INTERNATIONAL ATOMIC ENERGY AGENCY
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**EXPERIMENTAL WORKSHOP ON
HIGH TEMPERATURE SUPERCONDUCTORS
(11 - 22 April 1988)**

MICROSCOPIC ASPECTS OF HIGH T_c SUPERCONDUCTORS
TOWARDS A MICROSCOPIC THEORY OF MAGNETISM & SUPERCONDUCTIVITY
(I, II & III)

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MICROSCOPIC ASPECTS OF HI-TC SUPERCONDUCTORS. – TOWARDS A MICROSCOPIC THEORY

Magnetic Insulator becomes a Hi T_c Superconductor on doping

SOME OF THE ANOMALOUS PROPERTIES

T_c is high

Well defined magnetic moment in Cu^{2+}

Magnetic Insulator is anomalous: Spin Liquid (RVB)

Hall effect: +ve Hall const.

Resistivity: $\rho = aT$

$T_c = a_1 \delta$ (δ: concentration of Cu^{3+})

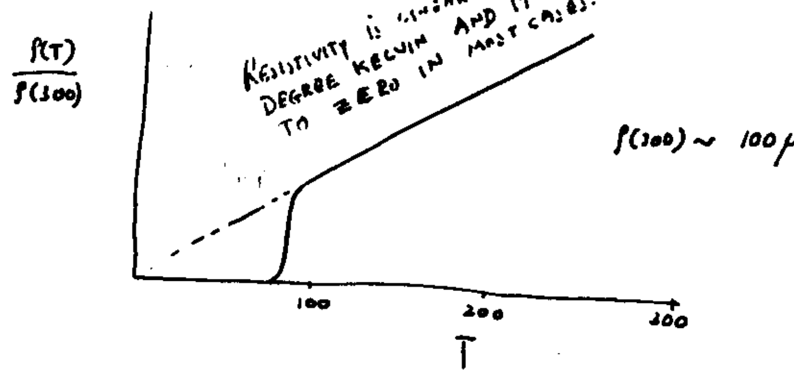
Tunnelling

Specific heat

Sound attenuation, Velocity

Unstable very high T_c's

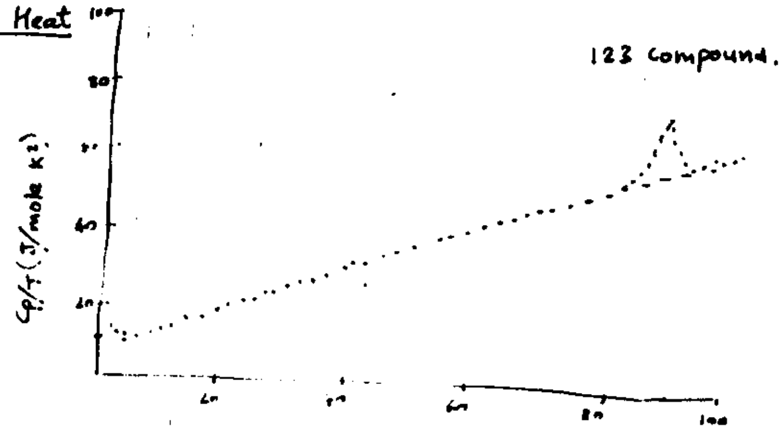
RESISTIVITY



$\rho(300) \sim 100\,\mu\Omega$..

Specific Heat

123 compound.

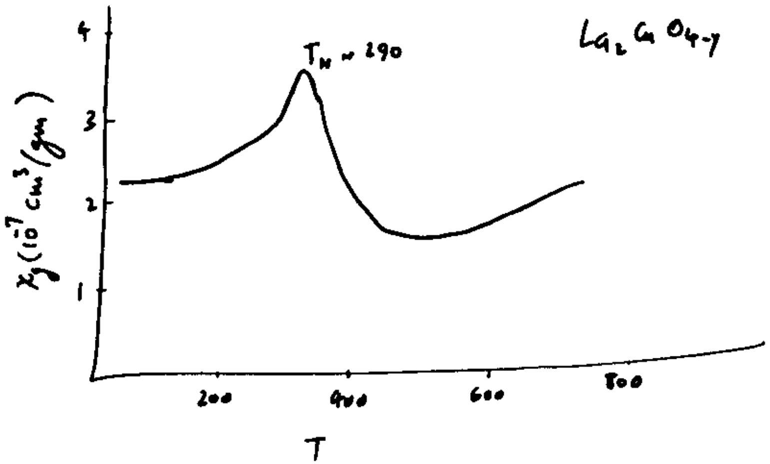


Is the linear sp. ht. at small T due to normal metal regions or due to some intrinsic novel excitations (spinon, pseudo fermi surface

$3 < T < 11K$: $C_p = \gamma T + \beta T^3$

$\gamma \sim 8\,mJ/mole\,K^2$

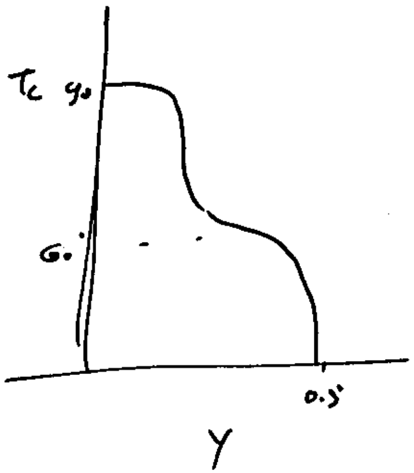
$\beta \sim 0.5\,mJ/mole\,K^4$



No essential qualitative or quantitative difference in susceptibility between doped La_2CuO_4 and 123 compounds

T_c as a function of oxygen vacancy y.

$Y_1Ba_2Cu_3O_{7-y}$



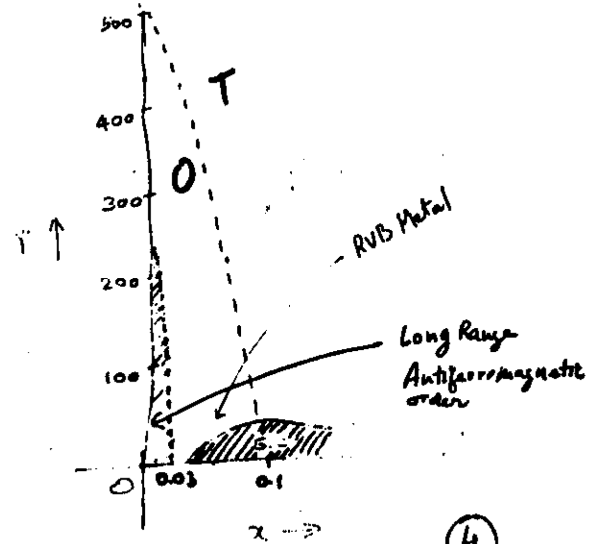
CuO BASED SUPERCONDUCTORS

Bednorz, Muller	$La_{2-x}Sr_xCuO_4$	$T_c^{max} \sim 42^\circ K$
Chu et.al.	$Y_1Ba_2Cu_3O_{7-y}$	$T_c^{max} \sim 94^\circ K$

unstable superconductivity has been seen in many systems upto $500^\circ K$ (?!)

SUPERCONDUCTIVITY IS IN THE VICINITY OF ANTIFERROMAGNETIC INSULATOR

(INSULATOR TO S.C. TRANSITION)

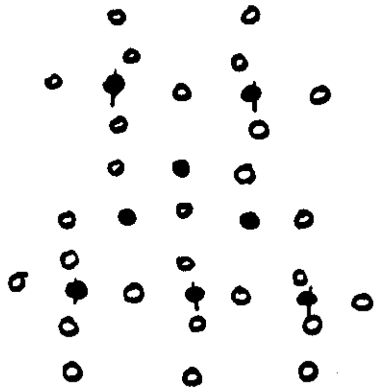


$YBa_2Cu_3O_7$ is electronically similar to $La_{2-x}Sr_xCuO_4$ (chains or not the high T_c superconductors)

$BaPb_xBi_{1-x}O_3$

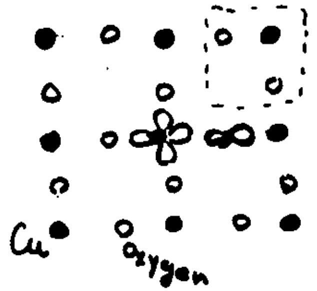
CRYSTAL STRUCTURE

La_2CuO_4



K_2NiF_4 Structure

Corner sharing octahedra form well separated planar network



BEDNORZ & MULLER

(Z. Phys. 64, 189 (86))

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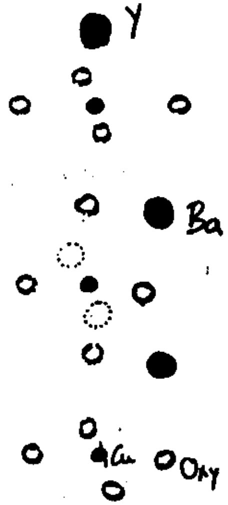
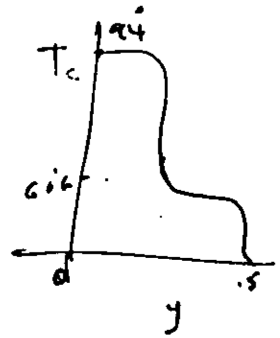
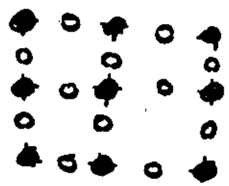


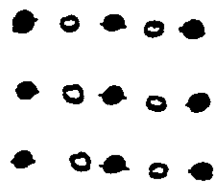
$YBa_2Cu_3O_{7-y}$

Gd ..

Eu ..

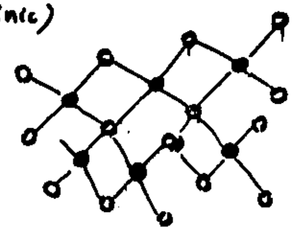






CuO (TENORITE)

(Monoclinic)



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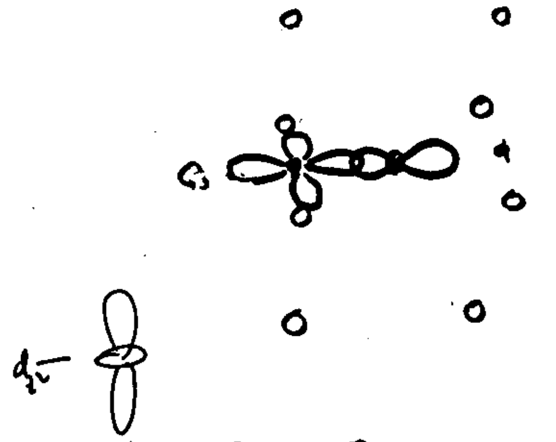
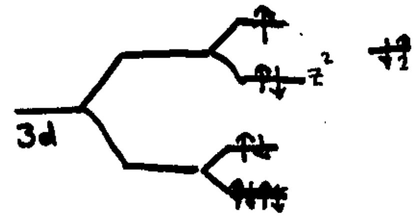
ELECTRONIC STRUCTURE





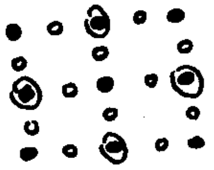
$La_{2-x}Sr_xCuO_4$

La: 3+

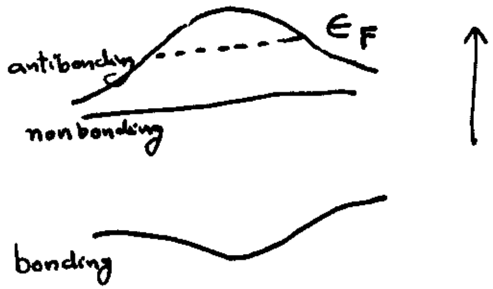
Cu: 2+ → $3d^9$

O: 2−

Sr: 2+ ⇒ $Cu^{2+} \to Cu^{3+}$



unit cell

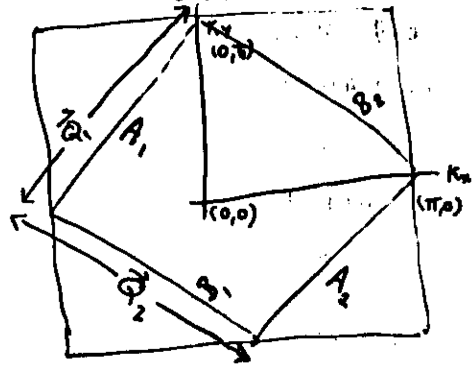


THERE ARE EXPTL. INDICATION THAT THE NON-BONDING & BONDING BANDS ARE NOT CRUCIAL FOR THE UNDERSTANDING OF TRANSPORT & STATISTICAL MECHANICAL PROPERTIES. THERE ARE MANY WHO BELIEVE THAT THE OXYGEN RICH BANDS ARE IMPORTANT. THIS QUESTION IS ACTIVELY BEING STUDIED AT PRESENT.

IS CDW ARISING FROM FERMI SURFACE NESTING RESPONSIBLE FOR HI-Tc SUPERCONDUCTIVITY? No.

NESTING

THE ANTIBONDING BAND CAN BE APPROXIMATED BY A SIMPLE TIGHT BINDING BAND OF A SQUARE LATTICE. THE CORRESPONDING WANNIER ORBITALS ARE ANTI-BONDING COMBINATION OF THE TWO OXYGEN p-ORBITALS AND ONE COPPER $d_{x^2-y^2}$ ORBITAL FROM THE UNIT CELL IN THE CuO_2 PLANE



THE PIECE OF FERMI SURFACE A_1 CAN BE TRANSLATED BY THE VECTOR $\vec{Q}_2$ TO OVERLAP ON TOP OF A_2. SIMILARLY B_1 & B_2 by $\vec{Q}_1$

THIS GEOMETRIC PROPERTY OF THE FERMI SURFACE IS CALLED NESTING.

THE NESTING PROPERTY IMPLIES THAT THE DENSITY PARTICLE-HOLE EXCITATION SPECTRUM HAS A STRONG SINGULARITY AT ZERO-ENERGY AND WAVE-VECTORS $\vec{Q}_1$ & $\vec{Q}_2$

IN THE ABSENCE OF STRONG ELECTRON-ELECTRON REPULSION THIS WOULD LEAD TO CDW'S WITH WAVE-VECTORS $\vec{Q}_1$ & $\vec{Q}_2$ AND CONSEQUENTLY GAPS AT THE FERMI SURFACE.

EXPERIMENTS SHOW NO SUCH DISTORTION FOR OUR SYSTEM. THE ORTHORHOMBIC DISTORTION HAS A DIFFERENT SYMMETRY AND DOES NOT LEAD TO A GAP AT THE FERMI SURFACE.

FERMI SURFACE NESTING CAN ALSO LEAD TO SDW WITH WAVE VECTORS $\vec{Q}_1$ and $\vec{Q}_2$.

THERE IS NO EXPERIMENTAL EVIDENCE FOR THIS EITHER. WHAT WE HAVE IS THE MOTT INSULATING ANTIFERROMAGNET.

IN A MOTT INSULATOR AFTER ANTIFERROMAGNE IS DESTROYED IT WILL REMAIN AN INSULATOR.

WHY DO WE HAVE A MOTT INSULATOR?

THE BAND WIDTH ~ 2eV.

The ON SITE ELECTROSTATIC REPULSION (HUBBARD) U ~ 5eV

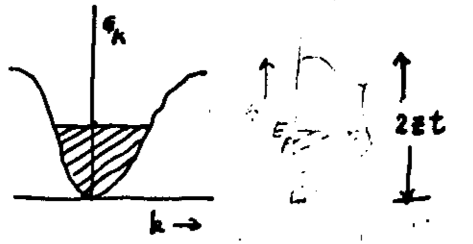
THUS IF ELECTRONS GAIN DELOCALISATION ENERGY (~ 2eV) THEY WILL LOOSE ENERGY DUE TO STRONG RUPULSION. THUS INT THE GROUND STATE THEY CHOOSE TO REMAIN LOCALISED ON THE SITES.

QUANTUM FLUCTUATIONS LEAD TO EXCHANGE INTERACTION LEADING TO NON-TRIVIAL MAGNETIC STATE (AFM ORDER or RVB).

MOTT INSULATOR $\frac{U}{t} \gg 1$

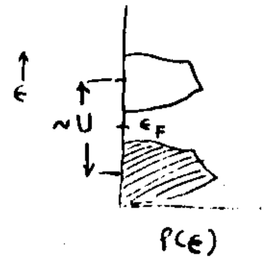
A SIMPLE TIGHT BINDING MODEL:
ONE ORBITAL PER SITE
ONE ELECTRON PER SITE

SIMPLE HARTREE-FOCK & FREE ELECTRON PICTURE

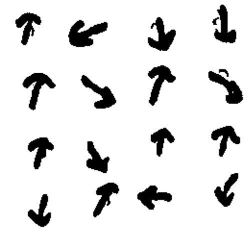


HALF-FILLED BAND METAL

MOTT-HUBBARD PI

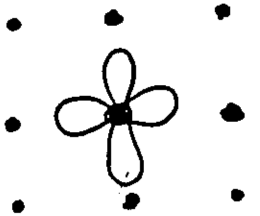


CHARGE EXCITATIONS HAVE A GAP ~ U - zt



THE 2^N DEGENERACY IS SPLIT BY THE EXCHANGE INTERACTION.

A ONE BAND HUBBARD MODEL DESCRIBES MAGNETIC & SUPERCONDUCTING PROPERTIES.



$$H = -t\sum c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + \mu \sum c^{\dagger}_{i\sigma} \ldots$$
$$+ U \sum n_{i\uparrow} n_{i\downarrow}$$

> ADMIXTURE OF Cu $d_{x^2-y^2}$ AND OXYGEN 2p ORBITALS HAS $d_{x^2-y^2}$ SYMMETRY

$t \sim 0.5\,eV$

$U \sim 5\,eV$

ANDERSON

HALF FILLED BAND —SUPER EXCHANGE→ HEISENBERG MODEL

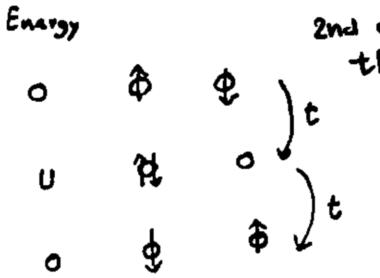
$\frac{U}{t} \gg 1$

MOTT INSULATOR

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

$$J = \frac{2t^2}{U}$$

2nd order perturbation theory



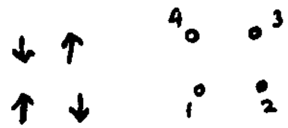
$$H = -J \sum b^{\dagger}_{ij} b_{ij}$$

$$b_{ij} = \frac{1}{\sqrt{2}}\left(c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}\right)$$

$$n_{i\uparrow} + n_{i\downarrow} = 1$$

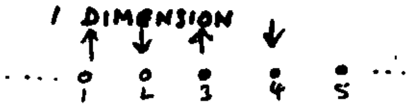
SINGLET GROUND STATES

IN LOWER DIMENSIONS THE ENERGY IS LOWERED BY FORMATION OF SINGLET PAIRS AND ALSO, BY RESONATING AMONG VARIOUS SINGLET CONFIGURATIONS.



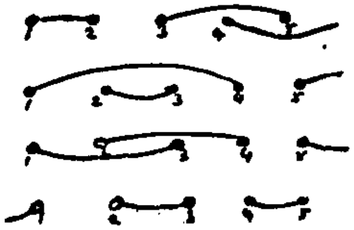
$|G\rangle = a$  $+\ b$

1 DIMENSION



$|G\rangle = \sum a(c)\,|c\rangle$

$|c\rangle$ $|1\rangle$ $|2\rangle$ $|3\rangle$ $|4\rangle$



RESONATING
VALENCE
BOND STATE

IN HIGHER DIMENSIONS (example $d = 3$) THE ENERGY IS GAINED BY FORMATION OF LONG RANGE NEEL TYPE AFM OR

GEOMETRIC FRUSTRATION OR OTHER DYNAMIC EFFECTS COULD EASILY DESTROY THE AFM ORDER AND GO INTO A SINGLET LIQUID STATE THEREBY RESTORING THE SYMMETRY

RVB (RESONATING VALENCE BOND STATE)

ANTIFERROMAGNET $\longleftrightarrow$ SPIN - CRYSTAL

QUANTUM PARAMAGNET $\longleftrightarrow$ QUANTUM LIQUID OF SINGLET PAIRS

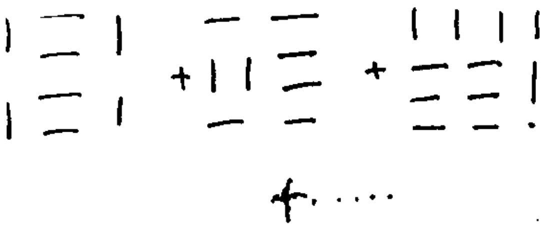
" " $\longleftrightarrow$ SOLID OF SINGLET PAIRS (Valence Bond state)

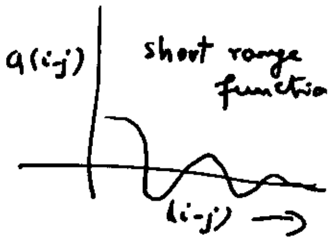
WELL DEFINED AND SIMPLE PHASE RELATION AMONG VARIOUS VALENCE BOND CONFIGURATIONS

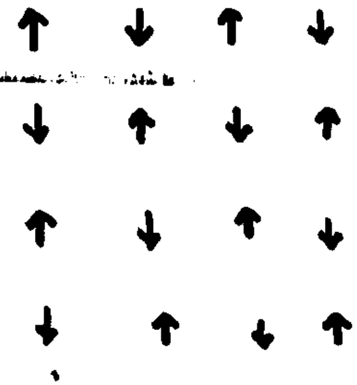
CREATE SINGLET PAIRS IN ZERO MOMENTUM STATE $\left(\sum_{ij} a(i-j)\left(c^{+}_{i\uparrow}c^{+}_{j\downarrow}-c^{+}_{i\downarrow}c^{+}_{j\uparrow}\right)\right)|0$

FILL THE LATTICE WITH N/2 SINGLET PAIRS $\left(\sum_{ij} a(i-j)\, b^{\dagger}_{ij}\right)^{\frac{N}{2}}|0\rangle$

PROJECT OUT STATES CONTAINING DOUBLE OCCUPANCIES $P_G\left(\sum a(i-j)\, b^{\dagger}_{ij}\right)^{\frac{N}{2}}|0\rangle$







FOR $S=\frac{1}{2}$ HEISENBERG ANTIFERROMAGNETS ON A SQUARE LATTICE THIS LONG RANGE ORDER IS **FRAGILE**

GEOMETRIC FRUSTRATIONS — ANDERSON; ANDERSON, FAZEKAS

&

DYNAMICAL EFFECTS ARISING FROM DOPING — NAGAOKA; ANDERSON, BASK[...] ZOU, HSU

COULD DESTROY THE ORDER

NAGAOKA: FOR $\frac{U}{t} >>> 1$ SMALL DOPING DESTROYS ANTIFERROMAGNETISM AND STABILISES FERROMAGNETIC ORDER

TWO ENERGIES

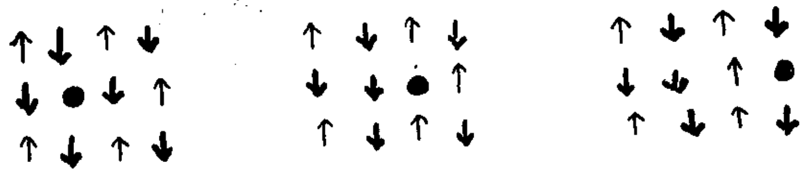
- DELOCALSATION ENERGY OF HOLES (GAIN

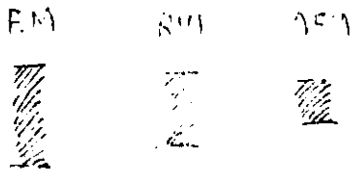
  $\sim \alpha t \delta$ — doping fraction

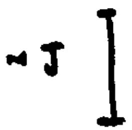
- BULK MAGNETIC ENERGY (LOSS)

  $\sim J$

depends on the magnetic state







$I \sim 0.1J$.

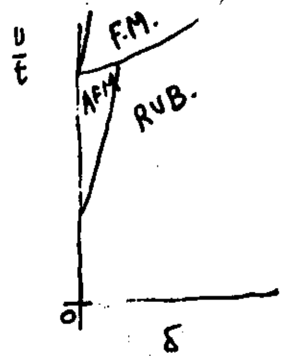
Anderson
Baskaran
Zou
Hsu

Small doping stabilises RVB rather than FM state for $U/t \sim 5$

Hole bandwidth is comparable to that in a F.M.

And $(E_{RVB} - E_{AFM}) < (E_{FM} - E_{AFM})$

Numerical verification by Shiba & Yokoyama



$$\alpha t \delta_c \approx E_{RVB} - E_{AFM} = 0.1J$$

$$\delta_c \approx \frac{0.1J}{\alpha t} \approx 0.03$$

ONE POSSIBLE CONSEQUENCE OF DOPING

SEA OF SINGLET PAIRS.

SINGLETS HOP IN THE INSULATOR

- ONLY SPIN CURRENT NO CHARGE CURRENT.

THE MOTT-HUBBAR GAP PREVENTS CHARGE FLUCTUATIONS.

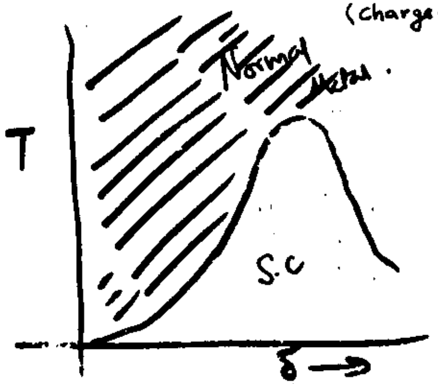
(ZERO ELECTRONIC COMPRESSIBILITY)

NO SUPERCONDUCTIVITY INSPITE OF SINGLET PAIRS

DOPE IT (example: Remove carriers)

Singlets in the vicinity of holes transport charge as they move

Small density of holes (charged pairs) ⇒ Large phase fluctuation



QUASI PARTICLES

FERMI LIQUID — dressed electron

charge and spin are carried by the same quasi particle.

Bogolubov Q.P. in Superconductors.

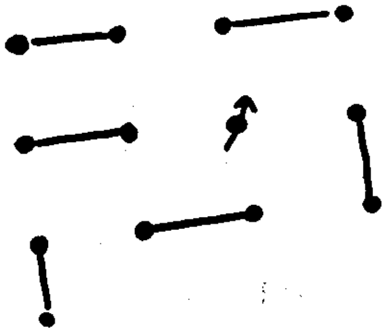
Fractional Q.H.E — Fractional charge & fractional spin

RVB — CHARGE - SPIN DECOUPLING

Holon (Boson) — Spinon (Fermion)

EXCITATIONS OF AN RVB STATE

Kivelson
Rokshar
Sethna

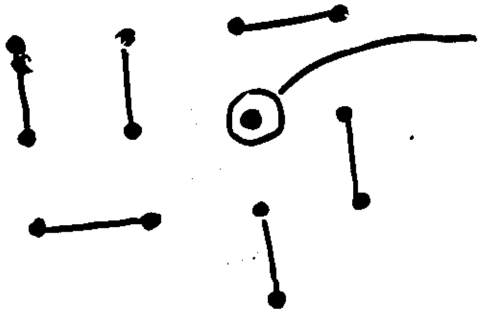


dangling Spin or SPINON

$S = \frac{1}{2}$ charge $Q = 0$

Fermion

J



hole (a charged Boson)

$S = 0$, $Q = +e$

density of charged valence bond increases with doping

They undergo Bose condensation

$$T_c \sim 1.7\times10^5 \left(\frac{\delta^3}{a^4 c^2 m_{vb}^2 m_z} \right)^{\frac{1}{3}}$$

THERMALLY PRODUCED SPINONS REDUCE THE DENSITY OF BOSONIC HOLES. THIS IS WHAT CHANGES THE SCALE OF T_c from $t\delta$ to J. WEAK 3D COUPLING FURTHER REDUCES THIS.

SPINON-HOLON SCATTERING – CONSEQUENCES

Anderson & Zou.

Holons are scattered by real spinons that are thermally produced. If the spinons have a pseudo fermi surface (or a small gap)

density of thermal spinons $\sim \frac{k_B T}{J}$

$\therefore$ holon life-time $\sim \frac{J}{k_B T}$

$\therefore$ Resistivity $\rho_{\parallel} \sim T$

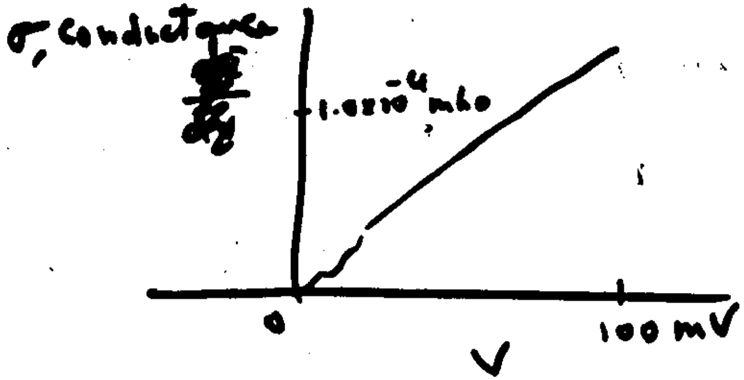
Anisotropic Conductivities

In the normal state, holon cannot tunnel from plane to plane. It has to wait for a spinon to join to become a fermion (electron).

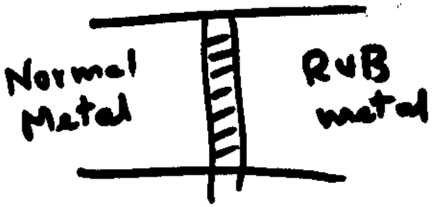
$$\therefore \quad \sigma \propto T$$

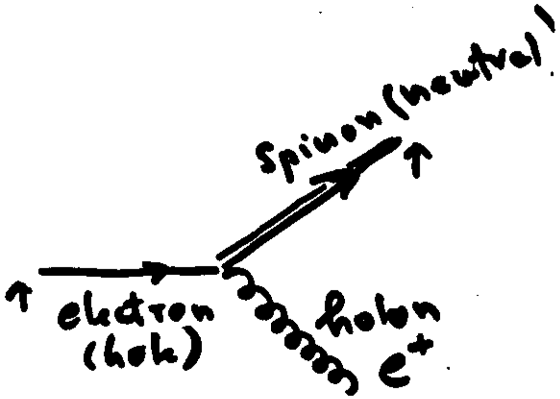
$$\therefore \rho_{\perp} \sim \frac{1}{T}$$

Tunnelling characteristics



$\sigma \propto V$

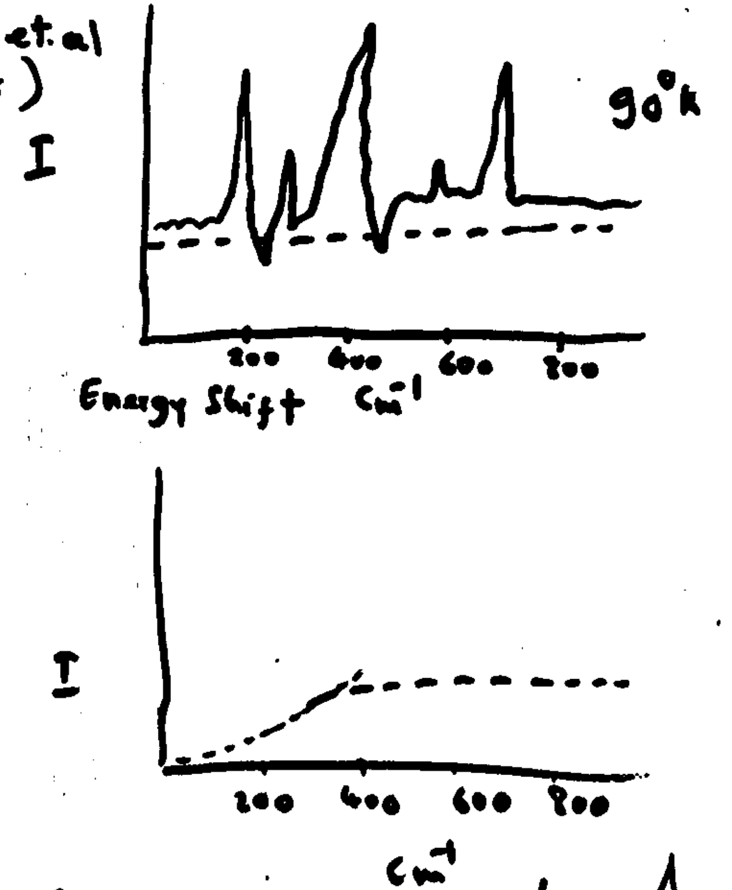


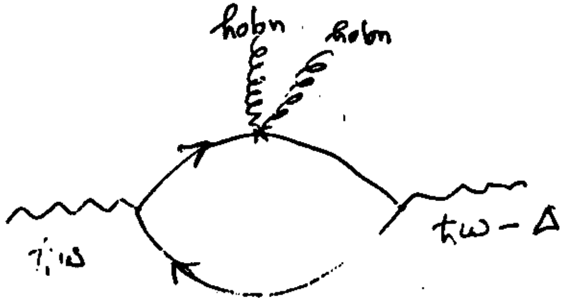


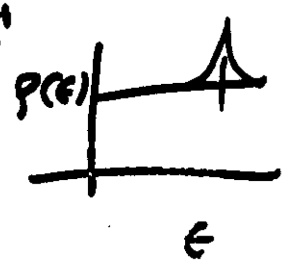
RAMAN EFFECT

(S.L. Cooper et. al Illinois)

G. BASKARAN

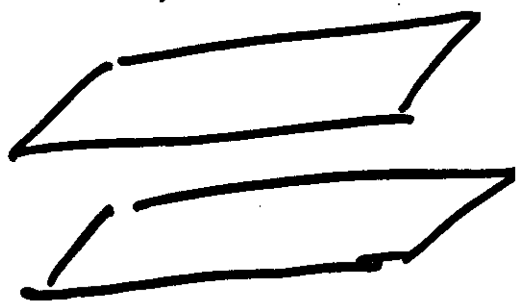






2d → 3d Superconductivity

2e or not 2e



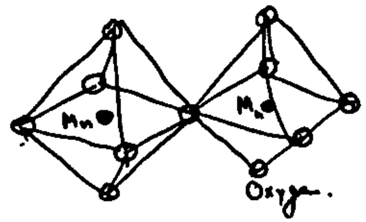
Holons cannot have ODLRO in 2-d (long wavelength fluctuations destroy it). Hence e^+ condensate is absent in the plane.

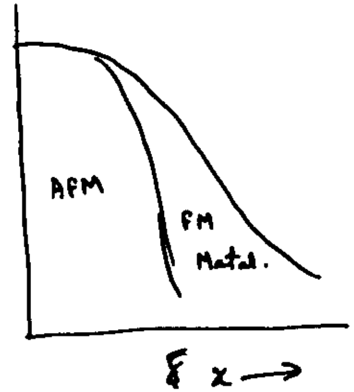
Pair tunnelling as opposed to independent particle tunnelling is more probable at low T, due to RVB correlations.

Thus pairs of holons of charge +2e tunnel and stabilise a 3-d condensate of charge +2e rather than e !

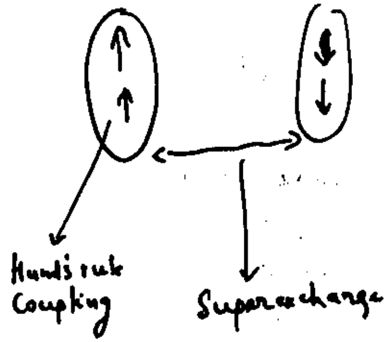
WHAT IS SPECIAL ABOUT CuO BASED CERAMICS ?
WHY ARE MANY OXIDES NON-SUPERCONDUCTING ?

THE CASE OF MANGANITE $La_{1-x}(Ca \text{ or } Sr)_x MnO_3$





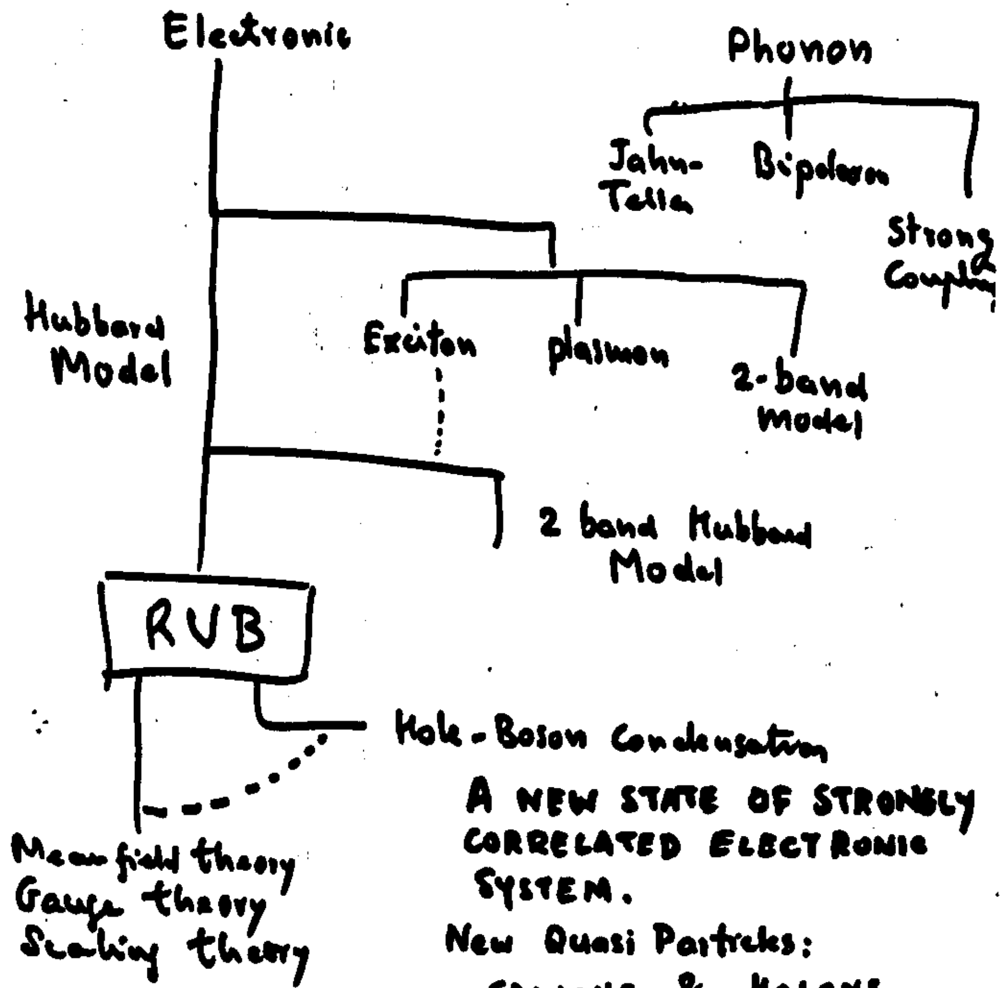
ZENER'S DOUBLE EXCHANGE



J_H Hund's rule exchange ~ 2eV
t, Hopping Integral ~ 0.5eV
J_S Super exchange ~ 0.1eV

THE SYSTEM LOOSES THE SMALL EXCHANGE ENERGY (J_S) TO GAIN A LARGER DELOCALISATION ENERGY (t) BY A FERROMAGNETIC POLARIZATION AROUND THE HOLE

Theories of Hi-Tc Superconductors.



A NEW STATE OF STRONGLY CORRELATED ELECTRONIC SYSTEM.

New Quasi Particles:

SPINONS & HOLONS