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SMR/455 - 14

EXPERIMENTAL WORKSHOP ON HIGH TEMPERATURE SUPERCONDUCTORS & RELATED MATERIALS (BASIC ACTIVITIES)

12 - 30 MARCH 1990

CURRENT STATUS OF HIGH-T_c THEORY

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

CURRENT STATUS OF HIGH-Tc THEORY

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ICTP, Trieste

* Basic Experimental Facts
  * Almost "BCS" Superconducting Properties
  * Anomalous Normal State Properties
    * Fermi Liquid vs Strong Coupling Behavior
    * Hall Measurements Confronting Angle-Resolved Photoemission
* Some Theoretical Understanding
  * Models
  * Ground State of Reference Compounds
  * Single Hole Problem
  * Finite Hole Concentration
* Possible Way Out from the Dilemma
  * Marginal Fermi Liquid (Varma)
  * 1D Hubbard Model and Possible Generalization (Anderson)
  * Fermi Liquid, Similar Story of Heavy Fermions?

"Almost" BCS Behavior

* Meissner effect
* Zero resistance
* 2e flux quantization, Andreev reflecti[on]
  ac & dc Josephson Tunn[eling]
* Excitation gap (Tunneling, IR, PE

  $\frac{2\Delta}{k_B T_c} \approx 2 \div 8$

* $\Delta C / \chi T_c$ roughly correct
  no jump for Bi-compound.
* Ginzburg-Landau theory "works"

  $\Delta(T)$, $H_c(T)$

  Anisotropy, short correlation length

  $\lambda_\parallel / \lambda_\perp \approx 5$

  $\xi_\parallel / \xi_\perp \approx 10$ → even smaller ~2

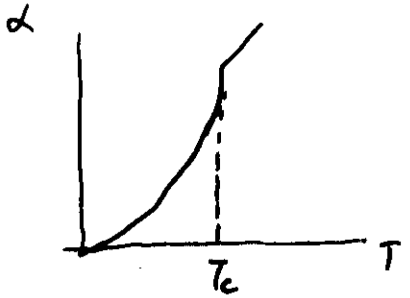
* $m^*/m \approx 3 \div 5$ determined from susceptibility and optical properties,

More subtle coherence effects

$\alpha_{k\uparrow} = u_k a_{k\uparrow} + v_k a^+_{-k\downarrow}$

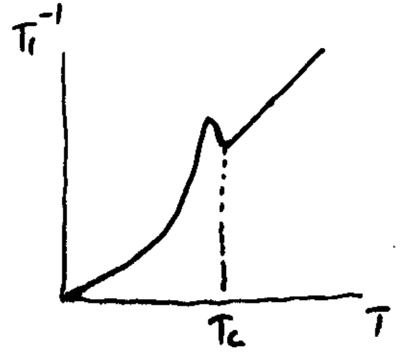
"Destructive effects"

e.g. Acoustic absorption



"constructive" effect

e.g. NMR relaxation



Hebel-Slichter resonance

It has not been observed.

damping effect?

Main features of Fermi-liquid behavior

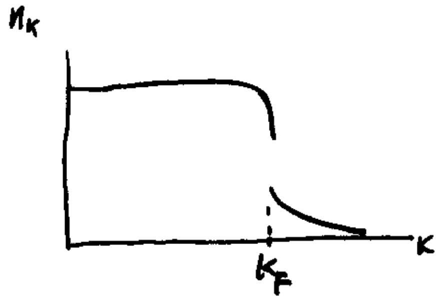
1) Well-defined quasiparticles

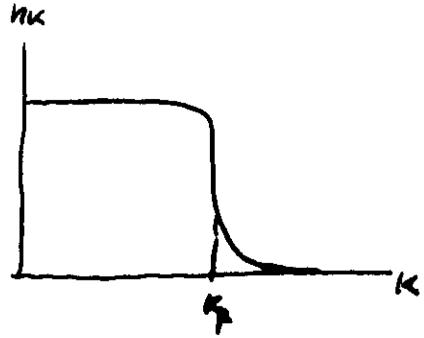
$$\mathrm{Re}\,\varepsilon \gg \mathrm{Im}\,\varepsilon$$

T, ω T^2, ω^2

2) Charge e and spin 1/2 are associated with each other

3) Luttinger theorem
volume of Fermi-surface ~ N





FL, jump ~ z

$$G \sim \frac{z}{\omega - \varepsilon_k + i0\,\mathrm{sgn}}$$

NFL, no jump

The difference is more subtle!

Anomalous "normal state"

Properties

* Resistivity

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

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

* Optical absorption

Drude component + Strong background $\sim \omega^{-1}$

$$\sigma(\omega) = \frac{ne^2\tau^*}{m^*} \frac{1}{1 - i\omega\tau^*}$$

From the width $(\tau^*)^{-1} \sim 2kT$

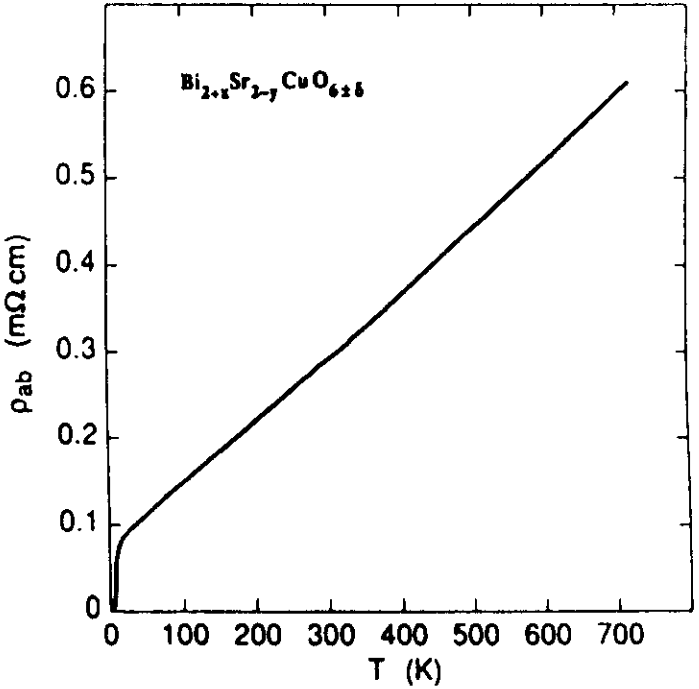
$\therefore$ the T dependence is lifetime effect, not due to n/m^*

also $\frac{n}{m^*} \sim \delta/m^*$ not $(1-\delta)/m^*$

* Strong background in Raman scattering up to 4000 cm^{-1}

metals: ~20 cm^{-1}
particle-hole

* Tunneling conductivity $G = g_0 + g_1 |V|$



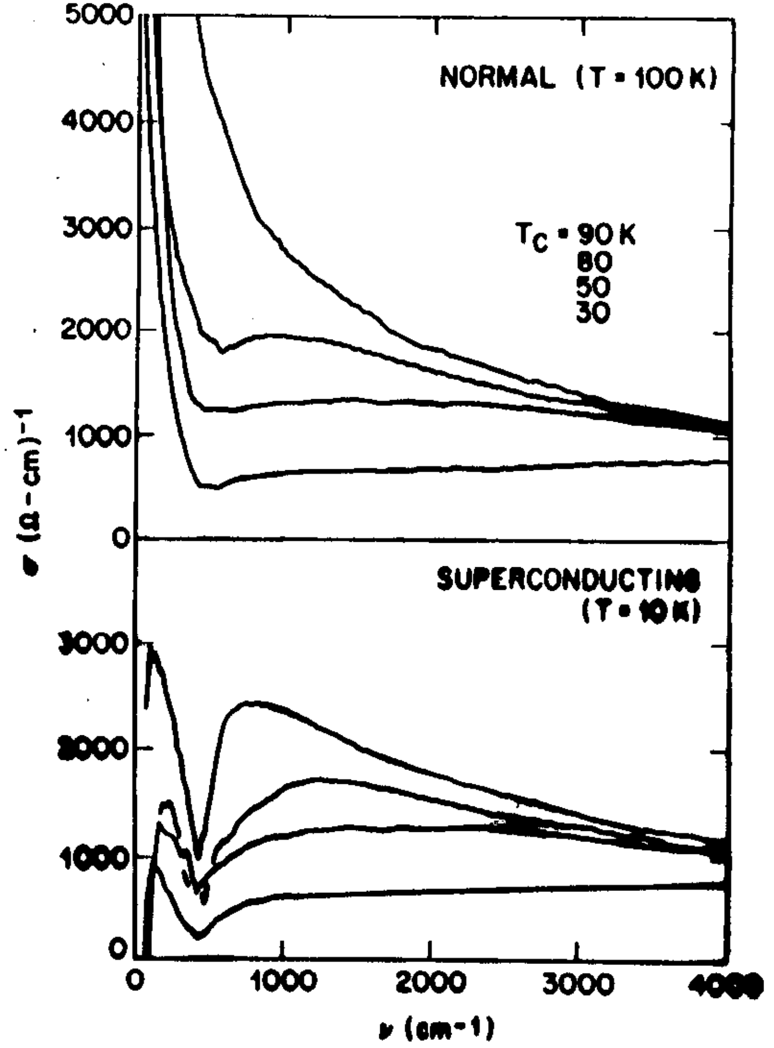
ig. (4): Resistivity of the single layer Bi superconductor. From Ref. (7), S. : al.

This rules out "phonon" interpretation.

$\rho \propto T$, $T > \Theta/4$

Optical Conductivity:
Orenstein, Thomas et. al.

(13)



3 Anomalous features in the Normal state.

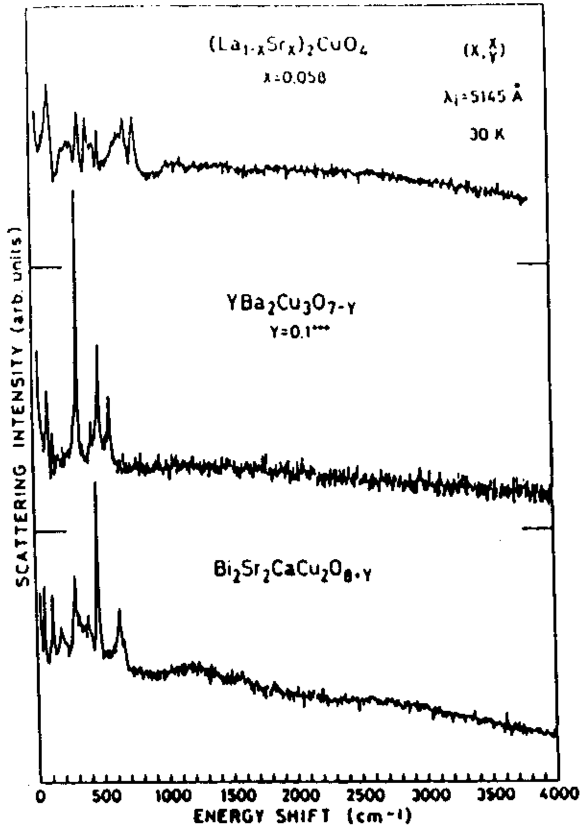


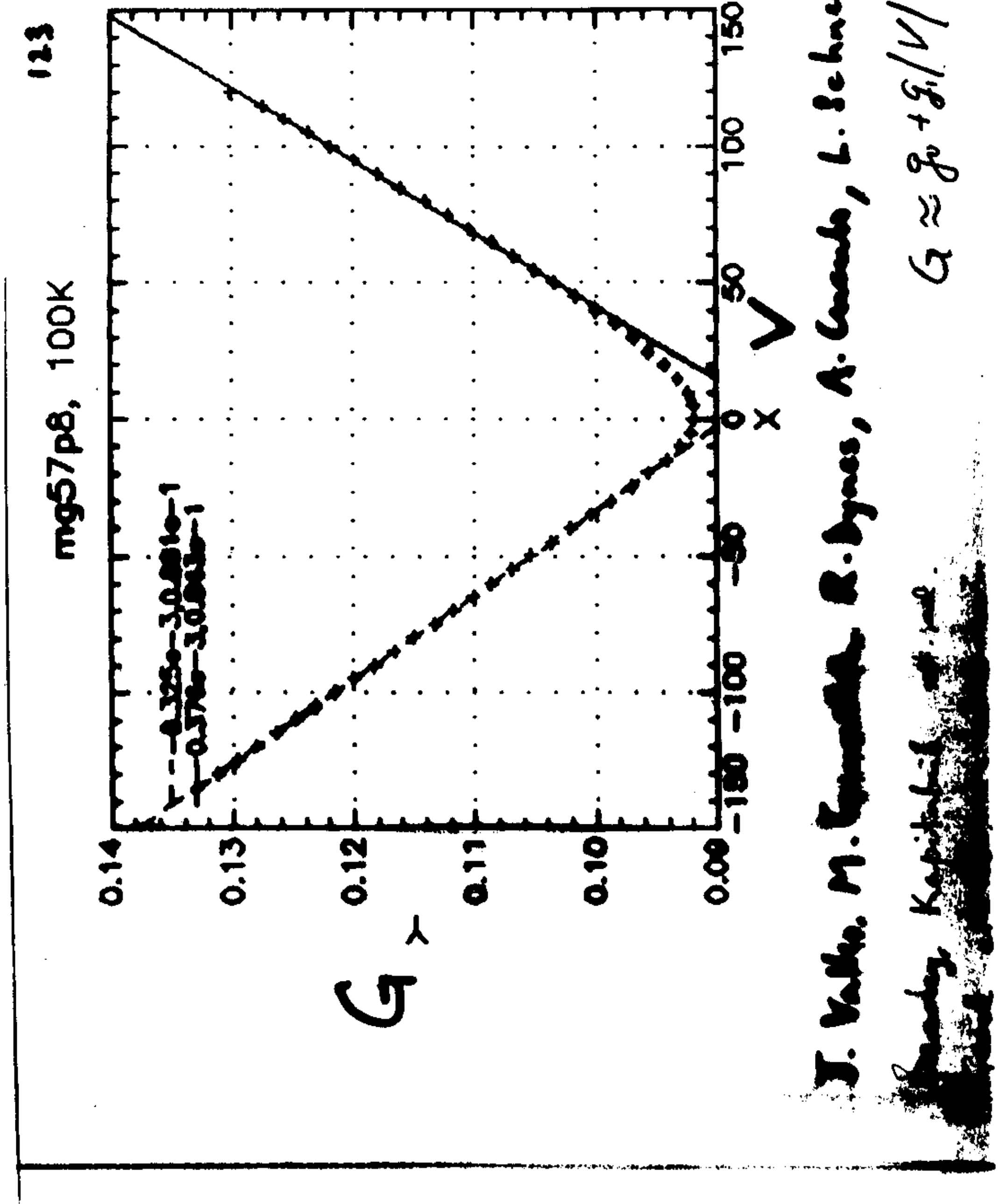
Fig. (9): Raman scattering intensity for various superconducting Cu-O compounds. From Ref. (14), Sugai et al.

hypothesis:

$\mathrm{Im}\,\chi(\omega)$ < $S_0\ \omega/T$ for $\omega < T$; S_0 for $\omega > T$

Klein et al.

due to continuum excitations



* NMR relaxation

^{89}Y, ^{17}O Korringa like

$T_1^{-1} \sim T$, $N(0) = const$
$T_1^{-1} \sim$ # of exci

^{63}Cu the same plane

not Korringa like

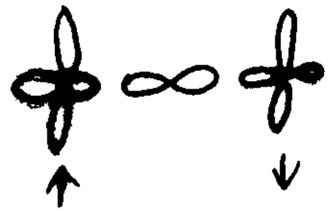
much faster

Millis et al. $\chi(\mathbf{k}, E)$ enhanced
AF correlations

^{63}Cu is sensitive to this part

^{17}O, ^{89}Y - not, due to symmetry

one component spin system



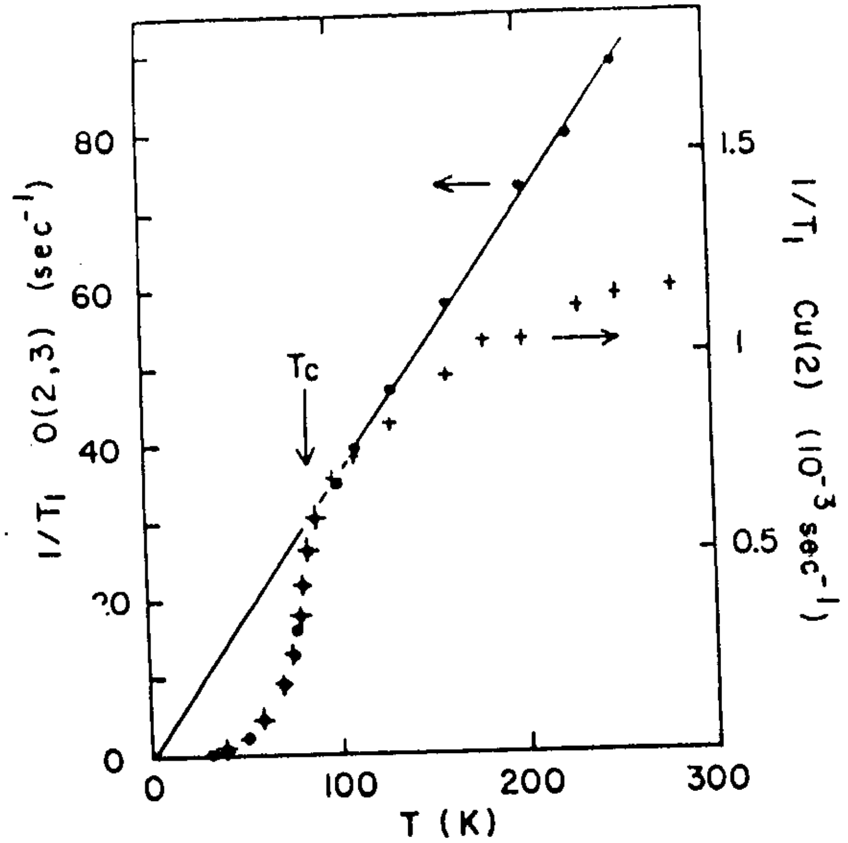


Figure 3. Temperature dependence of $1/T_1$ at the O(2,3) (solid dots) and the Cu(2) (crosses) sites.

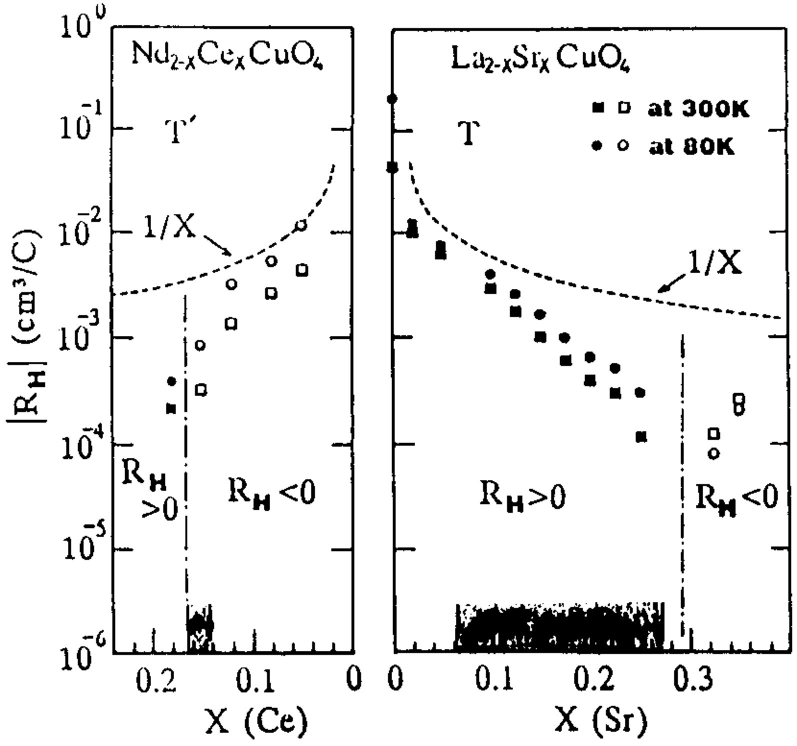


Fig. 8 The absolute value of the Hall coefficient as a function of Ce composition for reduced $Nd_{2-x}Ce_xCuO_{4-y}$. The same ploted for $La_{2-x}Sr_xCuO_4$ are show for composition. The shaded are a indicates composition region where superconductivity is observed.

Normal state: ^{17}O $\frac{1}{T_1} \sim T$ Korringa

^{63}Cu much larger, not Korringa

Superconducting state.
No Hebel-Slichter reso[nance]

$R_H \sim \frac{1}{nec}$

1) consistent with Mott-Hubbard pic[ture]
2) deviation from 1/X
3) consistent with disappearance of line law and magn. correlations

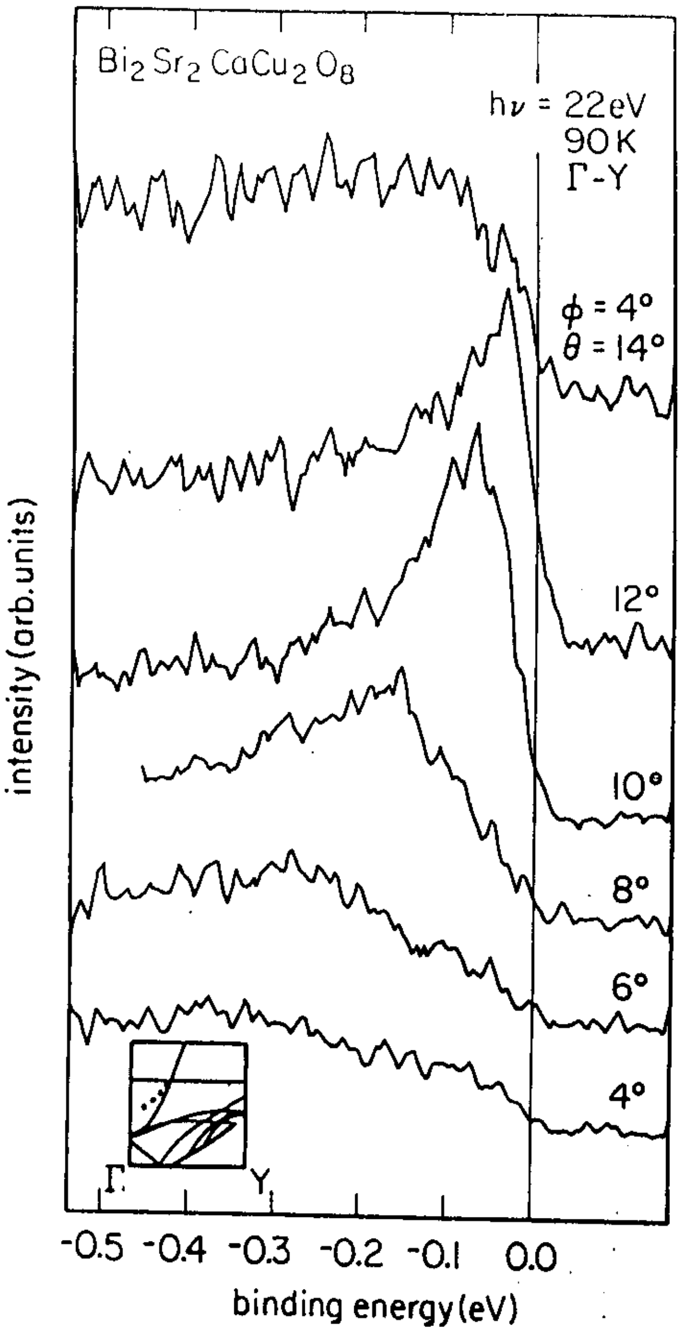


Fig. 1

Olson et al

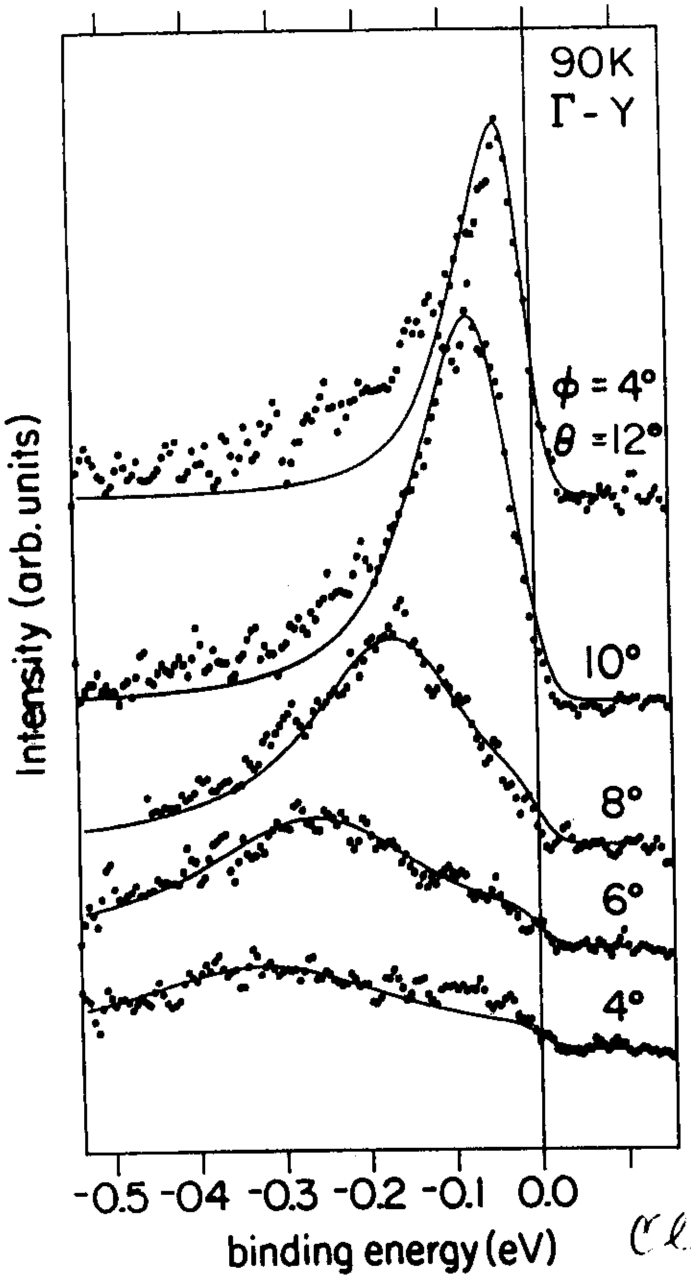
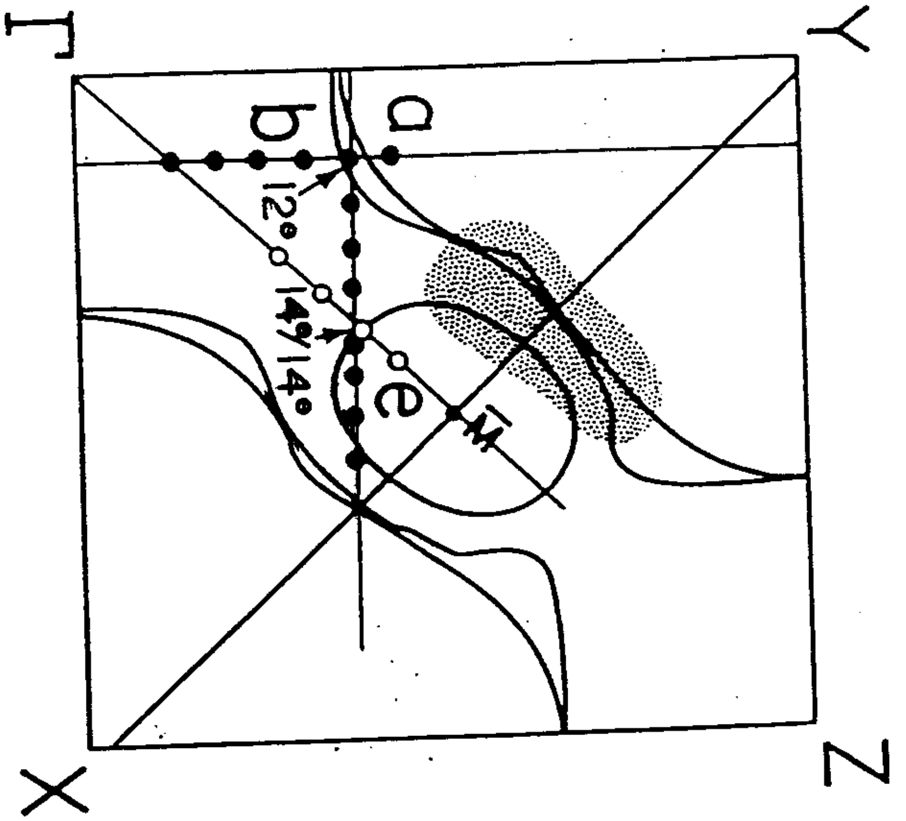


Fig. 5

Olson et al



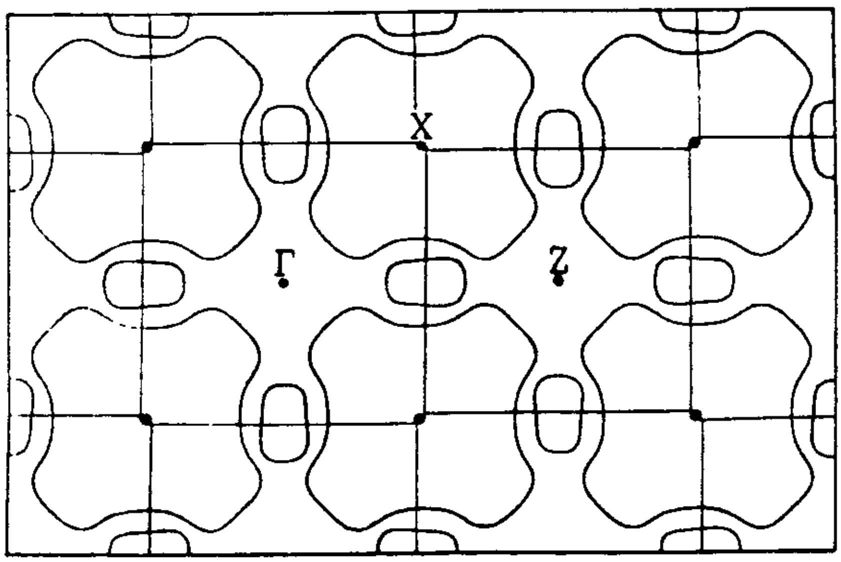
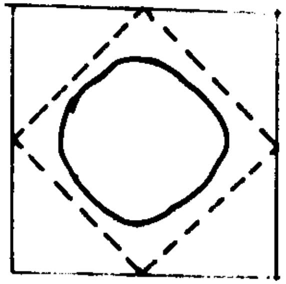
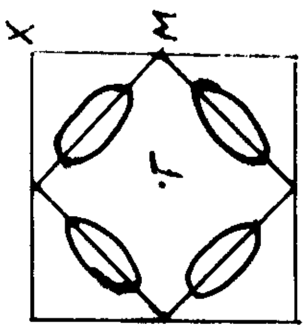


FIG. 3. Calculated Fermi surfaces in the (001) plane. For clarity, we show only one of the two large, nearly degenerate X-centered sheets arising from the Cu-O bonds. The small rounded rectangular electron pockets midway between Γ and Z arise from Bi-O states.



(b)



(a)

Summary of Experiments

Superconducting properties

BCS like

Normal state Propertie

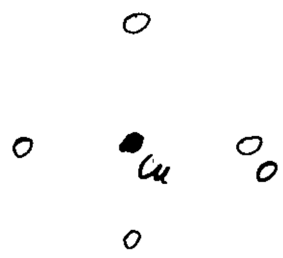
Abnormal

Non-FL behavior

Angle-resolved photoemission

Well-defined Fermi surface

Model Hamiltonian for CuO_2 plane



$$H = -\sum_{\langle i,l\rangle\sigma} t_{il}\left(d^{+}_{i\sigma} p_{l\sigma} + c.c.\right)$$

$$- \sum_{\langle ll'\rangle\sigma} t'_{ll'}\left(p^{+}_{l\sigma} p_{l'\sigma} + c.c.\right)$$

$$+ \epsilon_d \sum_{i,\sigma} d^{+}_{i\sigma} d_{i\sigma} + \epsilon_p \sum_{l\sigma} p^{+}_{l\sigma} p_{l\sigma}$$

$$+ U_d \sum_{i} n_{di\uparrow} n_{di\downarrow} + U_p \sum_{l} n_{pl\uparrow} n_{pl\downarrow}$$

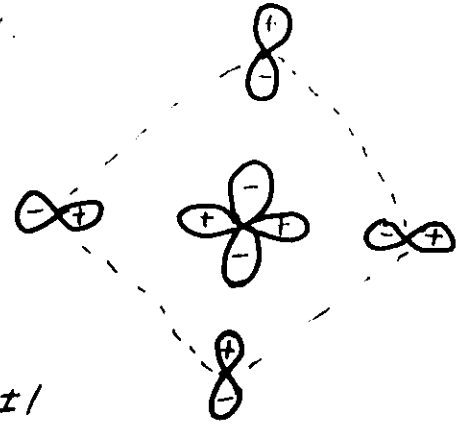
$$+ V \sum_{\langle il\rangle\sigma\sigma'} n_{di\sigma} n_{pl\sigma'}$$

$U_d = 5 \div 10$ eV, $U_p = 3 \div 6$ eV, $t = 1 \div 1.5$ eV

$t' = 0.5$ eV, $V \approx 1.5$ eV. $\Delta \equiv \epsilon_p - \epsilon_d \approx 3$ eV

Effective one band model.

Zhang & Rice



$$\hat{P}_i = \frac{1}{2}\sum_l \varsigma_{il} p_l \qquad \varsigma_{il} = \pm 1$$

$$\phi_i^{s,t} = \frac{1}{\sqrt{2}}\left(\hat{P}_{i\uparrow} d_{i\downarrow} \mp \hat{P}_{i\downarrow} d_{i\uparrow}\right)$$

$$E^t - E^s \approx 16 \cdot \frac{t_{pd}^2}{\Delta}$$

Wannier state of singlet

* Emery & Reiter. objection
Exact solution on FM background
Different from singlet, $\langle S\rangle \neq 0$

* Pang, Xiang, Su, Yu
"Exact" solution can be reproduced by combining singlet & triplet

* NMR seems to show one spin excitation

Hubbard model

$$\mathcal{H}_H = -t\sum_{\langle ij\rangle}(c_{i\sigma}^+ c_{j\sigma} + h.c.) + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

$U \gg t$. project out doubly occupied sites

$t - J$ model

$$\mathcal{H}_{t-J} = -t\sum_{\langle ij\rangle} P(c_{i\sigma}^+ c_{j\sigma} + h.c.) + J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j + t'\sum_{i,k\ n.n.n}(c_{i\sigma}^+ c_{k\sigma} + h.c.)$$

$$\vec{S}_i = c_i^+ \frac{\vec{\sigma}}{2} c_i$$

$$J = 2t^2/U$$

They are equivalent only if

$t > J$, or $U > t$

Ground State of Reference Compounds

2D . $T = 0$

1) Original RVB . BZA, Kotliar, Zhang, Rice ....

Slave boson

$$c_{i\sigma}^+ = S_{i\sigma}^+ e_i + \sigma S_{i-\sigma} d_i^+, \quad n_e + n_d + n_s = 1$$

pp and ph condensation

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

$$\xi_{ij} = \sum_\sigma c_{i\sigma}^+ c_{j\sigma}$$

$\Delta_x = \langle b_{i,i+\hat{x}}\rangle$, $\Delta_y = \langle b_{i,i+\hat{y}}\rangle$

$\xi_x = \langle \xi_{i,i+x}\rangle$, $\xi_y = \langle \xi_{i,i+\hat{y}}\rangle$

s-wave pairing $\Delta_x = \Delta_y = C$, $\xi_x = \xi_y = 0$

d-wave pairing $\Delta_x = -\Delta_y = C$ $\xi_x = \xi_y = C$

Kotliar flux phase $\Delta_x = i\Delta_y = C$, $\xi_x = \xi_y =$

~~Affleck~~-Marston phase $\Delta_x = \Delta_y = 0$, $\xi_x = -i\xi_y =$

degenerate due to SU(2) symmetry

[illegible] Heisenberg [illegible]

Energy is high

$$\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle \approx -.321$$

Problem: Marshall sign is not satisfied

$$b_{ij}^{+} = b_{ji}^{+}$$

How to cure?

(1) Guarantee marshall sign

Liang, Doucot, Anderson

(2) Introduce staggered magnetization

$$\langle S_{ij} \rangle = (-1)^{i} S$$

Lee, Feng

"Coexistence" Chen, Su, Yu

2) Quantum Antiferromagnetic State

Finite size calculation

AF LRO $\langle S_z \rangle \sim 0.3$ instead of ½

Neel state + Quantum Fluctuations

SPIN WAVE THEORY

1/S expansion

Nonlinear σ-model

$\langle \vec{S}_i \cdot \vec{S}_j \rangle$ correlation function

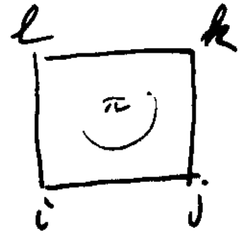
Chakravarty, Halperin, Nelson

$$\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle \approx -0.334$$

Finite hole concentration

1) Slave bosons

* Flux phase



$$|\xi|^4 e^{i\phi} = \xi_{ij}\xi_{jk}\xi_{kl}\xi_{li}$$

$\phi = \pi$

At finite concentration

$\pi \to (1+x)\pi$

flux per particle remains unchanged

Commensurate flux phase

Rice et al.

* Gap in the spectrum
* Breaks time-reversal symmetry
+ Like anyon superconductivity → Meissner effect & persistent current

However, energetically favorable only if $t \leq J$

* Staggered flux phase

$\phi = \pi \quad \Leftrightarrow \quad \phi = -\pi$

+ − +
− + −
+ − +

for $x \neq 0$

$\phi \to \pm\pi(1+x)$

No gap. Fermi surface → pockets near $(\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$ ÷ f.s.

⇒ Incommensurate spin-spin correlation functions

* Staggered Chirality

$\langle \vec{S}_1 \cdot (\vec{S}_2 \times \vec{S}_3) \rangle$

* Energetically better for $t \gtrsim J$

2) Slave fermion (Schwinger boson) method

* Gives good energy for undoped system. It treats "J" term well. Bosons — all occupy low energy state
* Has difficulty in treating "t" term — broad ferromagnetic region is spurious
* If minimum at $(\pm\frac{\pi}{2},\pm\frac{\pi}{2})$
  ⇒ dipolar distortion — Shraiman, Siggia
  ⇒ Spiral phase — Kane et al.

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle = \frac{3}{8} n_0^2 \cos[2\vec{K}_0 \cdot (\vec{r}_i - \vec{r}_j)]$$

$$K_0 a = \frac{\pi}{2} + 1.25 \frac{t}{J} \delta$$

Some indication, inelastic scattering

* How to get FL behavior?

* Phenomenological approach

Marginal FL behavior

C.M. Varma et al.

Ansatz: Polarization of charge or spin fluctuations

$$\mathrm{Im}\,\tilde{P}(\vec{q},\omega) \sim \begin{cases} -N(0)\,\omega/T, & \text{for } |\omega| < T \\ -N(0)\,\mathrm{sgn}\,\omega, & \text{for } |\omega| > T \end{cases}$$

independently of $\vec{q}$. generalization from Raman experiments

Self-energy:

$$\Sigma(\vec{k},\omega) \sim g^2 N(0)^2 \left(\omega \ln\frac{x}{\omega_c} - i\frac{\pi}{2}x\right)$$

$x = \max(T, |\omega|)$, ω_c cut-off

$$G(\vec{k},\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(\vec{k},\omega)} = \frac{Z_k}{\omega - E_k + i\Gamma_k} + G_{inc}$$

$$Z_k^{-1} = \left(1 - \frac{\partial \mathrm{Re}\,\Sigma}{\partial \omega}\right)_{\omega = E_k} \sim \ln|\omega_c/E_k|$$

$E_k \to 0$, $Z_k^{-1} \to \infty$

Marginal Fermi liquid !!

FL: $\mathrm{Re}\,\Sigma \sim \omega$

$\mathrm{Im}\,\Sigma \sim \omega^2$

Marginal FL $\mathrm{Re}\,\Sigma \sim \omega \ln \frac{\omega}{\omega_c}$

$\mathrm{Im}\,\Sigma \sim \omega$

Difference is measurable

* Explains "ALL" anomalies
* Linear dependence $\rho \sim T$
* Background in Raman
* Tunneling

$G \sim g_0 + g_1 |V|$

assuming

$N(\omega) \sim \sum_k A(k, \omega) \sim N_0 + N_1 |\omega|$

to get $g_1 > 0$. additional elastic scattering

* NMR

$T_1^{-1} \sim aT + b$

why the difference for ^{17}O and ^{63}Cu?

* Optical absorption

$\sigma(\omega) = \sigma_1(\omega) + \sigma_2(\omega)$

$\sigma_1(\omega) \propto \mathrm{Im} \frac{\omega_p^2}{\omega + i\Sigma(\omega)}$ Drude

$\sigma_2(\omega) \sim -\omega\, \mathrm{Im}\, \tilde{P}(0, \omega)$

Good fit

* Photoemission

More sensitive to angular aver

* Superconducting properties

S-wave

$2\Delta / k_B T \sim 8$

No Hebel-Slichter resonance

Life-time effects

Microscopic origin ??

* 1 D Hubbard model

Typical Non-FL behavior

at the same time - very similar to experimental observations

Bethe Ansatz solution

* Ogata & Shiba   cluster calc.

* Sorella, Parola, Parrinello, Tosatti

$U/t >> 1$

* Separation of charge and spin

holons, charge e, spinless fermion

$2K_F$

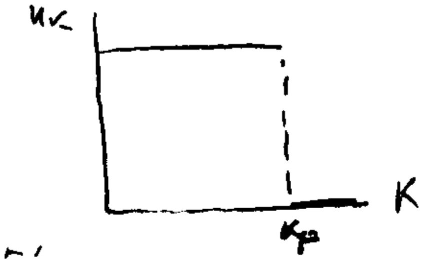
Spinons, $S = 1/2$, $Q = 0$

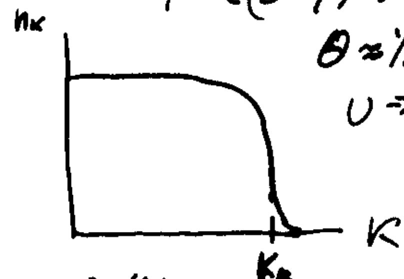
K_F

* n_K $1 - \mathrm{sgn}(\varepsilon - \varepsilon_F)$ $1 - C(\varepsilon - \varepsilon_F)^{\theta}\,\mathrm{sgn}(K - K_F)$

$\theta \approx 1/8$

$U \to \infty$





1 D HM

No singularity at $2K_F$

Weak singularity at $3K_F$

$Z_K \to 0$ at K_F, no charge

$$\langle C^{+}(0)\, C(r)\rangle \sim \frac{\sin K_F r}{r^{1+\theta}}$$

Continuity from $U < t \to U > t$

$$\langle \rho(0)\rho(r)\rangle \to K_2\, r^{-\alpha} \cos 2K_F r + K_4\, r^{-\beta} \cos 4K_F r + \cdots$$

$$\langle \vec{S}(0)\cdot\vec{S}(r)\rangle \to H_2\, r^{-\gamma} \cos 2K_F r + \cdots$$

$U = 0$, $\alpha = \gamma = 2$, $K_4 = 0$

$U \to \infty$, $\alpha = \gamma = 3/2$, $\beta = 2$, $\theta = 1/8$

Anderson's conjecture:

This is true also for 2D and higher dimensions. Luttinger Liquid vs Fermi Liquid

Infrared Catastrophe !!

* Fermi Liquid Theory

1) "Genuine" FL

BCS pairing, spin fluctuation

Schrieffer, Wen, Zhang, Spin bag

Kampf, Schrieffer, pseudo gap

No problem with FS

Normal state properties ?

Optical sum rule

$$\left(\frac{N}{m}\right)^* \sim \frac{x}{m_1}, \quad \text{not } \frac{1-x}{m^*}$$

2) Heavy fermion version

P.A. Lee et al. ...

Newns et al. ....

Anderson lattice model → slave boson

→ renormalization of Cu level, etc.

No problem with FS

Not so heavy! $m^*/m \approx 2$

concentration dependence of χ, σ

$\chi \sim 1/x$, but ↑

Anyon Superconductivity

* "Anyon gauge", multivalued wave function

$$\psi \to \psi e^{i\theta}$$

Generically $e^{i\theta} \neq e^{-i\theta}$

depends on the presence of other particles

Laughlin

Fetter, Hanna, Laughlin

Fradkin

Lee, Fisher

Canright

Wen, Zee

Chen, Wilczek, Witten, Halperin

Banks,

Mele, Voit

- - - -

* Single-valued wave function as for bosons or fermions

Fermions + flux tubes

$$H = \sum_{\alpha=1}^{N} \frac{|\vec{p}_\alpha - \vec{a}_\alpha|^2}{2m^*} + V$$

$$\vec{a}_\alpha = \left(\frac{\pi-\theta}{\pi}\right) \sum_{\beta\neq\alpha} \frac{\hat{z} \times \vec{r}_{\alpha\beta}}{|r_{\alpha\beta}|^2}$$

$$\vec{r}_{\alpha\beta} \equiv \vec{r}_\alpha - \vec{r}_\beta$$

$\because \quad \vec{\nabla}_\alpha \times \vec{a}_\alpha = \left(\frac{\pi - \theta}{\pi}\right) \sum_{\beta \neq \alpha} \delta(\vec{r}_\alpha - \vec{r}_\beta)$

$\vec{H}_{eff} = 0$, except for positions of other particles

Where to find?

① Fractional Quantum Hall Effect

Laughlin, Halperin ... direct measurement

② Vortices in thin films of ^3He-A

Volovik + Yamamoto

③ models of High Tc SC

Laughlin — analogy with FQHE

Chiral Spin liquid

$\theta = \pm \frac{\pi}{2}$, At, sym. broken but PT conserved

spinon

holon

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there is an effective long-range gauge force ⇒ pairing

pair of half-fermions ⇒ boson

$e^{i4\theta} = 1$

Dilute anyon gas

$\theta = \pi(1 - \frac{1}{n})$ n = integer

RPA.

1) Ground state is SC. with Meissner effect...

2) Quasiparticle excitations — charged vortices. with gap

3) Long-wave length collective ~~mode~~ - sound

4) At least two species of anyons

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Experimental Consequences of Broken T.P symmetry

Single layer

1. Intrinsic orbital magnetic moment

$\approx \frac{1}{4} \mu_B \frac{m}{m^*}$ per carrier

μSR ?

2. Optical Rotation at $\vec{B}=0$

Wen & Zee

absent in effective mass approx.

3. Righi-Leduc effect at $B=0$

(= Hall effect in thermal conductivity tensor

4. Spontaneous Hall effect at $\vec{B}=0$ in the normal state (CSL)

3D Ferromagn. or AF coupling?

Bulk or surface effect.

Local probe _ magnetic field

~10 Gauss

Concluding Remarks

* Constraints set by experiments

S-Wave pairing ...

Fermi Surface ...

Normal State anomalies

Optical sum rules ----

* All theoretical approaches have "successes" and "troubles"

Weak coupling

Strong coupling < slave boson / slave fermion / ....

Heavy fermions

Phenomenology - useful, but postpone difficulties