Title: Unconventional Magnetism and Superconductivity in 3 Dimensional Doped Mott Insulators

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Abstract: Utilizing a variety and also
constraints offered by quantum and solid

state chemistry, we discuss
possibilities of unconventional quantum

magnetism and superconductivity
in doped 3 dimensional Mott insulators.

Some of the possibilities are
quantum spin liquid states having pseudo

fermi surface coexisting with
long range magnetic order, 3 dimensional

emergent gauge fields and
unconventional superconducting order parameter

symmetry. We present a few
realistic models to illustrate this and use our

theory to understand anomalous
behavior of certain double perovskite

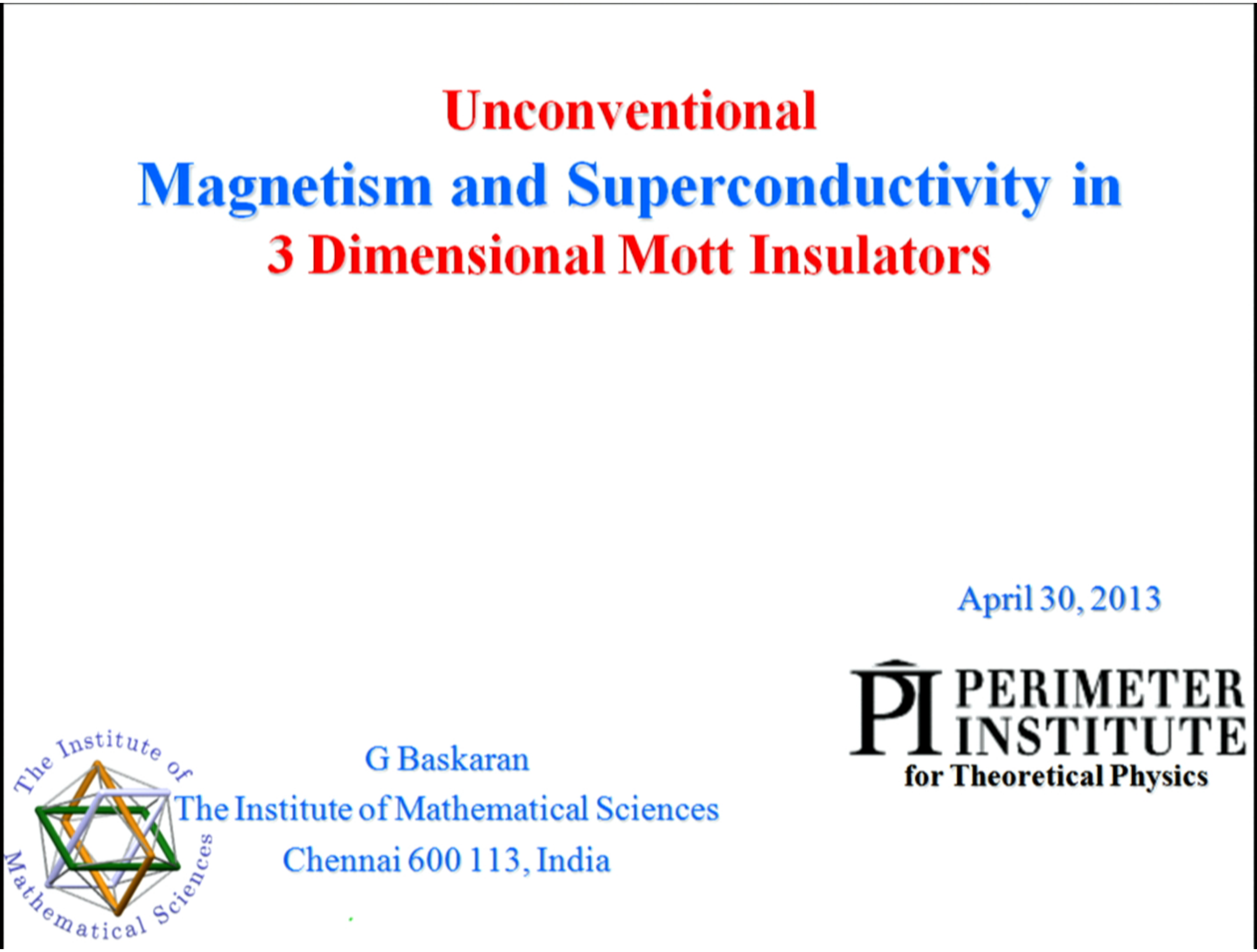
compounds.

Unconventional
Magnetism and Superconductivity in
3 Dimensional Mott Insulators

April 30, 2013

PERIMETER INSTITUTE
for Theoretical Physics

G Baskaran
The Institute of Mathematical Sciences
Chennai 600 113, India



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Mott Insulators as Seat of

Unconventional Magnetism & High Tc Superconductivity

Atomic - Molecular Orbitals, Jahn-Teller Effect , Dimensionality .

Materials Engineering

Cuprates, Iron Pnictides, Fullerites, Bismuthates, …

Two Examples in 3D: Rb_3C_{60} and Sr_2LaRuO_6 family

We are having an Exciting Time in the Field of Quantum Matter

We are witnessing an
Unexpected Richness in the Quantum World

Novel States, New Notions
New Theoretical Ideas, Mathematics and Tools

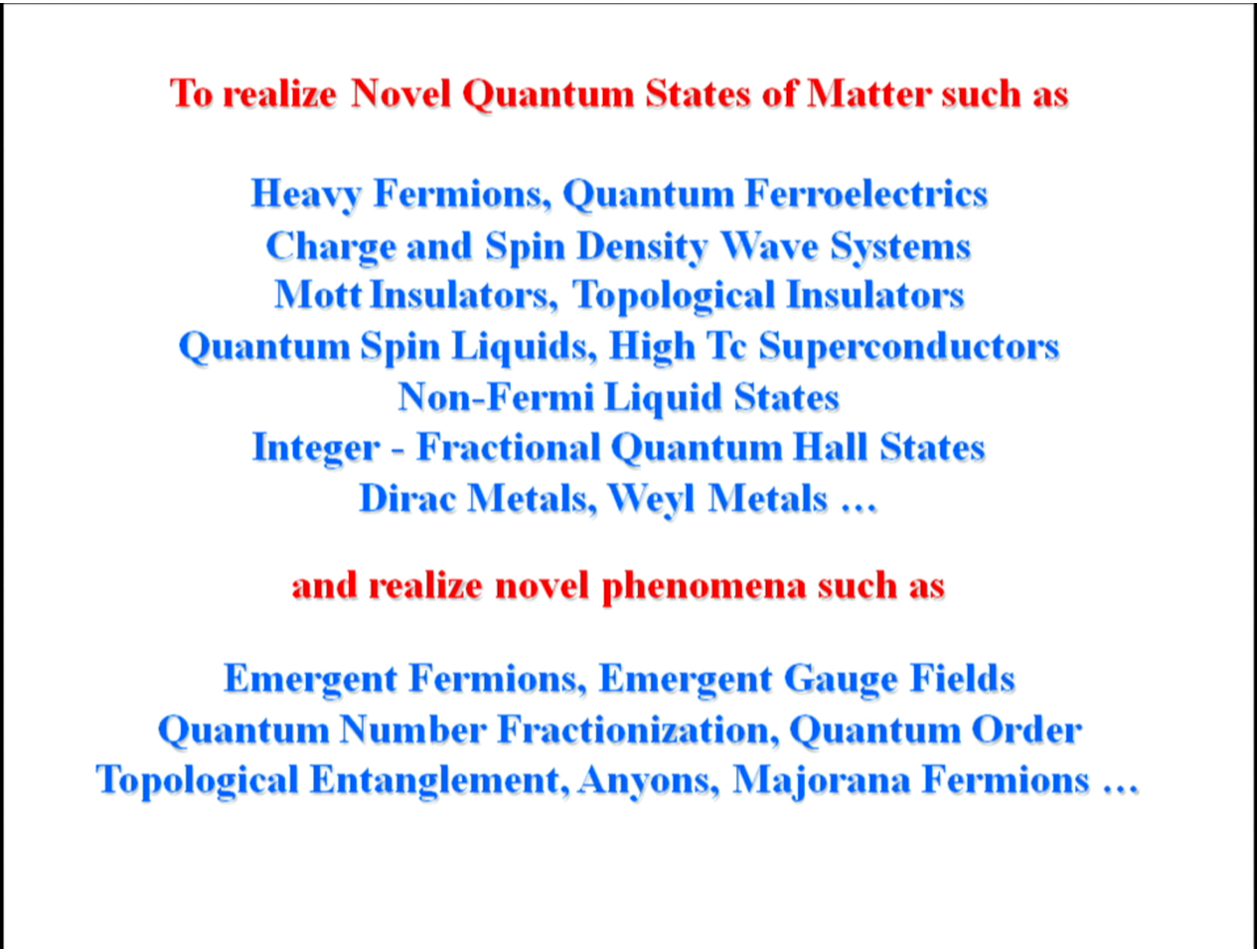
Help from Enlarged Hilbert Space, Parton Construction
Cohomology, DMFT, DMRG, Numerical Methods

Efficient Representations of Low Energy Quantum Many Body States
to gain new insights and address Strong Coupling Problems

MPS, Tensor Networks, MERA …
AdS/CFT Correspondence (an exciting route - full of mystery at the moment) …

To realize Novel Quantum States of Matter such as

Heavy Fermions, Quantum Ferroelectrics
Charge and Spin Density Wave Systems
Mott Insulators, Topological Insulators
Quantum Spin Liquids, High Tc Superconductors
Non-Fermi Liquid States
Integer - Fractional Quantum Hall States
Dirac Metals, Weyl Metals …



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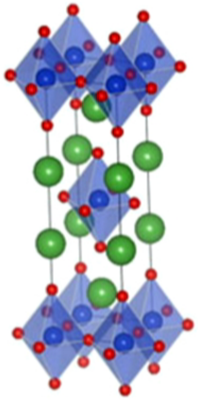
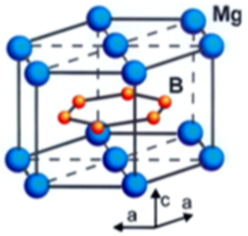
and realize novel phenomena such as

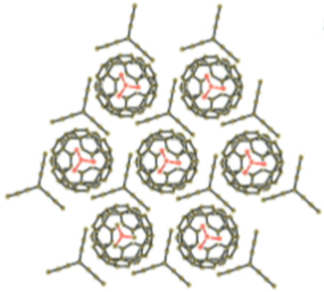
Emergent Fermions, Emergent Gauge Fields
Quantum Number Fractionization, Quantum Order
Topological Entanglement, Anyons, Majorana Fermions …



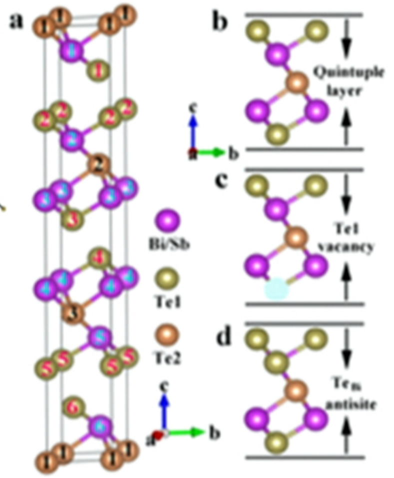
$La_{1-x}Ba_xCuO_4$



MgB_2

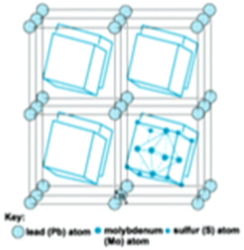


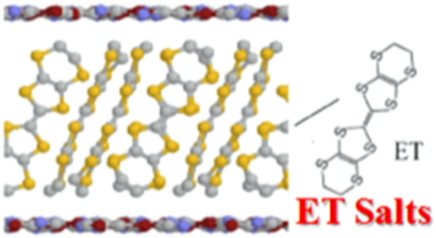
2D Fullerene Metal



Topological Insulator
Bi_2Se_3

Chevrel Phase

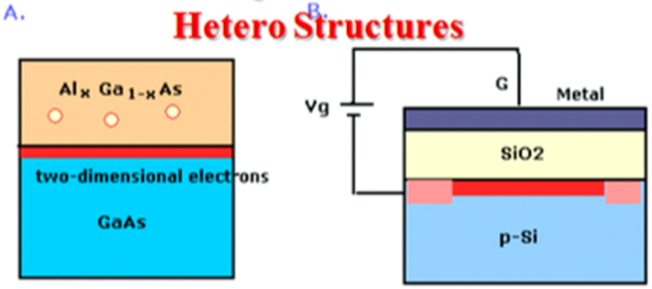




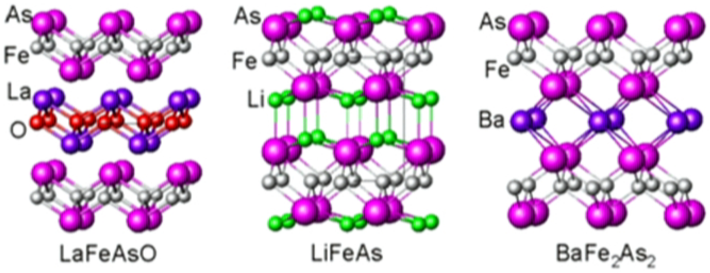
ET Salts

Quantum Spin Liquids and Superconductors

Fractional Quantum Hall Effect
Hetero Structures



Fe Pnictide Superconductor Family

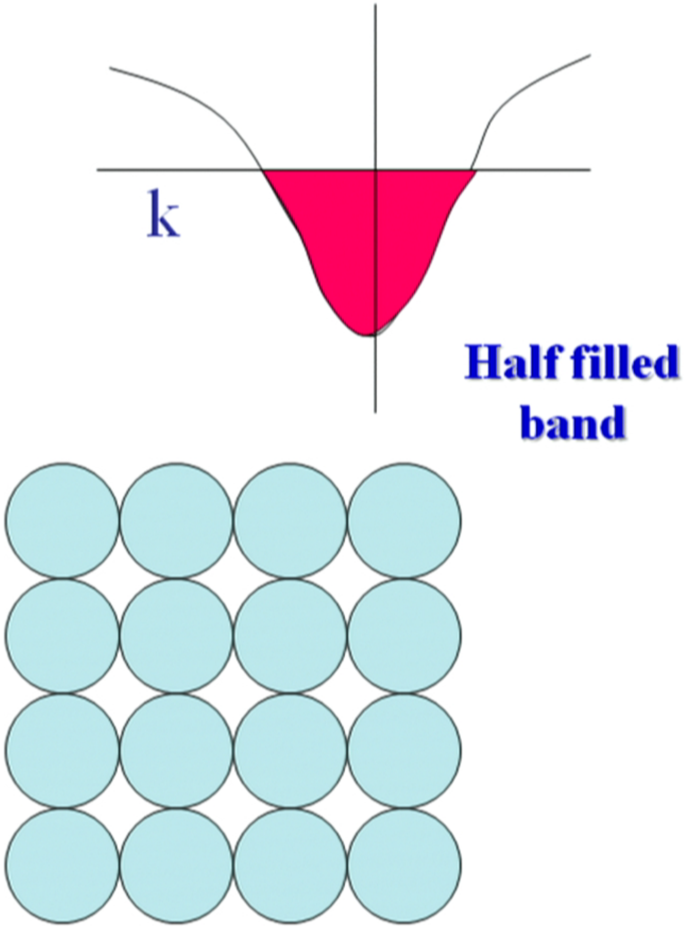


LaFeAsO

LiFeAs

$BaFe_2As_2$

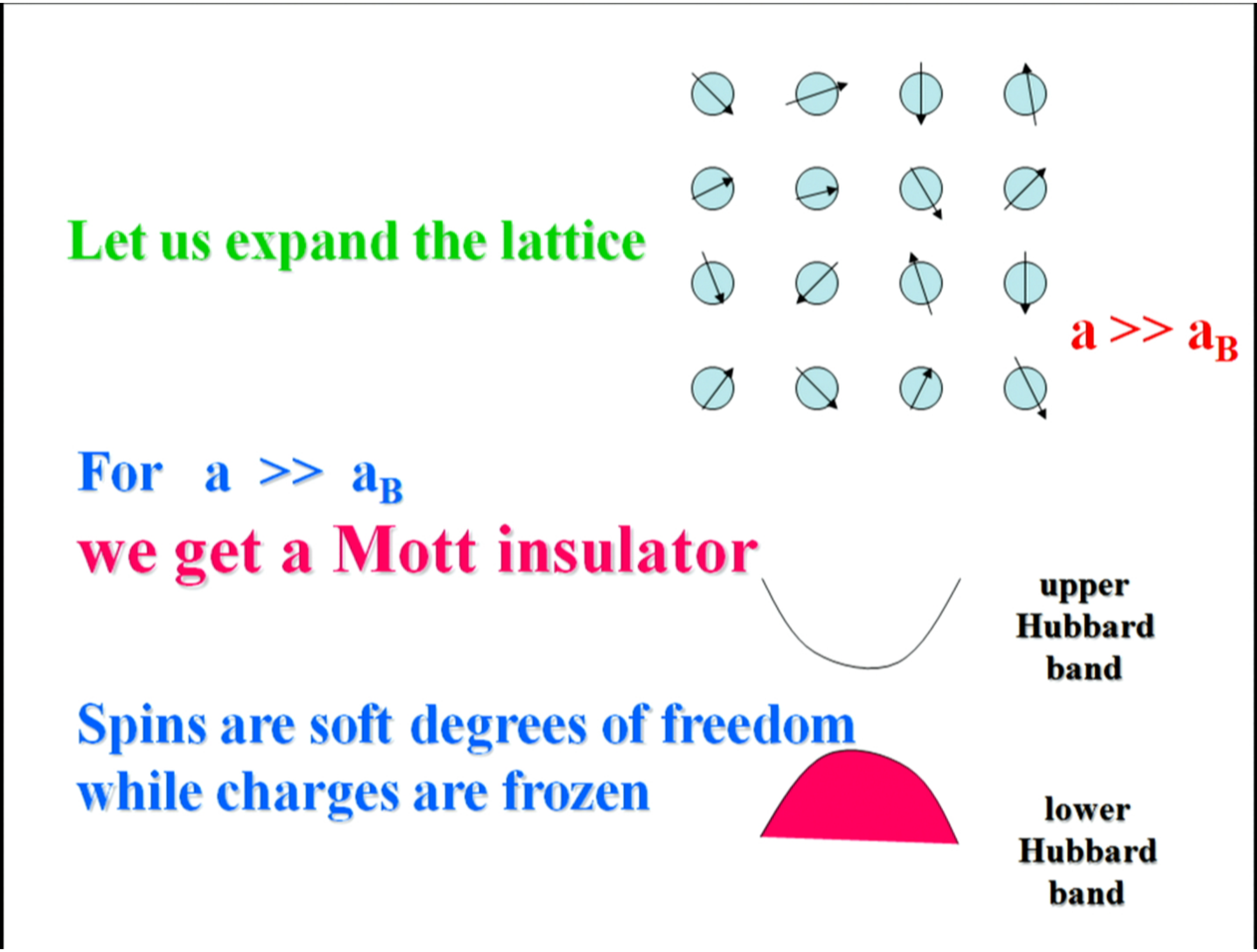
A collection of hydrogen atoms forming a hypothetical 3D lattice



1s atomic orbitals
of individual H-atoms
strongly overlap and
form a tight binding
half filled band
Made of 1s orbitals

It is a metal

a, lattice constant ~ a_B Bohr radius



Let us expand the lattice

$a >> a_B$

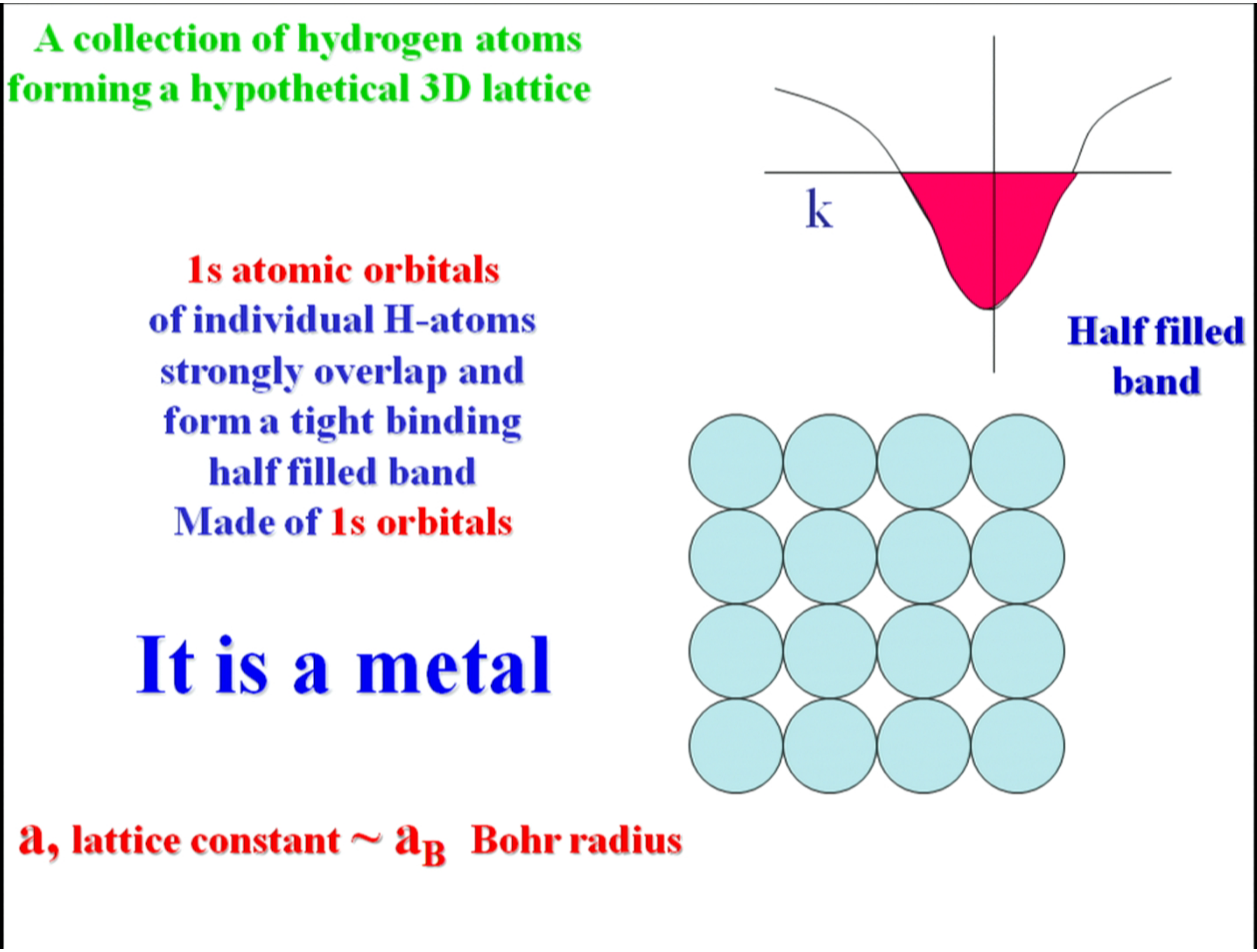
For $a >> a_B$

we get a Mott insulator

Spins are soft degrees of freedom
while charges are frozen

upper
Hubbard
band

lower
Hubbard
band



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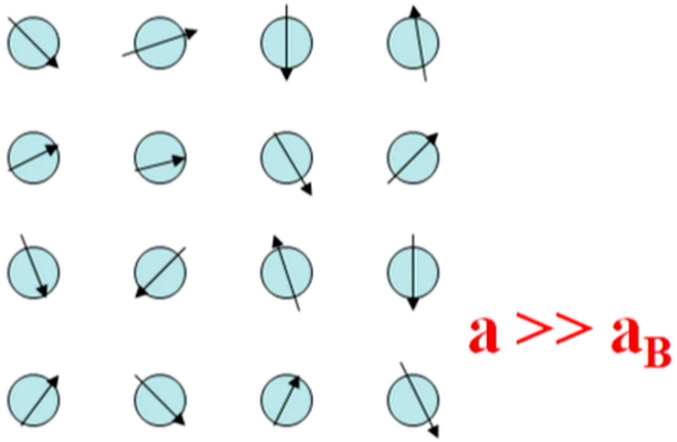

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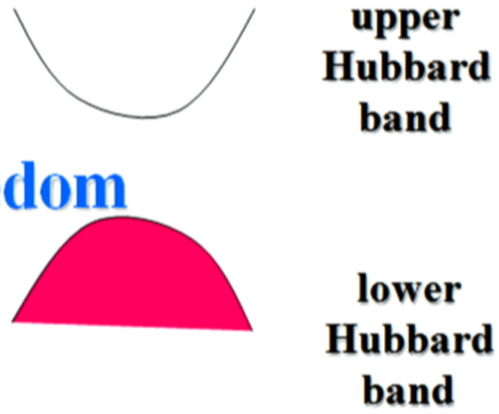

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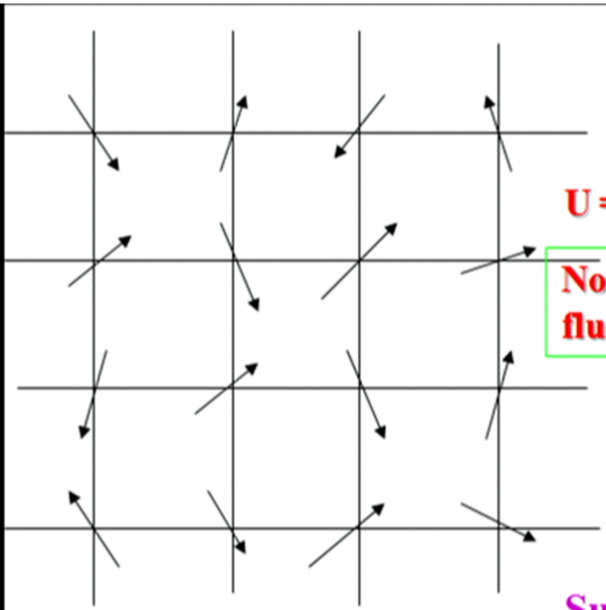
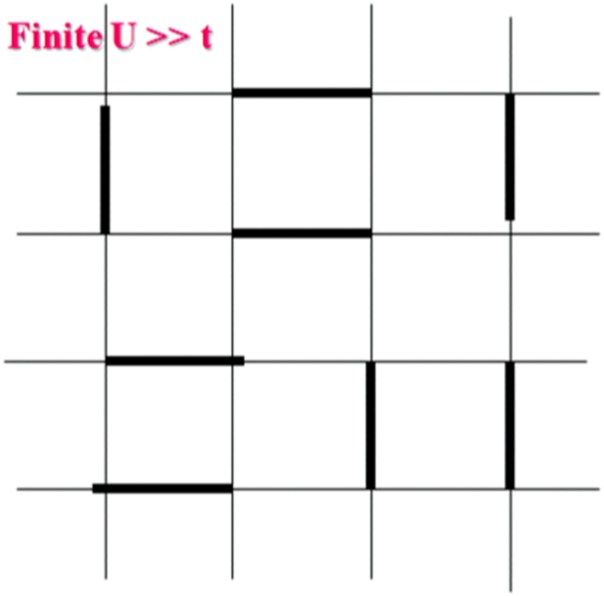
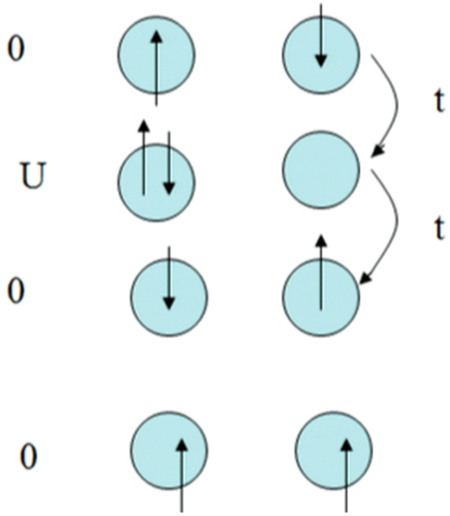


U = infinity

No quantum fluctuations

Finite U >> t





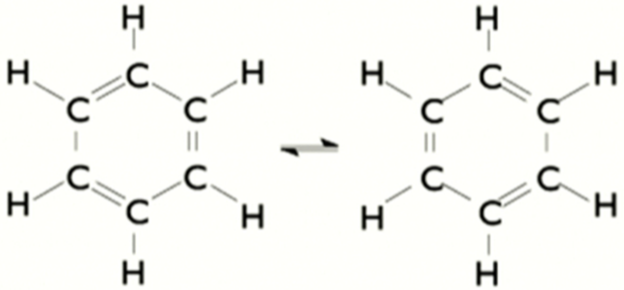
Superexchange or Kinetic exchange process

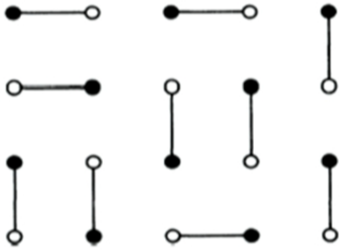
Energy gain = J = $\frac{-4t^2}{U}$

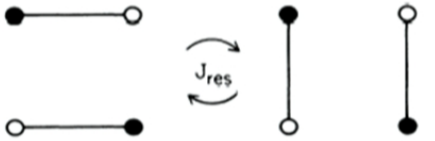
$▬ = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

$$H = J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4}\right)$$

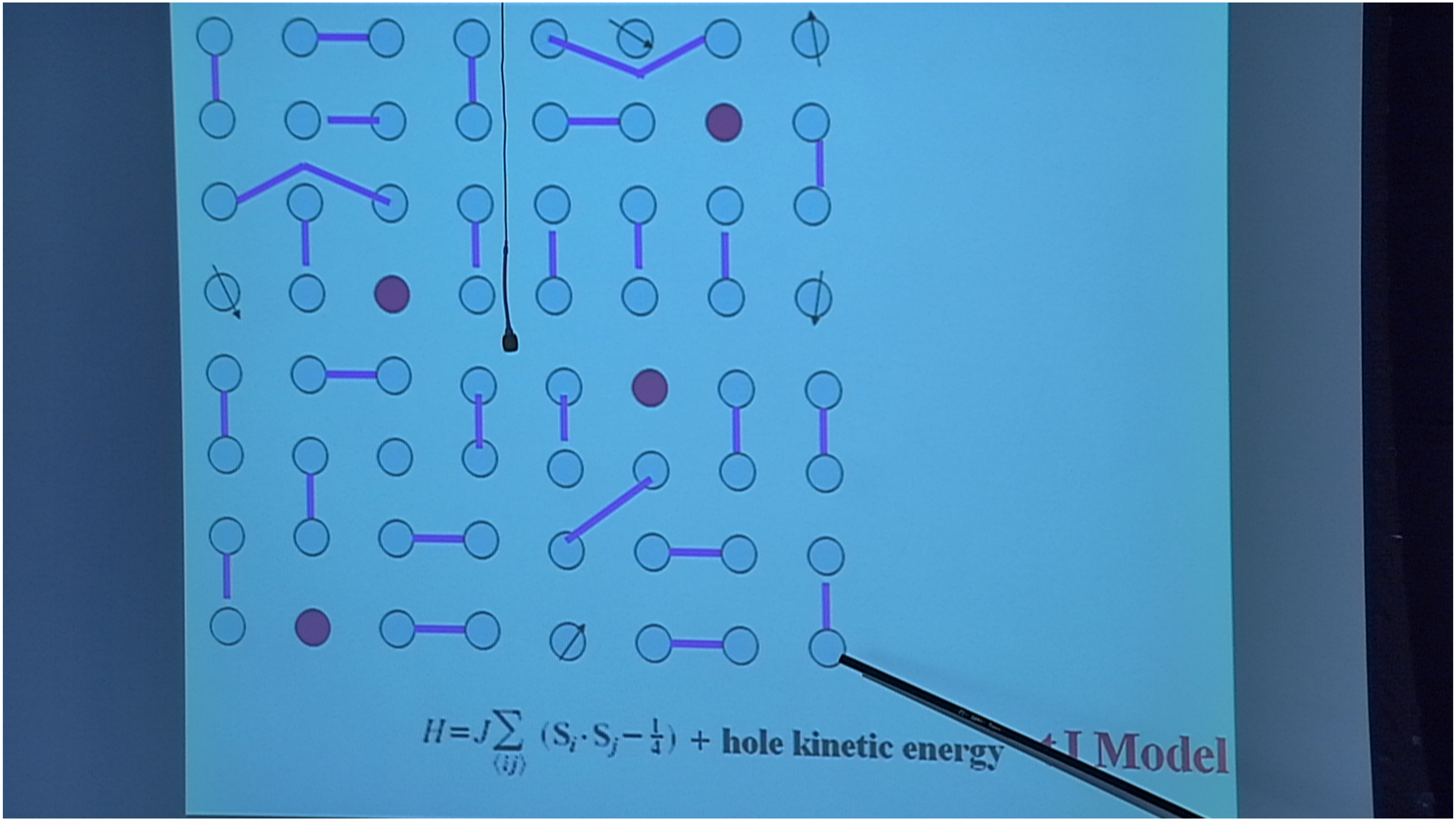
Energy gain = 0 !





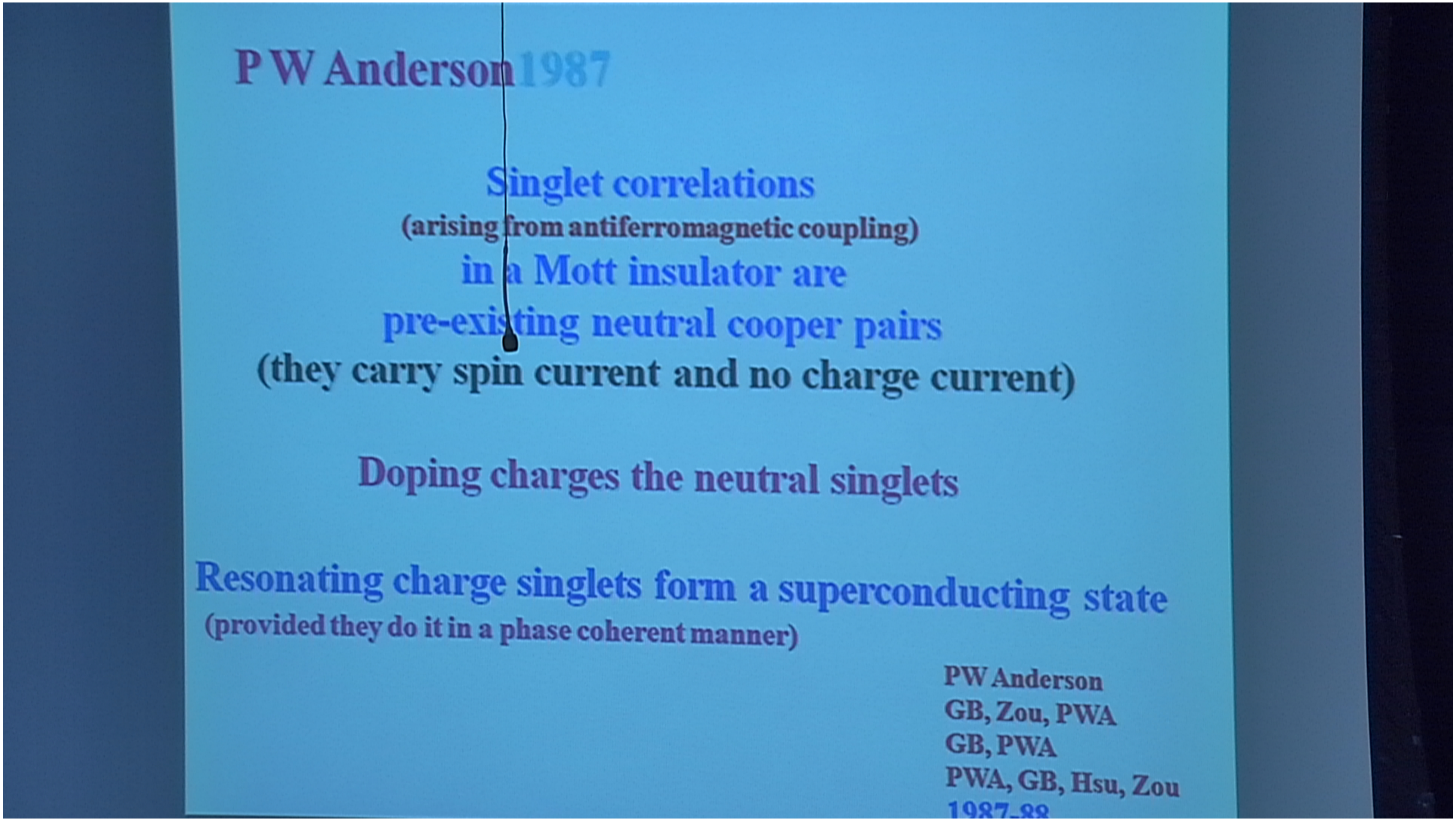


(b)



$$H = J\sum_{\langle ij\rangle} (\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4})$$ + **hole kinetic energy**

tJ Model



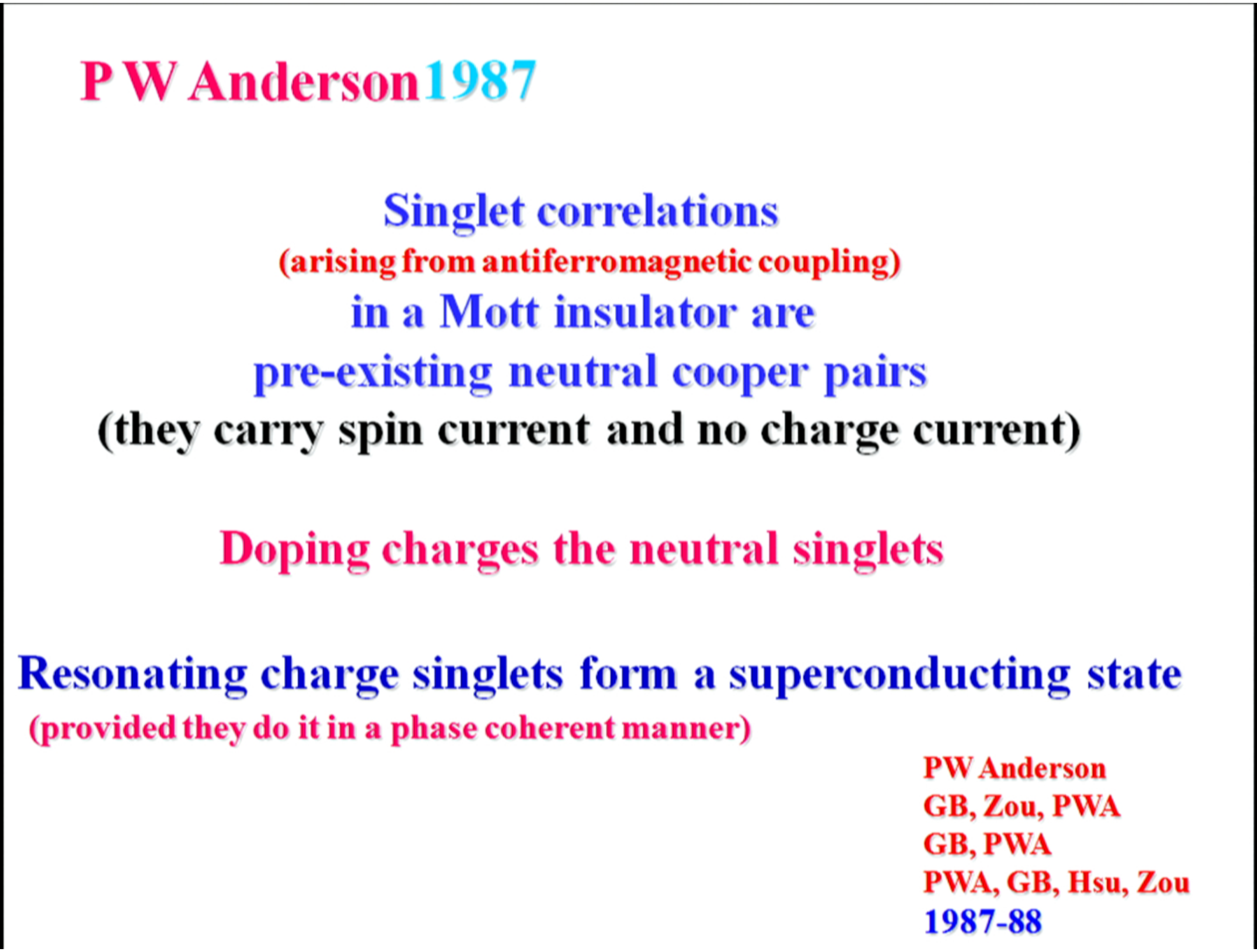
P W Anderson 1987

Singlet correlations
(arising from antiferromagnetic coupling)
in a Mott insulator are
pre-existing neutral cooper pairs
(they carry spin current and no charge current)

Doping charges the neutral singlets

Resonating charge singlets form a superconducting state
(provided they do it in a phase coherent manner)

PW Anderson
GB, Zou, PWA
GB, PWA
PWA, GB, Hsu, Zou
1987-88



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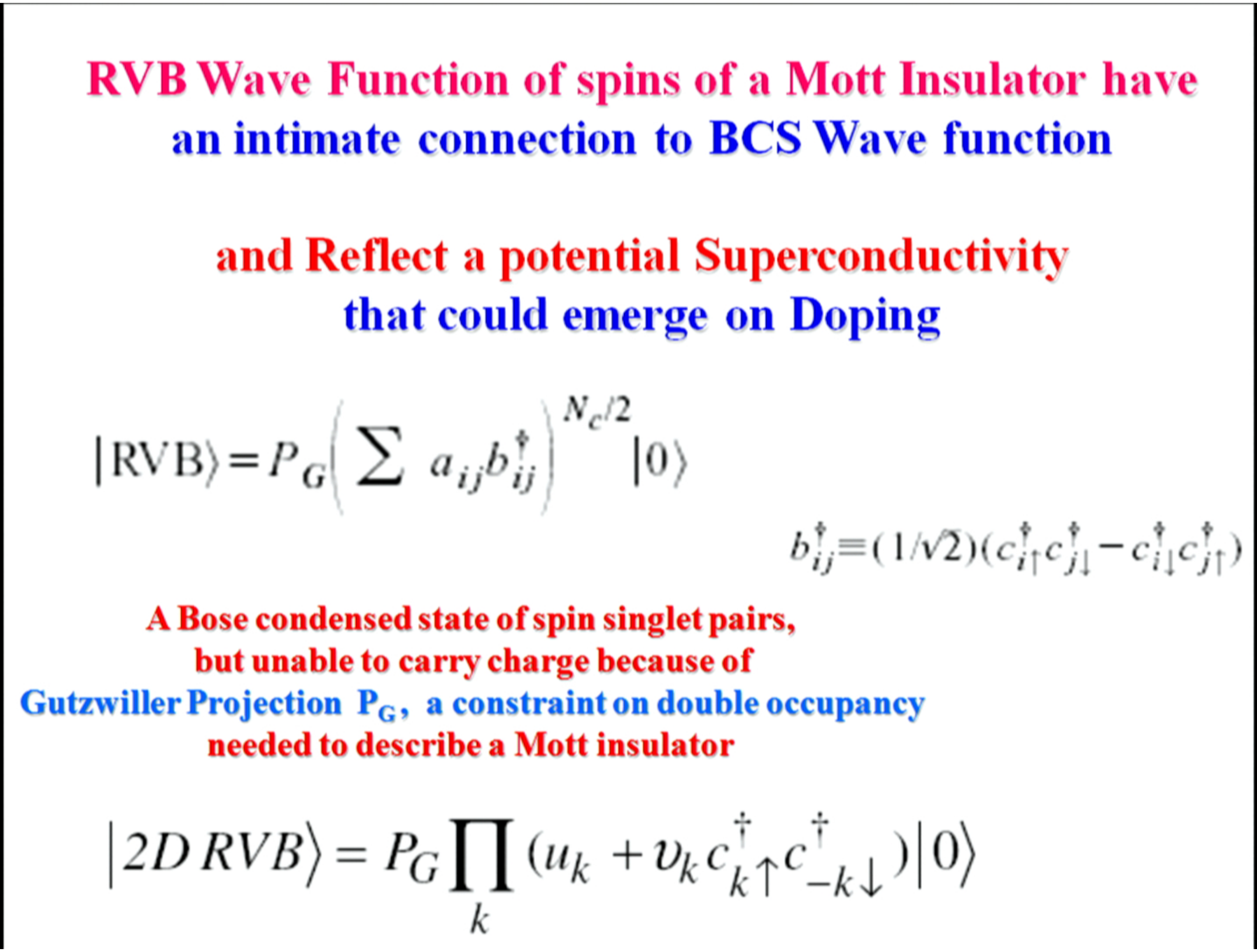
RVB Wave Function puts us in the correct corner of the Spin Liquid Hilbert Space

It is sufficiently general to
describe almost all known
Unconventional magnetic states such as

Z_2 , U(1), SU(2), Chiral … Spin liquids
and even AFM order
through a proper choice of the pair function a_{ij}

$$|\mathrm{RVB}\rangle = P_G \left(\sum a_{ij} b^{\dagger}_{ij} \right)^{N_c/2} |0\rangle \qquad b^{\dagger}_{ij} \equiv (1/\sqrt{2})(c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{j\uparrow})$$



RVB Wave Function of spins of a Mott Insulator have an intimate connection to BCS Wave function

and Reflect a potential Superconductivity that could emerge on Doping

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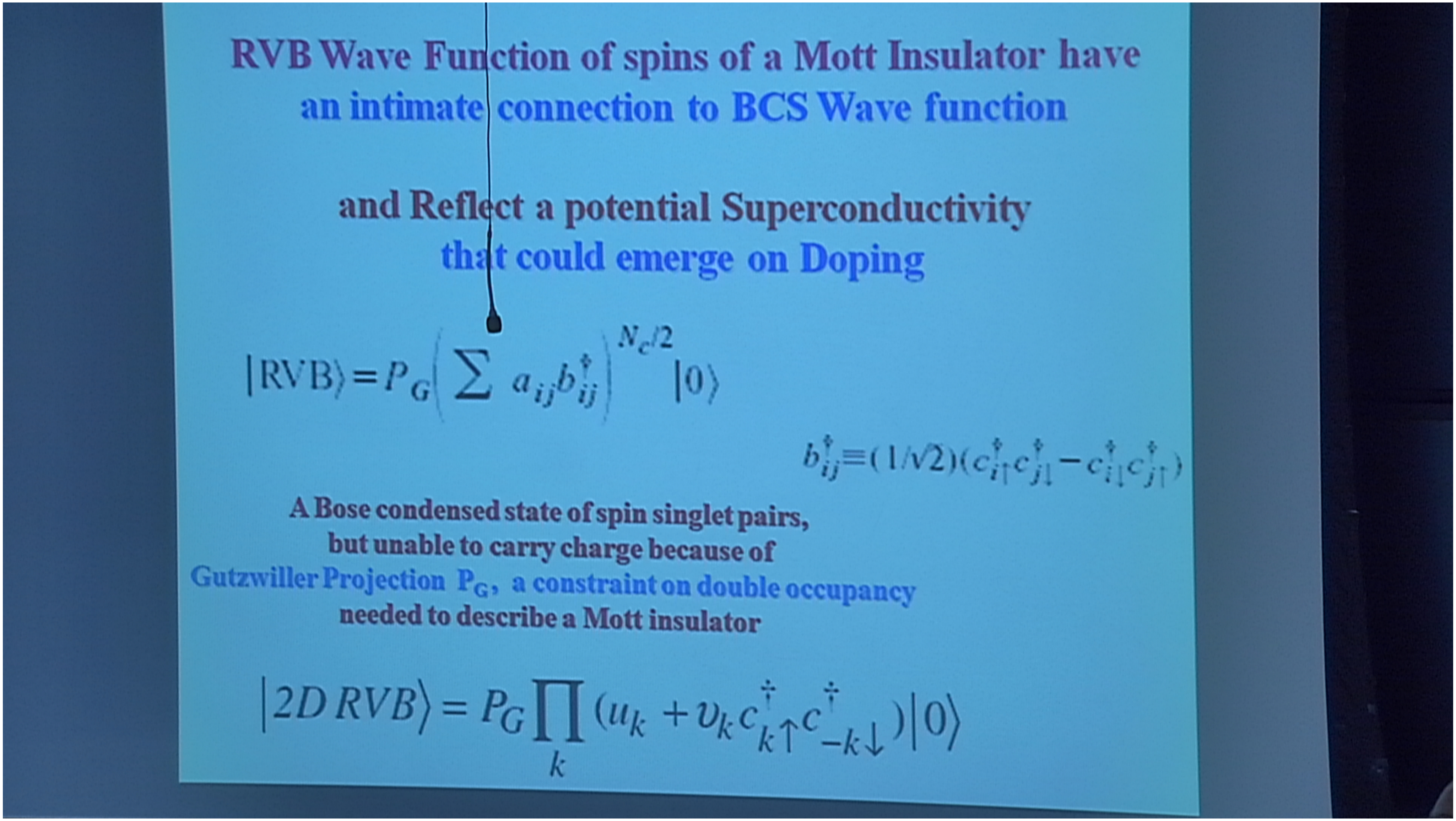
$$b_{ij}^{\dagger} \equiv (1/\sqrt{2})(c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} - c_{i\downarrow}^{\dagger} c_{j\uparrow}^{\dagger})$$

A Bose condensed state of spin singlet pairs,
but unable to carry charge because of
Gutzwiller Projection P_G, a constraint on double occupancy
needed to describe a Mott insulator

$$|2D\,RVB\rangle = P_G \prod_k (u_k + v_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger}) |0\rangle$$



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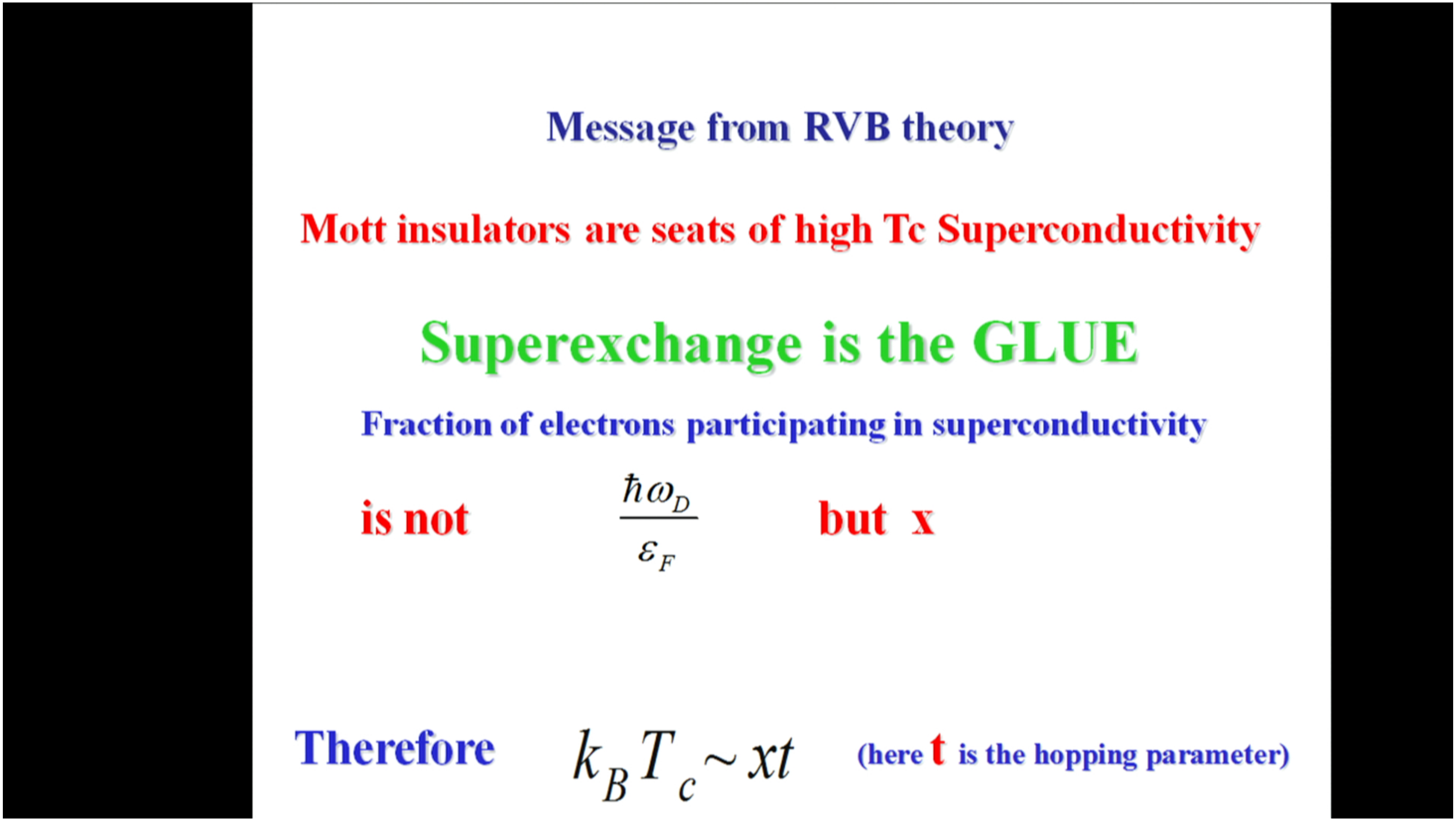


Message from RVB theory

Mott insulators are seats of high Tc Superconductivity

Superexchange is the GLUE

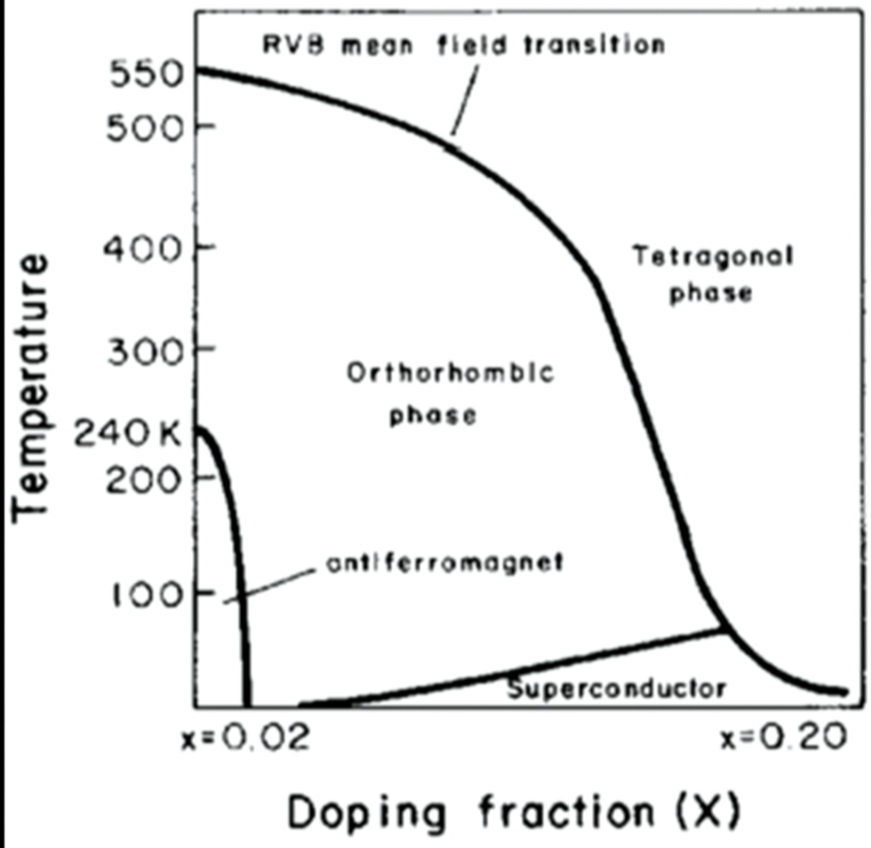
Fraction of electrons participating in superconductivity

is not $\frac{\hbar\omega_D}{\varepsilon_F}$ **but x**

Therefore $k_B T_c \sim xt$ **(here t is the hopping parameter)**

P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu

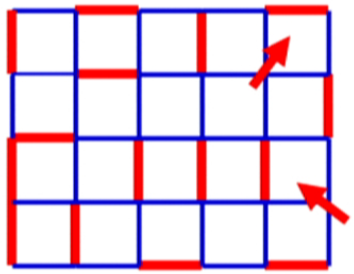
PRL June 1987



$$T_c \simeq (2\pi\hbar^2/m^*)(n-n_c)$$

Tc is independent of J
For n < $n_{optimal}$

Emergent Fermion and Pseudo Fermi Surface (GB, Zou, PWA 1987)
Emergent Gauge Fields (GB, PWA 1987)



Spinon and Holon as a Topological object (Kivelson, Rokhsar, Sethna 1987)

A Quantum Dimer Model & Topological Order (Kivelson, Rokhsar)
RVB Mean field solutions & Quantum Order (Wen)

Emergent Fermions from Localized Spins

RVB Meanfield Theory (GB, Zou, Anderson 1987)

$$J(\boldsymbol{S}_i . \boldsymbol{S}_j - \frac{1}{4} n_i n_j) \equiv -J \quad b^{+}_{ij} b_{ij}$$

$$\vec{S}_i \equiv C^{+}_{i\alpha} \vec{\sigma}_{\alpha\beta} C_{i\beta} \qquad n_{i\uparrow} + n_{i\downarrow} = 1$$

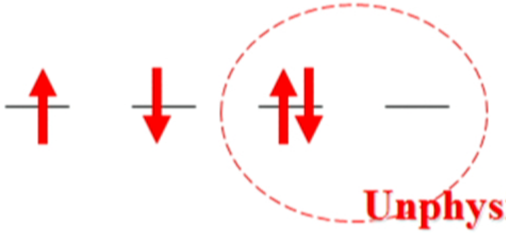
$$b^{+}_{ij} = \frac{1}{\sqrt{2}} (C^{+}_{i\uparrow} C^{+}_{j\downarrow} - C^{+}_{i\downarrow} C^{+}_{i\uparrow})$$

Two complex fermion Hilbert space

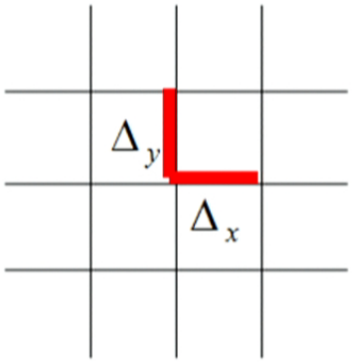
$$2^2 = 4$$

$$b^{+}_{ij} b_{ij} \to \langle b^{+}_{ij} \rangle b_{ij} + b^{+}_{ij} \langle b_{ij} \rangle$$

Δ^{*}_{ij}



Unphysical Hilbert space



Extended - S ⟶ $\Delta_x = \Delta_y$ **BZA**

Flux Phase ⟶ $\Delta_x = -\Delta_y$ **Kotliar, Affleck, Marston**

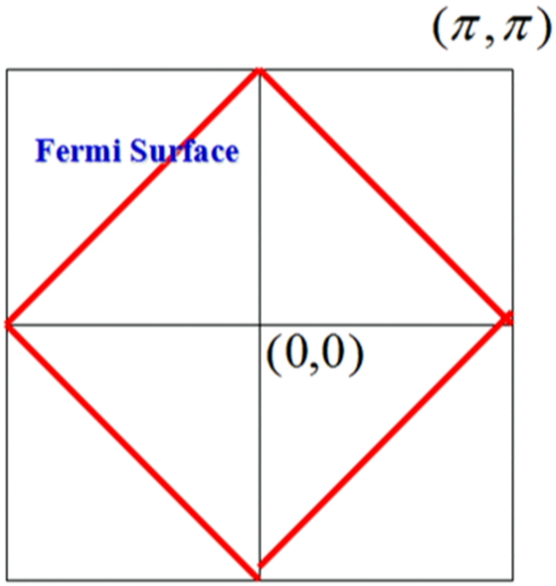
Extended - S $\longrightarrow \Delta_x = \Delta_y$

$$H_s = J\sum_{\langle ij\rangle}(S_i\cdot S_j - \frac{1}{4}) = -J\sum_{\langle ij\rangle} b_{ij}^{\dagger} b_{ij}$$

$$b_{ij}^{+} b_{ij} \to \langle b_{ij}^{+}\rangle b_{ij} + b_{ij}^{+}\langle b_{ij}\rangle$$

$$H_{pair} = -J\sum_{k,k'}\gamma(\mathbf{k}-\mathbf{k}')c^{\dagger}_{-k'\downarrow}c^{\dagger}_{k'\uparrow}c_{k\uparrow}c_{-k\downarrow}$$

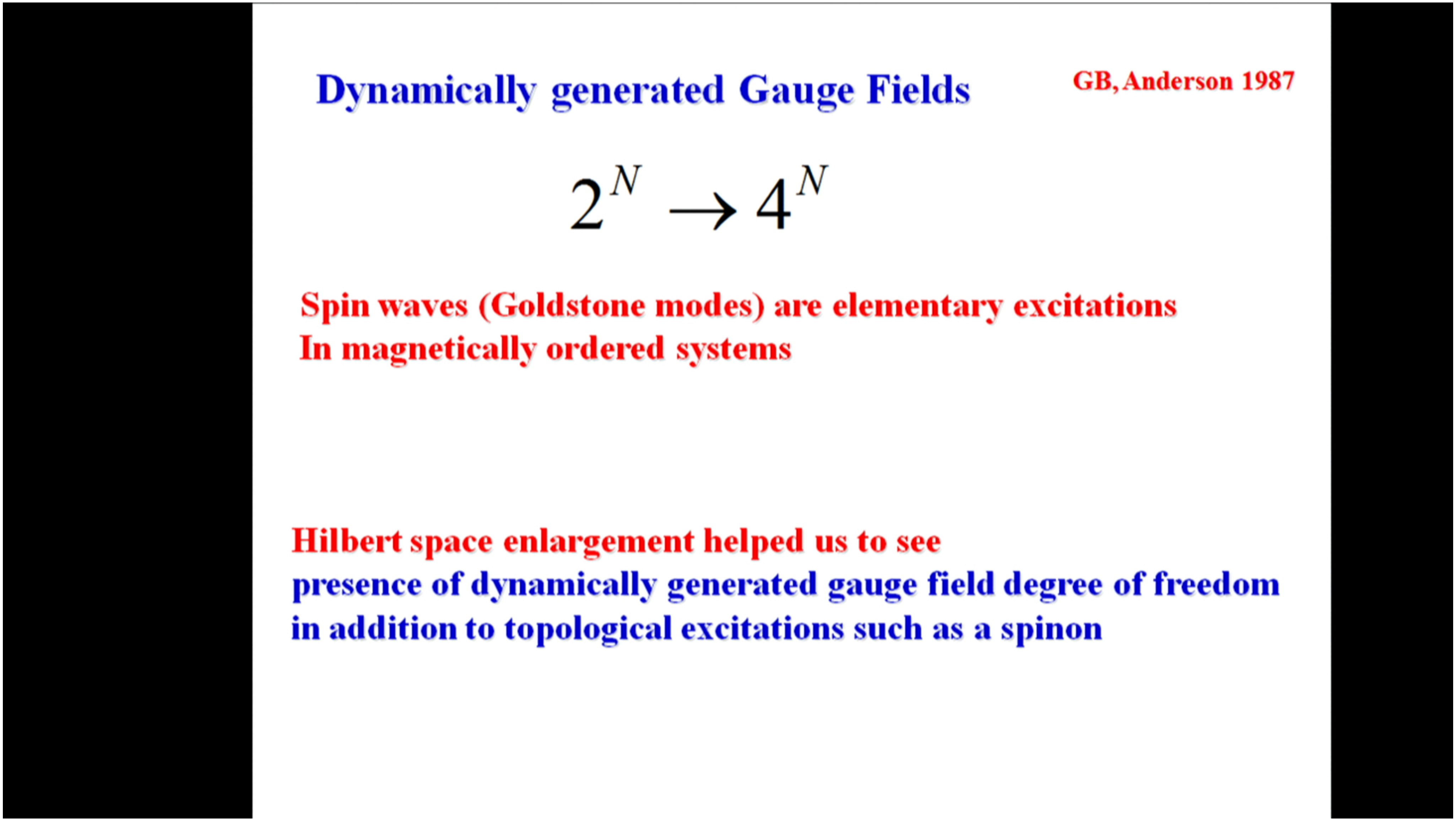
$$H_{mF} \sim J\sum_{k\alpha}|\cos k_x+\cos k_y|\ \alpha^{\dagger}_{k\sigma}\alpha_{k\sigma}$$



$$|2D\,RVB\rangle = P_G\prod_k(u_k+v_k c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow})|0\rangle$$

GB, Zou, Anderson 1987

Recent work by
Tao Li (2011) and Vishwanath et al. (2011) find long range AFM order



Dynamically generated Gauge Fields

GB, Anderson 1987

$$2^N \rightarrow 4^N$$

Spin waves (Goldstone modes) are elementary excitations
In magnetically ordered systems

Hilbert space enlargement helped us to see
presence of dynamically generated gauge field degree of freedom
in addition to topological excitations such as a spinon

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Systems described by a
Single Band Hubbard Model

$$H = -t \sum_{\langle ij \rangle} c^{+}_{i\sigma} c_{j\sigma} + h.c. + U \sum n_{i\uparrow} n_{i\downarrow}$$

are better suited for

Exhibiting Novel Quantum Spin Liquid behavior and High Tc Superconductivity

(Supported by phenomenology and RVB Theory)

Factors Detrimental for Quantum Spin Liquid behavior and High Tc Superconductivity are

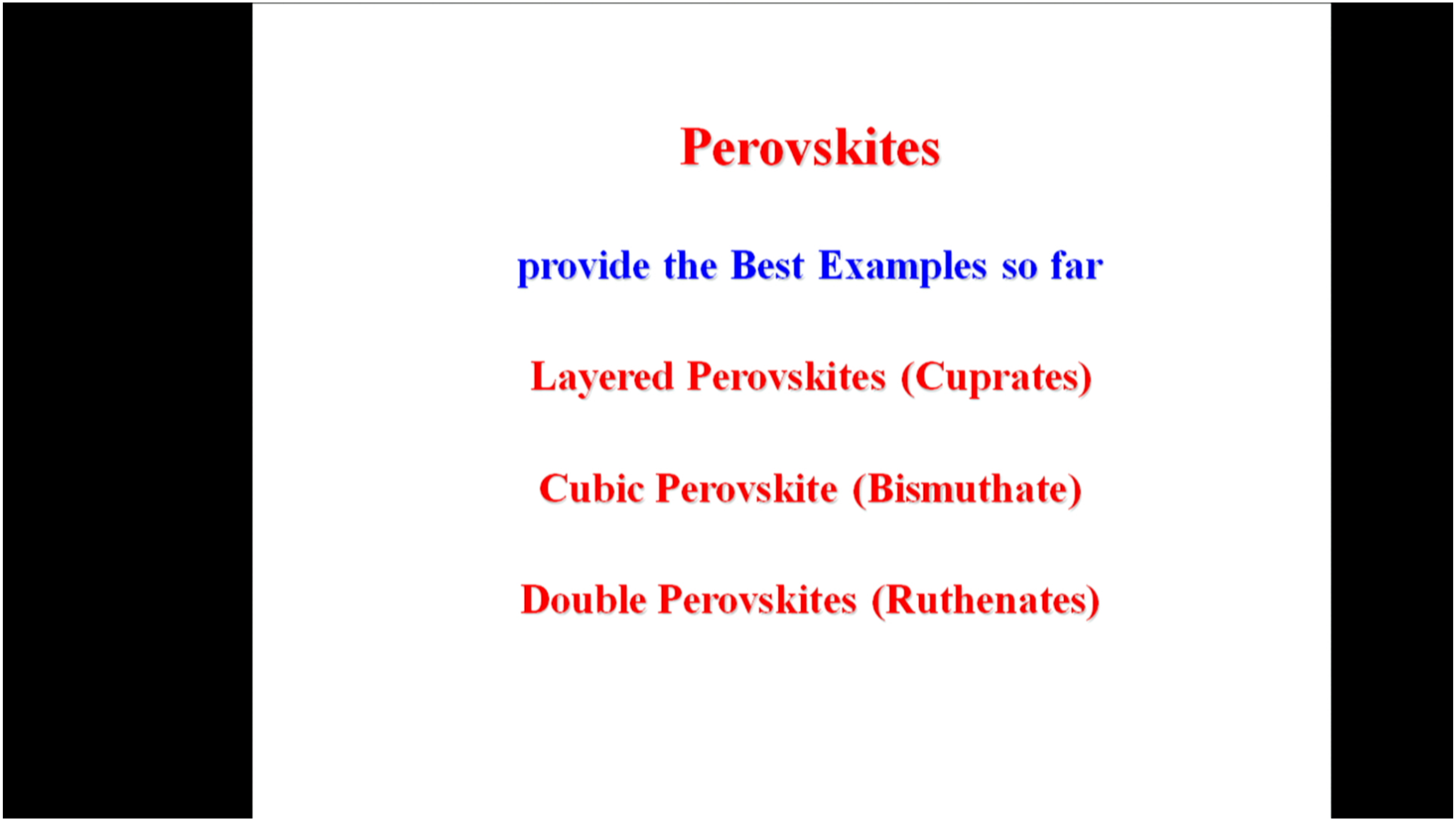
Orbital Degeneracy, Jahn-Teller Effect
Strong Electron-phonon coupling
Polaron formation (self trapping of charges)
Valence Bond Order (Frozen singlet bonds)
(Charge Stipe, CDW, Order)
Frozen Spins (AFM Order, SDW, Spin Stripe) …

Materials Engineering/Design

Choice of Atomic - Molecular Orbitals which facilitate Formation of a SingleTight Binding Band

Materials Engineering/Design
Depends critically on

Choice of Atomic - Molecular Orbitals
which facilitate Formation of a
SingleTight Binding Band



Perovskites

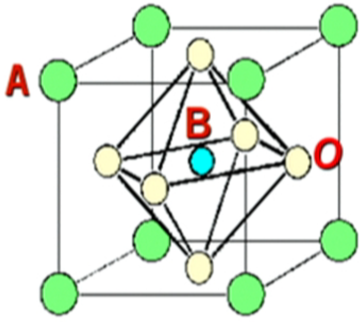
provide the Best Examples so far

Layered Perovskites (Cuprates)

Cubic Perovskite (Bismuthate)

Double Perovskites (Ruthenates)

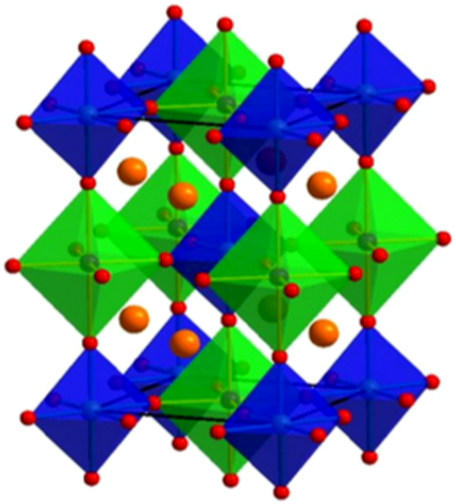
Cubic Perovskites
Double Perovskites
Layered Perovskites



ABO_3

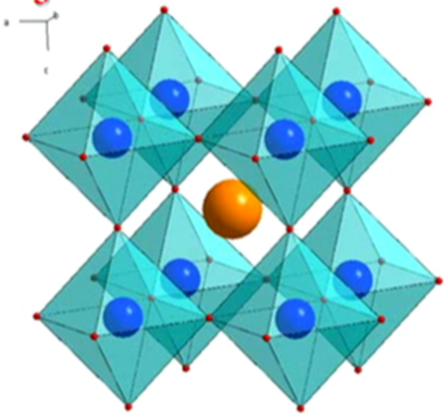
http://www.physics.ohio-state.edu/~trivedi/groupresearchb.html

Sr_2LaRuO_6



http://www.abdn.ac.uk/ncs/profiles/a.c.mclaughlin/

$SrRuO_3$



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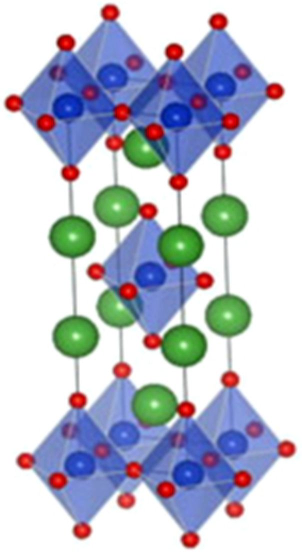
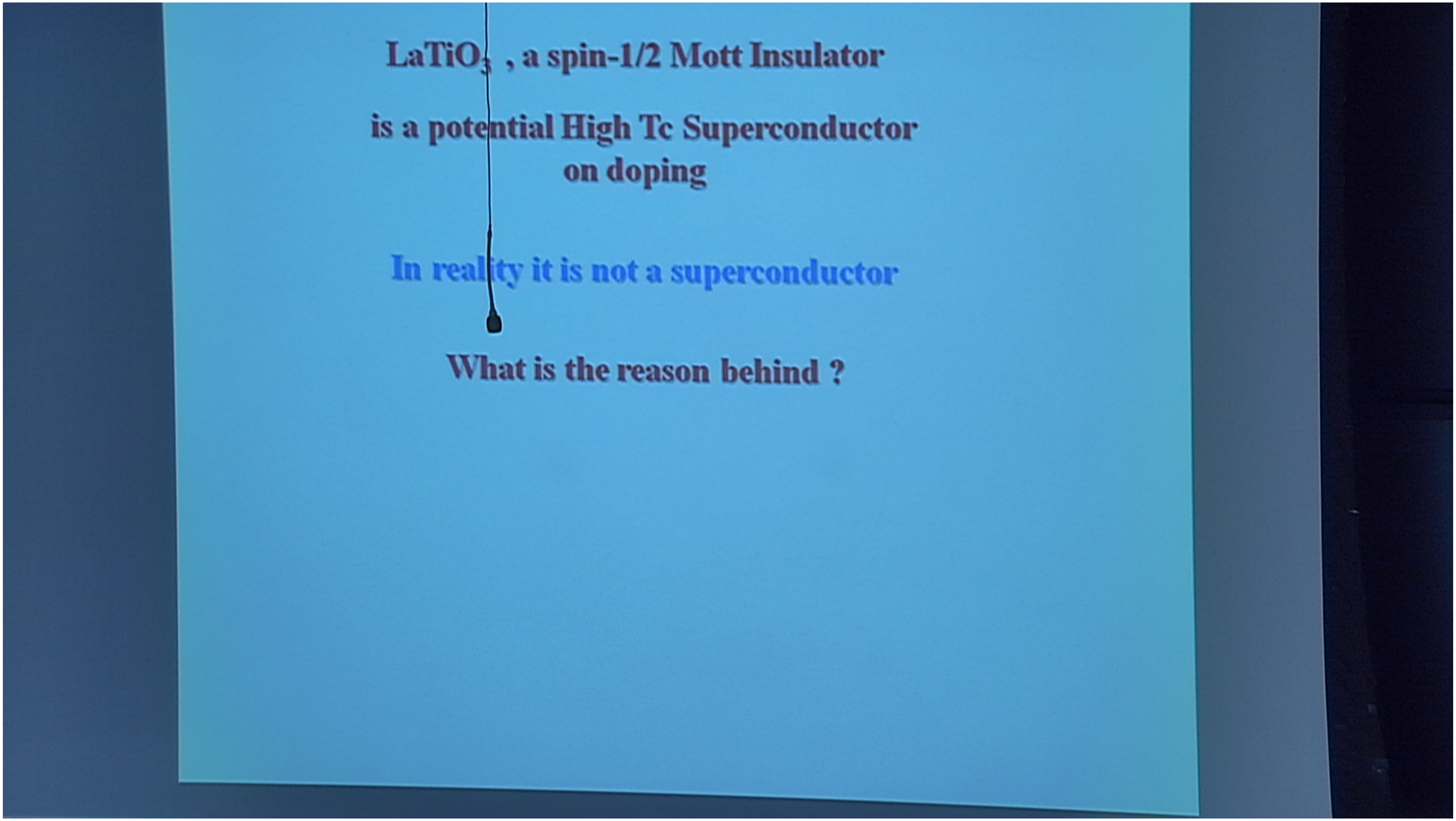


http://www.princeton.edu/~cavalab/tutorials/public/structures/perovskites.html



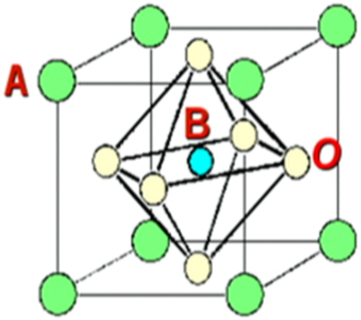
$LaTiO_3$, a spin-1/2 Mott Insulator

is a potential High Tc Superconductor
on doping

In reality it is not a superconductor

What is the reason behind ?

Crystal Field Splitting



ABO3

Consider an Octahedra in the cubic perovskite

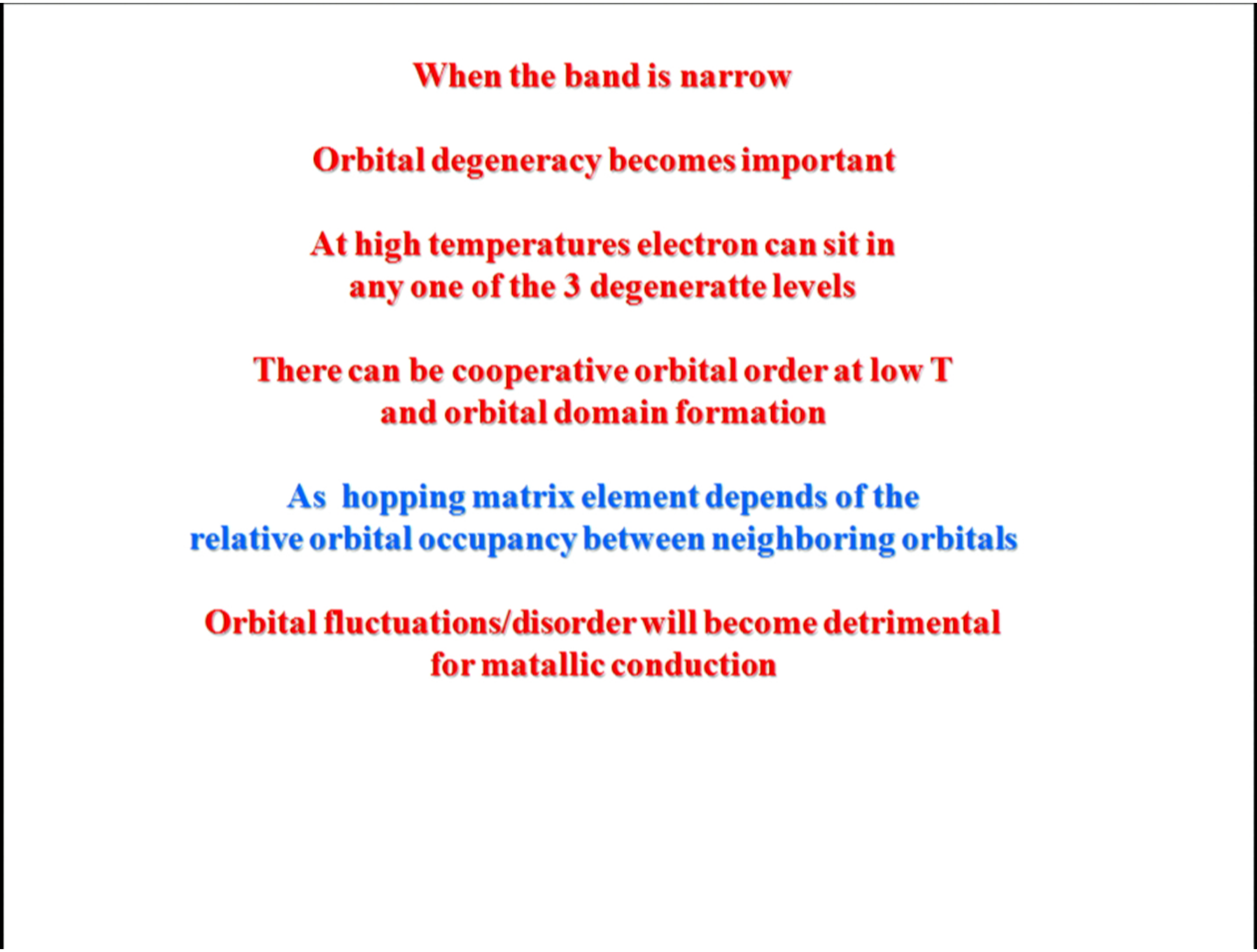
LaTi O_3 , a Mott Insulator

La $^{3+}$ Ti $^{3+}$ O_3 $^{6+}$

Cubic Crystal field splits the 5 fold degenerate 3d levels

Ti^{3+} : $3d^1$

3 orbitally degenerate ground states are possible



When the band is narrow

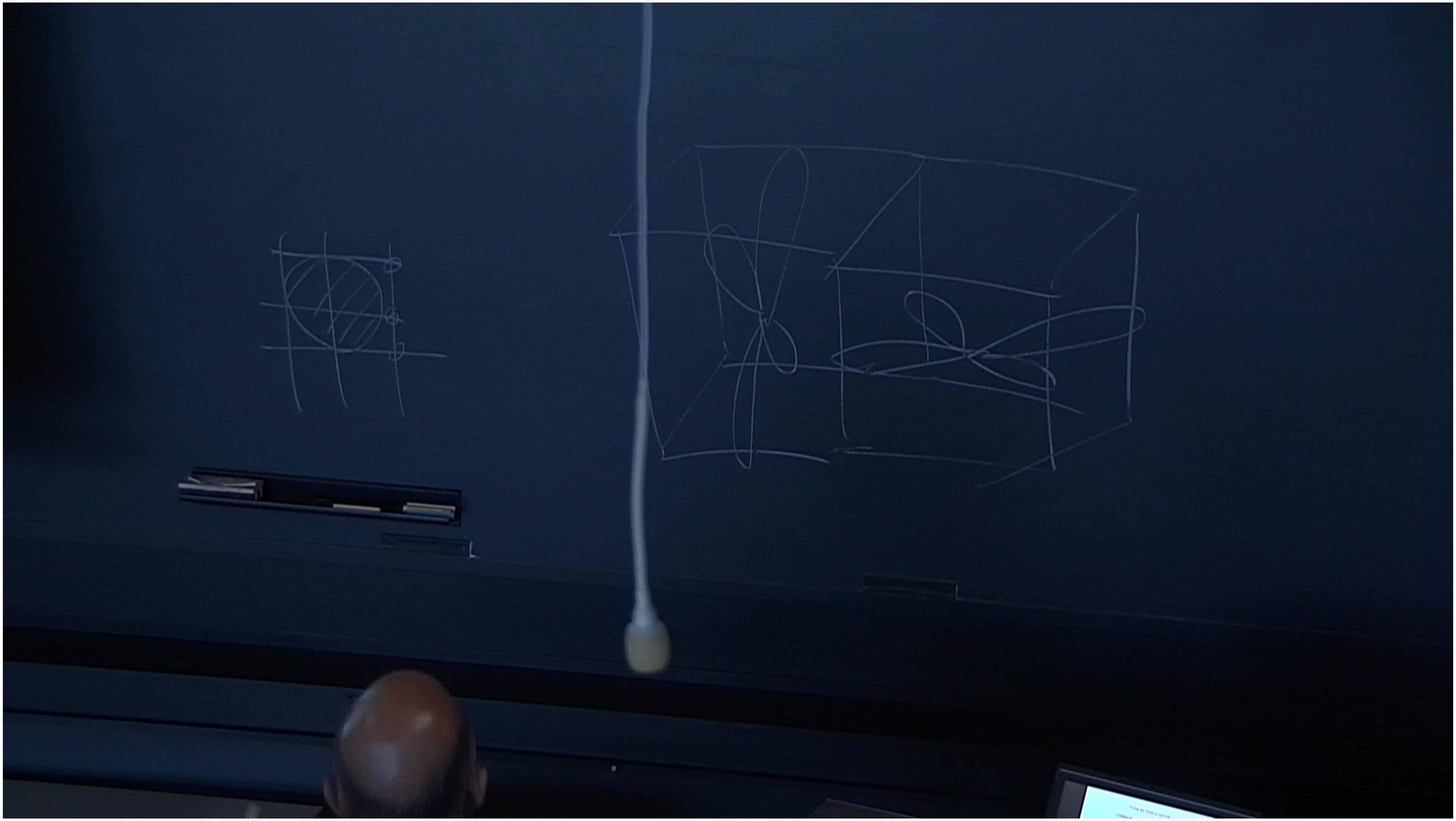
Orbital degeneracy becomes important

At high temperatures electron can sit in
any one of the 3 degeneratte levels

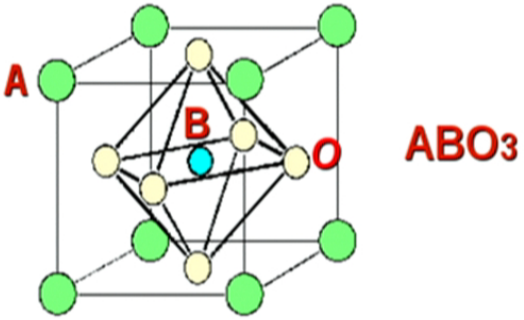
There can be cooperative orbital order at low T
and orbital domain formation

As hopping matrix element depends of the
relative orbital occupancy between neighboring orbitals

Orbital fluctuations/disorder will become detrimental
for matallic conduction



Crystal Field Splitting



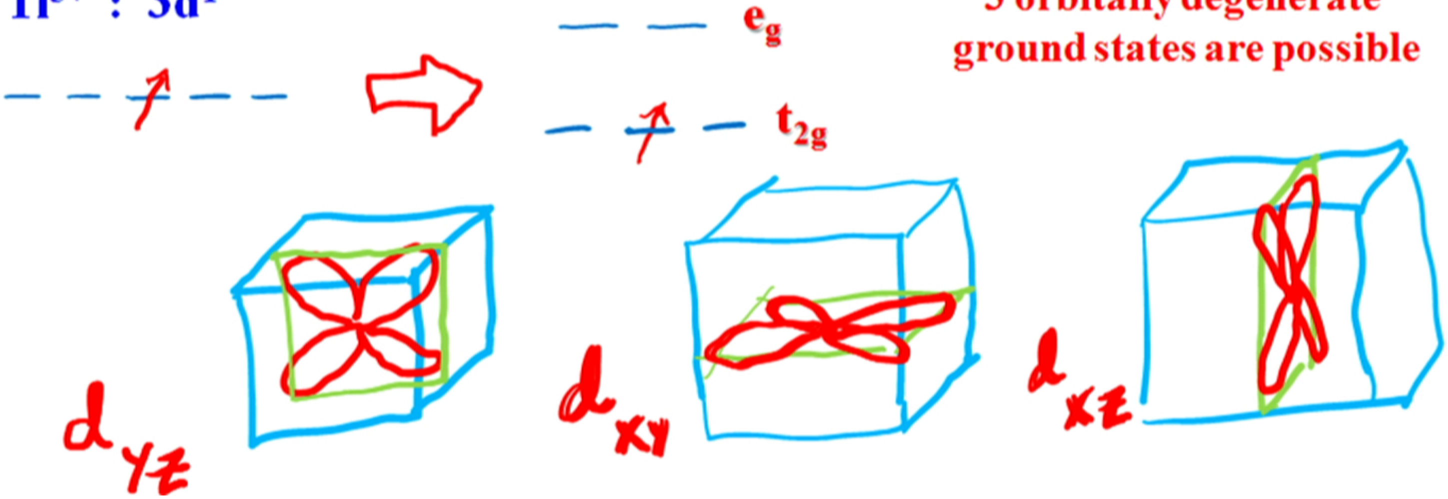
Consider an Octahedra in the cubic perovskite

LaTi O_3 , a Mott Insulator

La^{3+} Ti^{3+} O_3 $^{6+}$

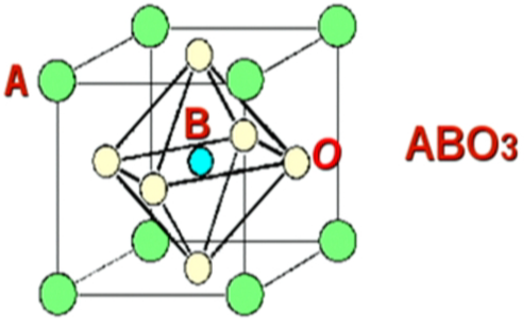
Cubic Crystal field splits the 5 fold degenerate 3d levels

Ti^{3+} : $3d^1$



3 orbitally degenerate ground states are possible

Jahn-Teller Effect



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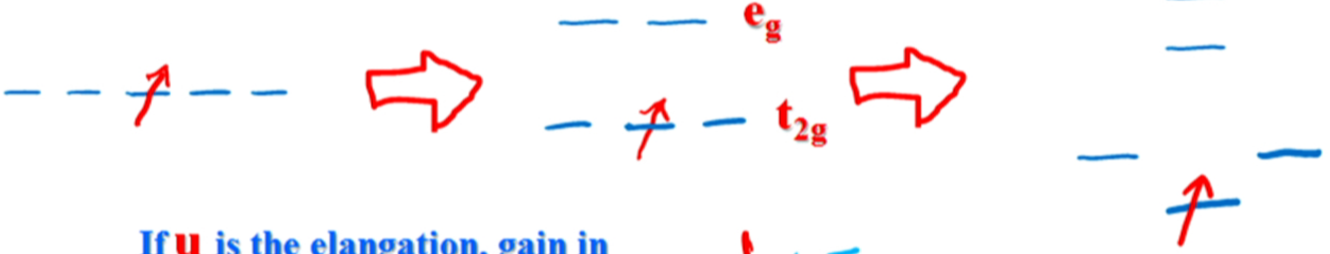
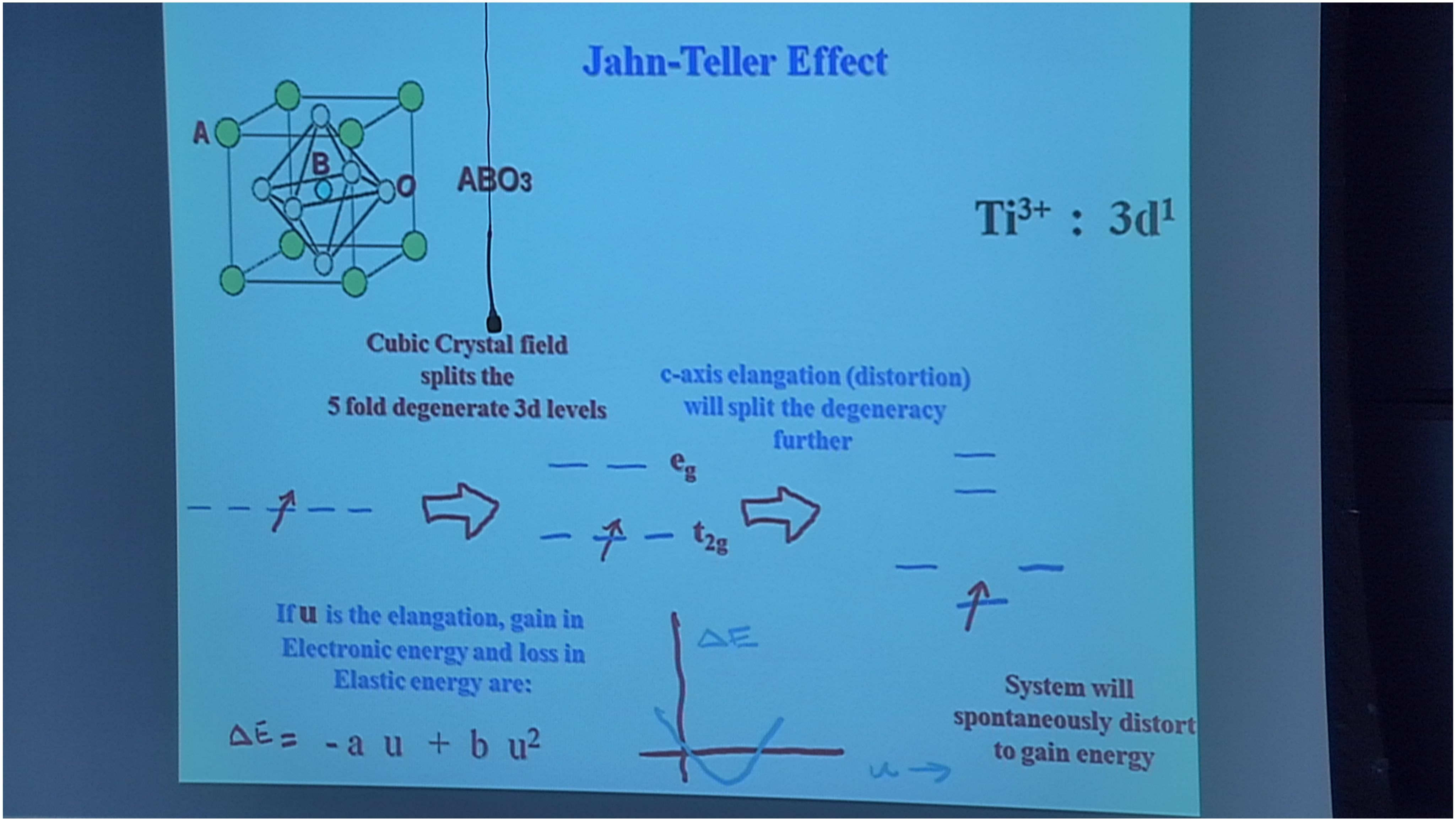


If **u** is the elangation, gain in
Electronic energy and loss in
Elastic energy are:

$$\Delta E = -a\ u + b\ u^2$$

System will
spontaneously distort
to gain energy



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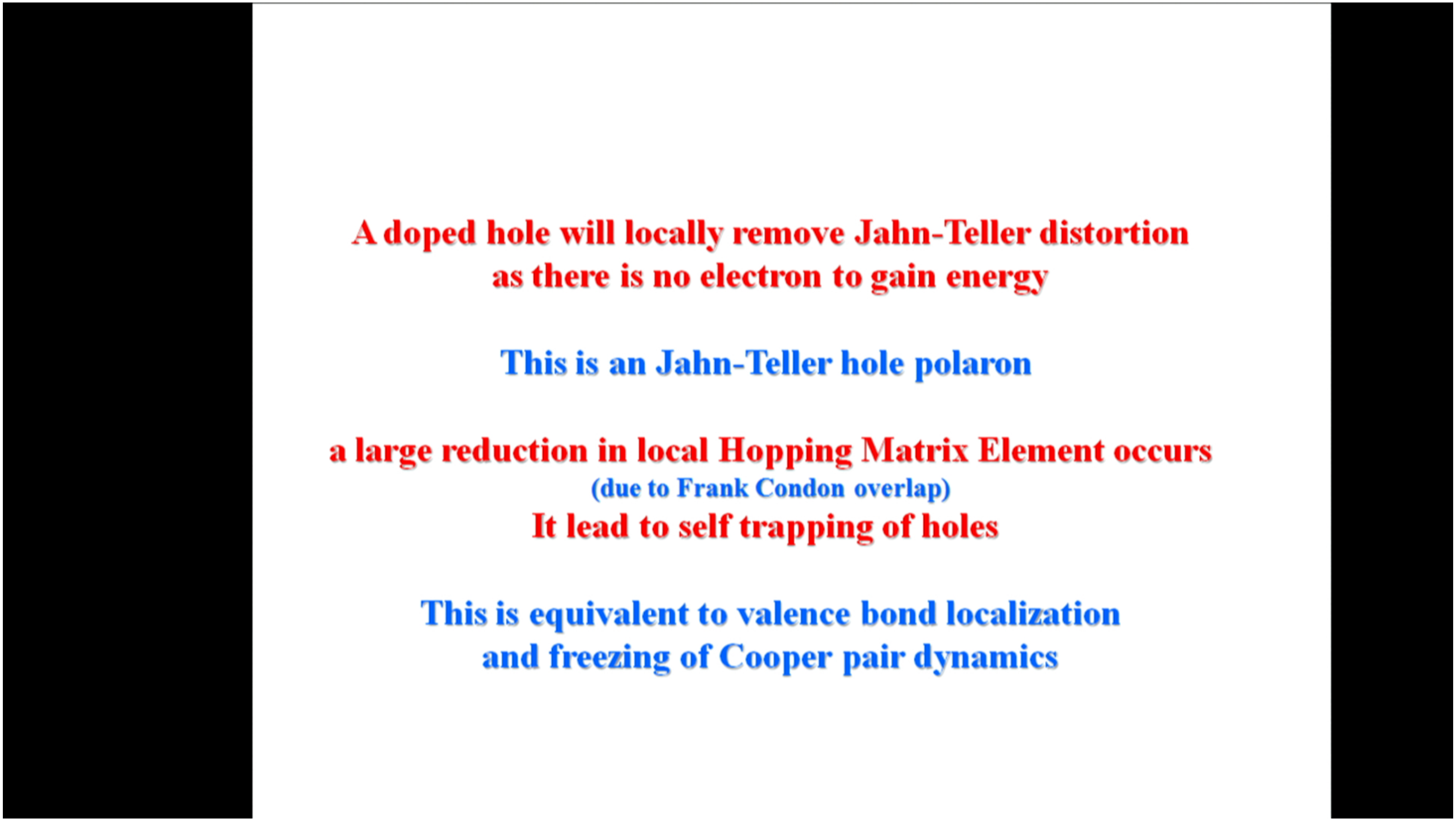
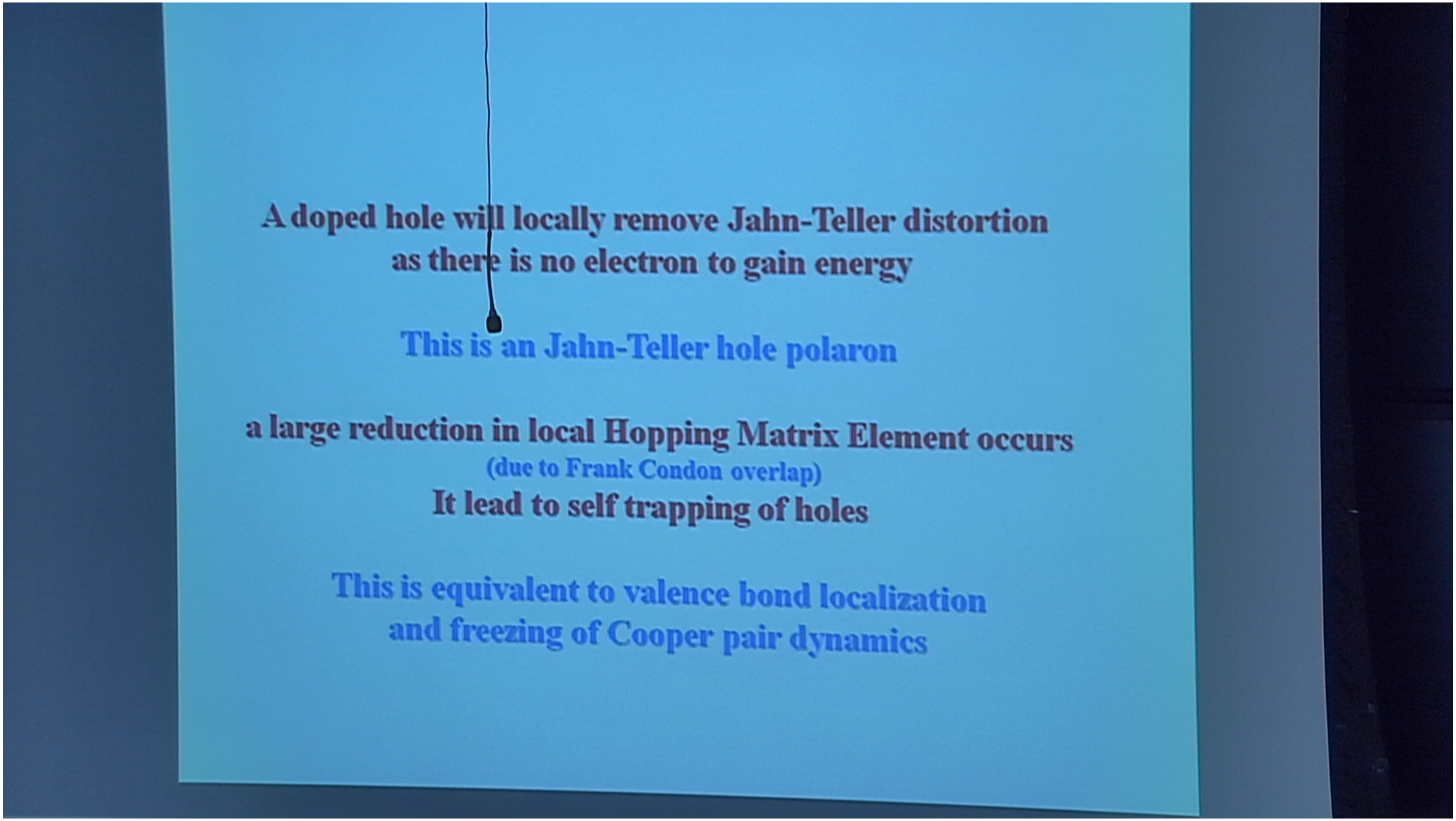


A doped hole will locally remove Jahn-Teller distortion
as there is no electron to gain energy

This is an Jahn-Teller hole polaron

a large reduction in local Hopping Matrix Element occurs
(due to Frank Condon overlap)
It lead to self trapping of holes

This is equivalent to valence bond localization
and freezing of Cooper pair dynamics



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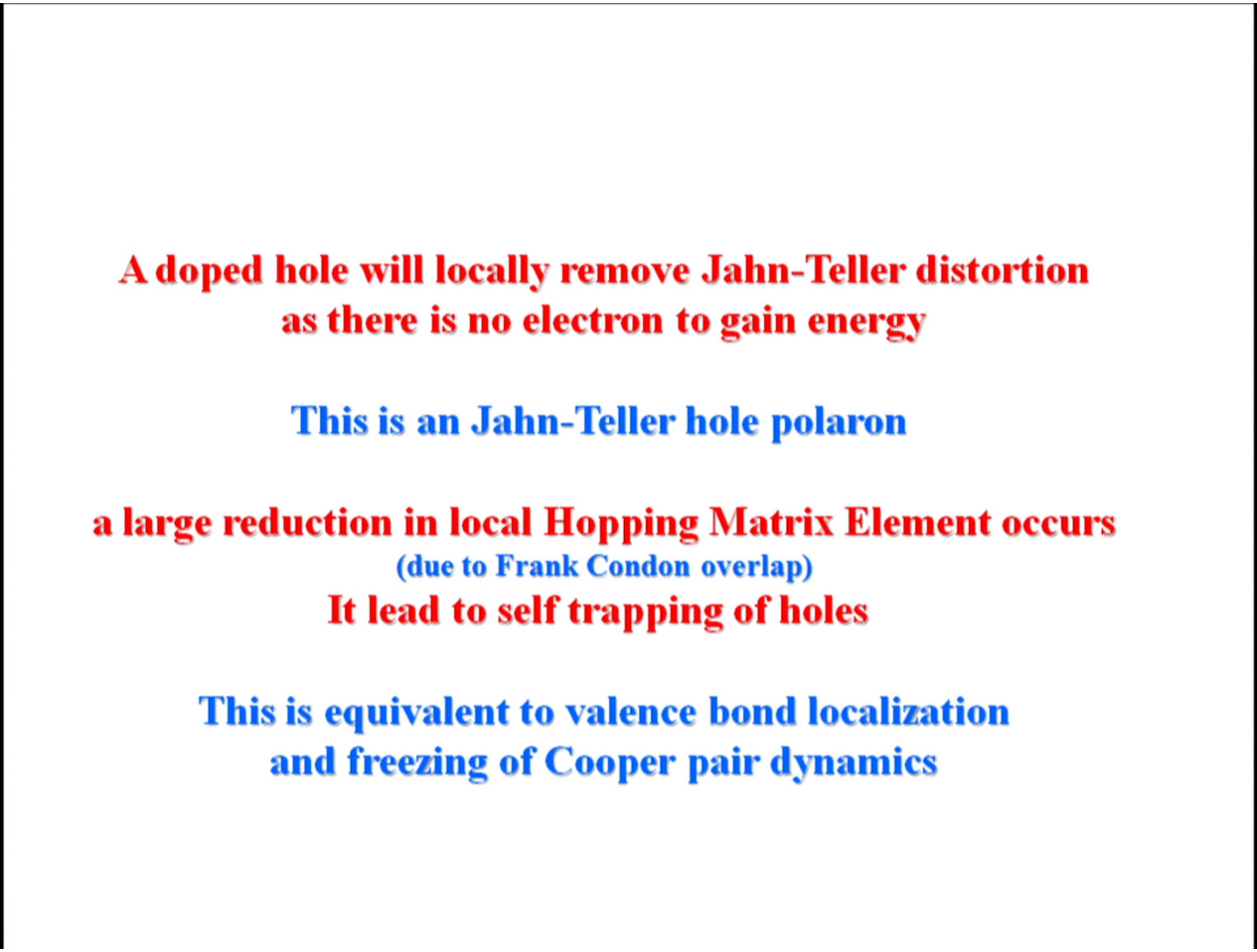
Two systems overcome these hurdles and manage to become High Tc Superconductors

Cuprates and Fe Pnictides

we will focus on Cuprates



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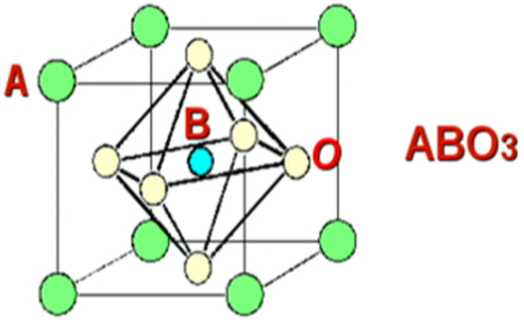

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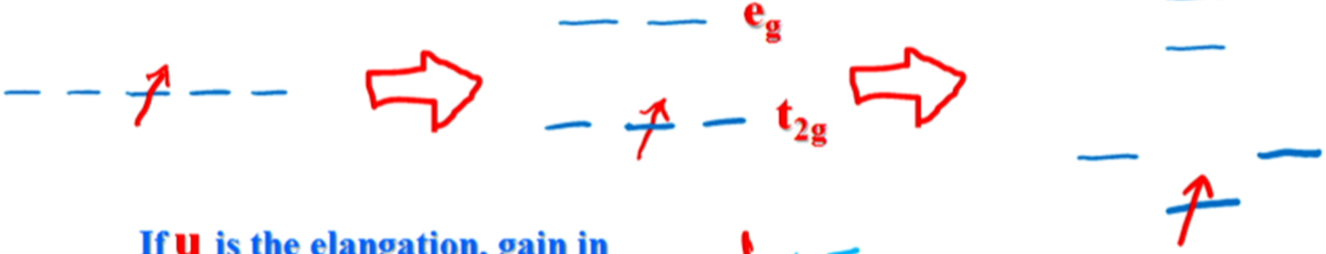

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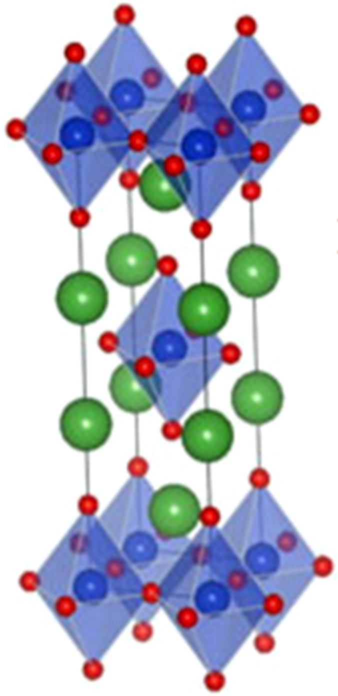
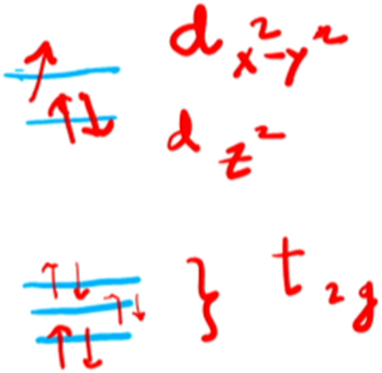
High Tc Cuprates (Bednorz and Muller 1986)



$La_{1-x}Ba_XCuO_4$

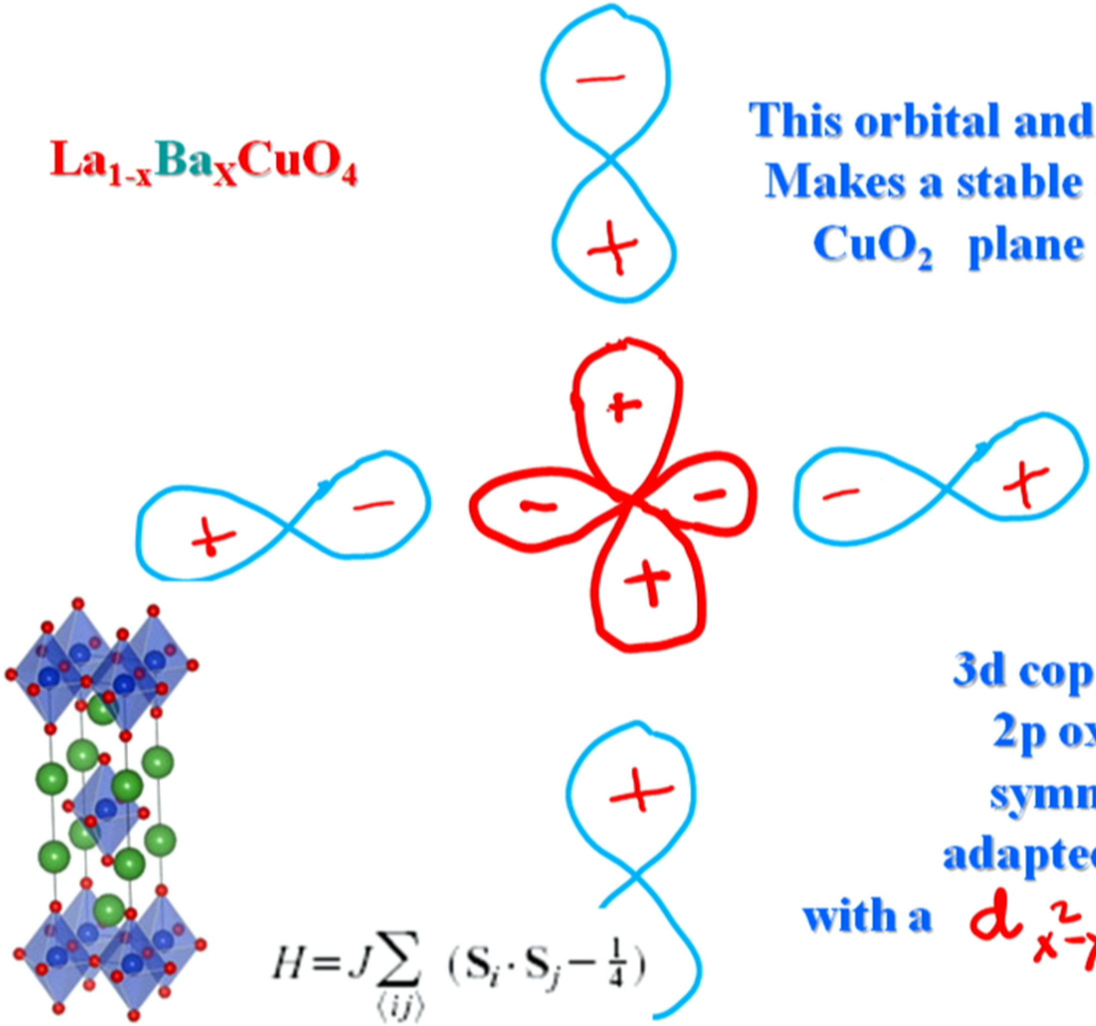
$La^{3+}\ Cu^{2+}\ O_4^{6-}$

Cu^{2+} : $3d^9$



It is an anisotropic crystal
with c-axis elangated octahedra
Not because of Jahn-Teller effect
But because of solid state chemistry

$La_{1-x}Ba_XCuO_4$



This orbital and their bonding
Makes a stable square lattice
CuO_2 plane in cuprates

3d copper and
2p oxygen
symmetery
adapted hybrid
with a $d_{x^2-y^2}$ symmetry

$$H = J\sum_{\langle ij\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})$$

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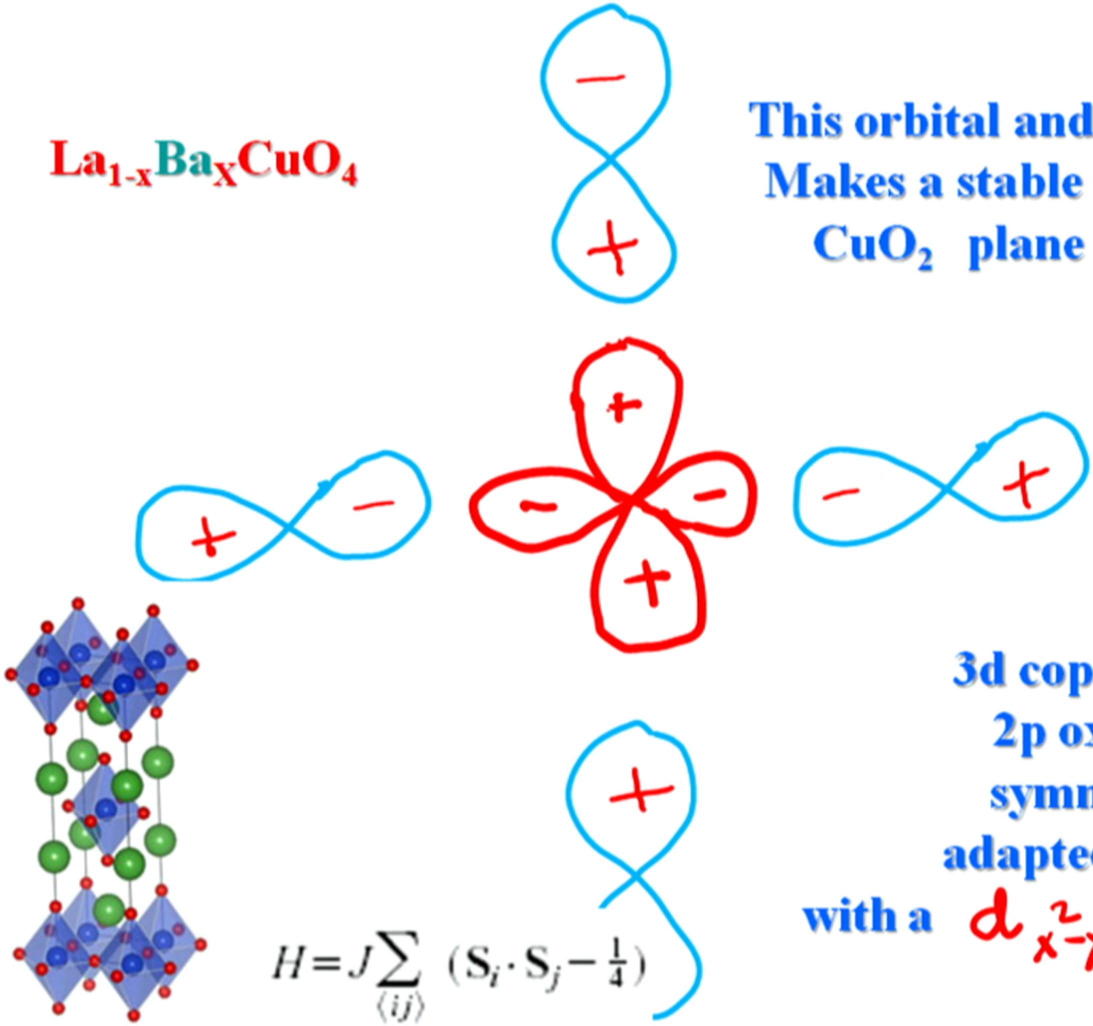

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with a $d_{x^2-y^2}$ **symmetry**

tJ Model

$$\boxed{n_{i\uparrow}+n_{i\downarrow}\neq 2}$$

$$H_{tJ} = -t\sum_{\langle ij\rangle} c^{\dagger}_{i\sigma}c_{j\sigma} + h.c + J\sum_{\langle ij\rangle}\left(\vec{S}_i\cdot\vec{S}_j - \frac{1}{4}n_i n_j\right)$$

$$= -t\sum_{\langle ij\rangle} C^{\dagger}_{i\sigma}C_{j\sigma} + h.c. - J\sum_{\langle ij\rangle} b^{\dagger}_{ij}b_{ij}$$

Now we look for 3 dimensional analogs

If we wish to avoid orbital degeneracy
One possibility is to have 's' orbital

Doped $BaBiO_3$ is an excellent example

In this case Tc is limited to 40 K
Because of Valence Bond order
arising frm strong spin phonon coupling

Chevral phase compounds, A15 compounds
suffer from multi orbital complications
(GB unpublished)

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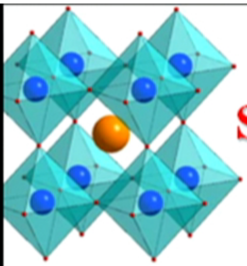
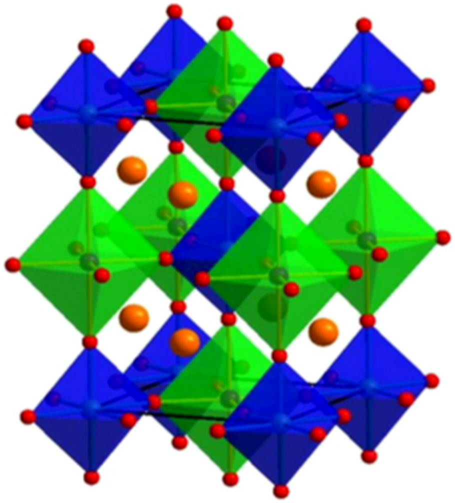


$SrRuO_3$

Double Perovskite

$Sr_2\,La\,Ru\,O_6$



Ru Octahedra form
fcc Lattice (Ru^{5+} is a $4d^{3+}$ system)

La Octahedra also form
fcc Lattice (La^{3+} is a closed shell atom)

All interesting electronic activities take place in the fcc lattice of Ru Octabedra

Hund Coupling &
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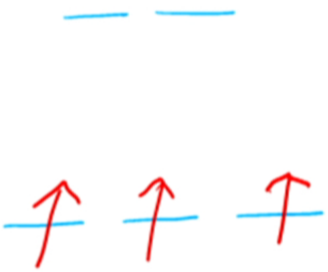
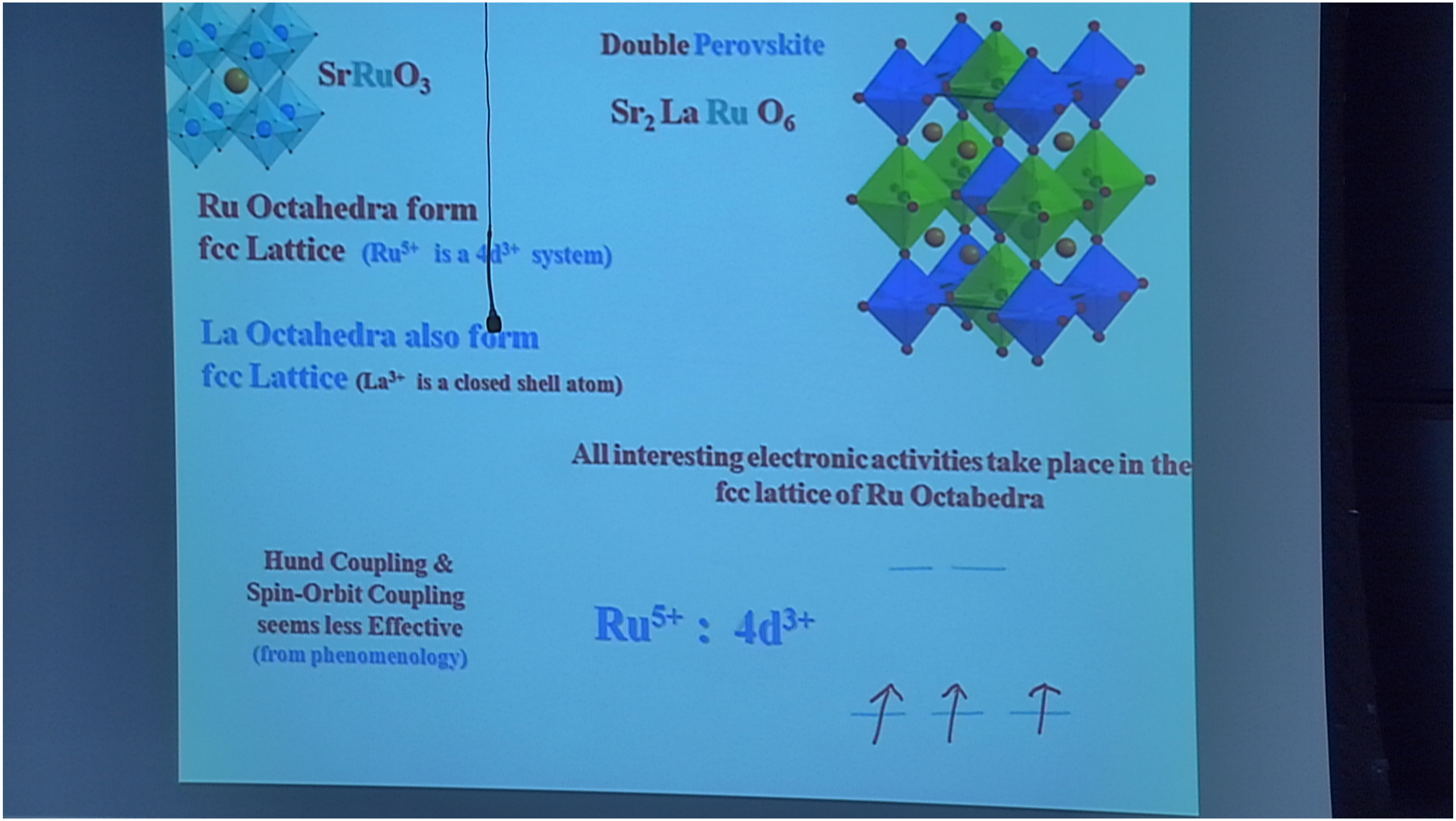
seems less Effective
(from phenomenology)

Ru^{5+} : $4d^{3+}$





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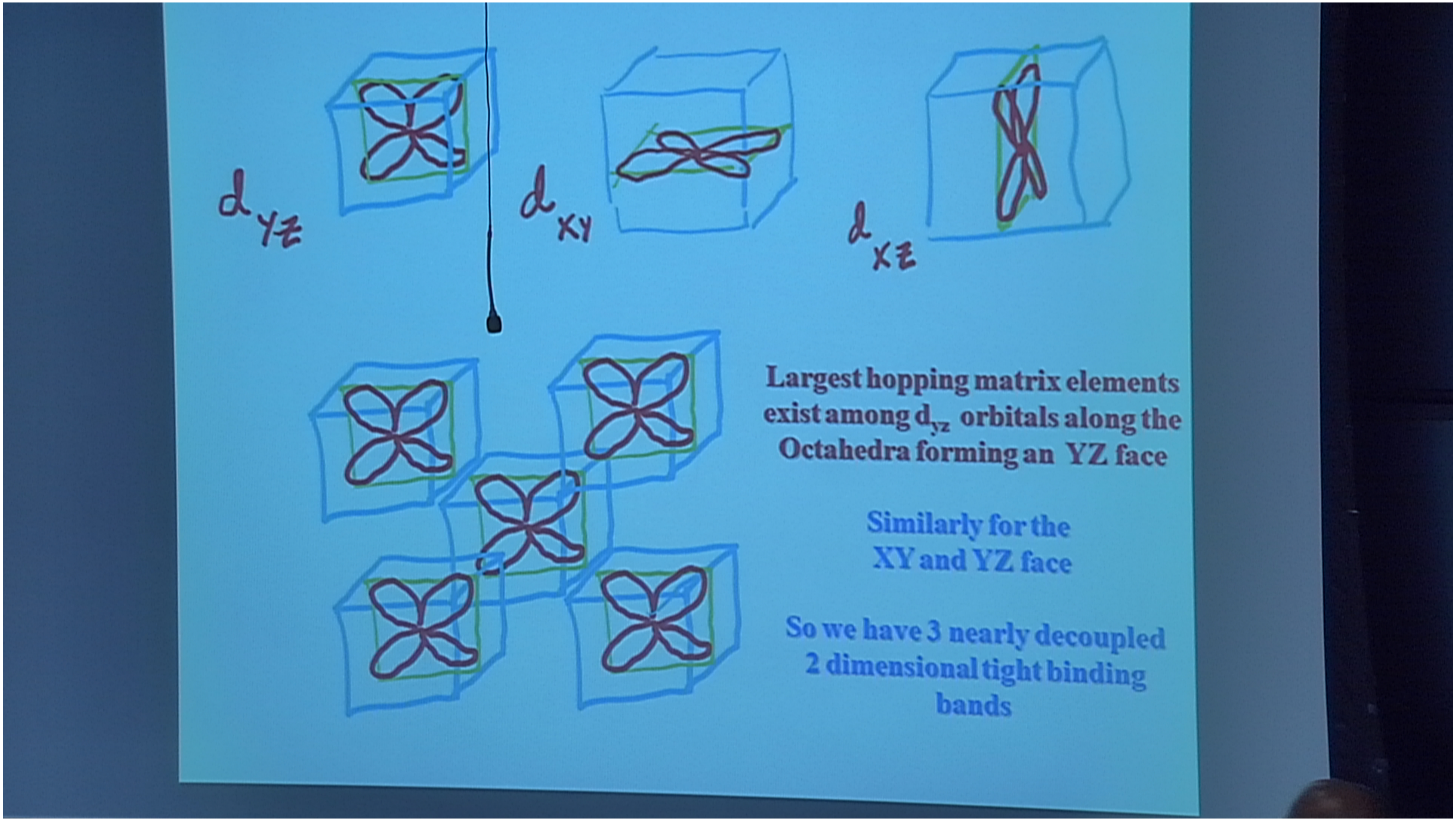
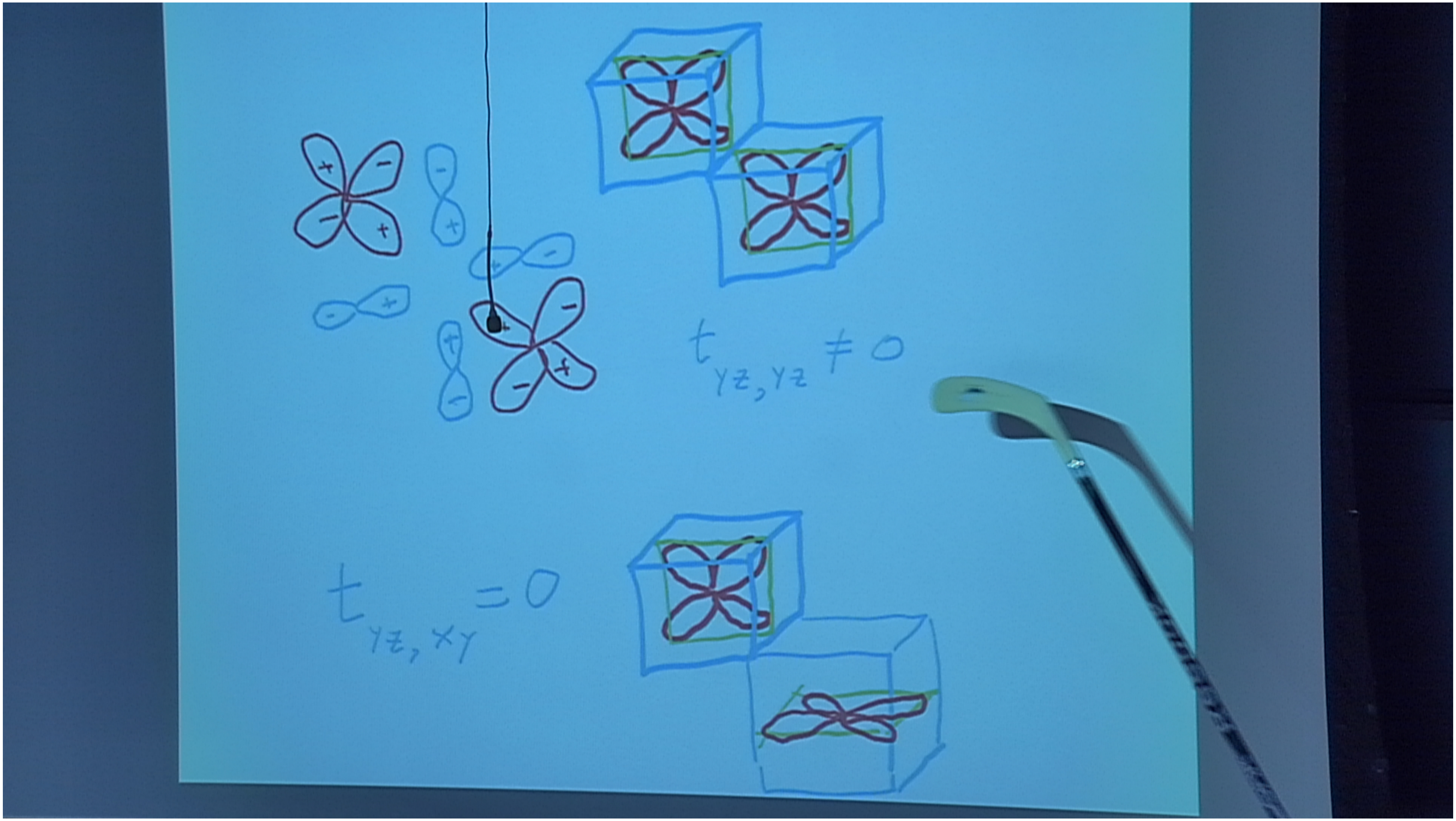
$\uparrow \; \uparrow \; \uparrow$



Largest hopping matrix elements exist among d_{yz} orbitals along the Octahedra forming an YZ face

Similarly for the XY and YZ face

So we have 3 nearly decoupled 2 dimensional tight binding bands



$t_{yz,yz} \neq 0$

$t_{yz,xy} = 0$

We have 3 nearly decoupled
2 dimensional tight binding bands

Three single Band Repulsive Hubbard Model
or tJ Model

Individual bands are similar to Cuprates
in terms of square lattice symmetry

Spin-orbit coupling, Hund Coupling, inter orbital U
are renormalized to small values (phenomenology)

$$H = H_{xy} + H_{yz} + H_{zx}$$

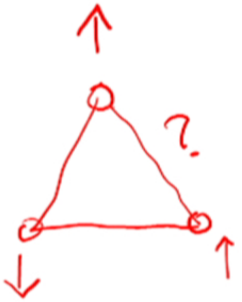
$$H = H_{xy} + H_{yz} + H_{zx}$$

individual bands form Mott insulatrs and exhibit
2 dimensional long Range Order

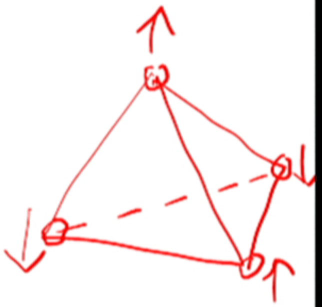
Fcc Lattice frustrates this long range order

and leads into interesting physics

End result is that
2 of them form long range AFM order &
third one forms a spin liquid state



Antiferromagnetic Order in FCC Lattice



3Dimensional FCC Lattice is the counterpart of
2Dimensional Triangular lattice

A given lattice site has 12 neighbors

We start with a nearest neighbor Ising or Heisenberg Antiferromagnetc Model
It is not possible to form an Antiferromagnetic Order
That will satisfy every bond

It is a frustrated Spin System
Ground state has a Macroscopic Degeneracy

In reality Order by Disorder and residual couplings
Choose Type-I or Type-III antiferromagnetic order

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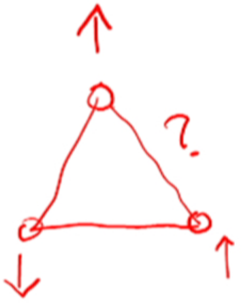

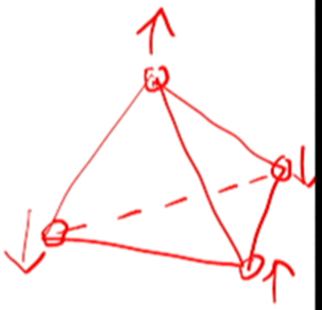

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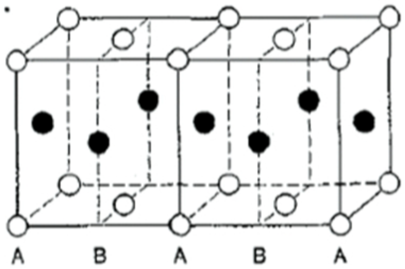
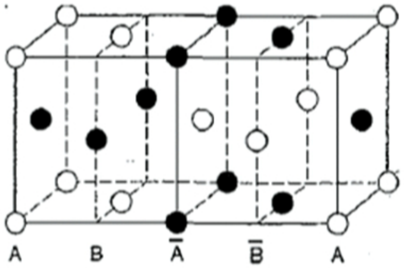
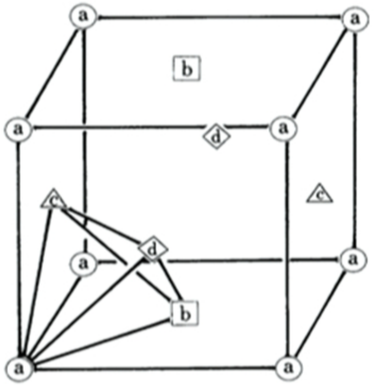
W Minor et al.
JOURNAL DE PHYSIQUE
Colloque C8, Supplément au n° 12, Tome 49, décembre 1988

Type I Antiferromagnetism.



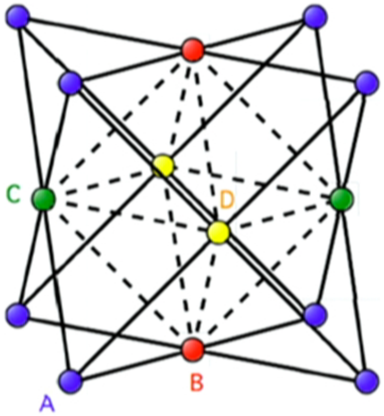
Type III Antiferromagnetism.





Oguchi et al 1985

Chen et al. PHYSICAL REVIEW B 82, 174440 (2010)



GB 2013 unpublished

Summary of the Results

Type-I Antiferromagnetism together
with a spin liquid state (gapped or ungapped)

This is obtained in RVB mean field theory

Two out of three 2d subsystems have AFM long range order
The third one continues to be a spin liquid

3D spinon fermi surface with partial AFM gap

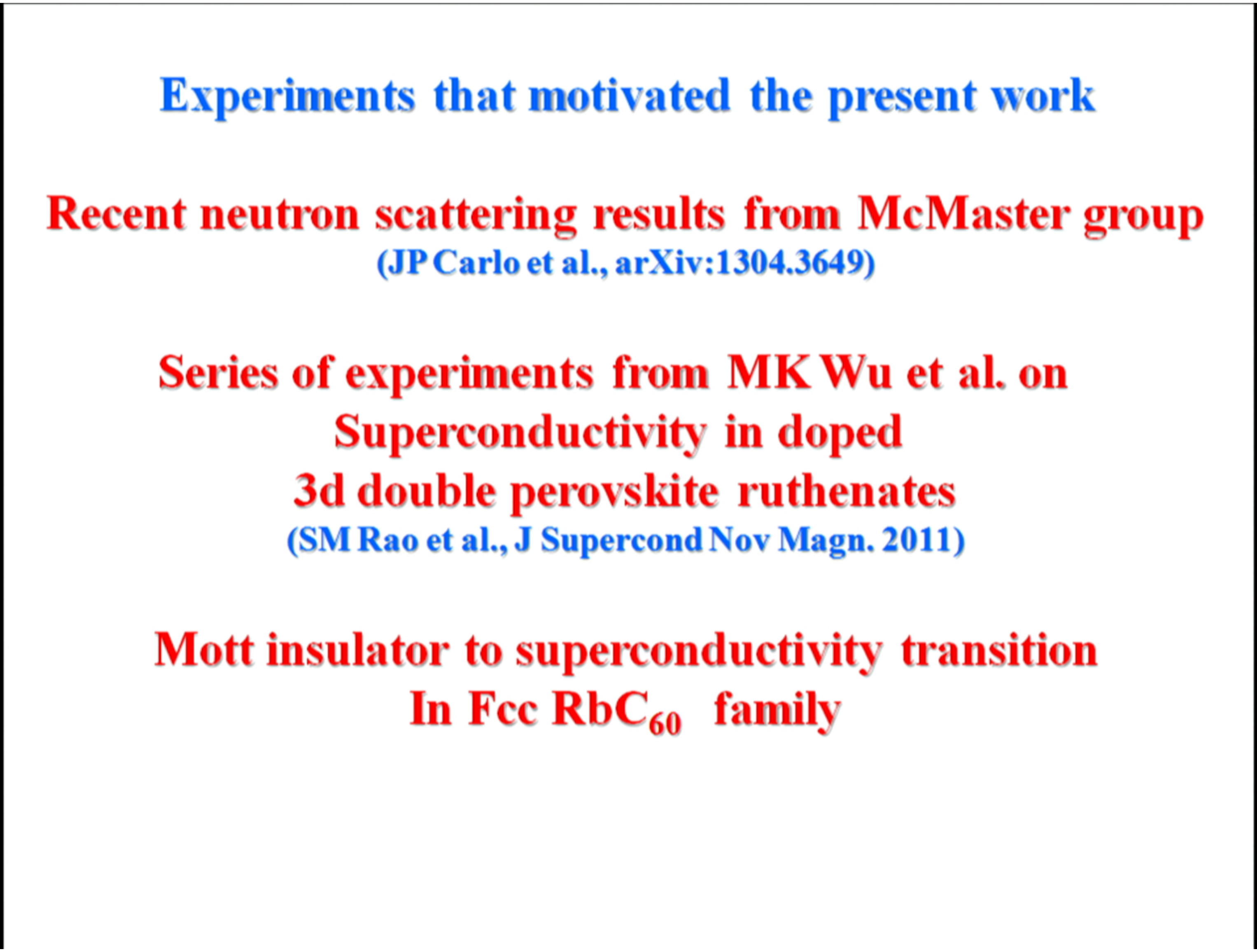
Low energy spinon spectrum coexists with
Goldstone antiferromagnetic modes

Doped Mott Insulator

Low doping dopes the 2D spin liquid subsystem
And leaves the two AFM subsystems untouched

Destruction of AFM order and superconductivity
at a critical doping

a superconducting dome



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Recent neutron scattering results from McMaster group
(JP Carlo et al., arXiv:1304.3649)

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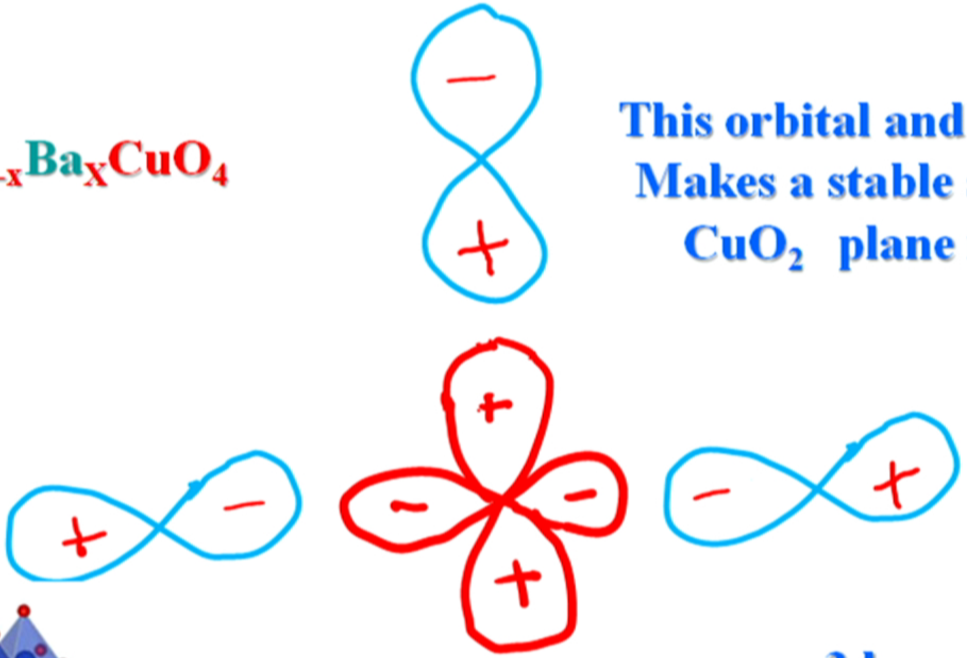

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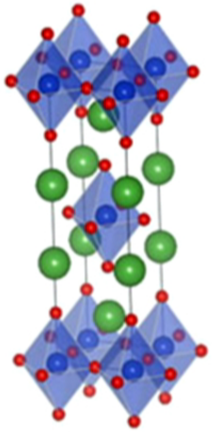

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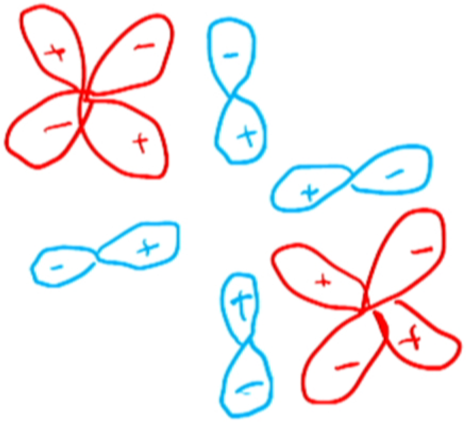

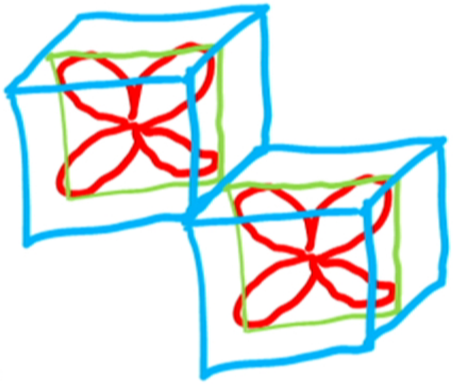

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