Motterials – 2007, some thoughts

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- ✓ Some thoughts – not a summary of the talks!
- ✓ General problems – but also with the motto:
  - How to make models realistic?
- ✓ Highlights:
  - 1. Orbitals
  - 2. Multiferroics
  - 3. Frustrations
  - 4. Interfaces / multilayers

  - ▲ a) Multiplets, $\lambda \vec{l}\vec{s}$
  - ▲ b) Negative charge transfer gaps & oxygen holes
  - ▲ c) General fundamental problems

1. Orbital physics

- ✓ Not a new topic ; active in ~1970 („Cooperative Jahn-Teller Effect")
- ✓ New life / fashionable : (HTSC) ; CMR
- ✓ Recent development :
  - reduced dimensionality due to orbital ordering
  - orbitals & frustrations
  - quantum effects

Fundamental questions ? → Quantum effects (∈ vibronic effects)

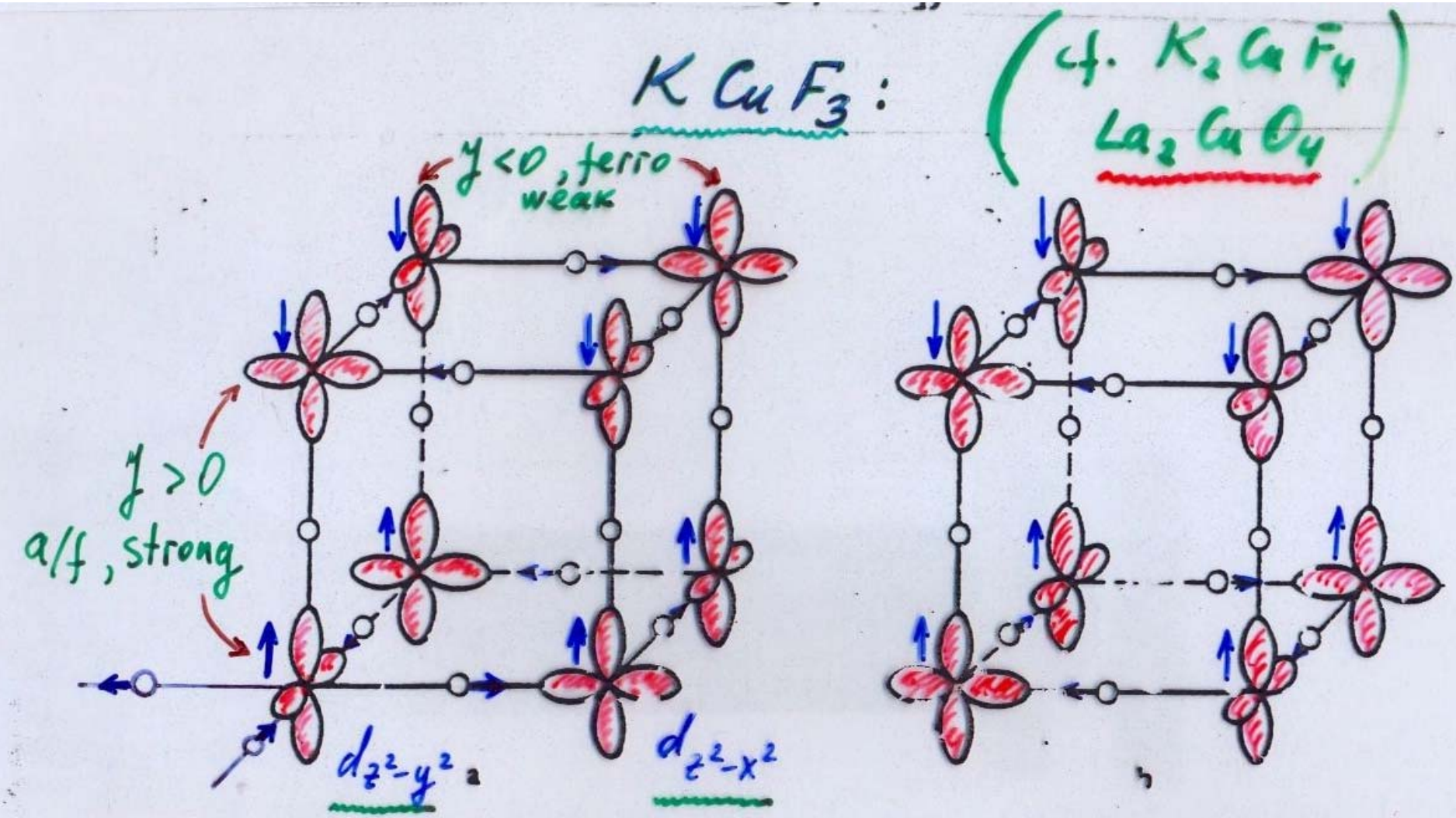
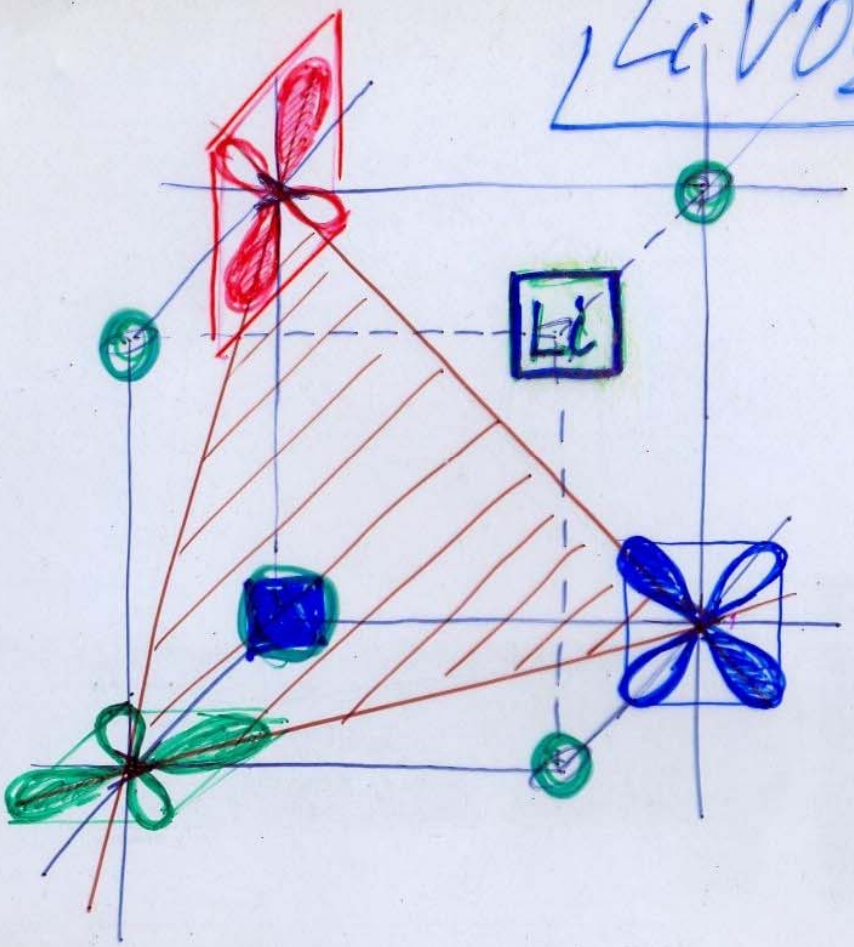


FIG. 3. Two equivalent types of ordering of singly-occupied orbitals in perovskites, obtained in the superexchange model. The figure shows the anion displacements produced for a hole orbital (Cu^{2+} ion).

- Nearly cubic, but 1-d antiferromagnet!

in the plane perpendicular to the c axis, the orbital

$LiVO_2$

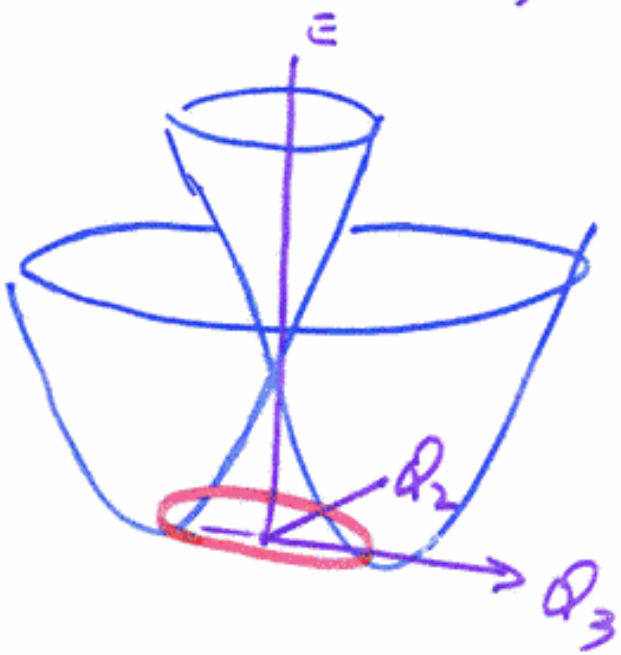


I order phase transition at 450 K
semiconductor - semiconductor,
spin gap opens at $T < T_c$

- Vibronic states

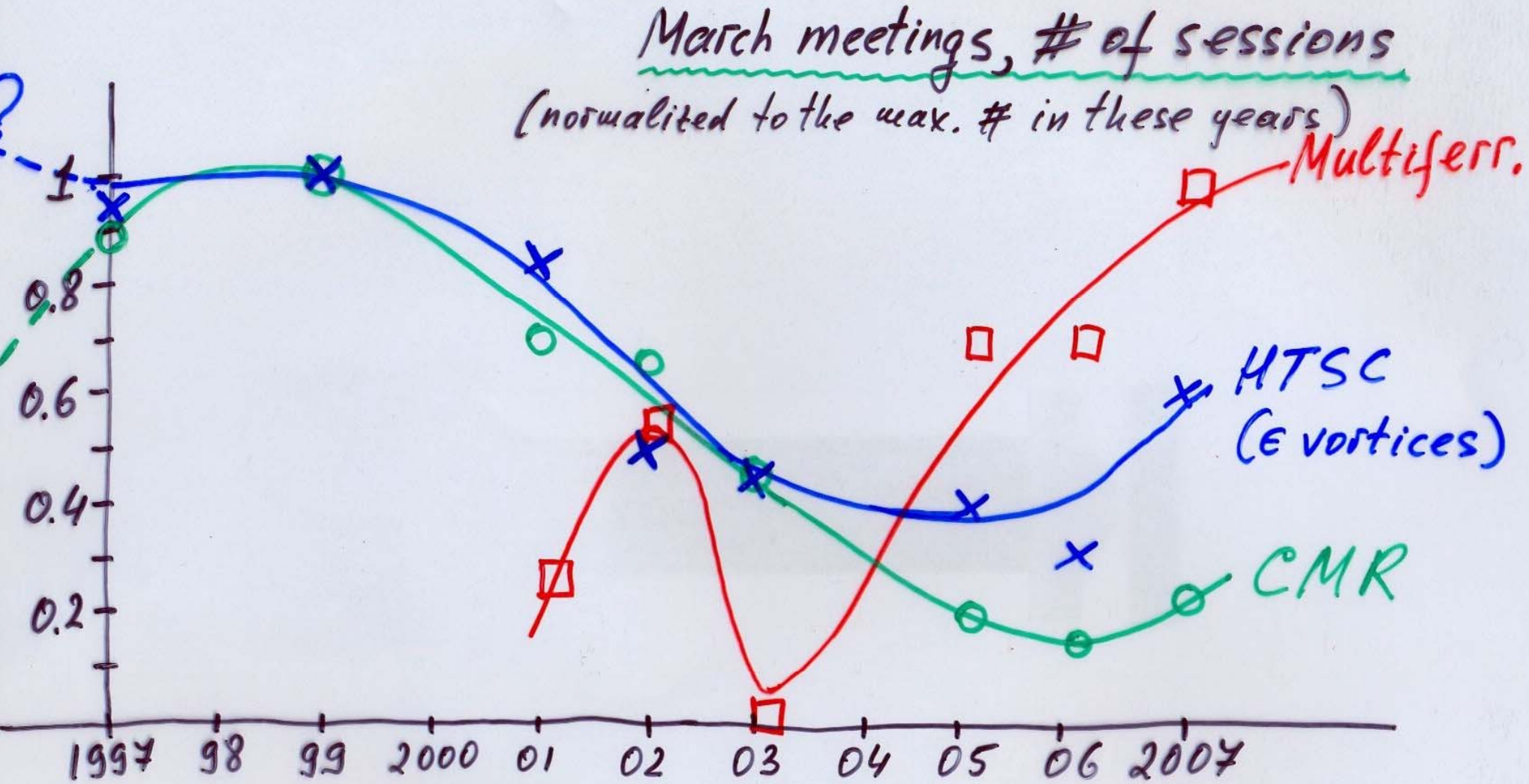
Adiabatic: $|1,2\rangle = |\psi_{1,2}\rangle \cdot |\varphi\rangle$

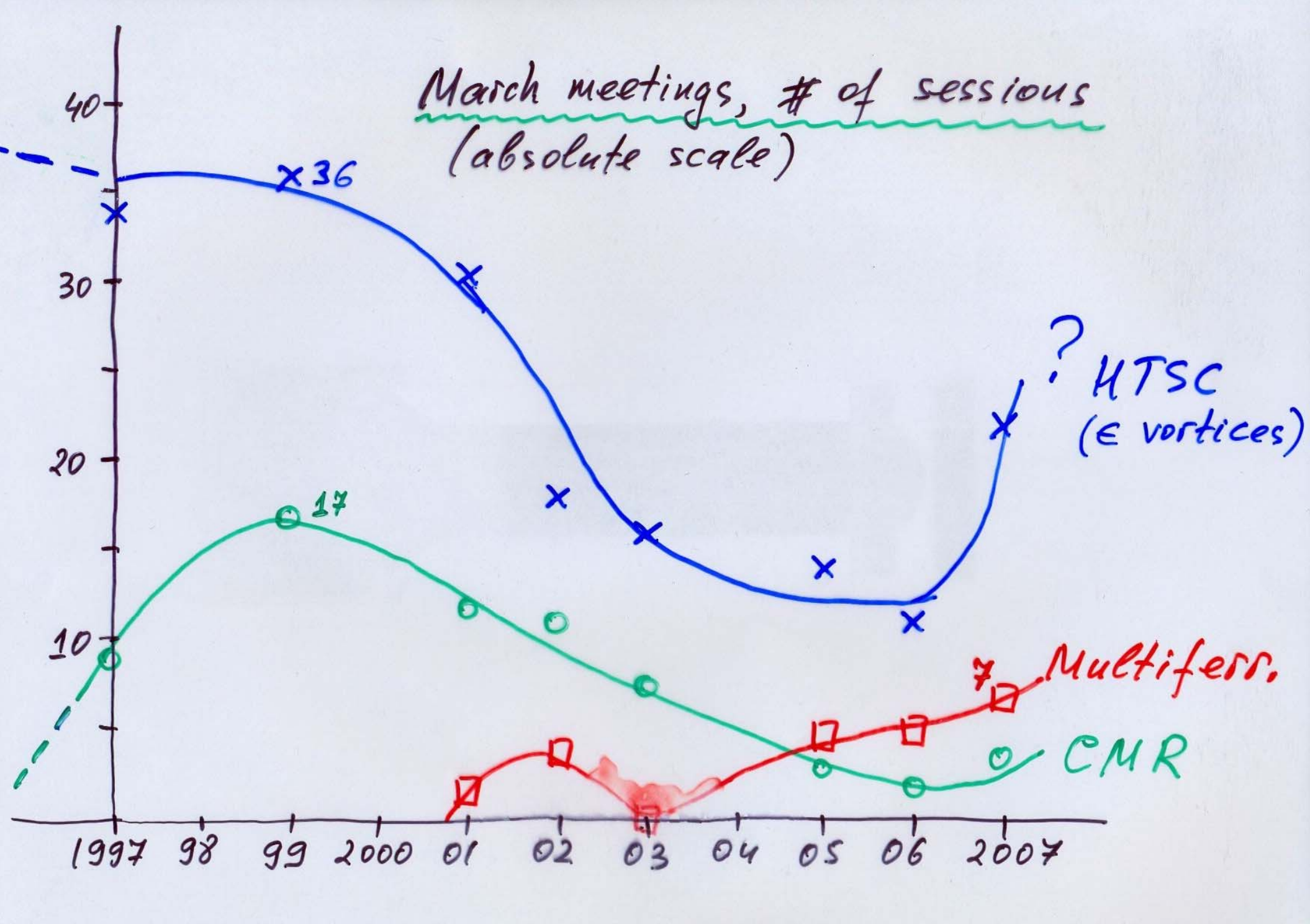
Vibronic: $|1,2\rangle = \begin{cases} |\psi_1\rangle|\varphi_1\rangle \\ |\psi_2\rangle|\varphi_2\rangle \end{cases}$



Rotational quantization, Berry phase, etc

Important for concentrated solids ?


March meetings, # of sessions
(normalized to the max. # in these years)
Multiferr.
HTSC
(ε vortices)
CMR
1
0.8
0.6
0.4
0.2
1997
98
99
2000
01
02
03
04
05
06
2007


March meetings, # of sessions
(absolute scale)
40
30
20
10
36
17
7
? HTSC
(∈ vortices)
Multifers.
CMR
1997
98
99
2000
01
02
03
04
05
06
2007

2. Multiferroics

✓ Also not a completely new story: 1960-1970-th, mostly in USSR

✓ Revival of interest - from ~2001

(even more exact date - goes back to (K)ITP, workshop on Quantum Spin Systems here in 1999)

✓ New life: from the discovery of magnetically-driven FE

($TbMnO_3$ - T. Kimura & Y. Tokura; $TbMn_2O_5$ - S.-W. Cheong)

✓ 2 types: • 1) „Independent" magnetic & FE subsystems

• 2) Magnetically-driven FE

▲ 2a) „Spirals", $\vec{P} \sim \vec{Q} \times \vec{e}$ (Katsura-Nagaosa; Mostovoy)

Mechanisms:

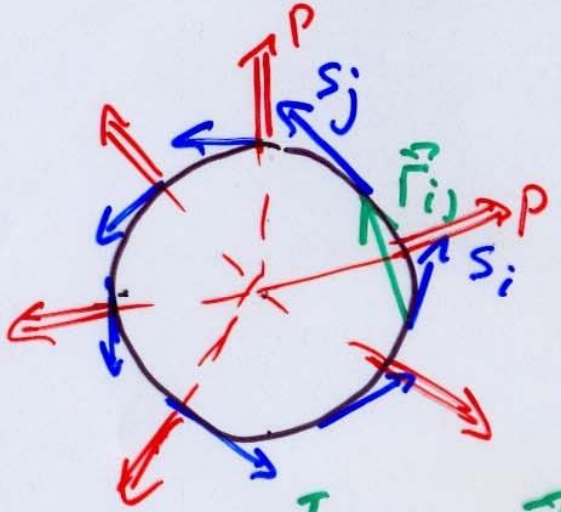
▲ 2b) Magnetostriction

Fundamental open questions ?

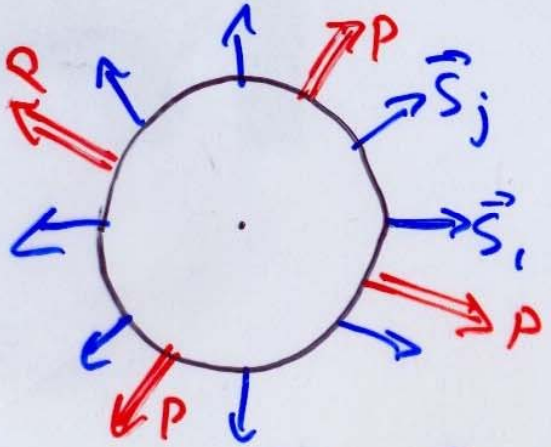
✓ May be (role of) toroidal moments ?

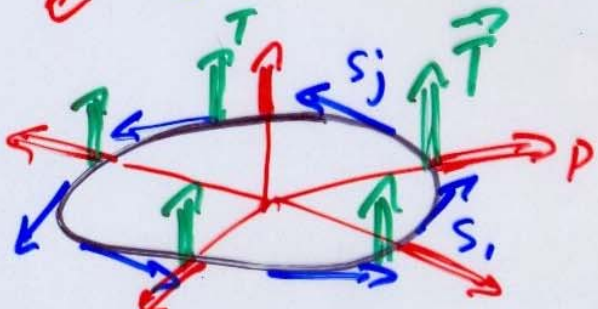
$\vec{\vec{T}} = \sum \vec{r}_i \times \vec{s}_i$, $\sim \vec{P}_i \times \vec{M}_i$; breaks P & T-invariance

↑ May depend on the choice of coordinates! (C. Ederer)



$\vec{P} \sim \vec{r}_{ij} \times [\vec{s}_i \times \vec{s}_j]$





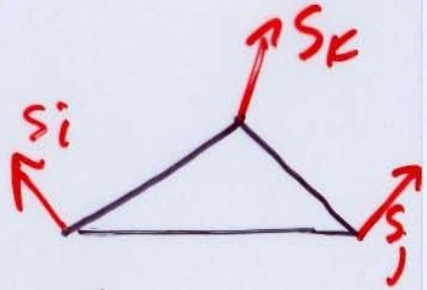
$\vec{\vec{T}} \neq 0$

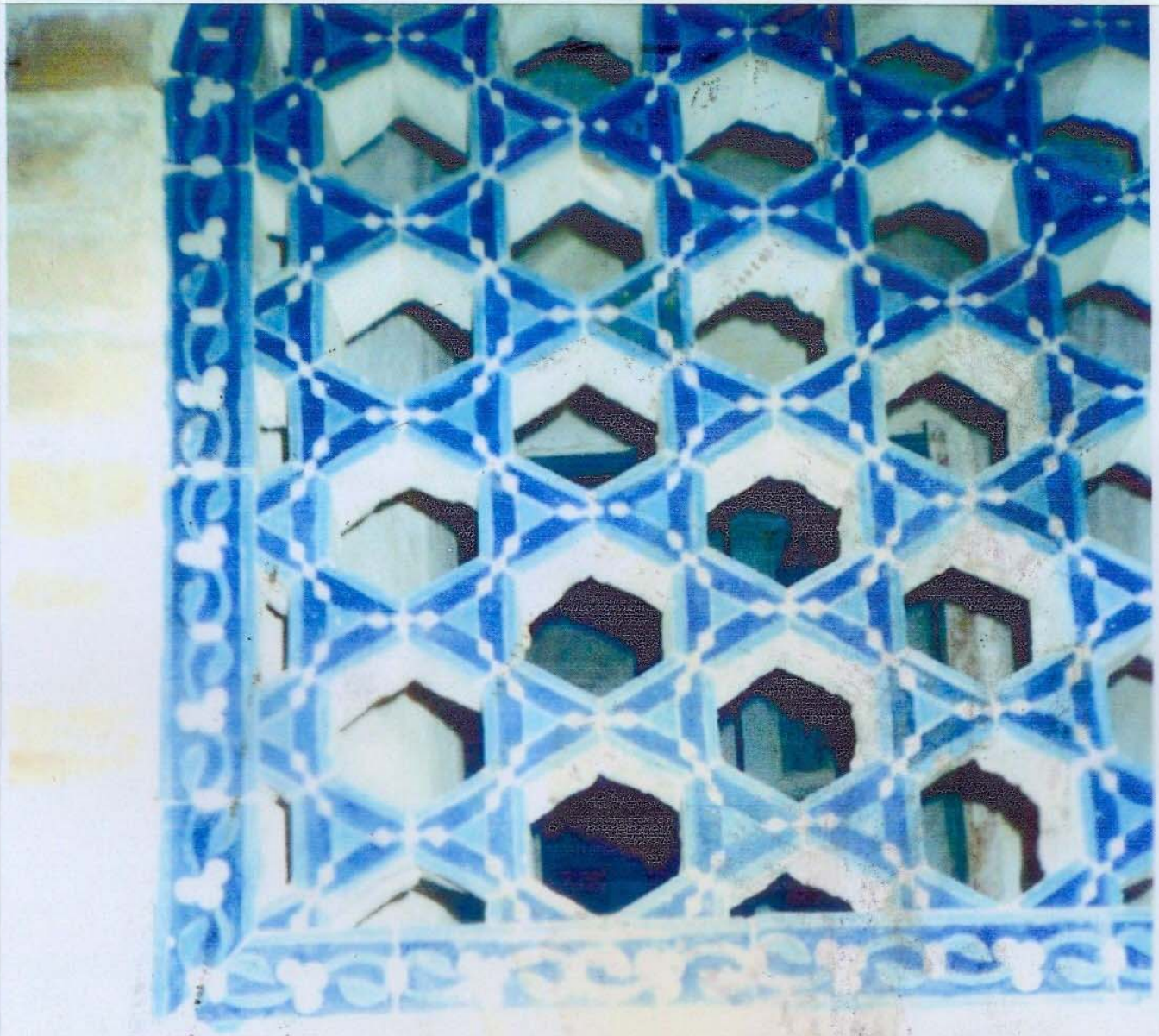
But here $\vec{\vec{T}}_i \sim \vec{P}_i \times \vec{S}_1 = 0$!

[No one-to-one correspondence with multiferroicity !]

3. Frustrations

- Really deep & open problems: type(s) of ground state? types of correlations? Spin-liquid state(s)? Unusual types of ordering? (e.g. chiral states)
- (Scalar) chirality: $\chi_{ijk} = \vec{S}_i \cdot [\vec{S}_j \times \vec{S}_k]$





Bukhara, „Kagome" window
(Uzbekistan) in medrese (1400-1500)

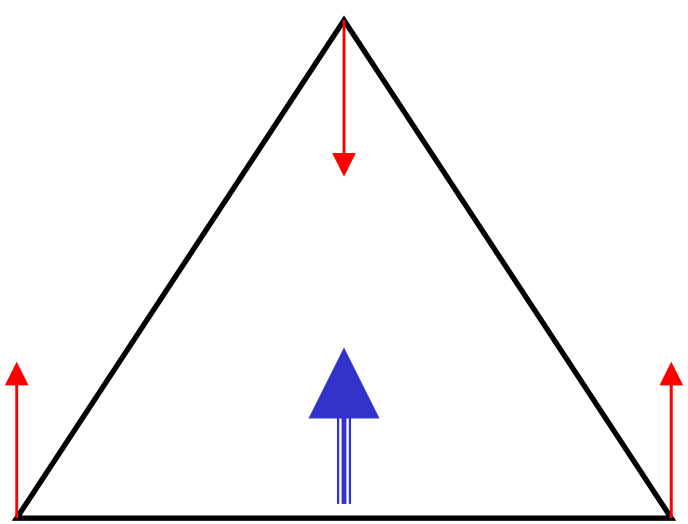
(L. Bulaevskii, Ch. Batista, M. Mostovoy & D. Kh.) : **Real electric effects** in (strong) Mott insulators $U \gg t$, $n = 1$

- Spontaneous circular electric currents (and corresponding orbital moments)

$$I \sim \frac{e}{\hbar} \frac{t^3}{U^2} \vec{S}_1 \cdot [\vec{S}_2 \times \vec{S}_3]$$

- Spin-driven charge redistribution (and possible dipole moments)

$$\delta Q_i \sim \frac{t^3}{U^2} [\vec{S}_1 (\vec{S}_2 + \vec{S}_3) - 2\vec{S}_2 \vec{S}_3]$$



4. Interfaces, multilayers etc

✓ A lot of possibilities, extra freedom

✓ Large part of the physics until now - classical
(polar surfaces & charge redistribution;
image charges; „2d screening" (but embedded into 3d!)

✓ Novel effects due to correlations ?
(magnetism; charge ordering; ..... ?)

a) Multiplet effects, spin-orbit coupling $\lambda \vec{l}\vec{s}$

✓ Often very important practically, but often ignored

$g_s = 2$, $g_e = 1 \Rightarrow \vec{M} = g_e \vec{l} \pm g_s \vec{S}$

- E.g. t_{2g}^1 (Ti^{3+}): $l_{eff} = -1$, $S = \frac{1}{2} \Rightarrow M = 0$!
  (or g-factor = 0)
  $L \neq 0$, $S \neq 0$
  - but nonmagnetic!
- Or: Ru^{4+} (=), $L = 1$, $S = 1$

$J = 3; 2; 1; 0$

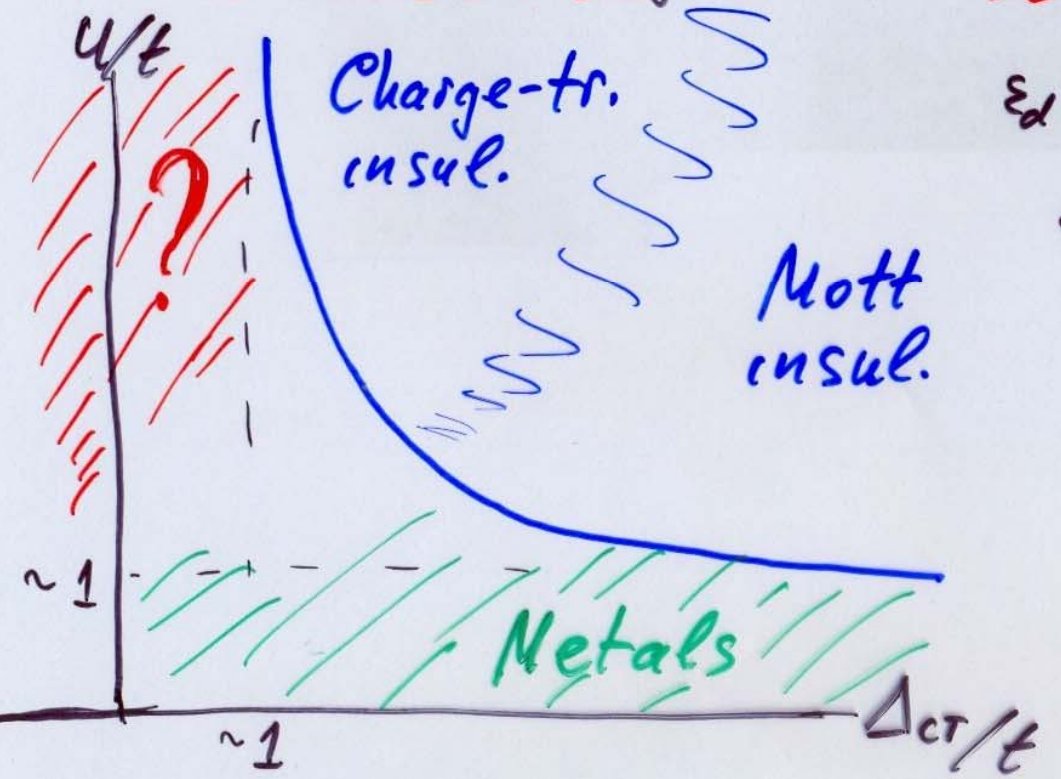
- and may be $J = 0$ ground state!

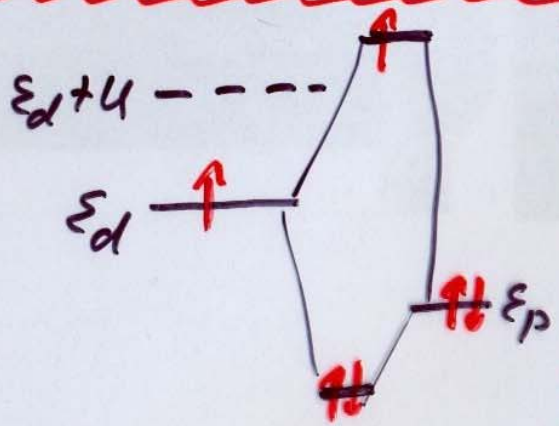
And many other similar effects

b) Small or negative Charge-transfer gaps; oxygen holes

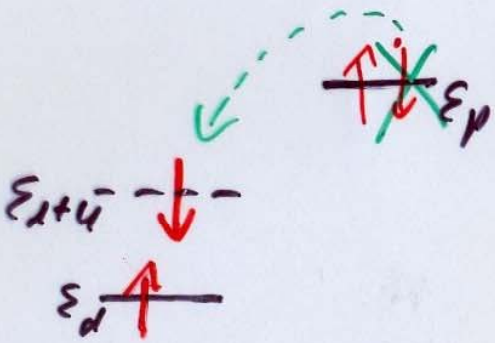
✓ ZSA: new paradigm; have to reconsider many previous interpretations

✓ Novel physics? Qualitative effects?





$\Delta_{CT} > 0$

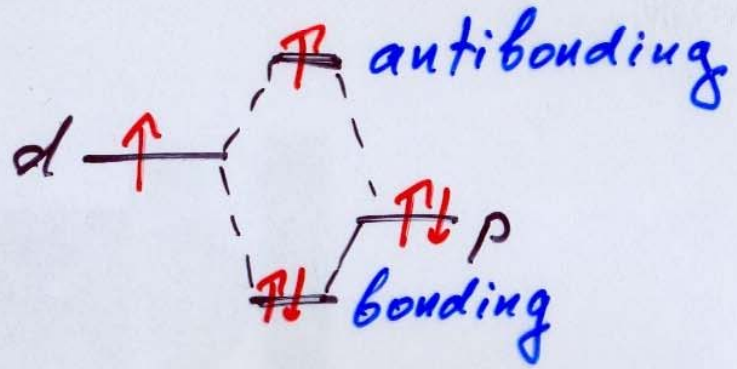


$\Delta_{CT} < 0$

⇒ oxygen holes (self-doping)

- Type of the ground state for $\Delta_{CT} \lesssim 0$?
  Metal? (Kondo-) insulator? Magnetic structure?
  (High-T_c) superconductor?

✓ Often quantitative effects :



$$|\Psi_{bond.}\rangle = \alpha|p\rangle + \beta|d\rangle$$

$$|\Psi_{antib.}\rangle = \beta|p\rangle - \alpha|d\rangle$$

Naively change of $\Delta_{CT} \Rightarrow$ change of relative weights $|\alpha|^2 \propto |\beta|^2$

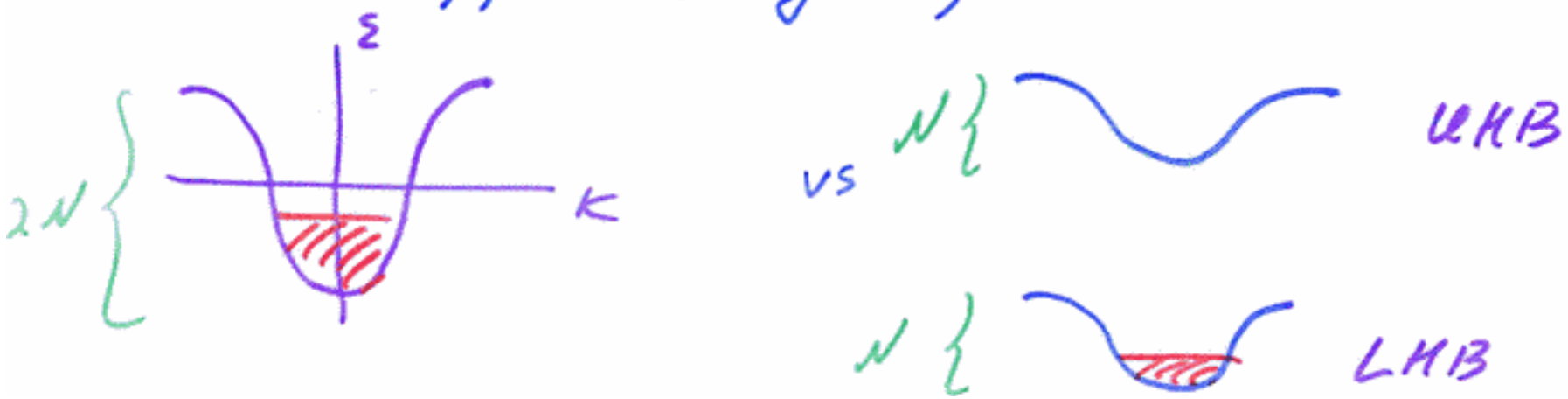
✓ Novel qualitative effects / states?
E.g. spontaneous charge disproportionation ($2Fe^{4+} \rightarrow Fe^{3+} + Fe^{5+}$ etc)

e) Fundamental (open) problems in Mott systems

- Ferromagnetism in simple Hubbard model? (or we need Hund's rule coupling?)
  - ▲ Nagaoka theorem ($U=\infty$, $N_e = N \pm 1$, bipartite) - but not thermodynamic case
  - ▲ Flat bands (Mielke, Tasaki) - rigorous. But very special case
  - ▲ In general?
- Superconductivity in pure Hubbard model?

Many different results, but (for me at least) still not clear

- Nature of single-particle excitations;
  - confinement? etc.; statistics!
  - Large vs small Fermi-surface
  - Hall effect (sign?)



- Order parameter? How to characterize Mott insulator state vs metal? Symmetry?

✓ Not the usual Landau paradigm

$\psi = \langle 0 | \hat{A} | 0 \rangle$; broken symmetry (Landau)

‖ Here: the difference is not just the property of the ground state, but rather of the lowest charge carrying excited states (gap or no gap?)

✓ (Pure) Mott transition: always Ising?

✓ Topological order? (M. Levin & X.-G. Wen; A. Kitaev; ...)

■ Deep questions still open