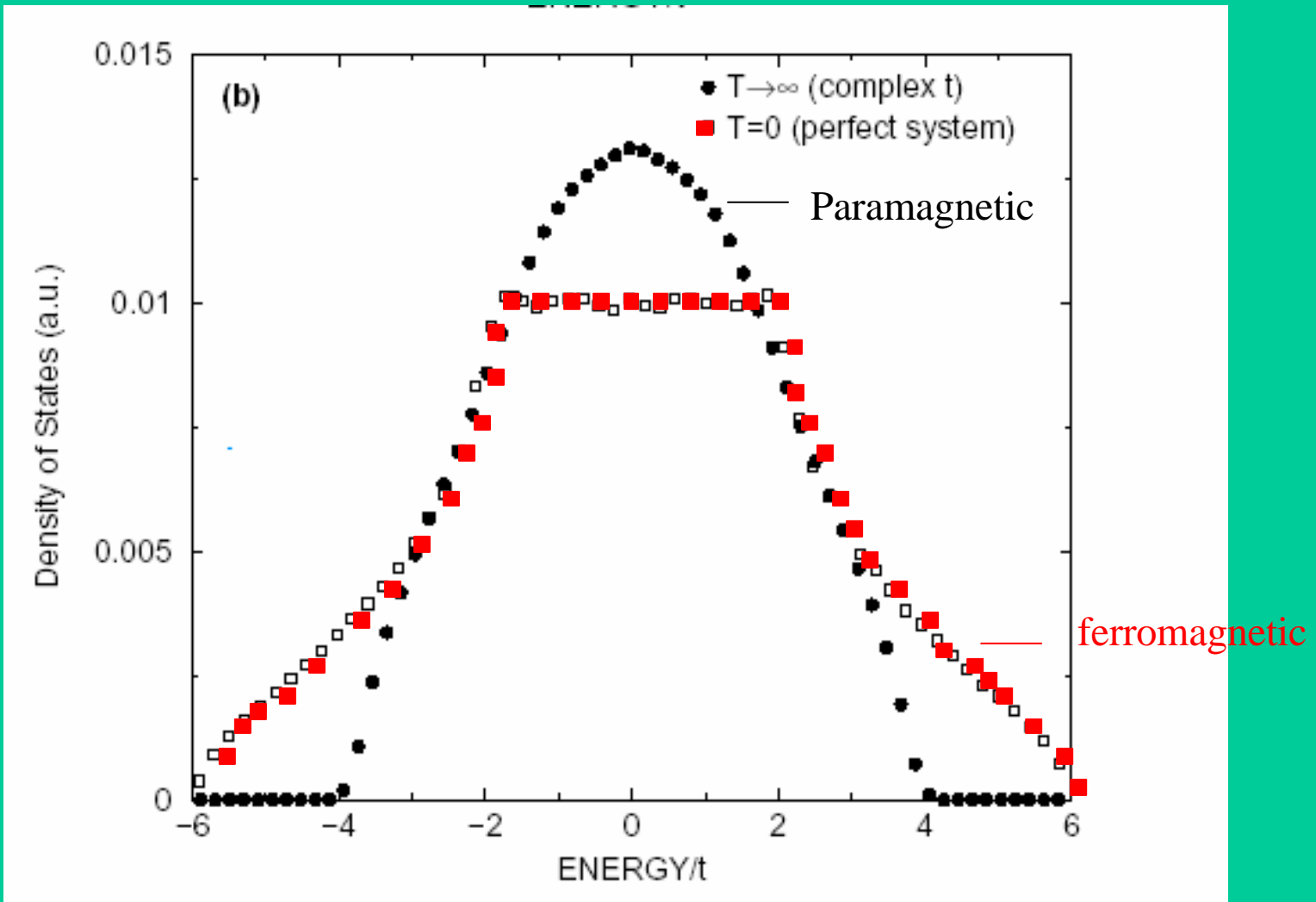
M.J.Calderón an L.Brey PRB '98

ELECTRONIC PROPERTIES AS A FUNCTION OF T IN THE DE MODEL

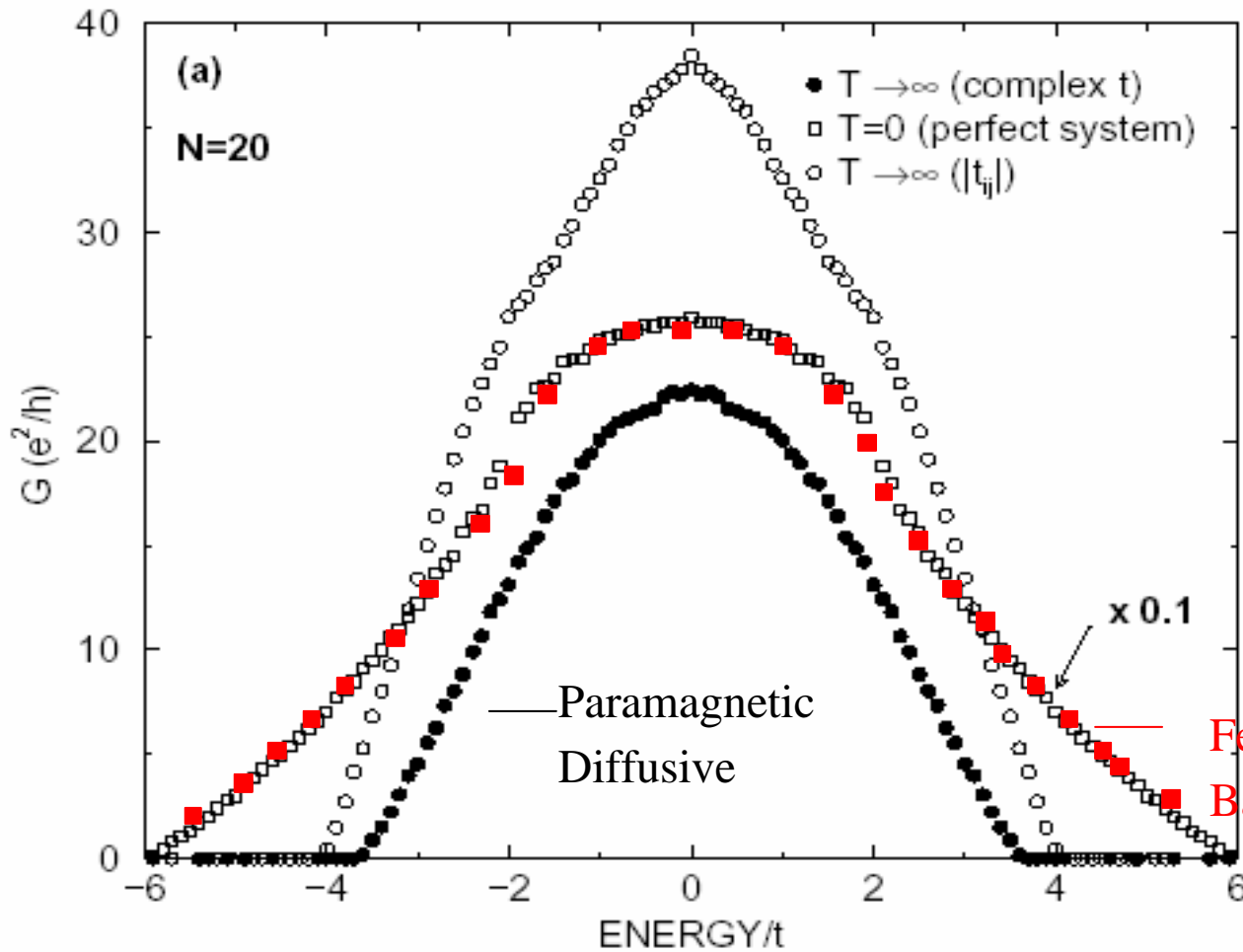


M.J.Calderón an L.Brey PRB '98

DENSITY OF STATES IN THE DE MODEL.



CONDUCTANCE IN THE DE MODEL.

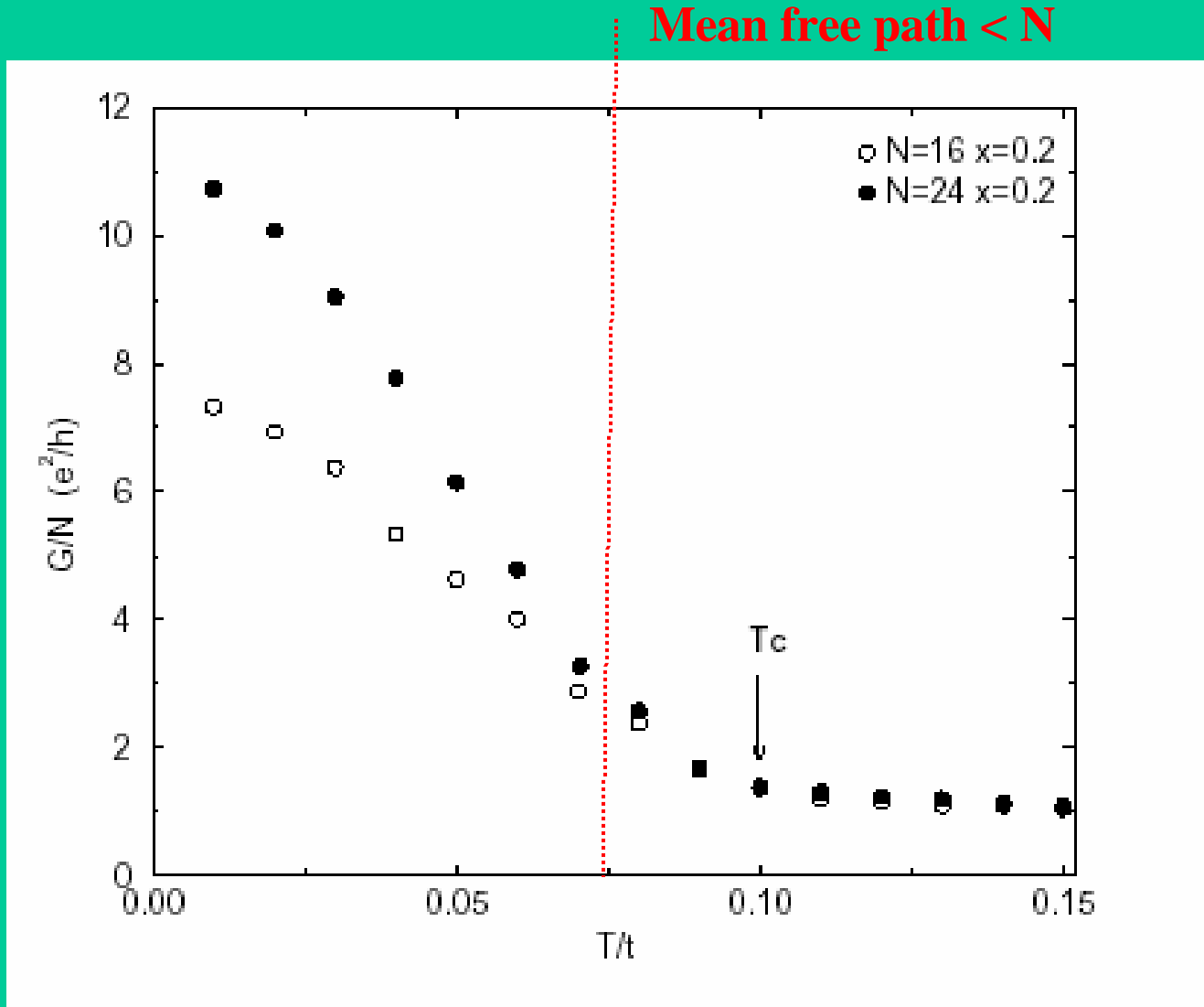


T[®] 8 Localized electro

$$-4t < E < -3.6t$$

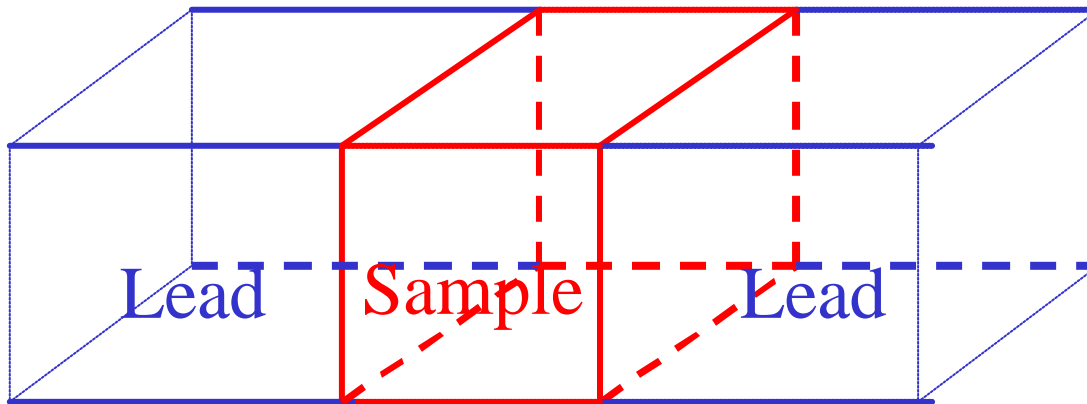
$$x \ll 0.1$$

Conductivity



M.J.Calderón, J.A.Vergés and L.Brey PRB '99

DC-CONDUCTANCE



KUBO FORMULA

$$G = \mathbf{s}_{zz}(0) = -2 \frac{e^2}{h} \text{Tr} \left[\hbar v_z \text{Im} \hat{G}(\mathbf{m}) \hbar v_z \text{Im} \hat{G}(\mathbf{m}) \right]$$

DUBLE EXCHANGE MODEL
ALONE CAN NOT EXPLAIN
T-DEPENDENT M-I TRANSITION.

A LATTICE-SPIN MECHANISM (1)

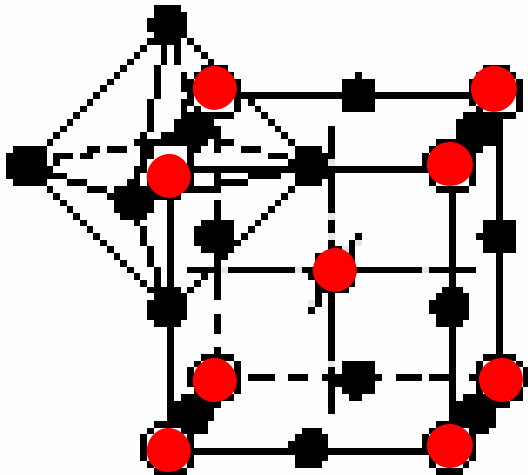
-Model-

$$H = K_{KE} + H_{HUND} + H_{e-ph} + H_{ph}$$

$$H_{KE} + H_{HUND} = -t \sum \cos \frac{\mathbf{q}_{ij}}{2} e^{i\mathbf{f}_{ij}/2} C_i^+ C_j$$

$$H_{ph} = t \sum (u_{i,a})^2$$

$$H_{e-ph} = -1t \sum \underbrace{(u_{i,-a} - u_{i,a})}_{\text{phonon}} \underbrace{C_i^+ C_i}_{\text{electron}}$$



CARRIERS COUPLED WITH CLASSICAL COOPERATIVE PHENON.

BREATHING MODES OF THE OXYGEN OCTAHEDRA.

$u_{i,a}$: are the oxygen displacements.

The carrier couples with the change of volume in the oxygen octahedra around it.

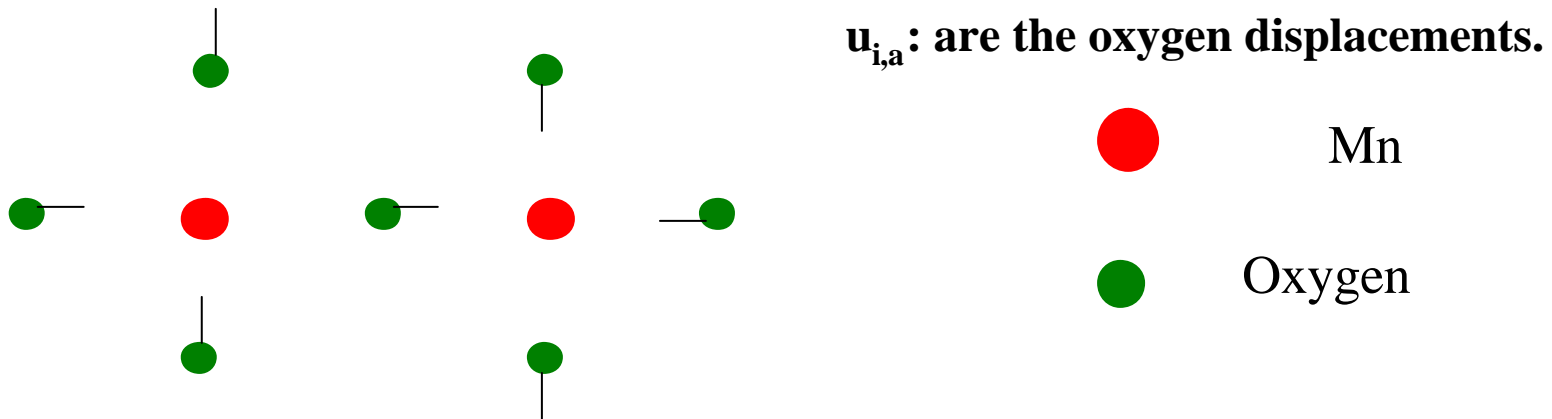
A LATTICE-SPIN MECHANISM (2)

$$H_{KE} + H_{HUND} = -t \sum \cos \frac{\mathbf{q}_{ij}}{2} e^{i\mathbf{f}_{ij}/2} C_i^+ C_j$$

$$H_{ph} = t \sum (u_{i,a})^2$$

$$H_{e-ph} = -1t \sum (u_{i,-a} - u_{i,a}) C_i^+ C_i$$

CARRIERS COUPLED WITH CLASSICAL COOPERATIVE PHENON. BREATHING MODES OF THE OXYGEN OCTAHEDRA.



Cooperative. Distortions are inhomogeneous.

A LATTICE-SPIN MECHANISM (3)

$$\frac{I}{\langle KE \rangle} \quad ,, \quad \langle KE \rangle (T)$$

T-dependent polaron formation

MONTE CARLO SIMULATIONS.

- Classical variables, S_i and $u_{i,a}$
- **INTERNAL ENERGY: KE of electrons. It is obtained by diagonalizing the Hamiltonian.**
- Lattice sizes 6x6x6. Checked with 4x4x4.
- Electrons at $T=0$.
- Kubo formula for electron conductance.

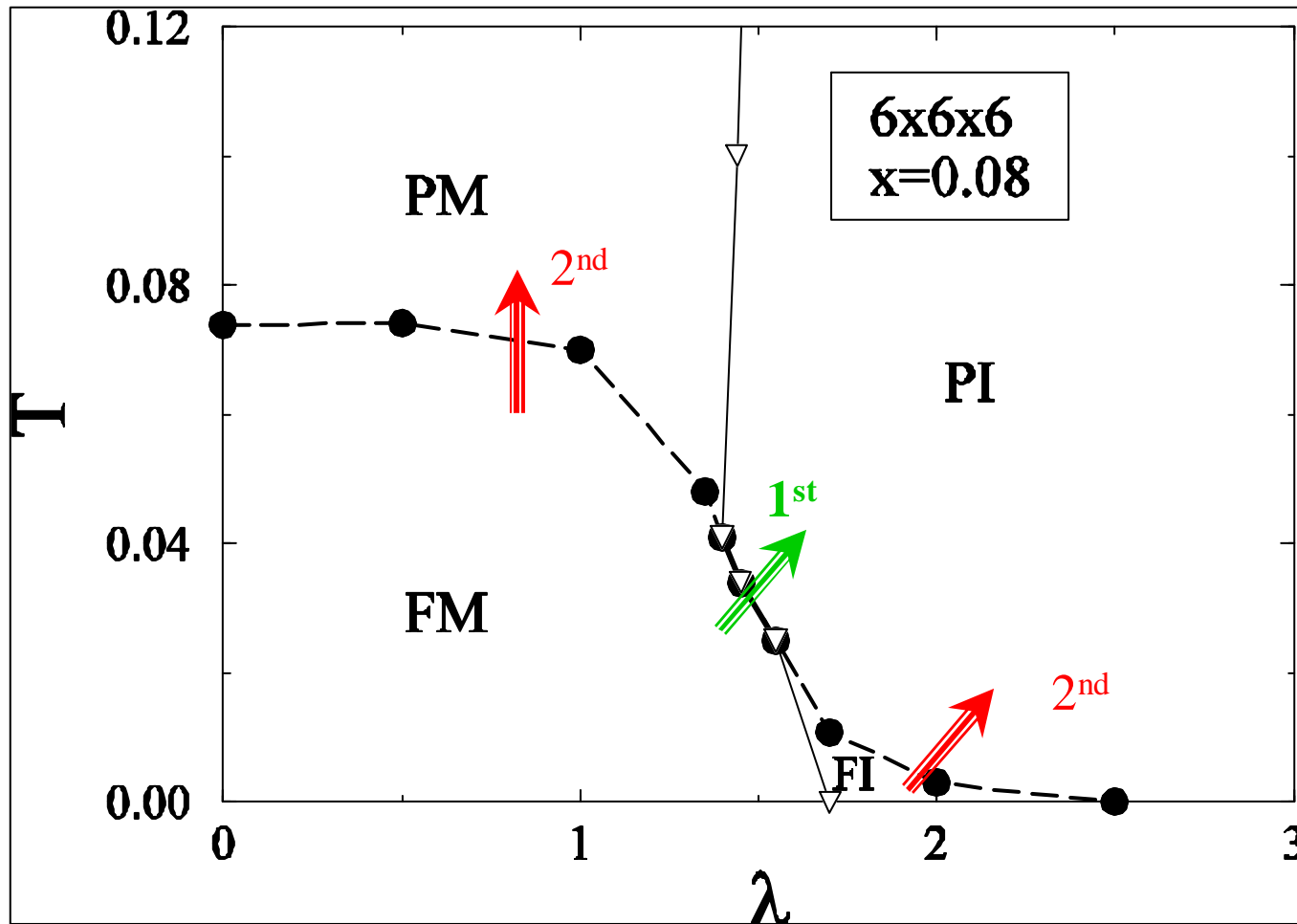
• **MAGNETIZATION.**

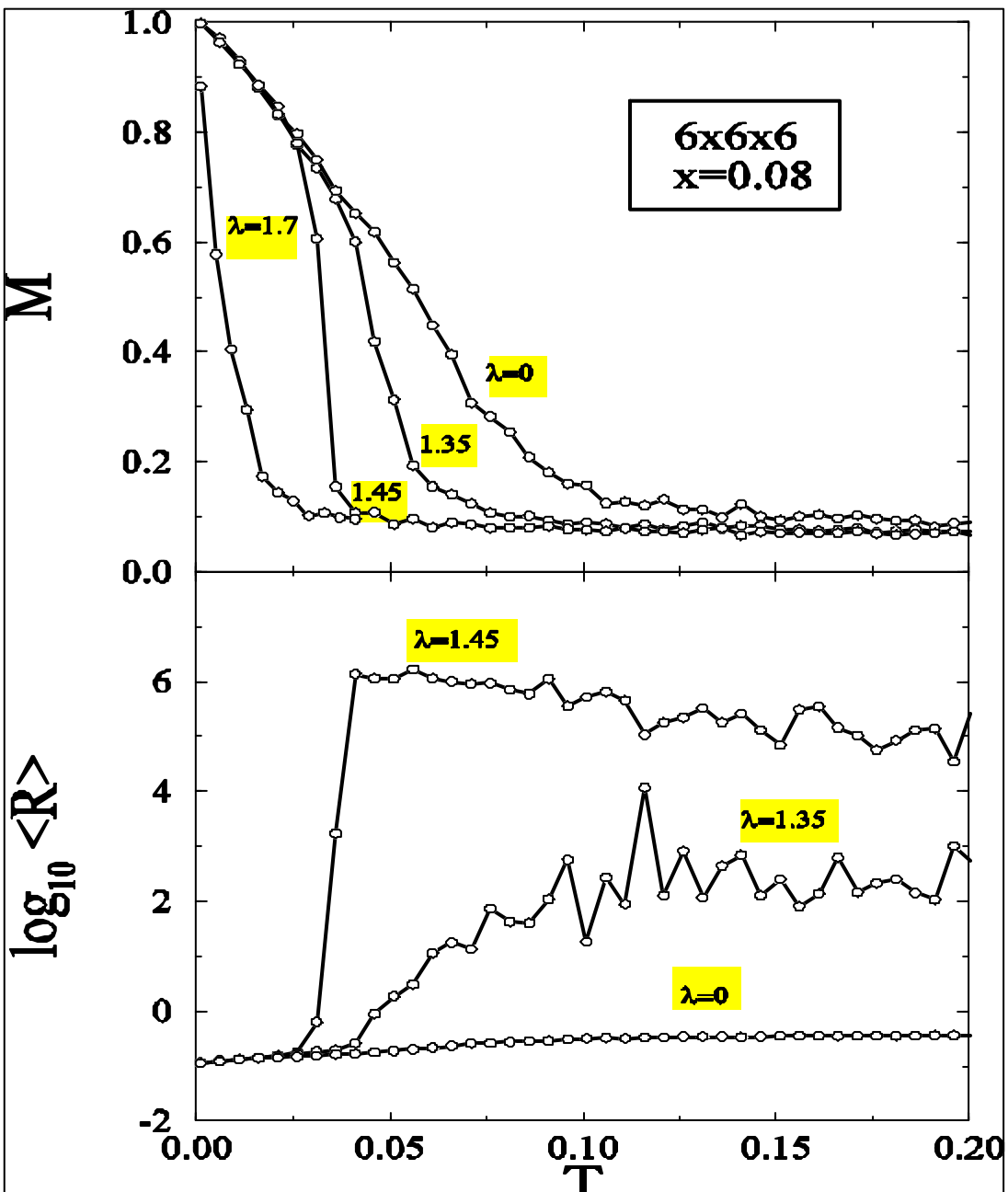
• **RESISTANCE.**

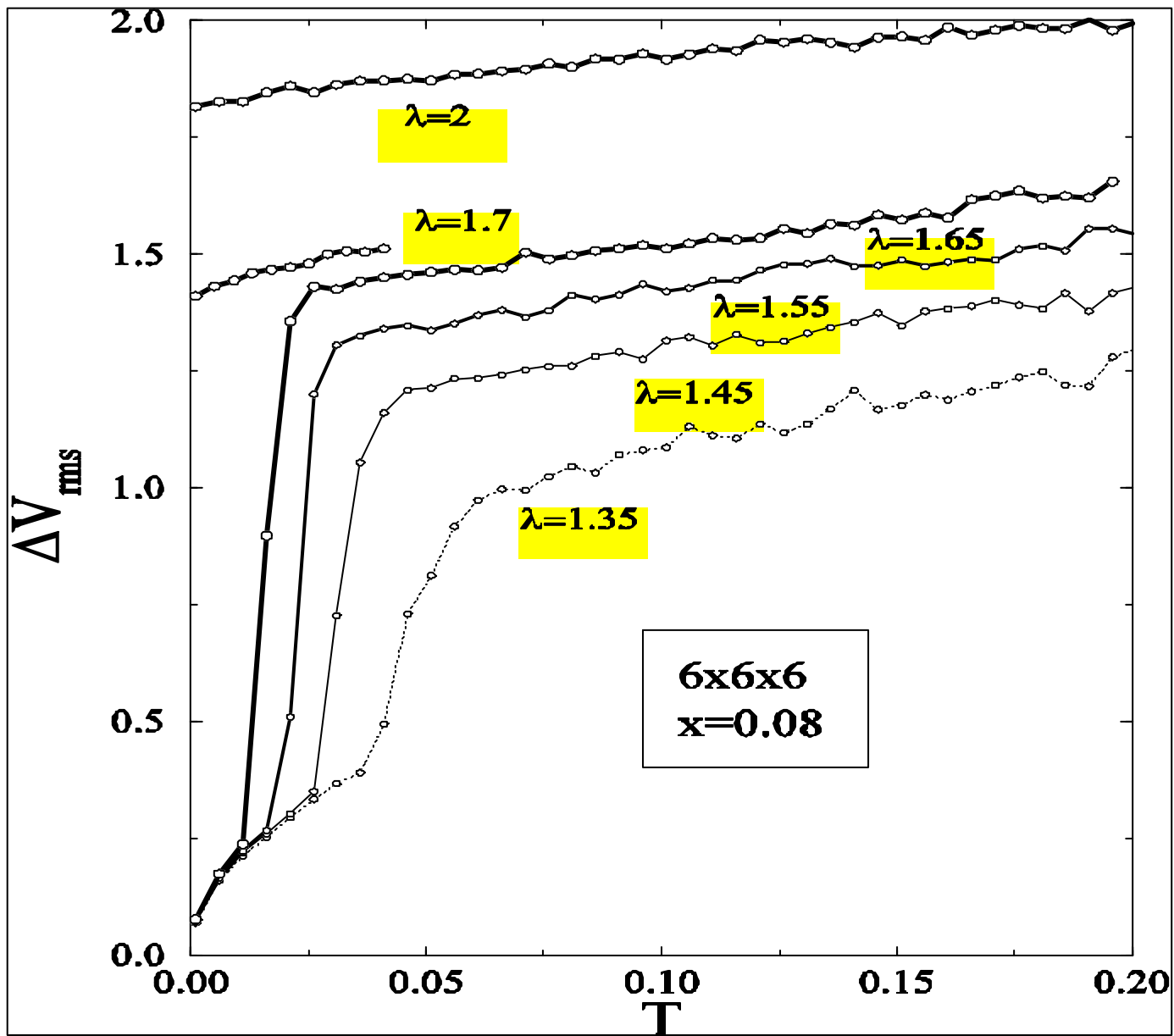
• **DOS.**

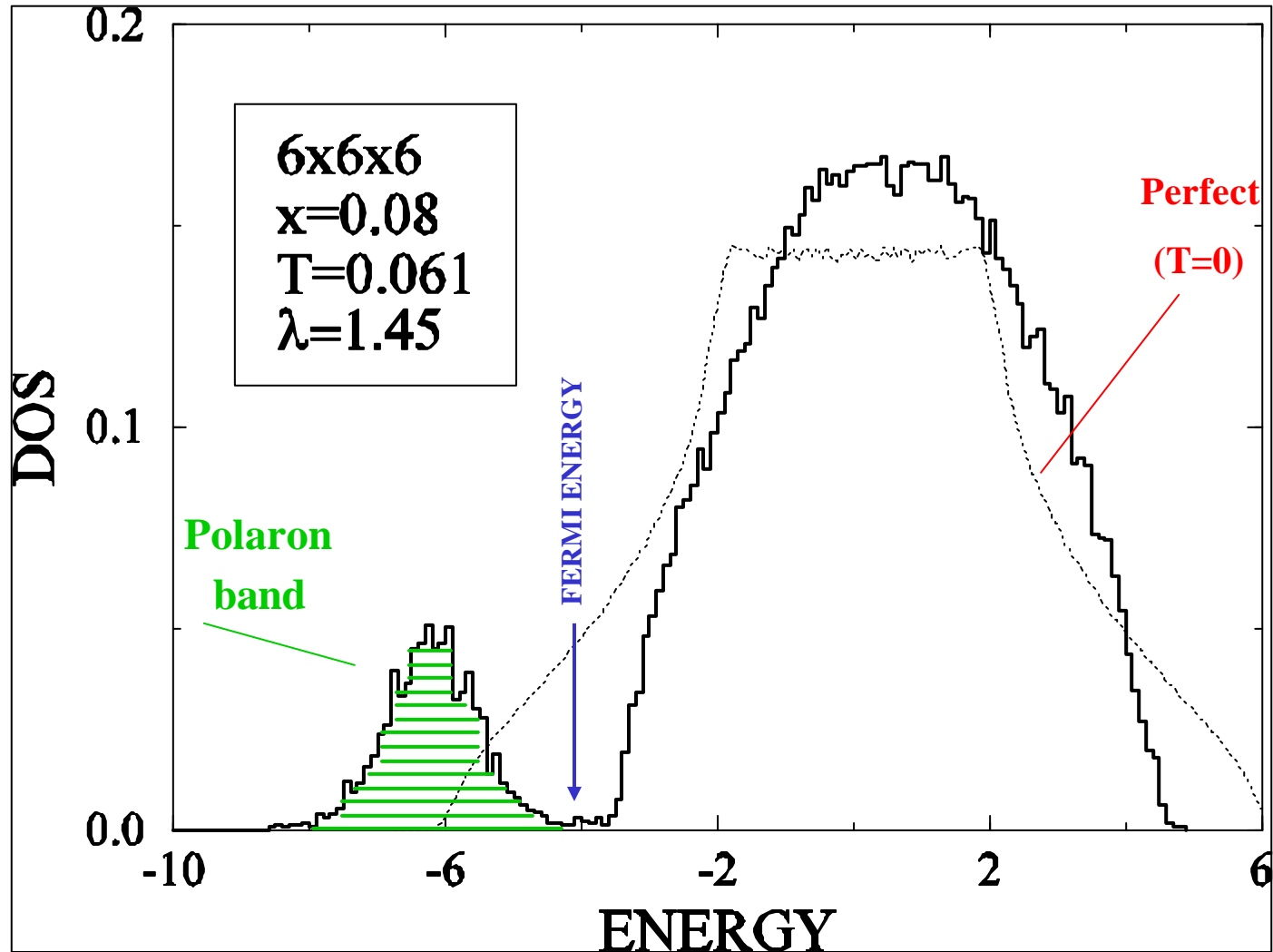
• **OCTAHEDRA DISTORTIONS.**

.....









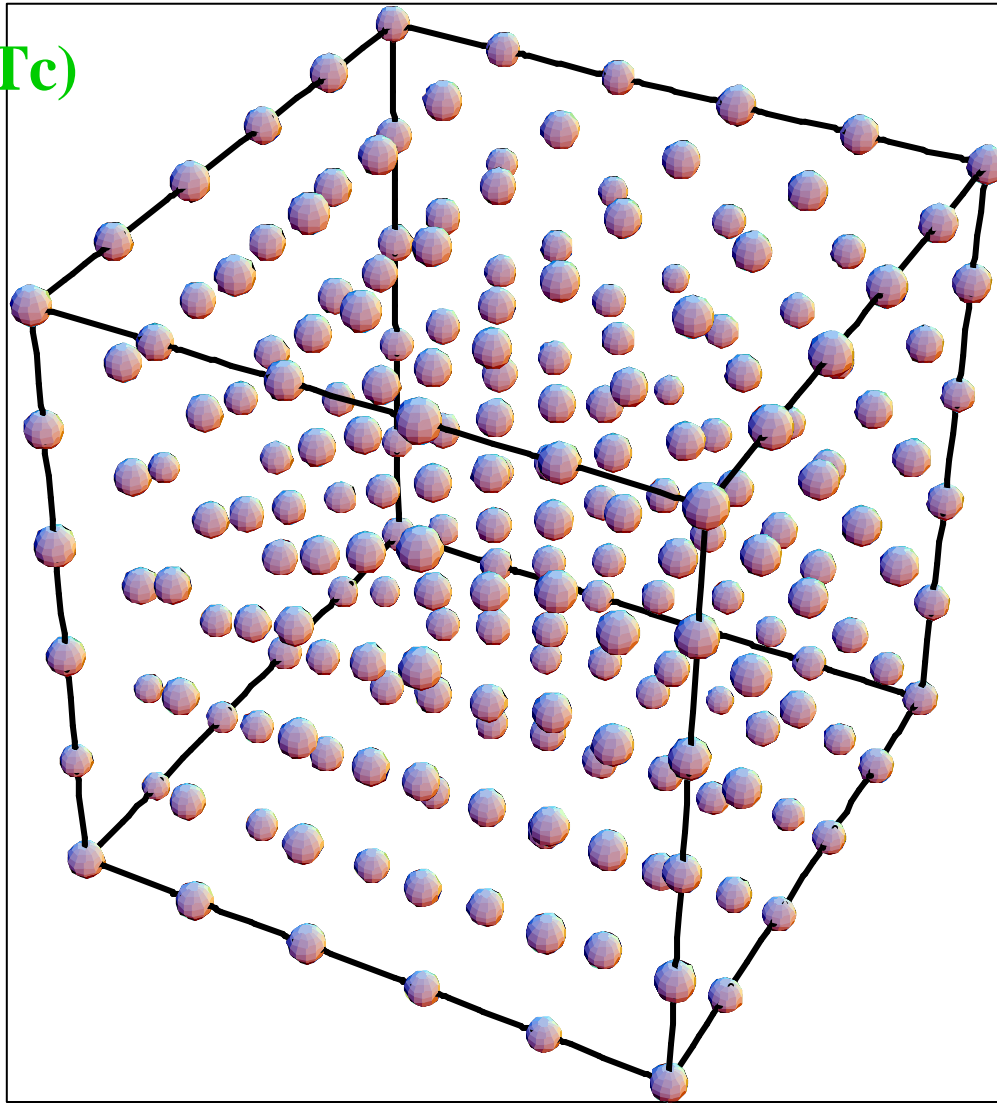
6 x 6 x 6

X=0.08 (17 electrons)

T=0.006 (T<T_c)

NO POLARONS

Ferromagnetic.



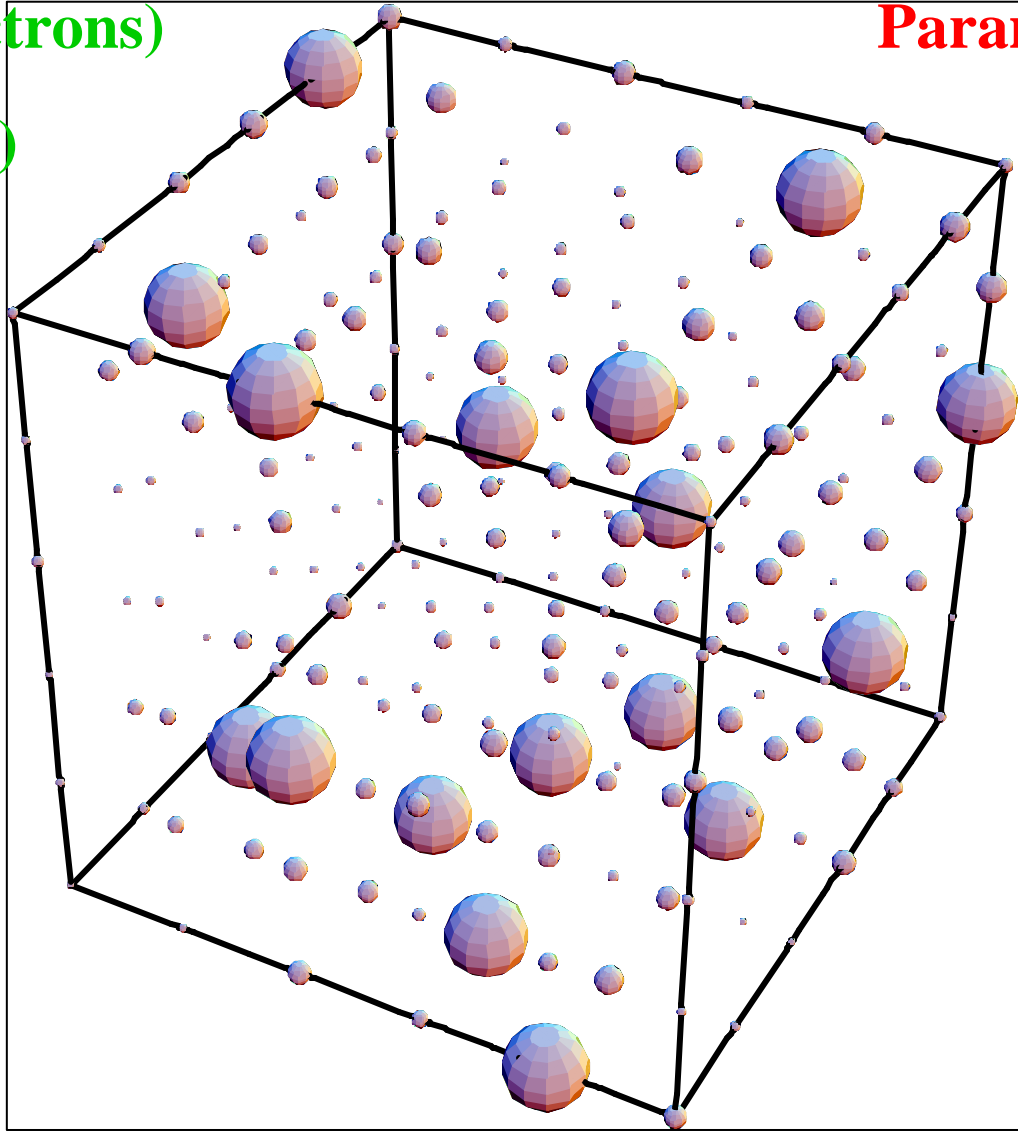
6 x 6 x 6

17 POLARONS

X=0.08 (17 electrons)

Paramagnetic.

T=0.121 (T>T_c)



WE STUDY A **DE** MODEL COUPLED WITH CLASSICAL COOPERATIVE PHONONS. (breathing modes of the oxygen octahedra)

•Monte Carlo Simulations.

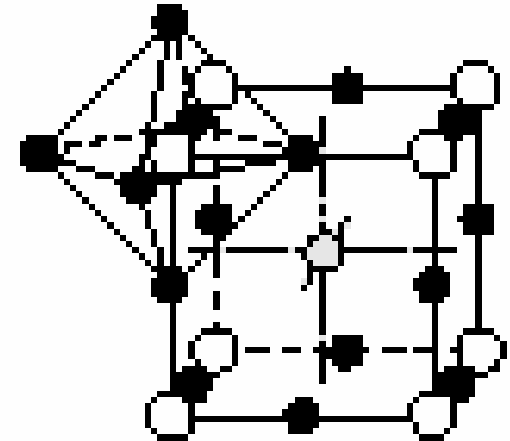
•MAGNETIZATION.

•RESISTANCE.

•DOS.

•OCTAHEDRA DISTORTIONS.

.....



CONCLUSIONS

•For a finite range of doping and el-phonon coupling constant, a first order **M-I** phase transition, that coincides with a **F-P** transition occurs.

•The insulating phase is due to the self-trapping of every carrier within an oxygen octahedron distortion. (**POLARON**)