INTERNATIONAL ATOMIC ENERGY AGENCY
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SMR. 767 - 9

MINIWORKSHOP ON STRONG CORRELATIONS
AND QUANTUM CRITICAL PHENOMENA
(4 - 22 July 1994)

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TRANSPORT AND AF IN DOPED 214 SYSTEM

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These are preliminary lecture notes, intended only for distribution to participants.

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Transport and AF in doped 214 system

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I Homogeneous doping

a) Phenomenology of small pockets

(Stability, AF vs doping)

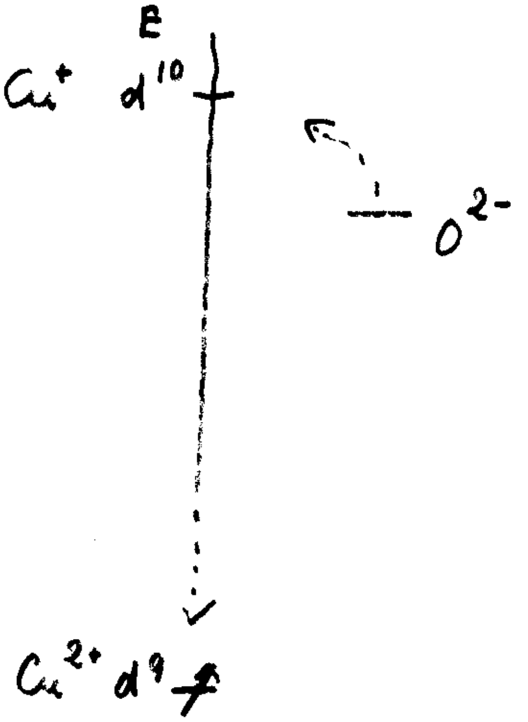
b) A discussion of the three band model

II Disorder + doping

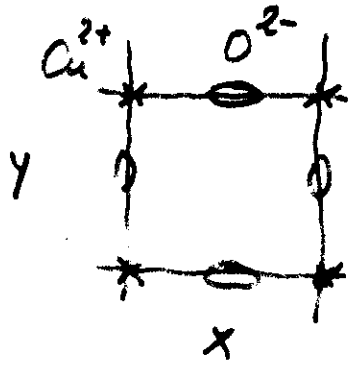
a) Experiments on conductivity at very small x

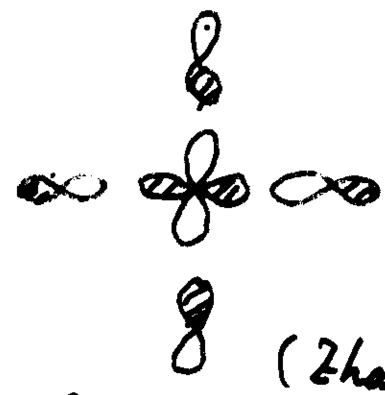
b) Phase separation in $La_2CuO_{4+\delta}$
vs $La_{2-x}Sr_xCuO_4$

Charge Transfer Insulator (Varma, Schmitt-Rink, Abrahams)



Three Band Model (Emery)





(Zhang, Rice)

$(-1)^6 t_0$

at homogeneous doping $\Rightarrow$ itinerant e, h.

$h = -e$ O^-, $\uparrow$

$e = d^{10}$ $\uparrow\downarrow$

Vacuum fluctuations/Cu:  $\sim -\frac{t_0^2}{\Delta}$ etc

any attempt to calculate bands ~ same scale

Range of parameters

From T.C. Leung et al '92

Δ : 1.5 – 4.0 eV

$U \equiv U_d$: 8.8 – 10.5 eV $[(d^{10} - d^8)]$

U_p : 4.0 – 6.0 eV

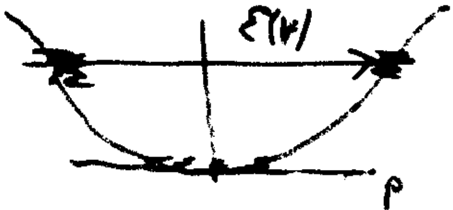
U_{dp} : 0.0 – 1.5 eV

$t_0 = t_{dp}$: 1.07 – 1.6 eV

t_{pp} : 0.3 – 0.65 eV

Phenomenological approach:

Assume that there is a band (h)



$$\varepsilon(p) \simeq \frac{p^2}{2m}$$

⊗ AF: $\vec{Q}$ mean field band

$$\left\{ \begin{aligned} H = &\sum \varepsilon_p a^+_{p\sigma} a_{p\sigma} + J' \sum \vec{m}_q \vec{\sigma}_{\sigma\sigma'} \hat{a}^+_{p\sigma} \hat{a}_{p-q\sigma'} \\ &+ \sum \Omega(q) (\alpha^+_q \alpha_q + \beta^+_q \beta_q) \end{aligned} \right.$$

$\cancel{\Omega(q) = c|q|}$ $\qquad \Omega(q) = \overset{Ja}{\downarrow}{s}|q|$

$$\hat{\alpha}, \hat{\beta} \Rightarrow \vec{L}_i - \vec{L}_{i+1} = \vec{\ell}_i \qquad \vec{M} = \vec{L}_i + \vec{L}_{i+1}$$

$$\vec{m}_q \propto \frac{d}{dt} \vec{\ell}_q$$

Stability: one hole (or e) dressed by spin-waves

$\downarrow$ $\psi_\sigma(\vec r)$

Minimizing over α, β: $n_\alpha \sim n_\beta \sim \frac{J'^2}{J^2(qa)} >> 1$

The Deigen-Pekar functional

$$\tilde H = \frac{1}{2m}\left\{\int \sum_\sigma |\nabla\psi_\sigma|^2 - 4c|\psi_\downarrow|^2|\psi_\uparrow|^2 d\vec r^2\right\}$$

$$\boxed{c \equiv \frac{m J'^2(qa)a^2}{2\sqrt2\,\Omega(q)} = \frac{J'^2}{JW}} \qquad \left(W = \frac{1}{2ma^2}\right)$$

2D - no barrier:

if $c < 2.88$ no saddle point (stable)

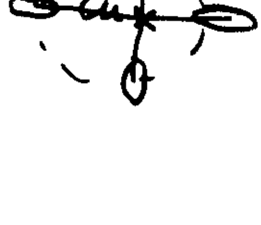
$c > 2.88$ the system forms polaron

(at $c >> 1$ — large ("Nagaoka") polaron)

To compare with Z.R. singlet:

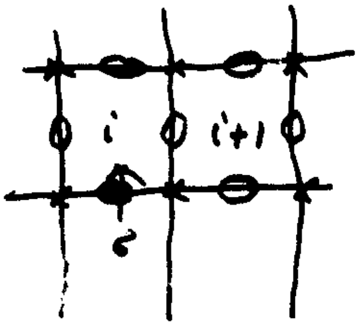
no t-J for holes
t-J for e

(?)

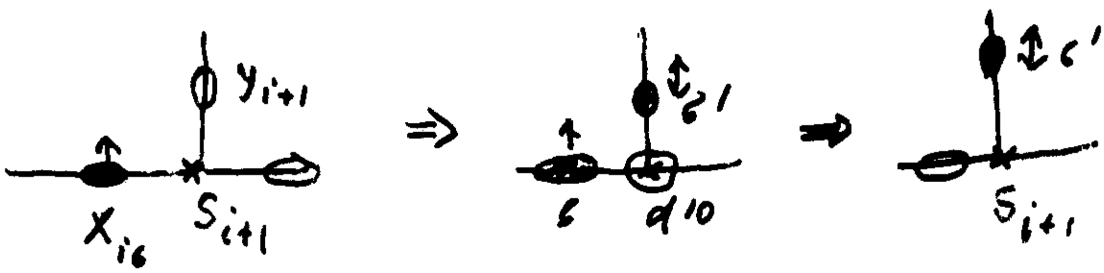


In the three band picture

$U = \infty$; Hamiltonian for holes:



$$X_{i\sigma} \Rightarrow Y_i \cdots + Y_{i\pm1} \cdots + X_i \cdots X_{i\pm1}$$



$$M_{i\,i\pm1} \propto (-)^{\sigma} \frac{t_0^2}{\Delta}\left\{1 + (\hat{\vec{\sigma}}\,\hat{\vec{S}}_{i+1})\right\}$$

$$\hat{S}_{i+1} \rightarrow \hat{S}_q \Rightarrow (-1)^i \mu + \hat{S}_q$$

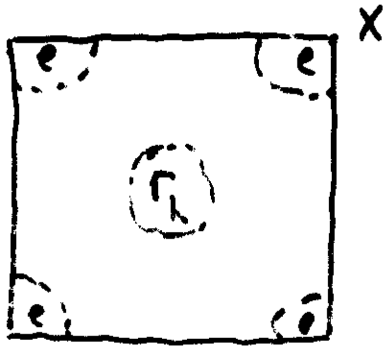
$$\mu \equiv \langle S_z \rangle_{Q_0} \qquad \mu = 0.6 \frac{\langle S_z \rangle}{\mu_B}$$

(?) Stability of the band:

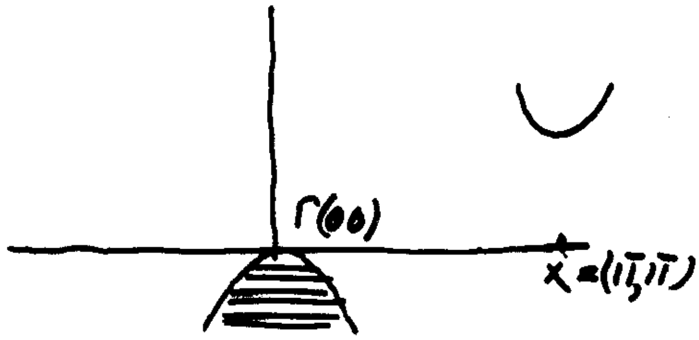
$$\frac{1}{(1-\mu^2)} \frac{U_p^2}{t_0^2} \frac{\Delta(2\Delta + U_p)}{(\Delta + U_p)^2} < 2.88$$

G. ? Kumar '93 (unpublished)

Band structure for holes and electrons



(in the old tetragonal band)



(the indirect gap)

if correct, is to be $< \Delta$!

Recall at $t_0 \ll \Delta$, $W \sim \frac{t_0^2}{\Delta}$!

- The charge transfer gap $\to 0$ $\Delta(x) \to 0$

The spill-over regime

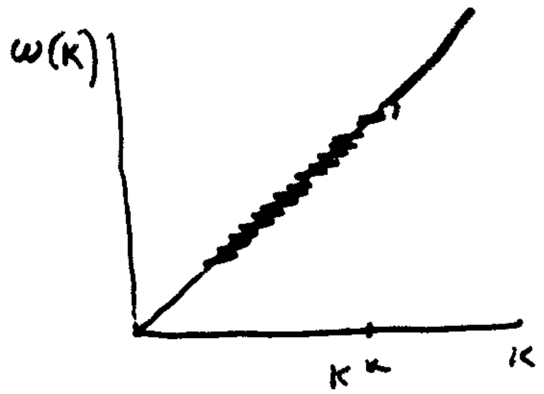
$R_H \sim \frac{1}{x}$ $x < 0.1$ (Ong'89)?
T-independent

$n_h \neq x$ at $x > 0.1$ T-dependent

AF vs doping in the homogeneous picture

Gan, Andrei, Coleman '91

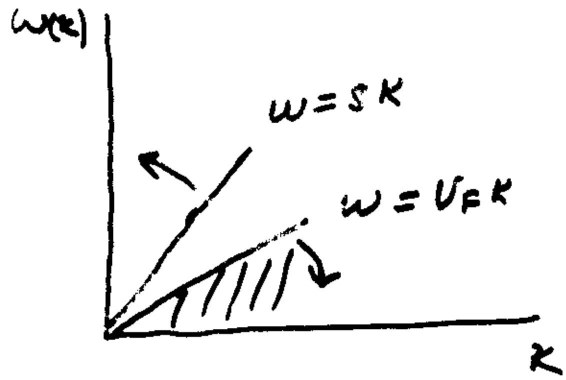
Balatsky '92



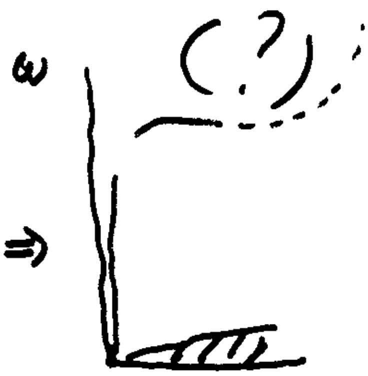
$K^* = 2ms$

$K^* - 2p_F < K < K^* + 2p_F$

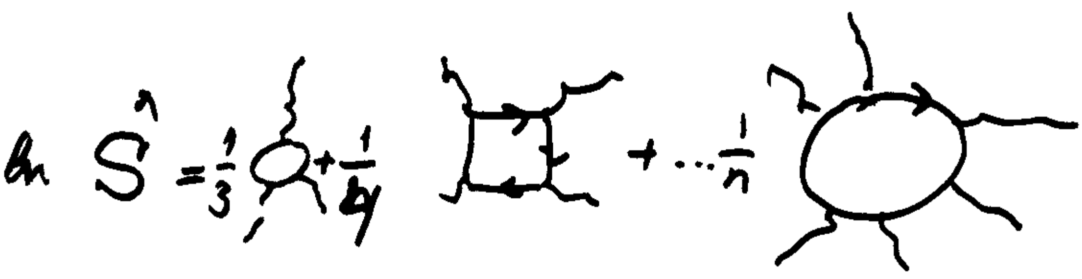
$$\bar{S} = S\left(1 + \frac{c}{\sqrt{1 - \frac{V_F^2}{S^2}}}\right)$$



$V_F \approx S \Rightarrow$



$\ln \hat{S} = \frac{1}{3}$ [diagram] $+ \frac{1}{4}$ [diagram] $+ \dots \frac{1}{n}$ [diagram]

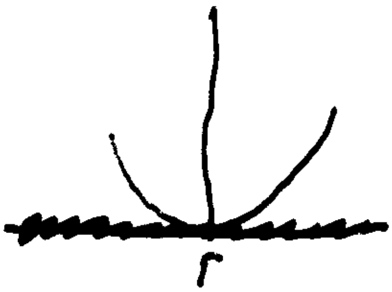


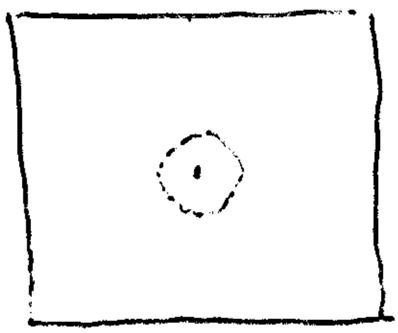
The need to consider $t_{pp} > 0$

$$- 2t_{pp} \cos\frac{p_x a}{2} \cos\frac{p_y a}{2}$$

in the hole representation

$t_{pp}=0$ dispersionless band →



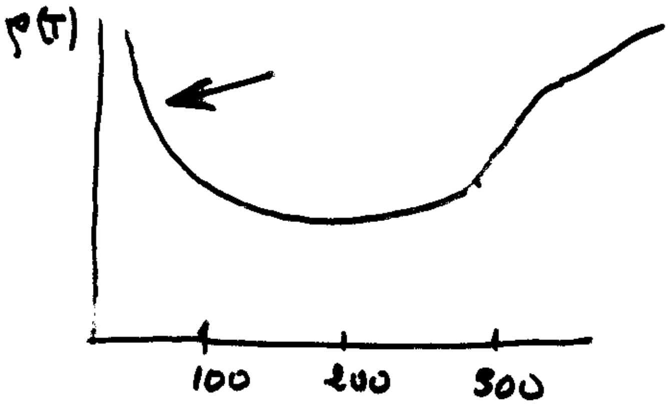


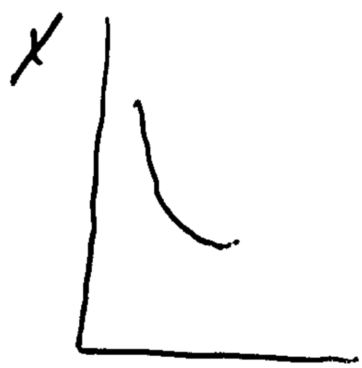
* $La_{2-x}Sr_x CuO_4$: $x = 0.025$

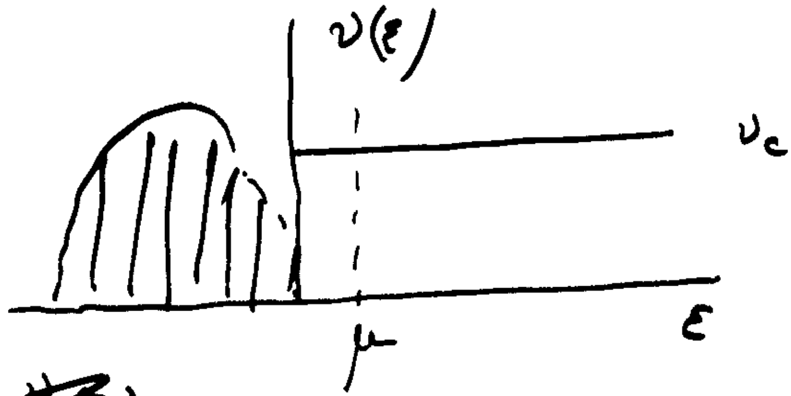
$x = 0.05$

? Doping ; Impurity Band, Screening of charge

Coulomb energy > 0.2 ev (the optical data)







$$\nu_e(\varepsilon) = \nu_0 \left(\frac{|\varepsilon|}{\Delta}\right)^{\alpha} e^{-\frac{|\varepsilon|}{\Delta}}$$

$$\left[\; \nu_0 \Delta \int_{-\infty}^{0} \frac{d\varepsilon}{\Delta}\left(\frac{|\varepsilon|}{\Delta}\right)^{\alpha} \frac{1}{e^{-\frac{|\varepsilon|}{T}-\frac{\mu}{T}}+1} + 2\nu_c \int_0^{\infty} \frac{d\varepsilon}{e^{\frac{\varepsilon-\mu}{T}}+1} = x \right.$$

$T=0 \qquad \varepsilon < 0$

$$\frac{2\nu_c}{\nu_0\,\Gamma(1+\alpha)} \int_0^{\infty} \frac{du}{e^{\frac{u}{t}-\frac{\tilde\mu}{t}}+1} =$$

$$= \int_0^{\infty} \frac{du\, u^{\alpha} e^{-u}\, e^{-\frac{u}{t}-\frac{\tilde\mu}{t}}}{e^{-\frac{u}{t}-\frac{\tilde\mu}{T}}+1}$$

$$t = \frac{T}{\Delta}, \quad \tilde\mu = \frac{\mu}{\Delta}$$

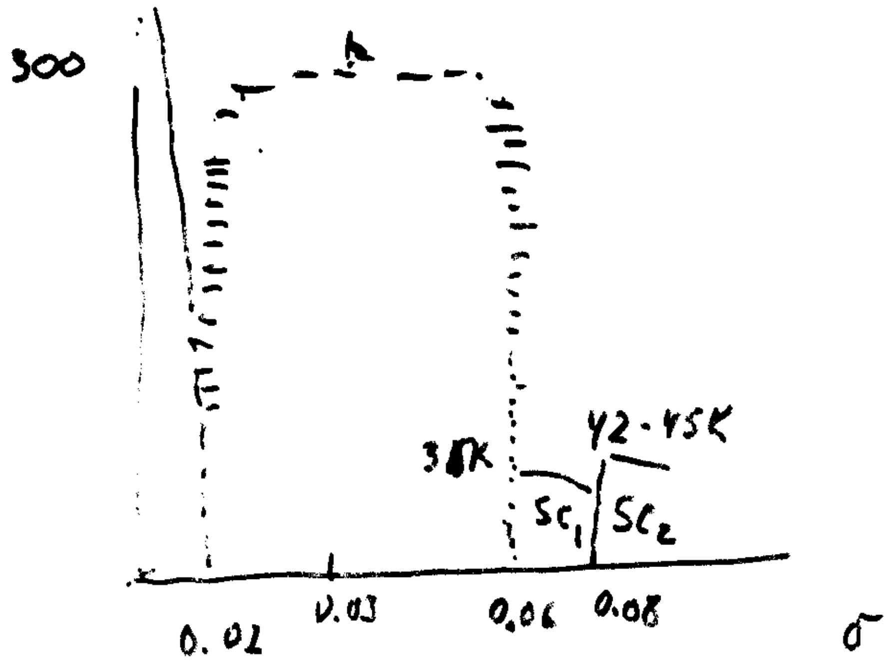
$$\sigma = \frac{n(T)\,e^2\,\tau}{m} \qquad \frac{1}{\tau} \simeq \frac{1}{\tau_0}$$

$\sigma(T) \propto n(T) \qquad (\sim T^{1+\alpha}$ at low $T)$

$\Delta \simeq 100K$

$La_2CuO_{4+\delta}$ 9.

δ



D. Johnston