QUANTUM 'IMPURITIES'

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UC DAVIS

OVERVIEW

LECTURE I JULY 14, 2003

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- C. KONDO MOLECULES

SOME KEY REVIEWS:

QMPT
GEORGES ET AL, REV MOD PHYS 68 13 (1996)
PRUSCHKE ET AL, ADV PHYS, 42, 187 (1995)

QUANTUM IMPURITIES
COX + ZAWADOWSKI, ADV PHYS 47, 599 (1997)

NON FERMI LIQUID METALS
STEWART, REV MOD PHYS 73 797 (2001)

QUANTUM DOT + RESTRICTED GEOMETRY KONDO

"KONDO EFFECT AND DEPHASING IN LOW-DIMENSIONAL METALLIC SYSTEMS," EDS. V. CHANDRASEKHAR ET AL, (KLUWER, DORDRECHT, 2001).

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N. GREWE & F. STEGLICH, HANDBOOK OF THE PHYSICS AND CHEMISTRY OF THE RARE EARTHS, VOL. 14, eds. K. GSCHNEIDNER AND L.L. EYRING (ELSEVIER, AMSTERDAM, 1991) p. 343 [REVIEW OF HEAVY FERMIONS]

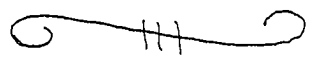
G.R. STEWART, REV. MOD. PHYS. 56, 755 (1984). [REVIEW OF HEAVY FERMIONS]

J. KONDO, SOLID STATE PHYSICS, VOL. 23, eds. F. SEITZ, D. TURNBULL, & H. EHRENREICH (ACADEMIC PRESS, NEW YORK, 1969), p. 183. [REVIEW OF KONDO EFFECT]

G. GRÜNER & A. ZAWADOWSKI, REP. PROG. PHYSICS 37, 1497 (1974); IN PROGRESS IN LOW TEMPERATURE PHYSICS, VOL. IIB, eds. D.F. BREWER (NORTH-HOLLAND, AMSTERDAM, 1978), p. 593 [REVIEWS OF KONDO EFFECT]

M.B. MAPLE, C.L. SEAMAN, D.A. GAJEWSKI, Y. DALICHAOUCH, V.B. BARBETTA, M.C. de ANDRADE, H.A. MOOK, H.G. LUKEFAHR, O.O. BERNAL & D.C. MACLAUGHLIN, J. LOW. TEMP. PHYS. 95, 225 (1994); M.B. MAPLE, M.C. de ANDRADE, J. HERMANN, Y. DALICHAOUCH, D.A. GAJEWSKI, C.L. SEAMAN, R. CHAU, R. MOVSOVICH, M.C. ARONSON, & R. OSBORN, J. LOW TEMP. PHYS. 99, 223 (1995). [EXPERIMENTAL REVIEWS OF NON-FERMI LIQUID PHYSICS IN HEAVY FERMION MATERIALS]

N.E. BICKERS, REV. MOD. PHYS. 59, 845 (1987). [REVIEW OF LARGE N APPROACHES TO ANDERSON/KONDO MODELS]



I. MATERIALS PHENOMENOLOGY

IN THESE LECTURES, I WILL FOCUS ON ARRIVING AT SOME UNDERSTANDING OF HEAVY FERMION (OR HEAVY ELECTRON) MATERIALS. THESE ARE RARE EARTH OR ACTINIDE BASED INTERMETALLIC ALLOYS AND COMPOUNDS. SOME EXAMPLES:

CERIUM BASED	YTTERBIUM	URANIUM
$CeAl_3$	$YbCuAl$	UPt_3
$CeCu_2Si_2$	$YbCu_2Si_2$	UBe_{13}
CeB_6	$YbBiPt$	U_2Zn_{17}
$CeAl_2$		URu_2Si_2

CRYSTAL STRUCTURES CAN BE QUITE COMPLEX -- LATER WE WILL DISCUSS HOW CRYSTAL STRUCTURE MAY AFFECT NORMAL METALLIC PROPERTIES, SUPERCONDUCTIVITY, AND MAGNETISM IN THESE MATERIALS.

THE TERM <u>HEAVY FERMION</u> REFERS TO THE GIANT EFFECTIVE MASS FOUND IN THESE SYSTEMS, AS MEASURED BY THE SPECIFIC HEAT. YOU MAY RECALL FOR FREE ELECTRONS THIS SIMPLE ARGUMENT:

<u>DEFINE</u> (1) $N(\varepsilon)$ = CONDUCTION ELECTRON DENSITY OF STATES (DOS) PER SPIN PER SITE

$$= \frac{1}{N_s} \sum_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}})$$

<u>WITH</u>: N_s = # SITES

$\varepsilon_{\vec{k}} = k^2/2m$ (I TAKE $\hbar = 1$ USUALLY!)

<u>S_0</u> : (2) $N(\varepsilon) = \frac{3}{4E_F}\sqrt{\frac{\varepsilon}{E_F}}$ IN 3D, $E_F = \frac{k_F^2}{2m}$ (FERMI ENERGY)

$\sim m$

$k_F = (3\pi^2 n)^{1/3}$

n = # ELS./UNIT VOLUME

NOW, FOR $T=0$, WE FILL TO E_F, AT $T>0$ WE SMEAR NEAR E_F

SO, <u>HEURISTICALLY</u>, THE ELECTRONIC SPECIFIC HEAT IS

(3) $C_{el} \approx \underset{(SPINS)}{2}\, k_B\, [\#_{EXCITATIONS\ PER\ EL.}] \cong 2k_B\,[N(E_F)(2k_BT)]$

$\approx 4k_B^2 N(E_F)\, T$ * LINEAR IN T * PROPORTIONAL TO $N(E_F) \sim m$

BASED ON SEMICLASSICAL (EQUIPARTION THEOREM) THINKING. MORE PROPERLY, FROM SOMMERFELD THEORY:

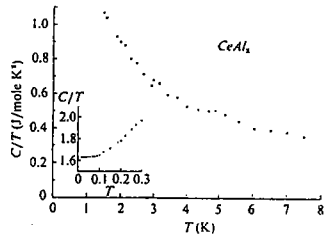
(4) $C_{el} = \frac{dE_{el}}{dT} = 2k_B \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right)[R(\varepsilon-\mu)]^2 N(\varepsilon) \underset{T\to 0}{\approx} \frac{2\pi^2}{3} k_B^2 N(E_F) T$

WHERE $\beta = (k_BT)^{-1}$, μ = CHEMICAL POTENTIAL, AND

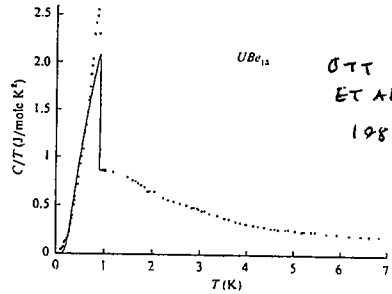
(5) $f(\varepsilon) = (e^{\beta(\varepsilon-\mu)}+1)^{-1}$ (FERMI-DIRAC DISTRIBUTION)

FOR A "FREE" ELECTRON METAL LIKE CU OR AL, WITH $E_F \approx 1\text{-}5$ eV, WE GET THE MOLAR SPECIFIC HEAT $\gamma \equiv \frac{N_0 C_{el}}{T} \approx 1\text{-}5$ mJ/mole-K^2 ($N_0 = 6.02\times10^{23}$ molec./mole)

BELOW ARE SPECIFIC HEAT DATA FOR $CeAl_3$ AND UBe_{13} NOTE THE MAGNITUDES OF $\approx$ 1 J/mole-K^2 !!



(LANDRES, GRAEBNER, OTT (1975)) PHYS REV LETT 52, 1979.



OTT ET AL, 1984.

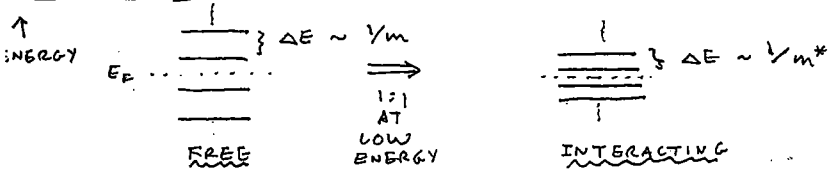
(H.R.OTT, H.RUDIGER, Z.FISK, J.L.SMITH, PHYSICA B 127, 359 (1984))

SINCE $C_{el}/T \sim m$, THIS SUGGESTS AN "EFFECTIVE" MASS $m^* \sim 1000\,m$. NOTE THE SUPERCONDUCTING TRANSITION IN UBe_{13} WITH $\Delta C_{el} \sim C_{el}$, IMPLYING <u>HEAVY FERMIONS</u> IN THIS MATERIAL SUPERCONDUCT! WE WILL BRIEFLY DISCUSS THIS IN LECTURE <u>III</u>. (<u>NB</u>: $m^* \sim 1000m \Rightarrow T_F^* \sim 10$ K)

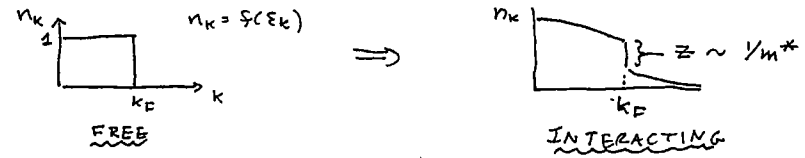
LANDAU, IN 1957, CONJECTURED THAT THE LOW LYING EXCITATIONS OF AN INTERACTING FERMI SYSTEM WOULD HAVE A 1:1 MAP TO THOSE OF A NON INTERACTING SYSTEM -- THESE "QUASIPARTICLE" EXCITATIONS WOULD HAVE AN ENHANCED MASS SINCE INTERACTIONS OF FERMIONS WITH OTHER FERMIONS WOULD RETARD MOTION.

[IT'S AMUSING TO LIKEN THIS TO CARS ON AN EMPTY HIGHWAY AND "QUASICARS" IN A SHTAU ... —]

ENERGY PICTURE:



DISTRIBUTION PICTURE:

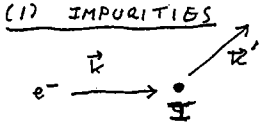


SO INTERACTIONS PRESERVE A SHARP FERMI SURFACE WHOSE VOLUME IS IN FACT THE SAME AS FOR FREE FERMIONS (LUTTINGER'S THEOREM) PROVIDED LANDAU THEORY HOLDS SELF-CONSISTENTLY. WE'LL DISCUSS THIS THEORY MORE IN LECTURE II.

RESISTIVITY AND SCATTERING

IN A TRUE FERMI GAS (NONINTERACTING) THE ELECTRICAL RESISTIVITY (IF CHARGED) IS ZERO -- NOTHING DEGRADES THE MOMENTUM! WE KNOW IN GOOD METALS LIKE Cu. THAT SCATTERING CAN COME FROM 3 SOURCES

(1) IMPURITIES



THESE BREAK TRANSLATIONAL INVARIANCE AND THUS MOMENTUM CONSERVATION, IF THE CONCENTRATION c IS DILUTE AND SCATTERING WEAK, WE MAY WRITE THE RESISTIVITY AS

$$(6)\quad \rho_{IMP} = \frac{m}{ne^2}\,\frac{1}{\tau_{tr}}$$

WITH $$(7)\quad \frac{1}{\tau_{tr}} \cong \frac{2\pi N(E_F)\, c}{\hbar} \int \frac{d\hat{k}'}{4\pi} |U_{\vec{k}\vec{k}'}|^2 (1-\hat{k}\cdot\hat{k}') \Big|_{|\vec{k}|=|\vec{k}'|=k_F}$$

WITH $U_{\vec{k}\vec{k}'}$ = SCATTERING POTENTIAL, THE TRANSPORT FACTOR $(1-\hat{k}\cdot\hat{k}')$ WEIGHTS AGAINST FORWARD SCATTERING THAT DOESN'T DEGRADE THE CURRENT. IF THE SCATTERING IS STRONG, WE SHOULD REPLACE $U_{\vec{k}\vec{k}'}$ BY THE T-MATRIX DEFINED BY THE BORN SERIES

$$(8)\quad t_{\vec{k}\vec{k}'}(\omega) = U_{\vec{k}\vec{k}'} + G^0_{\vec{k}} U_{\vec{k}\vec{k}'} G^0_{\vec{k}'} + \sum_{\vec{k}''} G^0_{\vec{k}} U_{\vec{k}\vec{k}''} G^0_{\vec{k}''} U_{\vec{k}''\vec{k}'} G^0_{\vec{k}'} + \dots$$

WHERE (ON-SHELL) THE GREENS' FUNCTION $G^0_{\vec{k}} = (\omega - \varepsilon_{\vec{k}})^{-1}$

IF SCATTERING IS (i) DOMINATED BY ONE ANGULAR MOMENTUM; (ii) STRONG

WE CAN PUT

$$(9)\quad U_{\vec{k}\vec{k}'} = \sum_{l=0}^{\infty} (2l+1)\, U_l\, P_l(\hat{k}\cdot\hat{k}') \approx (2l_0+1)\, U_{l_0}\, P_{l_0}(\hat{k}\cdot\hat{k}')$$

$$(10)\quad t_{\vec{k}\vec{k}'}(\omega) = \sum_{l=0}^{\infty} (2l+1)\, t_l(\omega) P_l(\hat{k}\cdot\hat{k}') \approx (2l_0+1)\, t_{l_0}(\omega) P_{l_0}(\hat{k}\cdot\hat{k}')$$

$$(11)\quad t_l = \frac{1 - e^{-2i\delta_l(\omega)}}{2\pi i N(\omega)} \qquad \delta_l(\varepsilon_k) = \tan^{-1}\left(\pi N(\varepsilon_k) U_{l_0}(\varepsilon_k)\right)$$

(PHASE SHIFT)

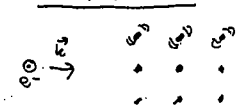
$e^{-2i\delta_l}$ = S-MATRIX (ONE-PARTICLE PROJECTION)

AND FIND

$$(12)\quad \frac{1}{\tau_{tr}} \approx \frac{1}{\tau} \approx \frac{2c}{\pi N(E_F)} (2l_0+1) \sin^2\delta_{l_0}(E_F)$$

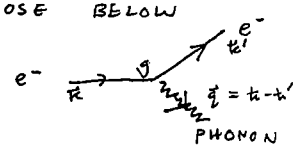
NOTE THIS SCATTERING IS T-INDEPENDENT.

(2) PHONONS AT FINITE TEMPERATURES, THE LATTICE OF IONS VIBRATES, DEVIATING FROM PERFECT PERIODICITY. (ZERO POINT MOTION AT T=0 PRACTICALLY AFFECTS ONLY THE $\vec{q}=0$ PHONON MODE WHICH HAS VANISHING PHASE SPACE AS $N_S \to \infty$).



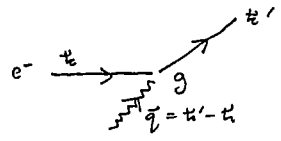
BLOCH NOTED THAT A STATIC PERIODIC LATTICE PRESERVES CRYSTAL MOMENTUM SO FREE ELECTRON WAVES CAN STILL

DIFFRACT THROUGH THE LATTICE "GRATING" AND THE RESISTIVITY $\rho = 0$. DEVIATIONS FROM PERIODICITY INDUCED BY QUANTIZED LATTICE VIBRATIONS (PHONONS) YIELD A RESISTIVITY. STANDARD TEXTS (E.G., MADELUNG SOLID STATE PHYSICS) DISCUSS THIS IN TERMS OF GOLDEN RULE DIAGRAMS LIKE THOSE BELOW



EMISSION (CERENKOV RADIATION) OF PHONONS; $v_F \gg s$ = SOUND VELOCITY

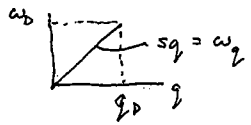
$\omega_{\vec{q}} = \varepsilon_k - \varepsilon_{k'}$



ABSORPTION

$\omega_{\vec{q}} = \varepsilon_{k'} - \varepsilon_k$

HERE $g_{\vec{q}} \approx \sqrt{\lambda \omega_{\vec{q}} / (N_3 N(0))}$ IS THE ELECTRON PHONON COUPLING, WITH $\lambda \sim 0.1$ (AL) TO ~ 2 (PB). IF WE ASSUME A DEBYE SPECTRUM



$G(\omega) = 3\omega^2/\omega_D^3$ = PHONON DOS

THEN THE LIFETIME OF AN EXCITED ELECTRON IS

$$(13)\quad \frac{1}{\tau(\varepsilon_k)} \approx \pi\lambda\omega_D \left[\left(\frac{\varepsilon_k}{\omega_D}\right)^3 + b\left(\frac{k_B T}{\omega_D}\right)^3 \right] \qquad \varepsilon_k, k_B T \ll \omega_D$$

$$\approx \pi\lambda\omega_D \qquad k_B T \ll \omega_D,\ \varepsilon_k \gtrsim \omega_D$$

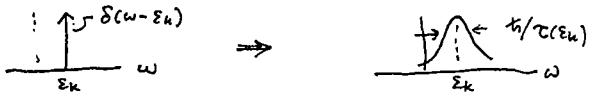
$$\approx \frac{3\pi}{2}\lambda \left(\frac{k_B T}{\hbar}\right) \qquad k_B T \gtrsim \omega_D$$

($b \sim O(1)$)

[NOTE THE ABSENCE OF FREQUENCY DEPENDENCE IN THE LAST CASE]

PRACTICALLY, THE ELECTRON "SPECTRAL FUNCTIONS" ARE BROADENED

FREE:



AND ONLY ASYMPTOTICALLY ($\varepsilon_k, T \to 0$) ARE PURE EXCITATIONS RECOVERED IN THE ELECTRON SYSTEM -- HOWEVER, FOR $\varepsilon_k, T \to 0$ OR $\varepsilon_k \gg 1/\tau$, THE EXCITATIONS ARE WELL DEFINED.

IN A BOLTZMAN EQUATION TRANSPORT TREATMENT, WE MUST WEIGHT THE GOLDEN RULE INTEGRAND BY $(1 - \hat{k}\cdot\hat{k}')^2 = (k - k')^2/k_F^2 \approx (\omega_q)^2/\omega_D^2$. THIS GIVES THE FAMOUS BLOCH-GRUNEISEN FORMULA ($d \sim O(1)$)

$$(14)\quad \rho(T) \approx \frac{m}{ne^2}\frac{1}{\tau_{tr}(T)} \approx \frac{m}{ne^2}\begin{cases} d\pi\lambda\omega_D \left(\frac{T}{\Theta_D}\right)^5 & T \ll \Theta_D \\ \frac{\pi\lambda}{4}\left(\frac{k_B T}{\hbar}\right) & T \gtrsim \Theta_D \end{cases}$$

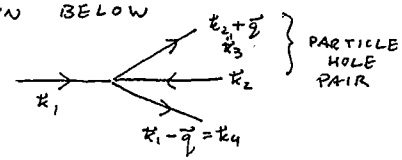
AT ROOM TEMPERATURE, TAKING $\lambda \sim 0.3$ FOR CU, WITH $n \sim 10^{22}$ el/cc WE GET

$$(15)\quad \rho(300K) \approx 6 \times 10^{-18}\ \text{sec (CGS)} \approx 6\,\mu\Omega\text{-cm (MKS)}$$

[10^{-18} sec (CGS) $\approx$ 1 $\mu\Omega$-cm (MKS OR SI)]

(3) ELECTRON-ELECTRON SCATTERING

THIS FOLLOWS BY A GOLDEN RULE PROCESS AS SHOWN BELOW



NAMELY, DECAY OCCURS VIA EMISSION OF A PARTICLE-HOLE PAIR. THE DECAY CAN ONLY OCCUR WITHIN ε_{k_1} OF THE FERMI ENERGY -- MOREOVER THE NUMBER OF PAIRS TO EXCITE IS ONLY OF ORDER ε_{k_1} (THE PAIR DENSITY OF STATES $\sim \varepsilon$) SO

$$(15)\quad \frac{1}{\tau(\varepsilon_k, T)} \approx A\frac{E_F}{\hbar}\left[\underbrace{\left(\frac{\varepsilon_k}{E_F}\right)^2}_{\text{ABOVE}} + \underbrace{\pi^2\left(\frac{T}{T_F}\right)^2}_{\text{DIMENSIONAL GROUNDS}}\right] \ll |\varepsilon_{k_1}| \quad \varepsilon_k, T \to 0$$

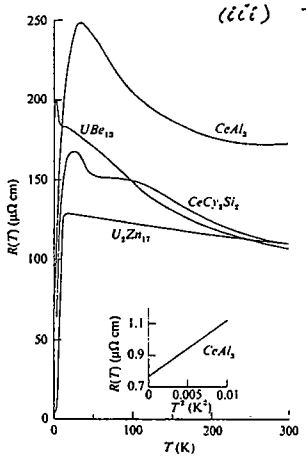
$A \sim O(1)$

IN A (VARIATIONAL) BOLTZMANN EQUATION TREATMENT, WE MUST DO A TRANSPORT AVERAGE WHICH INCLUDES A FACTOR $(\vec{k}_1+\vec{k}_2-(\vec{k}_1-\vec{q})-(\vec{k}_2+\vec{q}))^2$. IN A LIQUID, THIS VANISHES VIA MOMENTUM CONSERVATION, BUT CRYSTAL MOMENTUM IS CONSERVED ONLY TO WITHIN AN UMKLAPP VECTOR (RECIPROCAL LATTICE VECTOR), SO $1/\tau_{tr}$ ~ FRACTIONAL PROBABILITY FOR UMKLAPP SCATTERING ON THE FERMI SURFACE, AND STILL VARIES AS T^2.

THIS HAS BEEN OBSERVED IN THE mK REGIME IN ALKALI METALS. BECAUSE OF THE SMALL PREFACTORS (UMKLAPP PROBABILITY × $1/E_F$) IT IS ONLY IN THIS REGIME THAT IT EXCEEDS BLOCH-GRUNEISEN SCATTERING.

HEAVY FERMION RESISTIVITY

THE RESISTIVITIES FOR SEVERAL HEAVY FERMION COMPOUNDS ARE SHOWN BELOW. IT SHOULD BE NOTICED THAT: (i) THEY ARE NONMONOTONIC
(ii) THEY ARE HUGE (~ 100-200 μΩ-cm AT MAX)
(iii) THEY CAN SHOW HUGE T^2 COEFFICIENTS



FROM Z. FISK, H.R. OTT, T.M. RICE, J.L. SMITH, NATURE 320 124 (1986)

WE WILL GAIN A LIKELY UNDERSTANDING OF (i) TODAY.

HOW BIG IS "BIG"? LET US SIMPLIFY AND ASSUME SCATTERING IS DOMINANTLY IN ONE ANGULAR MOMENTUM CHANNEL, WHICH IS LIKELY HERE AS WE SHALL SEE SHORTLY,

TAKING THAT TO BE S-WAVE, THE MAXIMUM SCATTERER STRENGTH IS WHEN THE PHASE SHIFT $\delta_0(0) = \pi/2$ - SUPPOSE THERE IS ONE SCATTERER IN EACH UNIT CELL -- THEN AT RESONANCE OR AT "THE UNITARITY LIMIT" TAKE $C=1$ AND

$$(16)\quad \frac{1}{\tau_{UNITARY}} = \frac{1}{\hbar}\,\frac{2}{\pi N(0)}\,\sin^2\frac{\pi}{2} \approx \frac{E_F}{\hbar}$$

AND

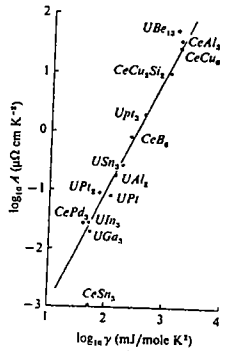
$$(17)\quad \rho_{UNITARY} = \frac{m}{ne^2}\,\frac{1}{\tau_{UNITARY}} \approx 200\,\mu\Omega\text{-cm} \qquad (n = 3\times10^{22}\ \tfrac{el's}{cc})$$

IF WE ARE DEALING WITH f-SCATTERING (LIKELY HERE DUE TO Ce, Yb (4f) OR U (5f) IONS) WE CAN PUSH THIS TO $7\,(=2l+1)\,\rho_{UNITARY} \approx 1400\,\mu\Omega$-cm. BUT THE POINT IS THAT THE SCATTERING IS CLOSE TO THE MAXIMUM POSSIBLE IN A METAL OF TYPICAL CARRIER CONCENTRATION! (NOTE: m^* DOES NOT APPEAR IN ρ -- IT CANCELS HERE FOR REASONS WE WILL CLARIFY IN LECTURE II)

HOW BIG IS THE T^2 COEFFICIENT? WELL, WE KNOW FOR Na, THE MEASURED VALUE IS $\lesssim 1.7\times10^{-9}\,\mu\Omega\text{-cm}/K^2$ [SEE J. BASS, W. PRATT JR., P.A. SCHROEDER, REV. MOD. PHYS. 63, 645 (1990)]

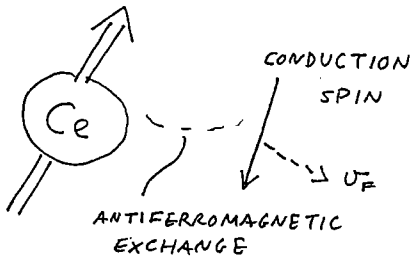
HERE, THE T^2 COEFFICIENT IS MUCH BIGGER MAINLY BECAUSE T_F IS DECREASED BY 3-4 ORDERS OF MAGNITUDE! INDEED, A GOOD EMPIRICAL TEST THAT THE RESISTIVITY AND SPECIFIC HEAT HAVE A COMMON ORIGIN IS TO COMPARE γ^2 TO $A = d\rho/dT^2$. KADOWAKI AND WOODS (SOL. ST. COMM. 58, 507 (1986)) HAVE DONE THIS FOR MANY MATERIALS -- THE CORRELATION IS EXCELLENT AS SEEN IN THE GRAPH ON THE NEXT PAGE.

[FOR $CeAl_3$, $T_F^* \approx 5K$, $A = d\rho/dT^2 \approx 34\,\mu\Omega\text{-cm}/K^2$
FOR Na, $T_F^* \approx 4\times10^4 K$ -- SO $\dfrac{A^{Na}}{A^{CeAl_3}} \cdot \left(\dfrac{T_F^{Na}}{T_F^{CeAl_3}}\right)^2 \approx 1.3$ -- CHECKS!]



SOURCE OF HEAVY FERMIONS: LOCAL MOMENTS

BY NOW IT IS CLEAR THESE SYSTEMS ARE INTERESTING -- WHAT CAUSES THIS PHYSICS? CLEARLY, IT IS THE Ce, Yb, U ATOMS. THESE ATOMS HAVE PARTIALLY FILLED 4f, 5f SHELLS, AND THE INTERACTIONS WITH ITINERANT ELECTRONS CAUSES THE UNIQUE BEHAVIOR. WE CAN GET ANTIFERROMAGNETIC COUPLING, AS WE SHALL SEE SHORTLY. (NB: ANALOGUES WITH LA, TH SHOW NOTHING!)



HIGH TEMPERATURE COUPLING OF Ce & CONDUCTION LOCAL MOMENTS

BECAUSE THE f-ORBITALS ARE TIGHTLY BOUND TO THE IONS, THEY ESSENTIALLY OBEY ATOMIC PHYSICS, SO IT IS APPROPRIATE TO APPLY HUNDS' RULES.

THESE TELL US

1) MAXIMIZE S (TO REDUCE EXCHANGE ENERGY)
2) MAXIMIZE L (TO PRODUCE NODES & THEREBYE REDUCE COULOMB REPULSION)
3) IF FOR A f^n SHELL: $n < 7$ MINIMIZE $\vec{J} = \vec{L} + \vec{S}$
   $n \geq 7$ MAXIMIZE $\vec{J} = \vec{L} + \vec{S}$
   (TO GET LOWEST SPIN ORBIT ENERGY)

BY APPLYING THESE RULES TO Ce^{3+}, Yb^{3+}, U^{4+}, U^{3+} WHICH ARE THE POSSIBLE VALENCES IN A METAL HOST, (SUBJECT TO VALENCE INSTABILITY, HOWEVER -- MORE LATER ...) AND USING THE CURIE LAW FORMULA FOR MAGNETIC SUSCEPTIBILITY (MOLAR) $\chi(T)$

$$(18)\quad \chi(T) = \frac{\mu_{eff}^2}{3k_BT} N_0 = -\frac{\partial^2 F}{\partial h^2}\Big|_{h=0} \qquad (h = \text{MAGNETIC FIELD})$$

$$(19)\quad \frac{\mu_{eff}}{\mu_B} = \sqrt{g_J J(J+1)}$$

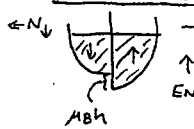
$$(20)\quad g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

WE OBTAIN THE TABLE BELOW FOR FREE IONS

ION	CONFIG.	L	S	J	g_J	$\frac{\mu_{eff}}{\mu_B}$	χ(100K) (emu/mole)	$2J+1 = N$
Ce^{3+}	$4f^1$	3	1/2	5/2	6/7	2.54	.0081	6
Yb^{3+}	$4f^{13}$	3	1/2	7/2	8/7	4.54	.026	8
U^{4+}	$5f^2$	5	1	4	4/5	3.58	.016	9
U^{3+}	$5f^3$	6	3/2	9/2	8/11	3.62	.016	11

HOW DO WE UNDERSTAND THE MAGNITUDE OF THESE χ VALUES?

1) NORMAL METAL, PAULI SUSCEPTIBILITY



RECALL FOR A NORMAL METAL, THE PICTURE AT LEFT GIVES

$$(21)\quad \chi = 2\mu_B^2 N(E_F) N_0 = 2N_0\mu_B \lim_{h\to 0} \frac{1}{h}\frac{n_\uparrow - n_\downarrow}{2(n_\uparrow + n_\downarrow)}$$

FOR $E_F \approx 1eV$, THIS GIVES $\chi \approx 6\times10^{-5}$ emu/mole (cc/mole) MUCH LESS THAN THE TYPICAL ~~FREE~~ LOW VALUES ABOVE

NOTICE THAT FOR FREE ELECTRONS, THE SO CALLED LANDAU-WILSON RATIO DEFINED BY

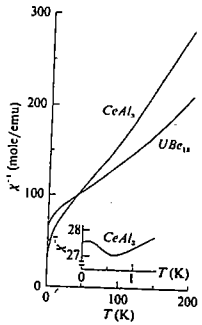
$$(22)\quad R = \frac{\pi^2 k_B^2}{\mu_{eff}^2}\,\frac{\chi(0)}{\gamma(0)}$$

IS EQUAL TO 1, DEVIATIONS FROM UNITY MEASURE THE STRENGTH OF MAGNETIC INTERACTIONS TO ZEROTH ORDER. BOTH χ & γ MEASURE m^*.

2) MEASURED χ, HEAVY FERMION METALS

Z. FISK, H. R. OTT, T. M. RICE, J. L. SMITH, NATURE 320, 124 (1986)

AT RIGHT WE SEE χ^{-1} FOR $CeAl_3$, UBe_{13}. WE NOTICE THAT FOR HIGH T, χ^{-1} IS ROUGHLY LINEAR IN T, CONSISTENT WITH A CURIE LAW. HOWEVER, IN EACH CASE $\chi(0)$ IS FINITE, AND ROUGHLY FOR HIGH T



$$(23)\quad \chi(T) \approx N_0 \frac{\mu_{eff}^2}{3(T+\theta)k_B}$$

WITH:

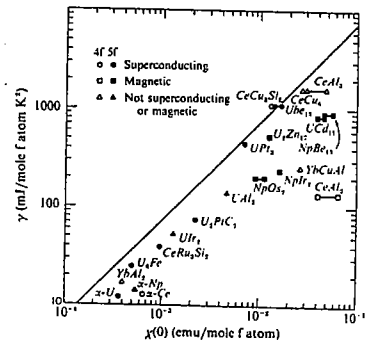
UBe_{13}:	$\mu_{eff} \approx 3.0\,\mu_B$	$\theta \cong 53K$	$\chi(0) \simeq 0.015$ emu/mole
$CeAl_3$:	$\mu_{eff} \approx 2.4\,\mu_B$	$\theta \cong 20K$	$\chi(0) \simeq 0.036$ emu/mole

THESE EFFECTIVE MOMENTS AGREE REASONABLY WITH OUR TABLE. THE $\chi(0)$ VALUES ARE ENORMOUS COMPARED TO FREE ELECTRONS! HOW DOES THE LANDAU-WILSON RATIO WORK OUT? ROUGHLY RIGHT -- THAT IS, WE CAN UNDERSTAND THE ENHANCEMENT OF $\chi(0)$ AS HAVING THE SAME ORIGIN AS $\gamma(0)$. FOR $CeAl_3$, $\gamma(0) = 1600$ mJ/mole-K^2, FOR UBe_{13} IT IS ≈ 1000 mJ/mole-K^2 (AT LEAST AT T_c, THE SUPERCONDUCTING TRANSITION) -- HENCE

UBe_{13}: $R \cong 0.37$

$CeAl_3$: $R \cong 0.86$

B. JONES HAS COMPILED A PLOT OF $\gamma(0)$ VS. $\chi(0)$ FOR HEAVY FERMION MATERIALS -- IT APPEARS BELOW -- THE CORRELATION IS QUITE GOOD CONSIDERING THAT IN A CRYSTAL WE DON'T KNOW ALWAYS WHAT μ_{eff} IS AS WE SHALL SEE A LITTLE LATER.



NOTICE THIS PECULIAR RESULT THOUGH: AT HIGH T, WE SEE LOCAL MOMENTS, AT LOW T? THEY GO AWAY! (THAT IS, $\chi(0) < \infty$), SINCE UBe_{13}, EG, DOES NOT MAGNETICALLY ORDER, THIS MOMENT LOSS IS NOT DUE TO ANTIFERROMAGNETISM (WHICH REDUCES χ). WE'LL SEE THAT SCREENING BY CONDUCTION ELECTRONS IS RESPONSIBLE!

HEAVY FERMIONS: LOCAL PHYSICS

SO FAR, WE HAVE FOCUSSED OUR ATTENTION ON CONCENTRATED SYSTEMS. IN FACT, HEAVY FERMIONS ARISE PURELY LOCALLY -- WE CAN SEE THIS IN EXPERIMENTS WHICH DOPE AWAY THE RARE EARTH OR ACTINIDE IONS.

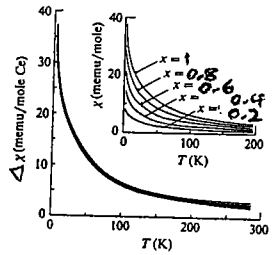
CONSIDER, FOR EXAMPLE, THE ALLOY SYSTEM $La_{1-x}Ce_xPb_3$*. La IS JUST LEFT OF Ce IN THE PERIODIC TABLE. HENCE La^{3+} HAS NO 4f ELECTRONS. WE DEFINE A DIFFERENCE PROPERTY SUCH AS THE SPECIFIC HEAT AS

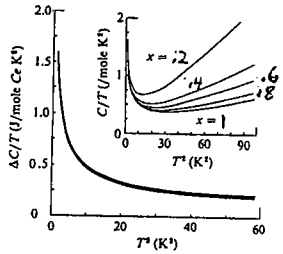
$$(24)\quad \Delta C_{el} = \frac{C_{el}(x) - C_{el}(x=0)}{x}$$

THIS MEASURES THE EXTRA SPECIFIC HEAT PER

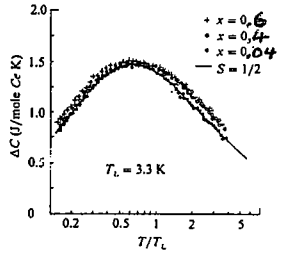
[* C. L. LIN ET AL, PRL 58, 1232 (1987)]

Ce^{3+} ION AS WE DOPE. WE CAN SIMILARLY DEFINE $\Delta\chi$. THE CURVES BELOW SHOW $\Delta C_{el}/T$ AND $\Delta\chi$ FOR A WIDE RANGE OF X VALUES -- CLEARLY THE CURVES DISPLAY <u>SINGLE ION SCALING</u>, I.E., INDEPENCE FROM X! THIS REMARKABLE BEHAVIOR IS NOT ISOLATED TO THIS SYSTEM -- IT IS ALSO SEEN IN $La_{1-x}Ce_xCu_6$, $La_{1-x}Ce_xSn_3$. THE LOW TEMPERATURE $\Delta\gamma$ VALUE OF $\approx$ 1.6 J/mole-K^2 IS CLEARLY <u>HEAVY</u>.



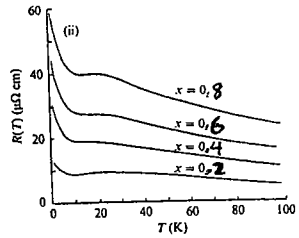


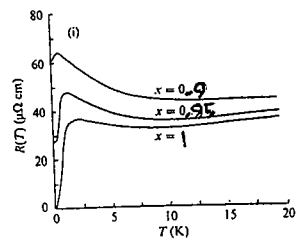
THE PLOT AT RIGHT PROVES THIS SCALING EVEN HOLDS TO THE DILUTE VALUE $x = 0.04$. THE SOLID LINE IS A FIT TO THE $S = 1/2$ KONDO THEORY WE SHALL EXPLAIN LATER.



HENCE TO UNDERSTAND THE <u>ORIGIN OF HEAVY FERMIONS</u>, IT IS APPARENTLY ENOUGH TO STUDY MODELS OF SINGLE IMPURITIES! THIS BY ITSELF, HOWEVER, WILL <u>NOT</u> EXPLAIN MAGNETIC ORDER (OBSERVED IN $CePb_3$), SUPERCONDUCTIVITY (EG, IN UBe_{13}), OR THE VANISHING RESISTIVITY OF, EG, $CeAl_3$, FOR $T \to 0$. THESE PROPERTIES ALL DEPEND UPON SOME KIND OF LATTICE "COHERENCE." NONETHELESS, CLEVER ROUTES EXIST TO LINK IMPURITY BEHAVIOR TO THESE AS WE SHALL SEE IN LECTURES II + III.

THE RESISTIVITY CURVES BELOW ILLUSTRATE THE EVOLUTION OF $\rho(T)$ FOR $La_{1-x}Ce_xPb_3$, DISPLAYING AN EVOLUTION FROM VANISHING RESISTIVITY AS $x \to 1$ TO FINITE AND LARGE RESISTIVITY AS $x \to 0$. [NOTE: GEOMETRY EFFECTS MAKE IT DIFFICULT TO SCALE $\Delta\rho$ PRECISELY IN CONTRAST TO ΔC_{el}, $\Delta\chi$]





"PUDGY FERMIONS" & CRYSTAL FIELDS

NOT ALL THE INTERESTING MATERIALS HAVE $C_{el}/T \sim 1000 \times$ (FREE ELECTRONS). $CePd_3$, FOR EXAMPLE, HAS $C_{el}/T \approx 40$ mJ/mole-K^2, OR $T_F^* \approx 700$ K, SAY. THIS IS AN IMPRESSIVE MASS ENHANCEMENT, BUT WARRANTS ONLY THE NAME "<u>PUDGY FERMION</u>".

THE SUSCEPTIBILITY OF $CePd_3$ IS ISOTROPIC AND AT HIGH T SEEMS TO SHOW THE FULL FREE ION BEHAVIOR OF EQ. (18) (PLUS TABLE II). NOW IT TURNS OUT THAT FROM NEUTRON SCATTERING MEASUREMENTS, THE GROUND STATE OF $CeAl_3$ IS <u>NOT</u> 6-FOLD DEGENERATE, UNLIKE, APPARENTLY, THE Ce IONS IN $CePd_3$ (HERE WE MEAN THAT THE ION HAS A DOUBLET OR SEXTET GROUND STATE WITHOUT COUPLING TO CONDUCTION ELECTRONS).

THIS ARISES FROM A COMBINATION OF CRYSTAL FIELD PHYSICS AND WHATEVER CAUSES HEAVY FERMIONS. WHAT DO I MEAN BY CRYSTAL FIELDS? THE FREE ION IS INVARIANT UNDER THE FULL SU(2) ROTATION GROUP (OR O(3) FOR INTEGER J).

BUT A CRYSTAL HAS ONLY DISCRETE ALLOWED ROTATIONS, WHICH MAKE THEMSELVES FELT THROUGH THE CRYSTALLINE ELECTRIC FIELD -- ONE MUST THEN FIND THE GOOD EIGENSTATES OF THE REDUCED SYMMETRY PROBLEM [- FOR A REFERENCE SEE M. TINKHAM, GROUP THEORY AND QUANTUM MECHANICS, (McGRAW-HILL, NEW YORK, 1964)]. WE FIND, FOR EXAMPLE --

Ce^{3+} $J = 5/2$ → $LaAl_3$ (HEXAGONAL) → $\pm 5/2$, $\pm 1/2$, $\pm 3/2$ } 3 DOUBLETS FROM $J = 5/2$

$\Delta_{CEF} \approx 60K$

Ce^{3+} $J = 5/2$ → $LaPb_3$ (CUBIC) → Γ_8 QUARTET, Γ_7 DOUBLET

$\Delta_{CEF} \approx 60K$

IN THE CASES OF $CePb_3$ ($T_F^* \approx 5K$) AND $CeAl_3$ ($T_F^* \approx 5K$), THE FERMI TEMPERATURE IS SMALL COMPARED TO THE CRYSTAL FIELD SPLITTING. IF IT IS LARGE, ($T_F^* >> \Delta_{CEF}$) THEN WE EXPECT THE FULL DEGENERACY, AS IN $CePb_3$.

WE NOTE HERE AN INTERESTING THEORETICAL IDEA: THE LARGE ORBITAL DEGENERACY OF THESE IONS COULD PROVIDE A PERTURBATION THEORY CONTROL (SMALL) PARAMETER: $1/N$! P.W. ANDERSON SUGGESTED THIS IN 1981, AND THE IDEA FLOURISHED IN THE 1980's -- WE SHALL USE IT IN THESE LECTURES

NON FERMI LIQUID METALS

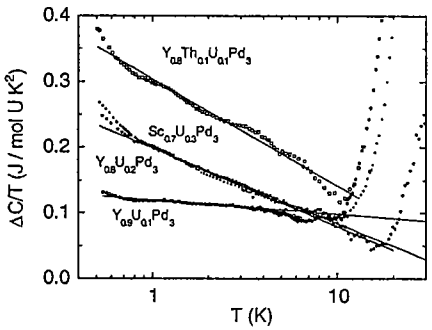
NOT ALL THE HEAVY FERMION MATERIALS DISPLAY SIMPLE PHYSICS SUCH AS $C_{el}/T \to$ CONST AS $T \to 0$, $\rho(T) \sim T^2$ AS $T \to 0$, AMONG BOTH CONCENTRATED AND DILUTE SYSTEMS, THERE ARE EXAMPLES WHERE

(25) $\frac{C_{el}}{T} \sim -\ln T$ $\qquad \rho(T) \approx \rho_0 + AT$

OVER EXTENDED TEMPERATURE REGIONS -- HERE A MAY BE POSITIVE OR NEGATIVE. WE DISPLAY SOME TYPICAL CURVES BELOW FOR BOTH CONCENTRATED AND DILUTE SYSTEMS.

SINCE THE LANDAU THEORY REQUIRES A 1:1 MAP OF LEVELS, A "LOG DIVERGING m^*" CLEARLY VIOLATES THIS -- MOREOVER, $\rho \sim T \sim \langle \varepsilon \rangle$ IMPLIES ILL DEFINED QUASI-PARTICLE STATES! APPARENTLY, THE CONVENTIONAL PICTURES FOR METALS MUST BREAK DOWN!

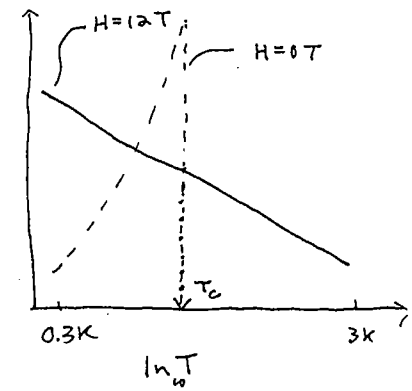
WE SHALL REACH ONE SCENARIO FOR "NON FERMI LIQUID" METALS IN THESE LECTURES.



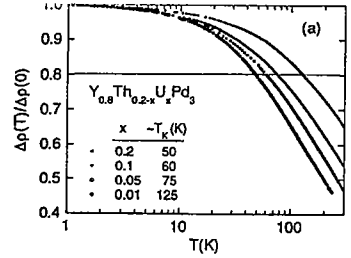
DILUTE

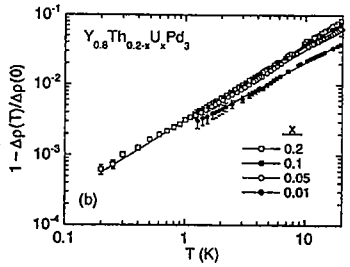
(SEE THE MAPLE ET AL. REVIEW REFERENCED AT THE FRONT OF THESE NOTES)

(H.R. OTT, UBe_{13} (STEGLICH GROUP, '89

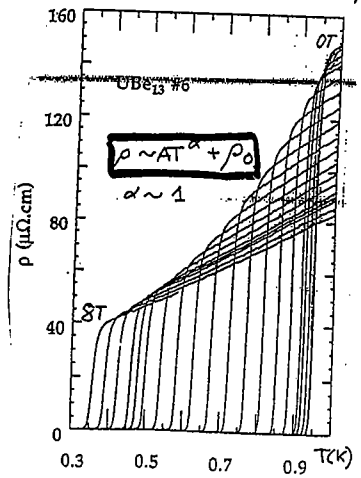


CONCENTRATED





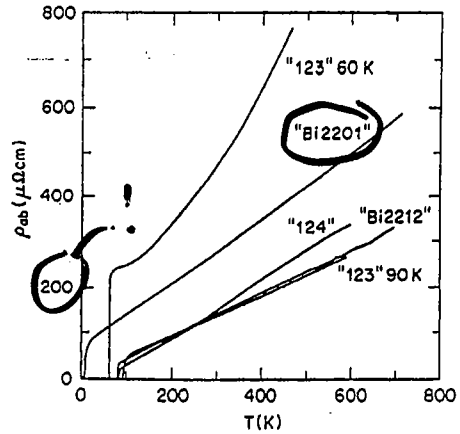
P. Gegenwart '95 (Steglich..)*



Cuprate High Temperature Superconductors

We note that early on Anderson (High Temperature Superconductivity, ds. K. Bedell, p. 3 (1990)) and Varma et al (PRL 63, 1996 (1989)) pointed out the apparent non-Fermi liquid behavior in the cuprates. Contemporaneously, Cox (PRL 59, 1240 [1987]) was suggesting the possibility in heavy fermion materials. The similarity of cuprate resistivity curves to those of nonFermiliquid heavy fermion systems is very intriguing -- namely, also $\rho \sim \rho_0 + AT$. We note that the scales are different -- apparently $T_F^* \gtrsim 1000$ K for the cuprates. This kind of comparison of heavy fermions to cuprates was initiated by K. Levin and collaborators (Physica C 175 499 (1991)).

* See also H.R. Ott



II Models: Strongly Correlated Electrons

Ionization / Addition Energies

We have argued that the heavy fermion metals have rare earth / actinide ions with local moments present (at least this is clear at high T!). For this to be true, the energies to add / remove electrons to the 4f / 5f shells must be large.

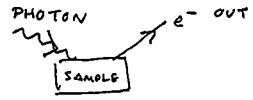
We can write these as (assuming a stable f^n configuration)

(26) $\Delta E_{\pm} = E(f^{n\pm1}) - E(f^n)$

For Ce^{3+}, Yb^{3+}, we have just one f electron or hole -- then for Ce^{3+} ΔE^- is equal to $-\varepsilon_f$, the one electron "binding" energy in the metal, and ΔE_+ is equal to $\varepsilon_f + U_{ff}$, where U_{ff} is the energy

OF COULOMB INTERACTION BETWEEN ELECTRONS (OR HOLES FOR YB^{3+}).

WE CAN MEASURE $\Delta E_\pm$ BY PHOTOEMISSION SPECTROSCOPY (PES)



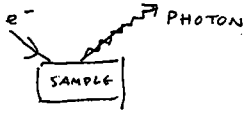
PES INTENSITY

$I(K_{EL} - K_{PHOTON})$ $\quad K$ = KINETIC ENERGY

$\sim N_{OCCUPIED}(K_{PHOTON} - K_{EL})$

OCCUPIED DOS

OR INVERSE PHOTOEMISSION (OR BIS)



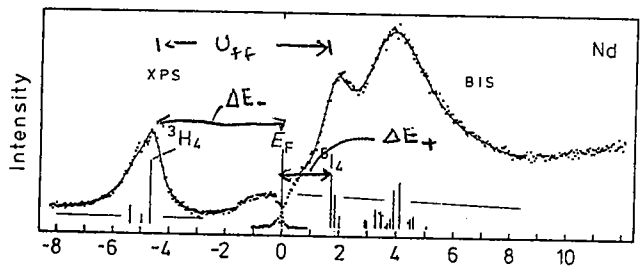
BIS INTENSITY

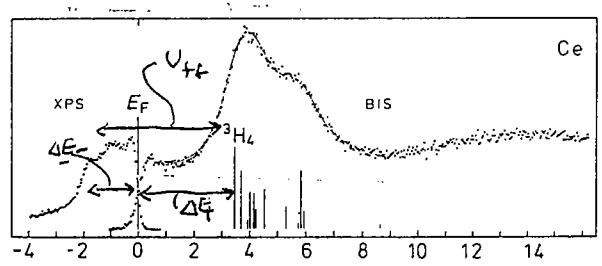
$I(K_{PHOTON} - K_{EL})$

$\sim N_{UNOCCUPIED}(K_{PHOTON} - K_{EL})$

EMPTY DOS

BELOW ARE PLOTS FOR ELEMENTAL CE AND ND FROM THE PIONEERING WORK OF LANG ET AL [JK LANG, Y BAER, PA COX, J PHYS F 11 121 (1981)] AT NEUCHATEL. $\Delta E_\pm$ ARE MARKED -- THOUGH CLEARLY ΔE_- HAS A LARGE ERROR BAR FOR CE! THE LINES REPRESENT MULTIPLET TRANSITION INTENSITIES DERIVED FROM ATOMIC THEORY.



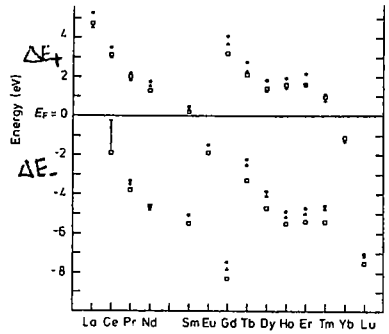


(ΔE_- HAS A BIG ERROR BAR HERE!)

$\Delta E_\pm$ MAY BE CALCULATED FROM A COUPLE OF METHODS

* RENORMALIZED ATOM: HERE THE RARE EARTH ION IS SUBSTITUTED IN A WIGNER SEITZ SPHERE OF 'JELLIUM' -- ENERGIES FOR DIFFERENT f-VALENCES ARE TO BE COMPUTED ALLOWING ENOUGH CONDUCTION CHARGE IN TO ASSURE LOCAL CHARGE NEUTRALITY (IE, CONDUCTION CHARGE SCREENING IS INCLUDED). [SEE JF HERBST, RE WATSON, JW WILKINS, PHYS REV B 13, 1439 (1976); 17, 3089 (1978)]
* SUPERCELL: IN THIS METHOD WHICH IS SENSITIVE TO MATERIAL CHANGE, THE TOTAL ENERGY DIFFERENCES OF IONIZED RARE EARTHS ARE COMPUTED FOR PERIODICALLY REPEATED ARRAYS OR "SUPERCELL" LATTICES, WITHIN THE LOCAL DENSITY APPROXIMATION. AS THE SUPERCELL SPACING GETS LARGE THIS APPROACHES A SINGLE SITE IONIZATION ENERGY [SEE A.J. FREEMAN ET AL, IN HANDBOOK OF THE PHYSICS AND CHEMISTRY OF THE RARE EARTHS VOL. 10, EDS. K.A. GSCHNEIDNER JR., L. EYRING, S. HÜFNER (1987, NORTH-HOLLAND, AMSTERDAM) p. 165]

THE AGREEMENT OF THE RENORMALIZED ATOM CALCULATIONS WITH EXPERIMENT IS QUITE GOOD, AS SHOWN ON THE PLOT OF THE NEXT PAGE FOR ELEMENTAL RARE EARTH METALS. NOTE THAT YB IS DIVALENT IN YB METAL.



• EXPT
□ THEORY (HEGBST + WILKINS)

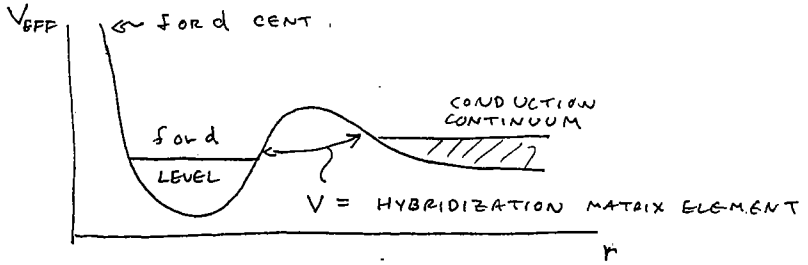
NOTE THAT "ANOMALOUS" RARE EARTHS WHICH DISPLAY HEAVY FERMION (OR OTHER EXOTIC) PHENOMENA HAVE EITHER $\Delta E_\pm$ CLOSE TO E_F ON THE SCALE OF 1-2 eV.

THE Cu^{2+} IONS IN CUPRATE SUPERCONDUCTORS ALSO HAVE LOCALIZED STATES ($3d^9$ IS THE OPEN SHELL). SIMILAR CALCULATIONS* THERE GIVE $E(d^9) - E(d^{10}) \equiv \varepsilon_d \simeq -1.5$ eV, $(E(d^8) - E(d^9)) - (E(d^9) - E(d^{10})) \equiv U_{dd} \approx 10$ eV. THE TABLE BELOW SUMMARIZES ADDITION AND REMOVAL ENERGY DATA FOR Ce, Yb, U, Cu ATOMS (TYPICAL VALUES)

ION	CONFIG (r^n r=f,d)	HOLE OR ELECTRON?	ε_f	U_{ff}
Ce^{3+}	$4f^1$	EL	-2 eV	5eV
Yb^{3+}	$4f^{13}$	HOLE	-1 eV	5eV
U^{4+}	$5f^2$	EL	-1 eV	3eV
Cu^{2+}	$3d^9$	HOLE	-1.5 eV	10eV

HYBRIDIZATION

DESPITE THE RATHER LOCALIZED ORBITALS FOR THESE ATOMS, HYBRIDIZATION IN THE CRYSTALLINE POTENTIAL IS POSSIBLE WITH ITINERANT ELECTRON STATES. IN A METAL LIKE $CeAl_3$, THESE COME FROM THE "LIGAND" Al ATOMS. THERE IS NEGLIGIBLE DIRECT f-f HOPPING BETWEEN Ce SITES.



THE PICTURE GIVES A LOOSE WAY TO VIEW THE HYBRIDIZATION MATRIX ELEMENT V. GENERALLY V WILL GO DOWN THE MORE TIGHTLY BOUND THE ORBITAL. 3d ORBITALS ARE LESS TIGHTLY BOUND THAN 5f's WHICH ARE LESS TIGHTLY BOUND THAN 4f's, 4f's ARE MORE TIGHTLY BOUND FOR INCREASING f NUMBER DUE TO THE "LANTHANIDE CONTRACTION" (ADDED f's SCREEN THE ADDED Z OF THE NUCLEUS POORLY!) THE TABLE BELOW GIVES A ROUGH FEEL FOR V MAGNITUDES AND ORIGINS

ION	MATERIAL	V	"BAND"
Cu^{2+}	La_2CuO_4	~ 1.5 eV	O 2p HOLES
U^{4+}	UBe_{13}	~ .3 eV	Be s-p BANDS
Ce^{3+}	$CeAl_3$	~ .25 eV	Al s-p BANDS
Yb^{3+}	YbCuAl	~ .15 eV	Cu, Al s, p BANDS

THE ORDER OF MAGNITUDE ENHANCED V FOR THE CUPRATES CAN EXPLAIN THE LARGER

*[A. K. McMahan, R. M. Martin, S. Satpathy, Phys Rev. B 38, 6650 (1988).]

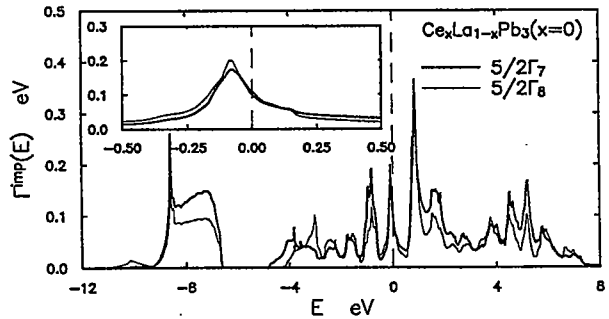
CHARACTERISTIC ENERGY THERE.

IN THIS PICTURE, V MEASURES THE KINETIC ENERGY OF THE LOCALIZED STATES -- IN ALL CASES THE COULOMB ENERGY IS LARGE COMPARED TO V. WE OPERATIONALLY DEFINE STRONGLY CORRELATED ELECTRONS AS THOSE FOR WHICH THE INTERACTION ENERGY EXCEEDS THE KINETIC ENERGY (AVERAGE).

A MORE USEFUL PARAMETERIZATION OF V IS TO CHOOSE INSTEAD $\Gamma = \pi N(0) V^2$.

THIS MEASURES THE GOLDEN RULE BROADENING OF THE LOCAL LEVEL -- THAT IS, PUT AN ELECTRON IN THE LOCAL STATE AND WITHIN A TIME OF ORDER $\hbar/\Gamma$ IT WILL TUNNEL OUT. THIS ACCOUNTS FOR THE BROADENING IN THE f-SPECTRA OF LANG ET AL. ON PP. 23-24.

NOTE THAT Γ, V ARE LIKELY TO BE ANYTHING BUT CONSTANT. THE PLOT BELOW SHOWS THE HYBRIDIZATION BROADENING $\Gamma(\varepsilon) = \pi N(\varepsilon) V^2(\varepsilon)$ VS. ENERGY FOR THE Γ_7, Γ_8 STATES (SEE P. 18) OF Ce^{3+} IN $LaPb_3$, CALCULATED BY J. HAN [J. HAN, M. ALOUANI, D.L. COX, SUBMITTED TO PRL, APRIL (1996)]. THE ENERGY DEPENDENCE IS IMPORTANT FOR UNDERSTANDING REALISTIC PROPERTIES (EG, CRYSTAL FIELD SPLITTING).



ANDERSON HAMILTONIAN: $S = 1/2$, $L = 0$

WHEN WE PUT THE LARGE CORRELATIONS TOGETHER WITH HYBRIDIZATION, WE HAVE THE KEY INGREDIENTS NEEDED TO EXPLAIN THE HEAVY FERMIONS, IN THE FORM OF THE CELEBRATED ANDERSON MODEL INTRODUCED BY PW ANDERSON IN 1961.

LET US RESTRICT ATTENTION TO $S = 1/2$, $L = 0$ FOR SIMPLICITY. THE HAMILTONIAN IS

$$(27)\quad H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \varepsilon_f \sum_\sigma f^\dagger_\sigma f_\sigma + U_{ff} n_{f\uparrow} n_{f\downarrow} + \frac{V}{\sqrt{N_s}} \sum_{k\sigma} \left(f^\dagger_\sigma c_{k\sigma} + c^\dagger_{k\sigma} f_\sigma \right)$$

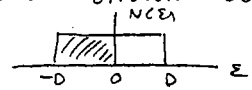
FOR ONE IMPURITY AT $\vec{R} = 0$

WHERE: $c^\dagger_{k\sigma}$ CREATES A CONDUCTION STATE OF MOMENTUM $\vec{k}$, SPIN σ

$f^\dagger_\sigma$ CREATES A LOCAL STATE OF SPIN σ

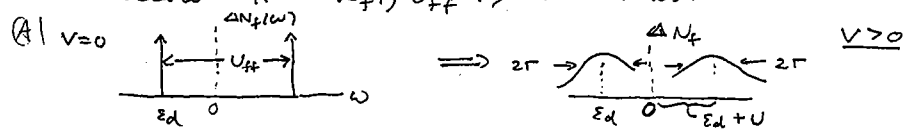
FOR SIMPLICITY, WE'LL ASSUME THAT V = CONSTANT, AND TAKE THE STEP DOS SHOWN BELOW

$$(28)\quad N(\varepsilon) = \frac{1}{2D}\,\theta(D - |\varepsilon|)$$



SO THAT $E_F = D$, THE CONDUCTION BANDWIDTH.

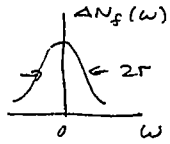
ROUGHLY, WE EXPECT A PICTURE LIKE THIS BELOW IF $|\varepsilon_f|, U_{ff} >> \Gamma = \pi N(0) V^2$



ΔN_f = EXTRA DOS FOR ADDING/REMOVING f-ELECTRONS

ON THE OTHER HAND, IF $\Gamma \gg |\varepsilon_f|, U_{ff}$, THEN WE JUST GET A SIMPLE RESONANCE CENTERED AT THE FERMI ENERGY

(B)



$\Delta N_f(\omega) \cong \Gamma/\pi(\omega^2+\Gamma^2)$

$\Gamma \gg |\varepsilon_f|, U_{ff}$

IN CASE (A), WE EXPECT LOCAL MOMENTS TO FORM -- IN CASE (B), THE RAPID CHARGE FLUCTUATIONS WIPE OUT ANY CHANCE TO GET LOCAL MOMENTS AND THE EXTRA SUSCEPTIBILITY IS JUST

$$(29)\quad \Delta\chi_f(T=0) = 2\mu_B^2\,\Delta N_f(0) = \frac{2\mu_B^2}{\pi\Gamma}$$

A QUESTION IS THIS: AS WE RAISE $|\varepsilon_f|, U_{ff}$ ABOVE Γ IN CASE (B) TO PASS TO (A), IS ANY THING LEFT OF THE RESONANCE AT $\omega=0$? WE'LL GET BACK TO THIS. FIRST, LET US CONSIDER THE LOCAL MOMENT QUESTION MORE CAREFULLY, BY CONSIDERING THE $V=0$ LIMIT; THEN FOR SIMPLICITY TAKE THE <u>SYMMETRIC CASE</u> $\underline{\varepsilon_f = -U_{ff}/2}$. THE EXTRA SUSCEPTIBILITY IS EASILY CALCULATED WITH BOLTZMANN STATISTICS:

$$(30)\quad \Delta\chi_f = +\frac{\partial^2}{\partial h^2}\, k_B T \ln Z_f(h)\Big|_{h=0}$$

WITH

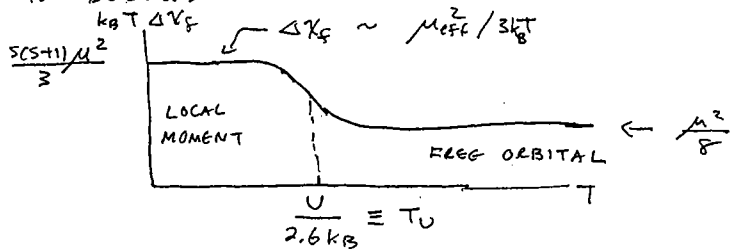
$$(31)\quad Z_f(h) = \underset{\uparrow}{2} + e^{\beta U/2 + \frac{\beta h \mu}{2}} + e^{\beta U/2 - \frac{\beta h \mu}{2}}$$

f^0, f^2

YIELDING

$$(32)\quad \Delta\chi_f(T) = \beta\frac{\mu^2}{4}\frac{e^{\beta U/2}}{1+e^{\beta U/2}} = \beta\frac{\mu^2 S(S+1)}{3}\frac{e^{\beta U/2}}{1+e^{\beta U/2}}$$

THIS GIVES A PLOT OF $k_B T\,\Delta\chi_f$ WHICH LOOKS AS BELOW:



BELOW T_U, A GOOD LOCAL MOMENT IS FORMED --- THE f^0 AND f^2 CONFIGURATIONS ARE SUPPRESSED IN OCCUPANCY. SO IF WE PASS TO THIS LIMIT, RATHER THAN WORK WITH THE FULL ANDERSON MODEL WHICH INCLUDES THESE CHARGE FLUCTUATIONS, IT IS CONVENIENT TO WORK WITH A MODEL INVOLVING THE LOCAL SPIN DEGREES OF FREEDOM ONLY.

MAPPING TO SPIN HAMILTONIAN

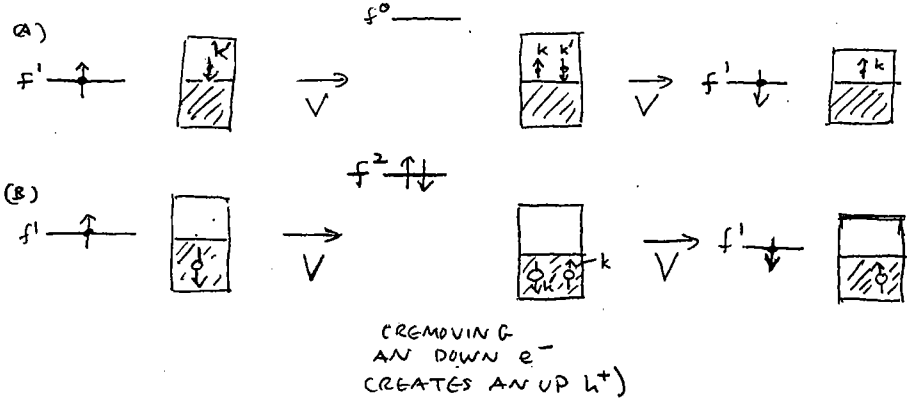
THE GENERAL IDEA HERE IS TO USE A CANONICAL TRANSFORMATION, FOLLOWING SCHRIEFFER & WOLFF (1966) AND COQBLIN & SCHRIEFFER (1969). TO PROCEED, WE SPLIT UP THE HAMILTONIAN INTO $H_0 + H_1$

$$(33)\quad H_0 = \sum_{k\sigma}\varepsilon_k n_{k\sigma} + \varepsilon_f\sum_\sigma n_{f\sigma} + U n_{f\uparrow} n_{f\downarrow}$$

$$(34)\quad H_1 = \frac{V}{\sqrt{N_S}}\sum_{k\sigma}\left(f_\sigma^\dagger c_{k\sigma} + \text{h.c.}\right)$$

THE TERM H_1 LINKS THE f^1 SPACE TO THE f^0, f^2 SPACES. WITHIN THE <u>TOTAL</u> SPACE OF (33), WE CAN SELECT OUT THE f^1 SPACE. WE WANT TO THEN ELIMINATE H_1 THROUGH 1ST ORDER TO GET AN EFFECTIVE HAMILTONIAN

JUST WITHIN THE f^1 + CONDUCTION SPACE. THIS MAKES SENSE -- SECOND ORDER IN V PROCESSES TAKE US FROM f^1 TO f^0, f^2 AND BACK TO f^1. FOR EXAMPLE, CONSIDER THE SEQUENCES BELOW WHICH SHOW A SPIN FLIP EXCHANGE BETWEEN THE f^1 AND CONDUCTION BAND:



THESE GIVE EFFECTIVE EXCHANGE INTERACTIONS OF ORDER $-\frac{V^2}{\varepsilon_f}$, $\frac{V^2}{\varepsilon_f + U_{ff}}$
(A) (B)

FORMALLY, WE WRITE THE CANONICAL TRANSFORMATION AS

$$\tilde{H}_{eff} = e^{-S}(H_0 + H_1)e^{S} = H_0 + (H_1 + [H_0, S]) + \left([H_1, S] + \tfrac{1}{2}[[H_0, S], S]\right) + \cdots \quad (32)$$

WE CAN CHOOSE THE TRANSFORMATION MATRIX S SO THAT

$$H_1 + [H_0, S] = 0 \quad (33)$$

WHICH GIVES

$$\tilde{H}_{eff} = H_0 + \tfrac{1}{2}[H_1, S] + \cdots = H_0 + H_2^{eff} + \cdots \quad (33)$$

IN TERMS OF EIGENSTATES OF H_0 $|a\rangle, |b\rangle$

$$\langle a|[H_0, S]|b\rangle = -\langle a|H_1|b\rangle \quad (34)$$

$$(\varepsilon_a - \varepsilon_b)\langle a|S|b\rangle \Rightarrow \langle a|S|b\rangle = \frac{\langle a|H_1|b\rangle}{\varepsilon_b - \varepsilon_a} \quad (|a\rangle \neq |b\rangle !)$$

SO

$$\tfrac{1}{2}[H_1, S_0] = \tfrac{1}{2}\sum_{a,b} |a\rangle\langle b| \langle a|[H_1, S]|b\rangle \quad (35)$$

$$= \tfrac{1}{2}\sum_{abc} |a\rangle\langle b| \left\{\frac{1}{\varepsilon_a - \varepsilon_c} + \frac{1}{\varepsilon_b - \varepsilon_c}\right\} \langle a|H_1|c\rangle \times \langle c|H_1|b\rangle$$

$$= H_2^{eff} \qquad (c \neq a, c \neq b)$$

NOW, LET'S APPLY THIS HERE -- WE WILL FOR SIMPLICITY TAKE $U_{ff} \to \infty$ BUT ASSUME $|\varepsilon_f| >> \Gamma$. THE RELEVANT STATES ARE

$$|a\rangle = |f^1\sigma, k'\sigma'\rangle \quad (36)$$
$$|b\rangle = |f^0, k\sigma\rangle$$
$$|c\rangle = |f^0, k'\sigma', k\sigma\rangle$$

$\varepsilon_a - \varepsilon_c = \varepsilon_f - \varepsilon_k \approx \varepsilon_f$
$\varepsilon_b - \varepsilon_c = \varepsilon_f - \varepsilon_{k'} \approx \varepsilon_f$
FOR $|\varepsilon_k|, |\varepsilon_{a,1}| << |\varepsilon_f|$

THEN: $\langle a|H_1|c\rangle = -\frac{V}{\sqrt{N_s}}$ (37)
$\langle c|H_1|b\rangle = +\frac{V}{\sqrt{N_s}}$

FOR $H_1 = \frac{V}{\sqrt{N_s}} \sum_{k\sigma} (|f^1\sigma\rangle\langle f^0| c_{k\sigma} + h.c.)$ (38)

WHERE WE USED $f_\sigma^+ \to |f^1\sigma\rangle\langle f^0|$, $f_\sigma \to |f^0\rangle\langle f^1\sigma|$ } $U_{ff} \to \infty$
($|f^0\rangle\langle f^1\sigma|$: PROJECTION OPERATORS)

THEN FOR $|\varepsilon_f| \gg \Gamma, \varepsilon_k, \varepsilon_{k'}$

(39) $$H_2^{eff} = \frac{-V^2}{N_s \varepsilon_f} \sum_{\substack{\sigma\sigma' \\ kk'}} |f'\sigma\rangle\langle f'\sigma'| \, c^\dagger_{k\sigma'} c_{k\sigma}$$

NOW WE CAN REWRITE THIS -- AS WE NOTE (SUPPRESSING k, k')

(40) $$|f'^\uparrow\rangle\langle f'\uparrow| c^\dagger_\uparrow c_\uparrow + |f'\downarrow\rangle\langle f'\downarrow| c^\dagger_\downarrow c_\downarrow + |f'\uparrow\rangle\langle f'\downarrow| c^\dagger_\downarrow c_\uparrow + |f'\downarrow\rangle\langle f'\uparrow| c^\dagger_\uparrow c_\downarrow$$

$$= 2\Big[\tfrac{1}{4}\big(|f'\uparrow\rangle\langle f'\uparrow| - |f'\downarrow\rangle\langle f'\downarrow|\big)\big(c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow c_\downarrow\big) + \tfrac{1}{4}\big(|f'\uparrow\rangle\langle f'\uparrow| + |f'\downarrow\rangle\langle f'\downarrow|\big)\big(c^\dagger_\uparrow c_\uparrow + c^\dagger_\downarrow c_\downarrow\big) + \tfrac{1}{2}\big(|f'\uparrow\rangle\langle f'\downarrow| c^\dagger_\downarrow c_\uparrow + |f'\downarrow\rangle\langle f'\uparrow| c^\dagger_\uparrow c_\downarrow\big)\Big]$$

$$= \underbrace{2\vec{S}_f \cdot \vec{S}_c}_{\text{SPIN EXCHANGE}} + \underbrace{\tfrac{1}{2} n_f n_c}_{\text{POTENTIAL SCATTERING}}$$

$$S_f^z = \tfrac{1}{2}\big(|f'\uparrow\rangle\langle f'\uparrow| - |f'\downarrow\rangle\langle f'\downarrow|\big)$$
$$S_f^+ = |f'\uparrow\rangle\langle f'\downarrow|$$
$$S_f^- = |f'\downarrow\rangle\langle f'\uparrow|$$

HENCE

(41) $$H_2^{EFF} = \frac{2V^2}{|\varepsilon_f|} \vec{S}_f \cdot \vec{S}_c(0) + \underbrace{\frac{V^2}{2|\varepsilon_f|}}_{U = \text{POTENTIAL SCATTERING}} n_f n_c(0)$$

$$\vec{S}_c(0) = \frac{1}{2N_s} \sum_{\substack{\sigma\sigma' \\ kk'}} c^\dagger_{k\sigma'} \underbrace{\vec{\sigma}_{\sigma'\sigma}}_{\text{PAULI MATRICES}} c_{k\sigma}$$

$$n_c(0) = \frac{1}{N_s} \sum_{\substack{\sigma \\ kk'}} c^\dagger_{k'\sigma} c_{k\sigma}$$

THE EFFECTIVE LOW ENERGY THEORY IS AN ANTIFERROMAGNETIC EXCHANGE BETWEEN THE f LOCAL MOMENT AND CONDUCTION STATES, WITH

(42) $$J = \frac{2V^2}{|\varepsilon_f|} > 0$$

[FOR $U_{ff} < \infty$, WE CORRECT THIS TO

$$J = \frac{2V^2}{|\varepsilon_f|} + \frac{2V^2}{\varepsilon_f + U_{ff}} \qquad U = \frac{V^2}{2|\varepsilon_f|} - \frac{V^2}{2(\varepsilon_f + U_{ff})}.$$

HENCE, IN THIS SPACE AFTER "INTEGRATING" OUT HIGH ENERGY CHARGE FLUCTUATIONS WE GET THE "KONDO HAMILTONIAN"

(43) $$\tilde{H}_{eff} = H_{COND} + \underbrace{J \vec{S}_f \cdot \vec{S}_c(0)}_{(H_2^{eff} = H_K)} + U n_f n_c(0)$$

$(\varepsilon_f \sum_\sigma |f'\sigma\rangle\langle f'\sigma|$ IS JUST A CONSTANT HERE!)

[NB: FOR THE SYMMETRIC ANDERSON MODEL, $\varepsilon_f = -U_{ff}/2 \Rightarrow J = \frac{8V^2}{U}$ $U = 0$]

DEGENERATE (ORBITALLY) ANDERSON MODEL

IN THE ABSENCE OF CRYSTAL FIELD SPLITTING, A Ce^{3+} ION (OR Yb^{3+}) HAS A LARGE ORBITAL DEGENERACY(N).

IN THIS CASE THE SIMPLEST HAMILTONIAN WE CAN WRITE DOWN IS

(44) $$H = \sum_{km} \varepsilon_k n_{km} + \varepsilon_f \sum_m f^\dagger_m f_m + \frac{U}{2} \sum_{m \neq m'} n_{fm} n_{fm'} + \frac{V}{\sqrt{N_s}} \sum_{km} \big(f^\dagger_m c_{km} + \text{h.c.}\big)$$

WHERE m RUNS OVER $-\frac{(N-1)}{2}, \ldots, \frac{N-1}{2}$

AND WE ASSUME N FOLD DEGENERATE CONDUCTION STATES. PHYSICALLY, THESE REALLY ARISE FROM A PARTIAL WAVE PROJECTION ABOUT THE IMPURITY SITE TOGETHER WITH SPIN ORBIT COUPLING.

FOR 4f/5f SYSTEMS, $\ell = 3$ SO FIRST:

$$(45) \quad C^+_{km_\ell\sigma} \approx \int \frac{d\hat{k}}{4\pi} \, C^+_{\vec{k}\sigma} \, Y_{3m_\ell}(\hat{k})$$

THEN ($j = 5/2$, SAY FOR Ce^{3+} OR $j = 7/2$ FOR Yb^{3+})

$$(46) \quad C^+_{km} = \sum_{m_\ell\sigma} \langle jm | 3m_\ell \tfrac{1}{2}\sigma \rangle \, C^+_{km_\ell\sigma}$$

THE ESSENCE OF (45) IS THAT WE MAY CHOOSE TO WORK IN A PLANE WAVE OR PARTIAL WAVE BASIS -- RECALL

$$(47) \quad e^{i\vec{k}\cdot\vec{r}} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) P_\ell(\hat{k}\cdot\hat{r}) \, j_\ell(kr)$$

SO THAT (45) PICKS OUT THE $\ell = 3$ SPHERICAL WAVES IN $C^+_{\vec{k}\sigma}$.

ONE MUST UNDERSTAND THAT THIS N-FOLD DEGENERACY IS PURELY LOCAL -- THAT IS, IF WE EXTEND OUR MODEL TO A LATTICE OF 4f SITES WE'LL NOT HAVE N-FOLD DEGENERATE BANDS, THOUGH THIS IS A CONVENIENT WAY TO ENVISION THINGS FOR CERTAIN THEORETICAL PURPOSES.

IF WE TAKE $U_{ff} \to \infty$, WE MAY WRITE

$$(47) \quad H = \sum_k \varepsilon_k n_{km} + \varepsilon_f \sum_{fm} |f^1 m\rangle\langle f^1 m| + \frac{V}{\sqrt{N_s}} \sum_{km} \left(|f^1 m\rangle\langle f^0| \, C_{km} + h.c. \right)$$

WE CAN FOLLOW THE SCHRIEFFER-WOLF TRANSFORMATION THROUGH AS BEFORE - HERE IT IS CALLED "COQBLIN-SCHRIEFFER". WE OBTAIN, FOR $|\varepsilon_f| >> \Gamma$

$$(48) \quad H_{cs} = \sum_{km} \varepsilon_k n_{km} + \frac{J_{cs}}{N_s} \sum_{kk'mm'} |f^1 m\rangle\langle f^1 m'| \, C^+_{k'm'} C_{km}$$

WITH $J_{cs} = V^2/|\varepsilon_f|$.

THIS IS CALLED THE COQBLIN-SCHRIEFFER (1969) MODEL, OR THE "SU(N)" KONDO MODEL BECAUSE (48) IS INVARIANT UNDER UNITARY* TRANSFORMATION AMONG THE N INDICES m, WHICH CORRESPONDS TO THE SYMMETRY GROUP $SU(N)$

EXTENSION TO THE LATTICE

TO DESCRIBE REAL HEAVY FERMION COMPOUNDS WE NEED TO EXTEND THESE IMPURITY MODELS TO THE LATTICE. HERE WE'LL JUST WRITE DOWN THE EXTENSIONS OF THE $S = 1/2$ MODELS

ANDERSON:

$$(49) \quad H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + \varepsilon_f \sum_{i\sigma} n_{i f\sigma} + U_{ff} \sum_i n_{i f\uparrow} n_{i f\downarrow} + \frac{V}{\sqrt{N_s}} \sum_{k i \sigma} \left(e^{i\vec{k}\cdot\vec{R}_i} f^+_{i\sigma} C_{k\sigma} + h.c. \right)$$

KONDO:

$$(50) \quad H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + \frac{J}{2N_s} \sum_{ikk'\mu\nu} \vec{S}_f(\vec{R}_i) \cdot \vec{\sigma}_{\mu\nu} \, C^+_{k\mu} C_{k'\nu} e^{i(k-k')\cdot R_i}$$

---

* UNIMODULAR

ASIDE FROM THE INTRODUCTION OF PERIODICITY, THE INTERESTING PHYSICS IN THESE MODELS IS THE INTERSITE COUPLING BETWEEN f-MOMENTS INDUCED BY CONDUCTION ELECTRONS!

KONDO EFFECT I: HIGH T

THEORY

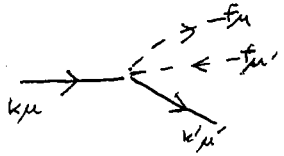
HAVING INTRODUCED THE LOW ENERGY MODELS DESCRIBING INTERACTIONS OF LOCAL MOMENTS (f) AND CONDUCTION ELECTRONS, LET'S NOW SEE WHAT PHYSICS CAN EMERGE.

BECAUSE $J = 2V^2/|\varepsilon_f| = 2\Gamma/\pi N(0)|\varepsilon_f|$ IN EQ. (43), AND $\Gamma/|\varepsilon_f| \ll 1$, THEN A SUITABLE DIMENSIONLESS COUPLING FOR DOING PERTURBATION THEORY WOULD APPEAR TO BE

$$(51) \qquad g = N(0)J = \Gamma/\pi|\varepsilon_f|$$

LET US FOLLOW THE FAMOUS WORK OF KONDO (1964) AND CALCULATE THE SCATTERING RATE OF CONDUCTION ELECTRONS OFF THE LOCAL MOMENT.

THE LOWEST ORDER (BORN APPROXIMATION) RESULT IS EASILY FOUND USING THE GOLDEN RULE. WE HAVE THE PROCESS



WHICH PROVIDES

$$(52) \quad \frac{1}{\tau_\mu(\varepsilon_k)} = \frac{2\pi}{\hbar} \frac{1}{\#\text{ OF IMPURITIES}} \sum_{k'\mu'} |\langle k'\mu', f'_{\mu'}| H_K |k\mu, f_\mu\rangle|^2 \delta(\varepsilon_{k'} - \varepsilon_k) \frac{e^{-\beta E_i}}{Z}$$

PRACTICALLY, THE THERMAL AVERAGE OVER INITIAL STATES JUST EFFECTS AN AVERAGE OVER INITIAL f-SPIN, IE $\frac{e^{-\beta E_i}}{Z} \Longrightarrow \frac{1}{2}$ SINCE THIS SCATTERING IS ONE-BODY IN CONDUCTION SPACE.

THE MATRIX ELEMENT IN (52) GIVES THE SPIN FACTORS (EINSTEIN NOTATION):

$$\sum_{\lambda\gamma} \sum_{\mu'} \underbrace{(S_f^\lambda S_f^\gamma)_{\mu'\mu'}}\ (S_c^\lambda S_c^\gamma)_{\mu\mu} \qquad (f,c \text{ ARE MNEMONIC LABELS})$$

$$\sum_{\lambda\gamma} \sum_{\mu'} \left\{ \left[\frac{\delta_{\lambda\gamma}}{4} \delta_{\mu'\mu'} + i \frac{\epsilon^{\lambda\gamma\rho}}{2} (S_f^\rho)_{\mu'\mu'} \right] \left[\frac{\delta_{\lambda\gamma}}{4} \delta_{\mu\mu} + i \frac{\epsilon^{\lambda\gamma\tau}}{2} (S_c^\tau)_{\mu\mu} \right] \right\}$$

($\mathrm{Tr}(S_f^\rho) = 0$)

$$= \frac{3}{8}$$

$$\underline{\underline{50}} \qquad (53) \quad \frac{1}{\tau_\mu(\varepsilon_k)} = \frac{2\pi}{\hbar} \frac{J^2 N_i}{N_s} \left(\frac{3}{16}\right) \frac{1}{N_s} \sum_{k'} \delta(\varepsilon_k - \varepsilon_{k'})$$

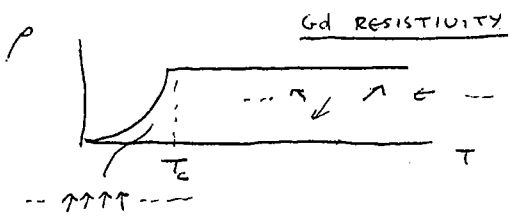
$$= \frac{2\pi}{\hbar} N(0) J^2 C \frac{1}{4} \left[\frac{3}{4}\right]$$

$$= \frac{\pi C}{2\hbar N(0)} g^2 S_f(S_f+1)$$

ABRIEF DIGRESSION:

[THIS RESULT IS KNOWN AS "SPIN-DISORDER" SCATTERING. GENERALIZED TO, EG, GD METAL, IT DESCRIBES THE RESISTIVITY ABOVE THE CURIE POINT QUITE WELL! FOR GD, $S_f = 7/2$

AND $c = 1$



THEN $\frac{\hbar}{\tau_{Gd}} \approx \frac{\pi}{2kN(0)} g_{GD}^2 \frac{63}{4} \approx \frac{47\pi}{N(0)} g_{GD}^2$

COMPARE THIS TO (16)

$$\frac{1}{\tau_{UNITARY}} \approx 2\pi^2 g_{GD}^2$$

EVEN FOR $g_{GD}^2 \approx 0.05$, $\tau_{GD} \sim \tau_{UNITARY}$ DUE TO THE LARGE GD SPIN! NONETHELESS, THE PERTURBATIVE EXPRESSION IS ADEQUATE----]

NOW, PRIOR TO KONDO, PEOPLE HAD STOPPED AT (53), ASSUMING NOTHING HAPPENED IN HIGHER ORDERS OF PERTURBATION THEORY.

KONDO WAS MOTIVATED TO LOOK AT HIGHER ORDERS BECAUSE OF A DESIRE TO EXPLAIN THE FAMOUS RESISTIVITY MINIMA OBSERVED IN METALS SINCE THE 1930's. A PICTURE APPEARS ON THE FOLLOWING PAGE FROM AN ARTICLE IN THE 30's.

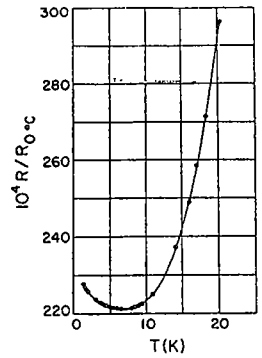
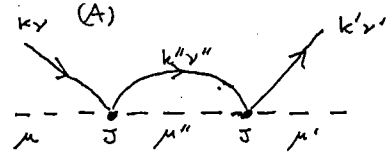


FIG. 1. Resistivity minimum in a noble metal (Au) with residual transition metal impurities, reproduced from the work of W. J. de Haas and G. J. van den Berg, Physica 3, 440 (1936). The curve shows the resistance of a Au wire, normalized by the value at 0° C. This represents one of the earliest observations of anomalous low-temperature effects in a dilute magnetic alloy. A number of excellent review articles discuss experiments on magnetic alloys from the 1930s through recent years (Ref. 1).

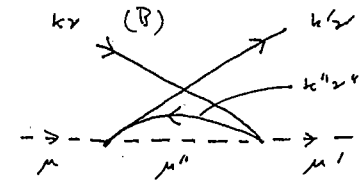
IT WAS FINALLY SUGGESTED THAT THIS MINIMUM HAD TO DO WITH TRACE AMOUNTS OF TRANSITION METAL IMPURITIES IN THE CASE OF, EG, AU. SINCE THESE HAVE MAGNETIC MOMENT KONDO LOOKED PAST LEADING ORDER.

A GOOD STRATEGY TO ORGANIZE THE PERTURBATION THEORY IS TO EXPAND IN THE EFFECTIVE INTGRACTION BETWEEN f MOMENTS AND CONDUCTION ELECTRONS, WE SHALL NOT DERIVE THE FORMAL PERTURBATION THEORY HERE BUT MOTIVATE IT IN TERMS OF DIAGRAMMATIC RULES. FOR A MORE EXTENSIVE DISCUSSION SEE THE REVIEW BY BICKERS.

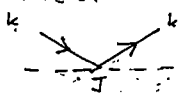
THE SECOND ORDER PROCESSES WHICH CONTRIBUTE TO THE "RENORMALIZED" COUPLING ARE SHOWN BELOW IN DIAGRAMS, WITH TIME RUNNING FROM LEFT TO RIGHT:



INTERMEDIATE PARTICLE



INTERMEDIATE HOLE STATE



[NOTE: THE "BARE" COUPLING HERE IS

TO GO FROM DIAGRAMS TO EXPRESSIONS FOLLOW THESE RULES:

① INCLUDE A FACTOR OF U/N_S FOR EVERY VERTEX, TOGETHER WITH SPIN ½ MATRICES $\sum_\delta (S_f^\delta)_{\mu\mu'} (S_c^\delta)_{\nu\nu'}$

② FOR EACH INTERNAL PARTICLE [HOLE] LINE, INCLUDE A FACTOR $f(-\varepsilon_k)$ $[f(\varepsilon_k)]$ REFLECTING THE OCCUPANCY OF THE STATE.

③ BETWEEN EACH PAIR OF VERTICES INCLUDE AN ENERGY DENOMINATOR $(\varepsilon_L - \sum_i \varepsilon_i)^{-1}$ WHERE ε_L IS THE SUM OF LEFT-MOST ENERGIES, AND $\sum_i \varepsilon_i$ IS THE SUM OF ENERGIES BETWEEN THE LINES, FOR HOLES INTERNALLY, $\boxed{\varepsilon_i = -\varepsilon_k}$

④ MULTIPLY BY $(-1)^{L+C}$ WHERE L IS THE NUMBER OF CLOSED CONDUCTION LOOPS AND C THE # OF CONDUCTION LINE CROSSINGS.

⑤ SUM OVER ALL INTERNAL CONDUCTION MOMENTA AND ALL INTERNAL SPIN INDICES.

IT IS INSTRUCTIVE TO EVALUATE (A), (B) IN THE CASE WHERE WE REPLACE THE SPIN DEPENDENT VERTEX BY POTENTIAL SCATTERING -- IE, IN ① WE INSTEAD USE $\frac{U}{N_S}\delta_{\mu\mu'}\delta_{\nu\nu'}$

THEN WITH THE RULES:

(A) GIVES: $\frac{U^2}{N_S^2} \sum_{\substack{k'' \\ \mu''\nu''}} \delta_{\mu\mu''}\delta_{\mu''\mu'}\delta_{\nu\nu''}\delta_{\nu''\nu'} \frac{1-f(\varepsilon_{k''})}{\varepsilon_k - \varepsilon_{k''}}$

$= \frac{U^2}{N_S^2}\left(\sum_{k''} \frac{1-f(\varepsilon_{k''})}{\varepsilon_k - \varepsilon_{k''}}\right)\delta_{\mu\mu'}\delta_{\nu\nu'}$

(B) GIVES: $-\frac{U^2}{N_S}\left(\sum_{k''} \frac{f(\varepsilon_{k''})}{\varepsilon_k - (-\varepsilon_{k''} + \varepsilon_k + \varepsilon_{k'})}\right)\delta_{\mu\mu'}\delta_{\nu\nu'}$

$= \frac{U^2}{N_S^2}\sum_{k''} \frac{f(\varepsilon_{k''})}{\varepsilon_{k''} - \varepsilon_{k'}}$

IN THE GOLDEN RULE, WE WOULD THEN REPLACE $\frac{U}{N_S}$ BY

$$\frac{U}{N_S} \to \frac{U}{N_S}\left[1 + \frac{U}{N_S}\sum_{k''}\left(\frac{1-f(\varepsilon_{k''})}{\varepsilon_k - \varepsilon_{k''}} + \frac{f(\varepsilon_{k''})}{\varepsilon_{k'} - \varepsilon_{k''}}\right)\right]$$

BUT THE GOLDEN RULE FIXES $\varepsilon_k = \varepsilon_{k'}$. SO "ON SHELL"

$$(54)\quad U_{eff} = U\left[1 + \frac{U}{N_S}\sum_{k''}\frac{1-f(\varepsilon_{k''}) + f(\varepsilon_{k''})}{\varepsilon_k - \varepsilon_{k''}}\right]$$

ALL MANY BODY ASPECTS CANCEL. INDEED, THE SECOND TERM IS JUST THE SECOND ORDER BORN APPROXIMATION FOR SINGLE PARTICLE SCATTERING OFF THE IMPURITY!

FOR SPIN-DEPENDENT SCATTERING, THE MANY BODY EFFECTS DON'T CANCEL OUT! TURNING NOW TO THE KONDO COUPLING, WE GET:

$$(A) \Rightarrow \frac{J^2}{N_S^2}\sum_{k''}\sum_{\substack{\lambda\delta \\ \mu''\nu''}}\left\{\left[S_f^\lambda)_{\mu\mu''} S_c^\lambda)_{\nu\nu''} S_f^\delta)_{\mu''\mu'} S_c^\delta)_{\nu''\nu'}\right] \times \frac{1-f(\varepsilon_{k''})}{\varepsilon_k - \varepsilon_{k''}}\right\}$$

USING EINSTEIN NOTATION, THE SPIN ALGEBRA GIVES

$$S_f^\lambda)_{\mu\mu''} S_f^\gamma)_{\mu''\mu'} = \frac{\delta^{\lambda\gamma}}{4}\delta_{\mu\mu'} + \frac{i\epsilon^{\lambda\gamma\rho}}{2} S^\rho_{\mu\mu'}$$

$$S_c^\lambda)_{\nu\nu''} S_c^\gamma)_{\nu''\nu'} = \frac{\delta\lambda\gamma}{4}\delta_{\nu\nu'} + \frac{i\epsilon^{\lambda\gamma\tau}}{2} S^\tau_{\nu\nu'}$$

SO

$$\left[S_f^\lambda)_{\mu\mu''} S_c^\lambda)_{\nu\nu''} S_f^\gamma)_{\mu''\mu'} S_c^\gamma)_{\nu''\nu'}\right] = \frac{3}{16}\delta_{\nu\nu'}\delta_{\mu\mu'} - \frac{1}{2} S_f^\rho)_{\mu\mu'} S_c^\rho)_{\nu\nu'}$$

WHERE WE USED

$$(i\epsilon^{\lambda\alpha\rho})(i\epsilon^{\lambda\gamma\tau}) = -\delta_{\rho\tau}[\delta_{\alpha\gamma} - \delta_{\alpha\rho}\delta_{\gamma\tau}] = -2\delta_{\rho\tau}$$

THE FIRST TERM CORRESPONDS TO INDUCED POTENTIAL SCATTERING, THE SECOND TO SPIN EXCHANGE FROM (B)

$$(B) \Rightarrow -\frac{J^2}{N_S^2}\sum_{k''}\sum_{\lambda\mu''\gamma''}\Big\{\Big[S_f^{\lambda})_{\mu\mu''}\, S_f^{\gamma})_{\mu''\mu'}\, S_c^{\gamma})_{\nu\nu''}\, S_c^{\lambda})_{\nu''\nu'}\Big] \times \frac{f(\varepsilon_{k''})}{\varepsilon_{k''} - \varepsilon_{k'}}\Big\}$$

NOTICE THE INTERCHANGE OF γ, λ RELATIVE TO (A) FOR THE CONDUCTION SPINS! BECAUSE THESE SPIN MATRICES DON'T COMMUTE WE'LL GET A NEAT RESULT! WITH EINSTEIN NOTATION

$$S_f^{\lambda})_{\mu\mu''}\, S_f^{\gamma})_{\mu''\mu'}\, S_c^{\gamma})_{\nu\nu''}\, S_c^{\lambda})_{\nu''\nu'} = \frac{3}{16}\delta_{\nu\nu'}\delta_{\mu\mu'} + \frac{1}{2}S_f^{\rho})_{\mu\mu'}\, S_c^{\rho})_{\nu\nu'}$$

PUTTING (A), (B) TOGETHER WITH $\varepsilon_k = \varepsilon_{k'}$ WE FIND

(55) $$J_{eff}(T) = J\left[1 + \frac{J}{2N_S}\sum_{k''}\frac{1-2f(\varepsilon_{k''})}{\varepsilon_{k''} - \varepsilon_k}\right]$$

NOW: $\frac{1}{2N_S}\sum_{k''}\frac{1-2f(\varepsilon_{k''})}{\varepsilon_{k''} - \varepsilon_k}$ WE SHALL EVALUATE IN TWO LIMITS.

(1) $\varepsilon_k \ll k_BT \Rightarrow$ SET $\varepsilon_k = 0$ IN (55)

(56) $$\frac{1}{2N_S}\sum_{k''}\frac{1-2f(\varepsilon_{k''})}{\varepsilon_{k''}} = N(0)\int_{-D}^{D}d\varepsilon\,\frac{\tanh\beta\varepsilon/2}{2\varepsilon} \approx 2N(0)\int_{k_BT}^{D}\frac{d\varepsilon}{2\varepsilon} = N(0)\ln\frac{D}{k_BT}$$

[EXACT: $N(0)\ln\frac{1.130}{k_BT}$]

(2) $\varepsilon_k \gg k_BT \Rightarrow$ SET ~~T~~ $= 0$ IN (55)

(57) $$\frac{1}{2N_S}\sum_{k''}\frac{1-2f(\varepsilon_{k''})}{\varepsilon_{k''} - \varepsilon_k} = \frac{N(0)}{2}\,P\int_{-D}^{D}\frac{d\varepsilon''\,\mathrm{sgn}(\varepsilon'')}{\varepsilon'' - \varepsilon} = N(0)\ln\frac{D}{|\varepsilon|}$$

SO: (58) $$J_{eff}(\varepsilon, T) = J\left[1 + N(0)J\ln\frac{D}{MAX[|\varepsilon|, T]}\right] = J\left[1 + g\ln\frac{D}{MAX[|\varepsilon|, T]}\right]$$

COMMENTS ON THIS RESULT:

(1) $g > 0$: $|J_{eff}| > |J| \Rightarrow$ J GROWS! (ANTIFERRO)
$g < 0$: $|J_{eff}| < |J| \Rightarrow$ $|J|$ SHRINKS! (FERRO)

(2) BACK TO RESISTANCE MINIMUM -- IN (53) REPLACE g BY $g(T, \varepsilon)$ WITH $\varepsilon = 0$ (ONLY FERMI SURFACE SCATTERING IMPORTANT)

$$g(T) = \underbrace{g_0}_{N(0)J} + g_0^2\ln\frac{D}{k_BT}$$

AND TO LEADING ORDER IN g_0

(59) $\frac{1}{\tau_{KONDO}(T)} \approx \frac{\pi c}{2kN(0)} g_0^2 \left[1 + 2g_0 \ln \frac{D}{k_B T}\right] S_f(S_f+1)$

ADD THIS TO THE BLOCH-GRUNEISEN LAW

(60) $\rho(T) \approx \frac{m}{ne^2}\left[\underbrace{\frac{1}{\tau_{th}(T)}}_{\sim AT^5} + \frac{1}{\tau_{KONDO}(T)}\right]$

FOR $g_0 > 0$, THE LOGARITHMIC RISE OF (59) COMPETING WITH THE T^5 FALL OF $1/\tau_{th}(T)$ AS $T \to 0$ WILL PRODUCE A MINIMUM AT $T_{MIN} \sim C^{1/5}$.

CONTROLLED DOPING EXPERIMENTS CONFIRMED THIS CONCENTRATION DEPENDENCE & KONDO'S THEORY!

(3) BREAKDOWN OF PERTURBATION THEORY

FOR $g_0 > 0$, WHEN THE SECOND TERM IN 58 EQUALS THE FIRST, WE HAVE

(61) $1 = g_0 \ln \frac{D}{k_B T_K}$ ← KONDO SCALE

$$\Rightarrow \boxed{k_B T_K = D \exp\left(-\frac{1}{g_0}\right) = D \exp\left(-\frac{1}{N(0)J}\right)}$$

THIS IS A CHARACTERISTIC TEMPERATURE SCALE WHICH DETERMINES THE REGION OVER WHICH HIGH TEMPERATURE (WEAK COUPLING PERTURBATION THEORY HOLDS.

IT IS A GOOD CANDIDATE SCALE FOR T_F^* IN HEAVY FERMIONS -- IF SO, THE EXPONENTIAL SMALLNESS COMPARED WITH D CAN EXPLAIN THE SMALLNESS OF T_F^*! INDEED, NEXT LECTURE WE'LL PROVE THIS.

(4) RENORMALIZATION / SCALING

NOTICE THAT IF WE CHANGE THE BAND WIDTH FROM $D \to D'$, WE GET A SCALING RELATION TO THIS ORDER IN PERTURBATION THEORY -- SPECIFICALLY

$$g(D,T) = g_0\left[1 + g_0 \ln \frac{D}{T}\right] = g_0\left[1 + g_0 \ln \frac{D}{D'} + \ln \frac{D'}{T}\right)\Big]$$

$$\approx \underbrace{g_0\left[1 + g_0 \ln \frac{D'}{T}\right]}_{g(D',T)}\left[1 + g_0 \ln \frac{D}{D'}\right]$$

SO $g(D,T) - g(D',T) = \delta g = g_0^2 \ln\left(\frac{D'}{D}\right)$

FOR $\frac{D'}{D} \to 1$, $\ln \frac{D'}{D} = \delta \ln D$

$$\Rightarrow (62)\quad \frac{\partial g}{\partial \ln D} = g^2 + O(g^3) + \cdots$$

WHAT IS THE PHYSICAL MEANING OF RESCALING? WE DERIVE AN EFFECTIVE COUPLING AT ENERGY SCALES $|\xi| < D'$ (RUNNING COUPLING) WITH PROCESSES HAVING ENERGY $> D'$ TREATED VIRTUALLY IN THEIR RENORMALIZATION OF g. EQUIVALENTLY, WE LOOK AT LONGER LENGTH SCALES, SINCE

$$D = v_F \underbrace{k_F}_{1/\text{SMALLEST LENGTH}}, \quad D' = v_F \underbrace{k_F'}_{1/\text{SMALLEST LENGTH}}$$

(62) IS EASY TO SOLVE -- WE GET

$$\frac{1}{g(D)} = \frac{1}{g_0} + \ln \frac{D}{D_0}$$

$$\Rightarrow \quad g(D) = \frac{g_0}{1 + g_0 \ln \frac{D_0}{D}} = \frac{1}{\ln\left(\frac{D}{k_B T_K}\right)} \qquad (63)$$

$$k_B T_K = D_0 \exp(-1/g_0)$$

NOTE: (i) THIS CORRESPONDS TO A SUMMATION OF A SUBSET OF PERTURBATION PROCESSES TO ALL ORDERS -- SO CALLED "LEADING LOGS" GOING AS $\sim g_0^{n+1} \ln^n \frac{D}{k_B T}$

(ii) THIS DISPLAYS UNIVERSALITY: IF, FOR EXAMPLE PLUGGED INTO EQ (53) AND THEN $\rho(T)$, WE GET

$$\rho(T) \sim \underbrace{\rho_0}_{\text{AMPLITUDE}} f\left(\frac{T}{T_K}\right)$$

IDENTIFYING $k_B T_K$ WITH D_-

(iii) PERT. THEORY IS AGAIN BROKEN AT T_K.

(iv) THIS DISPLAYS ASYMPTOTIC FREEDOM:

$g(D) \rightarrow$ SMALL, $D \rightarrow D_0$

$\rightarrow$ BIG $D \rightarrow k_B T_K \ll D_0$

JUST AS IN NONABELIAN GAUGE THEORIES SUCH AS QCD!

[FOR $g_0 < 0$, IT IS LIKE QED WHERE PERT. THEORY BREAKS AT HIGH ENERGY SCALES]

LECTURE II

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[SEE ALSO THE BICKERS AND HEWSON REFERENCES OF LECTURE I]

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[A REVIEW ARTICLE IS IN PREPARATION BY D.L. COX AND A. ZAWADOWSKI -- UPON REQUEST, COPIES WILL BE SENT AT COMPLETION]
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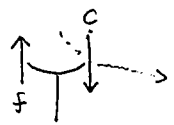
[SEE ALSO ABOVE ARTICLES BY COX & RUCKENSTEIN, KIM & COX)

KONDO II:
STRONG COUPLING KONDO THEORY

HEURISTIC OVERVIEW

PERTURBATIVE CALCULATIONS FAIL AT THE KONDO SCALE T_K. THE FIRST RELIABLE NONPERTURBATIVE CALCULATION TO GO WELL BELOW T_K WAS THE NUMERICAL RENORMALIZATION GROUP THEORY OF K.G. WILSON [REV. MOD. PHYS. 47, 773 (1975).] WE SHALL NOT GO INTO THIS WORK IN DETAIL HERE, BUT RATHER WILL SUMMARIZE THE KEY RESULTS. IN PERTURBATIVE RG THEORY, A "RUNNING COUPLING" $g(T, \omega, \ldots)$ WAS DEVELOPED THAT DIVERGES AT $T_K = T$ OR ω OR $\ldots$. IN THE NRG, THIS DIVERGENCE IS PUSHED TO $T=0$, THE PICTURE IS:

HIGH $T \sim T_F$
SMALL $L \sim k_F^{-1}$ (LENGTH SCALE)

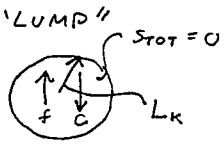


$g(T) \approx g_0 = N(0) J_0$

LOCAL MOMENT

$T \ll T_K$

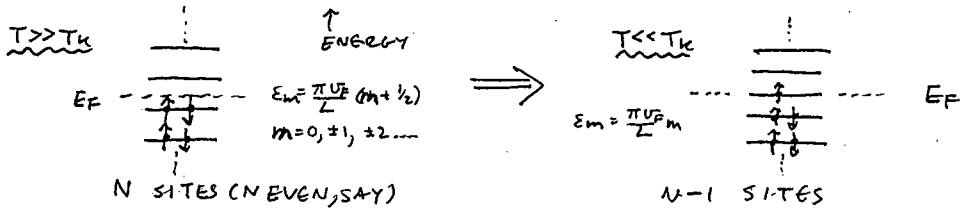
$L \gg L_K = \frac{\hbar v_F}{k_B T_K}$



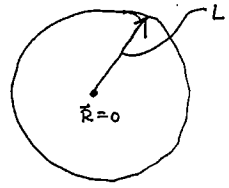
$g(T) \to \infty$

LOCAL MOMENT DISAPPEARS

ONE UNIT OF CONDUCTION SPIN IS BOUND OUT AS $g(T) \to \infty$, HENCE, IF AT HIGH T WE HAVE N-SITES, AT LOW T WE HAVE N-1 SITES, SO THE LEVEL SPECTRUM OF ELECTRONS SHIFTS:



THIS ENERGY SHIFT CAN BE READILY DESCRIBED BY A PHASE SHIFT.... TO UNDERSTAND, CONSIDER S-WAVE RADIAL QUANTIZATION



WALL BOUNDARY CONDITION:

$\psi_n(L) \approx A \frac{\sin k_n L}{k_n L} = 0 \Rightarrow k_n = (n + \frac{1}{2})\frac{\pi}{L}$ $n = 0, 1, \ldots$

$\Rightarrow \varepsilon_n = (m + \frac{1}{2})\frac{\pi}{L} v_F$ $m = 0, \pm 1, \ldots$

$= v_F(k_n - k_F)$

$(m = n - n_F)$

$g = 0$ -- IMPURITY AT ORIGIN

WITH $g \to \infty$ WE GET A 'LUMP' AT THE ORIGIN, AND ELECTRONS ARE SCATTERED, SO WE NEED A PHASE SHIFT:

$$\psi_n(L) \approx A \frac{\sin(k_n L + \delta(k_n))}{k_n L} \Rightarrow k_n = \frac{\pi}{L}\left(n + \frac{1}{2} + \frac{\delta(k_n)}{\pi}\right)$$

$$\Rightarrow \varepsilon_n = \frac{\pi v_F}{L}\left(m + \frac{1}{2} + \frac{\delta(\varepsilon_n)}{\pi}\right)$$

STRO COUPLI

TO SHIFT THE SPECTRUM BY ½ UNIT AS IN THE PREVIOUS FIGURE REQUIRES

$$\delta(\varepsilon_n) \to \frac{\pi}{2} \quad \text{FOR } \varepsilon_n \to 0.$$

THAT IS, THE FACT $g(T \to 0) \to \infty$ IMPLIES THE DEVELOPMENT OF RESONANT SCATTERING OFF OF THE SINGLET "LUMP"! THIS IMPLIES THE RESISTIVITY PER IMPURITY IS AT THE UNITARITY LIMIT AND SO $\propto \ln$!!

SLAVE BOSON MEAN FIELD THEORY

A SIMPLE WAY TO ACCESS THE STRONG COUPLING "FIXED POINT" IS WITH A NOVEL KIND OF MEAN FIELD THEORY, BEST DESCRIBED BY READ + NEWNS. IN 1983,

SINCE THE ($U_{ff} \to \infty$) ANDERSON + KONDO MODELS HAVE EQUIVALENT LOW ENERGY PHYSICS WHEN $g_0 = \Gamma/\pi|\varepsilon_f| \ll 1$, WE SHALL WORK WITH THE (MORE FUNDAMENTAL) ANDERSON MODEL; WE SHALL ALLOW THE DEGENERACY N TO BE ARBITRARY: ($m \in \{-\frac{(N-1)}{2}, \ldots, +\frac{(N-1)}{2}\}$)

(1) $H = \sum_{km} \varepsilon_k n_{km} + \varepsilon_f \sum_m |f^1 m\rangle\langle f^1 m| + \frac{V}{\sqrt{N_s}} \sum_{km} (|f^1 m\rangle\langle f^0| c_{km} + h.c.)$

THIS HAMILTONIAN CONTAINS PROJECTION OR "HUBBARD" OPERATORS WHICH ARE "UGLY" TO WORK WITH BECAUSE THEY OBEY NONCANONICAL COMMUTATION RELATIONS.

EG: $f^+_m \xrightarrow[U_{ff}\to\infty]{} |f^1 m\rangle\langle f^0|$

AND: $|f^1 m\rangle\langle f^0|\, |f^0\rangle\langle f^1 m'| + |f^0\rangle\langle f^1 m'|\, |f^1 m\rangle\langle f^0|$

$= \delta_{mm'} |f^0\rangle\langle f^0| + |f^1 m\rangle\langle f^1 m'|$

FOR THE PURPOSES OF ORGANIZING PERTURBATION THEORY, SEE BARNES [J PHYS F6, 1375 (1976)] AND LATER P. COLEMAN [PHYS. REV. B29, 3035 (1984)] INTRODUCED "SLAVE BOSON" AND "SLAVE FERMION" OPERATORS TO AVOID THIS NASTINESS. INTUITIVELY, THINK OF THE EMPTY STATE AS BEING A BOSON AND THE SINGLY OCCUPIED STATE A FERMION -- THEN

(2)
$\|f^1 m\rangle\langle f^1 m'\| \longrightarrow$	$\tilde{f}^+_m \tilde{f}_{m'}$	$\{\tilde{f}_m, \tilde{f}^+_{m'}\} = \delta_{mm'}$
$\|f^1 m\rangle\langle f^0\| \longrightarrow$	$\tilde{f}^+_m b$	$[b, b^+] = 1$
$\|f^0\rangle\langle f^0\| \longrightarrow$	$b^+ b$	

TRY THIS WITH

(3) $\{|f^1 m\rangle\langle f^0|, |f^0\rangle\langle f^1 m'|\} = \{\tilde{f}^+_m b, b^+ \tilde{f}_{m'}\}$

$= \tilde{f}^+_m b b^+ \tilde{f}_{m'} + b^+ \tilde{f}_{m'} \tilde{f}^+_m b$

$= \tilde{f}^+_m \tilde{f}_{m'} + \delta_{mm'} b^+ b + b^+ b (\tilde{f}^+_m \tilde{f}_{m'} - \tilde{f}^+_{m'} \tilde{f}_m)$

$= \tilde{f}^+_m \tilde{f}_{m'} + \delta_{mm'} b^+ b = |f^1 m\rangle\langle f^1 m'| + |f^0\rangle\langle f^0|$ ✓

BUT THIS IS INCOMPLETE -- THE LOCAL HILBERT SPACE IS RESTRICTED SO THAT

(4) $1 = \sum_m |f^1 m\rangle\langle f^1 m| + |f^0\rangle\langle f^0| = \sum_m \tilde{f}^+_m \tilde{f}_m + b^+ b = Q_f$

IF WE PUT

(5) $H_{SLAVE} = \sum_{km} \varepsilon_k n_{km} + \varepsilon_f \sum_m \tilde{f}^+_m \tilde{f}_m + \frac{V}{\sqrt{N_s}} \sum_{km} (\tilde{f}^+_m b c_{km} + h.c.)$

THEN IT IS EASY TO CHECK THAT

(6) $[H_{SLAVE}, Q_f] = 0$

WHICH SAYS IF WE START WITH $Q_f = 1$ (IE, SINGLY OCCUPIED ($|f^0\rangle$ OR $|f^1 m\rangle$) WE'LL STAY THERE. HENCE, WE NEED TO ADD A FICTITIOUS CHEMICAL POTENTIAL OR LAGRANGE MULTIPLIER λ TO CONSTRAIN $Q_f = 1$:

(7) $\tilde{H}_{SLAVE} = \sum_{km} \varepsilon_k n_{km} + \varepsilon_f \sum_m \tilde{f}^+_m \tilde{f}_m + \frac{V}{\sqrt{N_s}} \sum_{km} (\tilde{f}^+_m b c_{km} + h.c.) - \lambda \left(\sum_m \tilde{f}^+_m \tilde{f}_m + b^+ b - 1 \right)$

WE ARE NOW IN A POSITION TO DO MEAN FIELD THEORY.

[[THESE OPERATORS ALSO ALLOW FEYNMAN-DYSON PERTURBATION THEORY IN V -- TECHNICALLY, THE SUCCESS OF FEYNMAN-DYSON THEORY RESTS UPON THE ABILITY TO PERTURB AROUND A BARE HAMILTONIAN WHICH IS QUADRATIC IN FERMI/BOSE FIELDS SO THAT WICK'S THEOREM HOLDS. THIS WORKS HERE -- AFTER EACH DIAGRAM EVALUATION ONE TAKES $\lambda \to -\infty$ TO PROJECT TO $Q_f = 1$]]

MEAN FIELD THEORY

OUR TREATMENT HERE IS QUITE ANALOGOUS TO THE BOGULUBOV THEORY OF SUPERFLUIDS AND SUPERCONDUCTORS AND THE MEAN FIELD THEORY OF CHARGE DENSITY WAVE SOLIDS BASED UPON THE SU-SCHRIEFFER-HEEGER MODEL. THE STRATEGY IS TO DERIVE AN EFFECTIVE ONE MODEL WITH PARAMETERS TO BE DETERMINED SELF CONSISTENTLY.

HEREWE REPLACE b, b^+ BY AVERAGE VALUES:

(8) a) $b \to \langle b\rangle + (b - \langle b\rangle) = \underbrace{b_0}_{\text{C-NUMBER}} + \underbrace{\delta b}_{\text{OPERATOR}}$

b) $b^+ \to \langle b^+\rangle + (b^+ - \langle b^+\rangle) = b_0 + \delta b^+$

c) $\lambda \to \langle\lambda\rangle + (\lambda - \langle\lambda\rangle) = \lambda_0 + \delta\lambda$

[WHILE λ IS A C-NUMBER, STRICTLY SPEAKING WE MUST INTEGRATE OVER A DISTRIBUTION OF λ TO COMPUTE PROPERTIES -- FOR EXAMPLE, IN EQ (7) THE HAMILTONIAN $\tilde{H}_{SLAVE}$ IS APPROPRIATE TO THE GRAND ENSEMBLE OF Q_f -- THE PHYSICAL PARTITION FUNCTION IS

(9) $$Z(Q_f = 1) = \int_{\bar\lambda - i\pi/\beta}^{\bar\lambda + i\pi/\beta} \frac{d\lambda}{2\pi}\, e^{-\beta\lambda}\, Z_{GRAND}(\lambda, \tilde{H}_{MF})$$

8(c) CORRESPONDS TO A STEEPEST DESCENTS EVALUATION OF (9)]]

WITH THE SUBSTITUTION OF 8(a,b,c) INTO (7), WE OBTAIN THE MEAN FIELD HAMILTONIAN

(10) $$\tilde{H}_{MF} = \sum_{km} \varepsilon_k n_{km} + \tilde{\varepsilon}_f \sum_m \tilde{f}_m^+ \tilde{f}_m + \frac{\tilde{V}}{\sqrt{N_s}} \sum_{km} \left(\tilde{f}_m^+ C_{km} + h.c.\right) - \lambda(b_0^2 - 1)$$

WITH (11) $\tilde{\varepsilon}_f = \varepsilon_f - \lambda_0$

$\tilde{V} = V\langle b\rangle$

AND WITH TERMS OF ORDER $\delta\langle b\rangle$, $\delta\lambda$ IGNORED.

(10) HAS THE FORM OF A "RESONANT LEVEL MODEL" IN WHICH CONDUCTION ELECTRONS HOP INTO A LOCAL NONINTERACTING LEVEL. SINCE IT IS A QUADRATIC OR ONE BODY HAMILTONIAN, IT CAN BE SOLVED EXACTLY. THIS CAN BE DONE WITH SCATTERING STATES, THOUGH IT IS FAIRLY MESSY. WE'LL USE GREEN'S FUNCTIONS HERE. DEFINE THE RETARDED OR CAUSAL GREEN'S FUNCTIONS

a) $G_{ff} = -i\theta(t) \left\langle \{\tilde{f}_m(t), \tilde{f}_m^+(0)\}\right\rangle$

(12) b) $G_{kk'} = -i\theta(t) \left\langle \{C_{km}(t), C_{k'm}^+(0)\}\right\rangle$

c) $G_{kf} = -i\theta(t) \left\langle \{C_{km}(t), \tilde{f}_m^+(0)\}\right\rangle$

d) $G_{fk} = -i\theta(t) \left\langle \{\tilde{f}_m(t), C_{km}^+(0)\}\right\rangle$

OUR MAIN GOAL IS TO CALCULATE THE EXTRA DENSITY OF STATES INDUCED BY THE LOCAL LEVEL. THIS WILL BE GIVEN BY THE IMAGINARY PART OF G_{ff} -- THE PROOF IS SKETCHED IN THE BOX BELOW:

$$G_{ff} = -i\theta(t) \left\langle \{\tilde{f}_m(t), \tilde{f}_m^+(0)\}\right\rangle$$

$$= -i\theta(t) \sum_M \frac{e^{-\beta E_M}}{Z_{MF}} \langle M|\{\tilde{f}_m(t), \tilde{f}_m^+(0)\}|M\rangle \qquad \tilde{H}_{MF}|M\rangle = E_M|M\rangle$$

$$= -i\theta(t) \sum_{M,N} \frac{e^{-\beta E_M}}{Z_{MF}} |\langle M|\tilde{f}_m|N\rangle|^2 \left[e^{i(E_M - E_N)t} + e^{i(E_N - E_M)t}\right]$$

SO $$G_{ff}(\omega) = \int dt\, e^{-i\omega t}\, G_{ff}(t)$$

$$= \sum_{M,N} \frac{1}{Z_{MF}} |\langle M|\tilde{f}_m|N\rangle|^2 \left\{\frac{e^{-\beta E_M}}{\omega + E_N - E_M + i\eta} + \frac{e^{-\beta E_N}}{\omega + E_N - E_M + i\eta}\right\}$$

$$= \sum_{M,N} \frac{(e^{-\beta E_M} + e^{-\beta E_N})}{Z} |\langle M|\tilde{f}_m|N\rangle|^2 \frac{1}{\omega + E_N - E_M + i\eta}$$

AND

$$-\frac{1}{\pi} \mathrm{Im}\, G_{ff}(\omega) = \sum_{M,N} \left\{ \frac{e^{-\beta E_M}}{Z} |\langle N|\tilde{f}_m^+|M\rangle|^2 \delta(\omega + E_N - E_M) \right\} \text{ADDITION DOS}$$

$$+ \frac{e^{-\beta E_N}}{Z} |\langle M|f_m|N\rangle|^2 \delta(\omega + E_N - E_M) \Big\} \text{REMOVAL DOS}$$

$$= \Delta N_f(\omega) \quad \text{EXTRA DOS FOR ADDING/REMOVING } \tilde{f} \text{ "ELECTRONS"}$$

TO SOLVE, WE USE EQUATIONS OF MOTION -- EG

(13) a) $i\dot{G}_{ff} = \delta(t) \langle \{\tilde{f}_m, \tilde{f}_m^+\} \rangle + i\theta(t) \langle \{[H_{MF}, f_m](t), f_m^+\} \rangle$

$= \delta(t) + \tilde{\varepsilon}_f G_{ff} + \frac{\tilde{V}}{\sqrt{N_s}} \sum_k G_{kf}$

b) $i\dot{G}_{kf} = \varepsilon_k G_{kf} + \frac{\tilde{V}}{\sqrt{N_s}} G_{ff}$

c) $i\dot{G}_{kk'} = \delta(t)\delta_{kk'} + \varepsilon_k G_{kk'} + \frac{\tilde{V}}{\sqrt{N_s}} G_{fk'}$

d) $i\dot{G}_{fk'} = \tilde{\varepsilon}_f G_{fk'} + \frac{\tilde{V}}{\sqrt{N_s}} \sum_{k''} G_{k''k'}$

BY FOURIER TRANSFORMING, ONE MAY EASILY SOLVE THESE EQUATIONS -- IN PARTICULAR

(14) a) $(\omega - \tilde{\varepsilon}_f) G_{ff} = 1 + \frac{\tilde{V}}{\sqrt{N_s}} \sum_k G_{kf}$

b) $(\omega - \varepsilon_k) G_{kf} = \frac{\tilde{V}}{\sqrt{N_s}} G_{ff}$

c) $(\omega - \varepsilon_k) G_{kk'} = + \frac{\tilde{V}}{\sqrt{N_s}} G_{fk}$

d) $(\omega - \tilde{\varepsilon}_f) G_{fk'} = \frac{\tilde{V}}{\sqrt{N_s}} \sum_{k''} G_{k''k'}$

SO:

(15) a) $\therefore G_{ff}(\omega) = \left[\omega - \tilde{\varepsilon}_f - \frac{\tilde{V}^2}{N_s} \sum_k \frac{1}{\omega - \varepsilon_k + i\eta} \right]^{-1}$

$\approx \frac{1}{\omega - \tilde{\varepsilon}_f + i\tilde{\Gamma}}$ $\quad (\tilde{\Gamma} = \pi N(0) \tilde{V}^2)$

b) $G_{kk'}(\omega) = \frac{\delta_{kk'}}{\omega - \varepsilon_k + i\eta} + \frac{\tilde{V}^2}{N_s} \frac{1}{\omega - \varepsilon_k + i\eta} \left(\sum_{k''} \frac{G_{k''k'}}{\omega - \tilde{\varepsilon}_f + i\eta} \right)$

$\Rightarrow G_{kk'}(\omega) \approx \underbrace{\frac{\delta_{kk'}}{\omega - \varepsilon_k + i\eta}}_{G_k^0} + \frac{1}{N_s} \underbrace{\frac{1}{\omega - \varepsilon_k + i\eta}}_{G_k^0} \underbrace{\frac{\tilde{V}^2}{\omega - \tilde{\varepsilon}_f + i\tilde{\Gamma}}}_{\tilde{V}^2 G_{ff}} \underbrace{\frac{1}{\omega - \varepsilon_{k'} + i\eta}}_{G_{k'}^0}$

FROM (15), WE INFER TWO IMPORTANT THINGS:

(16) $\Delta N_f(\omega) = -\frac{1}{\pi} \mathrm{Im}\, G_{ff}(\omega) = -\frac{1}{\pi} \mathrm{Im} \frac{1}{\omega - \tilde{\varepsilon}_f + i\tilde{\Gamma}} = \underbrace{\frac{1}{\pi} \frac{\tilde{\Gamma}}{(\omega - \tilde{\varepsilon}_f)^2 + \tilde{\Gamma}^2}}_{\text{LORENTZIAN D}}$

(17) $\underbrace{t_1(\omega)}_{\substack{\text{ONE PARTICLE} \\ \text{CONDUCTION} \\ t\text{-MATRIX}}} = \frac{\tilde{V}^2}{\omega - \tilde{\varepsilon}_f + i\tilde{\Gamma}} = \frac{e^{-i\delta(\omega)} \sin\delta(\omega)}{\pi N(0)}$

(18) $\delta(\omega) = \tan^{-1} \frac{\tilde{\Gamma}}{\omega - \tilde{\varepsilon}_f} = \frac{\pi}{2} + \tan^{-1} \frac{\tilde{\varepsilon}_f - \omega}{\tilde{\Gamma}}$

$=$ PHASE SHIFT.

~~HOW TO PROCEED~~

HENCE, THE LOCAL FERMIONS INDUCE RESONANT SCATTERING AT INCIDENT ELECTRON ENERGY $\omega (= \varepsilon_k) = \tilde{\varepsilon}_f$. THE SCATTERING RATE, BY THE OPTICAL THEOREM, IS, PER IMPURITY

(18) $\Delta\left(\frac{1}{\tau(\varepsilon_k)}\right)_z - 2\,\mathrm{Im}\, t_1(\omega = \varepsilon_k) = \frac{2}{\pi N(0)} \sin^2\delta(\omega)$

$= \frac{2}{\pi N(0)} \frac{\tilde{\Gamma}^2}{(\omega - \tilde{\varepsilon}_f)^2 + \tilde{\Gamma}^2}$ BREIT-WIGNER FORM!

NOW, LET'S GET THE THERMODYNAMICS. SINCE THE MEAN FIELD SYSTEM IS FERMIONIC, THE EXTRA FREE ENERGY PER IMPURITY IS

$$(19)\quad \Delta F_{MF} = -k_B T N \int_{-D}^{D} d\omega \frac{\tilde{\Gamma}}{\pi[(\omega-\tilde{\varepsilon}_f)^2+\tilde{\Gamma}^2]} \ln(1+e^{-\beta\omega}) + \lambda_0(1-b_0^2)$$

WE DEMAND A MINIMUM OF ΔF_{MF} WITH RESPECT TO OUR MEAN FIELD PARAMETERS:

$$(20)\quad \frac{\delta \Delta F_{MF}}{\delta b_0} = 0 = \frac{\delta \Delta F_{MF}}{\delta \lambda_0}$$

SO $(21)\quad \frac{\delta \Delta F_{MF}}{\delta b_0} = 0 \Rightarrow 2\lambda_0 b_0 = \frac{2\Gamma N b_0}{\pi} \int_{-D}^{D} d\omega \frac{\omega-\tilde{\varepsilon}_f}{(\omega-\tilde{\varepsilon}_f)^2+\tilde{\Gamma}^2} f(\omega)$

$$\Rightarrow \lambda_0 \underset{T=0}{\approx} \frac{N\Gamma}{\pi} \ln \frac{\sqrt{\tilde{\varepsilon}_f^2+\tilde{\Gamma}^2}}{D}$$

$$\Rightarrow \sqrt{\tilde{\varepsilon}_f^2+\tilde{\Gamma}^2} = D\exp\left(\frac{\pi\lambda_0}{N\Gamma}\right) \approx D\exp\left(-\frac{\pi|\varepsilon_f|}{N\Gamma}\right) = k_B T_K \quad \{\!\{ \text{KONDO SCALE}$$

THAT IS -- THE RESONANCE SCALE IS SET BY T_K!!

NEXT: $(22)\quad \frac{\delta \Delta F_{MF}}{\delta \lambda_0} = 0 \Rightarrow 1-b_0^2 = \underbrace{\frac{N}{\pi} \int d\omega \frac{\tilde{\Gamma}}{(\omega-\tilde{\varepsilon}_f)^2+\tilde{\Gamma}^2} f(\omega)}_{n_f = f \text{ OCCUPANCY!}}$

$$\Rightarrow 1 = b_0^2 + n_f$$

INTEGRATING AT $T=0$ WE SEE

$$(23)\quad \frac{N}{\pi}\tan^{-1}\frac{\tilde{\Gamma}}{(\tilde{\varepsilon}_f)} = \frac{N\delta(0)}{\pi} = 1-b_0^2 = n_f$$

$$\Rightarrow \boxed{\frac{N\delta(0)}{\pi} = n_f}$$

FRIEDEL SUM RULE: VALENCE IS RELATED TO PHASE SHIFT!

[PHYSICAL INTERPRETATION: WITH PHASE SHIFT

$$\tilde{\varepsilon}_m = (m+\tfrac{1}{2})\frac{\pi v_F}{R} - \frac{\delta(\tilde{\varepsilon}_m)v_F}{R} = \frac{(m+1/2)}{\Delta\varepsilon} - \frac{\delta(\tilde{\varepsilon}_m)}{\pi\Delta\varepsilon}$$

$$\Delta N(\varepsilon) = \frac{1}{N_s}\left(\frac{1}{\Delta\tilde{\varepsilon}} - \frac{1}{\Delta\varepsilon}\right) = \frac{1}{N_s\Delta\varepsilon}\left[\frac{d\varepsilon}{d\tilde{\varepsilon}} - 1\right]$$

$$\approx \frac{1}{\pi}\frac{d\delta}{d\varepsilon}$$

SO $N\int_{-\omega}^{0} d\varepsilon \frac{1}{\pi}\frac{d\delta}{d\varepsilon} = \underbrace{\Delta n}_{\text{\# OF ELECTRONS ADDED}} = \frac{N\delta(0)}{\pi}$ (TAKING $\delta(-\omega)=0$)

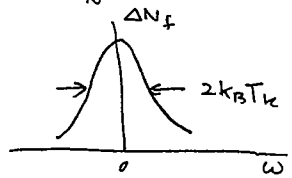
HERE $\frac{1}{\pi}\frac{d\delta}{d\varepsilon} = \frac{\tilde{\Gamma}}{(\varepsilon-\tilde{\varepsilon}_f)^2+\tilde{\Gamma}^2}$]

IF WE NOW SOLVE FURTHER; FOR $b_0^2 << 1$, $n_f \approx 1$

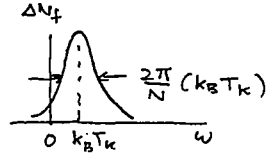
$$\delta(0) \approx \frac{\pi}{N} \Rightarrow \tilde{\Gamma} \approx \tilde{\varepsilon}_f \tan\frac{\pi}{N}$$

$$k_B T_K \approx \tilde{\varepsilon}_f \sec\frac{\pi}{N} \approx \tilde{\Gamma}\csc\frac{\pi}{N}$$

<u>N=2</u>: $\tilde{\varepsilon}_f \approx 0$, $\tilde{\Gamma} \approx k_B T_K$



<u>N>>1</u>: $\tilde{\varepsilon}_f \approx k_B T_K$ $\tilde{\Gamma} \approx \frac{\pi(k_B T_K)}{N}$



THE WIDTH SHRINKS TO ZERO AS $N \to \infty$!

PHYSICAL PROPERTIES

THERMODYNAMICS: FROM THE EXTRA DOS ΔN_f, WE MAY READILY COMPUTE

$$(24)\quad \frac{\Delta C}{T} \underset{T\to 0}{\approx} \frac{N\pi^2}{3} k_B^2 \Delta N_f(0) = \frac{\pi^2}{3} k_B^2 \frac{N\tilde{\Gamma}}{\pi(\tilde{\varepsilon}_f^2 + \tilde{\Gamma}^2)}$$

$$\approx \frac{\pi^2}{3} k_B^2 \frac{2}{\pi k_B T_K} \qquad N = 2$$

$$\approx \frac{\pi^2}{3} k_B^2 \frac{1}{k_B T_K} \qquad N \gg 1$$

SO THE KONDO SCALE, WHICH APPEARS AS A CROSSOVER SCALE FROM HIGH T, SERVES AS AN EFFECTIVE FERMI TEMPERATURE HERE!

THE SUSCEPTIBILITY IS

$$(24)\quad \Delta\chi \underset{T\to 0}{\approx} \frac{NS(S+1)}{3} \mu^2 \Delta N_f(0)$$

IMPLYING THAT THE LANDAU-WILSON RATIO AT MEAN FIELD LEVEL IS

$$(25)\quad \frac{3}{\mu^2 S(S+1)} \frac{\pi^2 k_B^2}{3} \frac{\Delta\chi}{\Delta\gamma} = 1.$$

TRANSPORT

A BOLTZMANN EQUATION SOLUTION FOR TRANSPORT RELATES RELEVANT TRANSPORT COEFFICIENTS TO "FERMI SURFACE" AVERAGES OF THE TRANSPORT LIFETIME -- SUCH AS

$$(26)\quad \ll \varepsilon^n \tau_{+\nu}(\varepsilon) \gg \equiv \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) \varepsilon^n \tau_{+\nu}(\varepsilon)$$

(SEE, EG, CH. 16 OF ASHCROFT + MERMIN)

FOR SCATTERING DOMINANT IN ONE ANGULAR MOMENTUM CHANNEL, $\tau_{+\nu} = \tau$, AND HERE (PER SPIN)

$$(27)\quad \frac{1}{\tau(\varepsilon)} = \frac{2c(N/2)}{\pi N(0)} \sin^2\delta(\varepsilon) = \frac{2c}{\pi N(0)} \left(\frac{N}{2}\right) \frac{\tilde{\Gamma}^2}{(\varepsilon - \tilde{\varepsilon}_f)^2 + \tilde{\Gamma}^2}$$

ACCORDINGLY, WE MAY COMPUTE:

(A) RESISTIVITY: IN BOLTZMANN THEORY

$$\rho(T) = \frac{m}{n e^2 \ll \tau \gg}$$

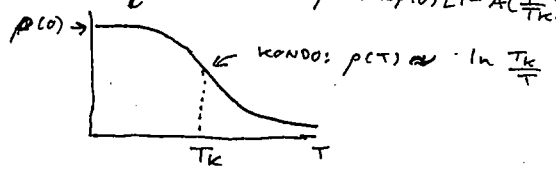
$$\ll \tau(\varepsilon) \gg = \frac{\pi N(0)}{2c\tilde{\Gamma}^2} \frac{2}{N} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) ((\varepsilon - \tilde{\varepsilon}_f)^2 + \tilde{\Gamma}^2)$$

$$= \frac{\pi N(0)}{2c\tilde{\Gamma}^2} \frac{2}{N} \left[\tilde{\Gamma}^2 + \tilde{\varepsilon}_f^2 + \frac{\pi^2}{3}(k_B T)^2\right]$$

$$= \frac{\pi N(0)}{Nc} \frac{\left[(k_B T_K)^2 + \frac{\pi^2}{3}(k_B T)^2\right]}{\tilde{\Gamma}^2}$$

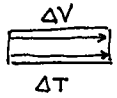
$$\Rightarrow \rho(T) \underset{T\to 0}{\approx} \frac{m}{ne^2} \frac{Nc}{\pi N(0)} \frac{(\tilde{\Gamma}/k_B T_K)^2}{1 + \frac{\pi^2}{3}\left(\frac{T}{T_K}\right)^2} \qquad (28)$$

MEAN FIELD: $\rho(T) \approx \rho(0)\left[1 - A\left(\frac{T}{T_K}\right)^2\right]$



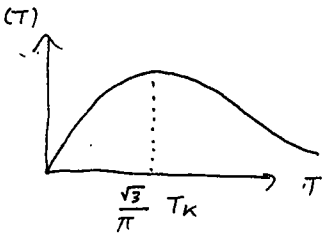
$\rho(0)$ = UNITARITY LIMIT PER IMPURITY WHEN $N = 2$!

(B) THERMOPOWER THE THERMOPOWER MEASURES THE PARTICLE-HOLE ASYMMETRY.



$S = \frac{\Delta V}{\Delta T} = \frac{\text{INDUCED VOLTAGE}}{\text{APPLIED TEMPERATURE DIFFERENCE}}$ AT ZERO ELECTRICAL CURRENT FLOW.

PHYSICALLY, ΔT COUPLES TO BOTH ELECTRONS AND HOLES -- IF HOLES MOVE TO THE RIGHT MORE QUICKLY THAN ELECTRONS TO THE LEFT A VOLTAGE DIFFERENCE WILL BE SET -- THE SIGN FLIPS IF WE REVERSE THE DIFFUSION SPEED OF $e^- + h^+$.



IN BOLTZMANN THEORY

(29) $$S(T) = \frac{-1}{eT} \frac{\langle\langle \varepsilon\, \tau(\varepsilon) \rangle\rangle}{\langle\langle \tau(\varepsilon) \rangle\rangle}$$

FOR OUR RESONANCE,

(30) $$S(T) = \frac{2\pi^2}{3}\left(\frac{k_B}{e}\right) \frac{\tilde{\varepsilon}_f (k_B T)}{\tilde{\varepsilon}_f^2 + \tilde{\Gamma}^2 + \frac{\pi^2}{3}(k_B T)^2}$$ } INDEPENDENT OF c!

THE SCALE OF S IS SET BY ITS MAX VALUE, WHICH OCCURS AT

(31) $$T_{max} = \frac{\sqrt{3}}{\pi} T_K \sim \tfrac{1}{2} T_K$$

THE MAX VALUE IS

(32) $$\frac{2\pi}{\sqrt{3}} \frac{\tilde{\varepsilon}_f}{2k_B T_K} \frac{k_B}{e} \approx \left(\cos\tfrac{\pi}{N}\right) \frac{\pi}{\sqrt{3}} \left(\frac{k_B}{e}\right) = 156 \frac{\mu V}{K} \times \cos\frac{\pi}{N}$$

THIS IS BIG! FOR TYPICAL METALS $|S| \lesssim 1\,\mu V/K$.

NOTES ON S(T):

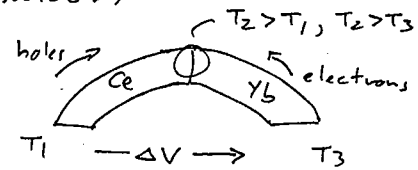
(1) IF $N = 2$, $S(T) \approx 0$ ... ONLY TO THE EXTENT $n_f \neq 1$ DOES S_{MAX} ACQUIRE A NONZERO VALUE

$$\sim \frac{\pi}{2}(1 - n_f) \frac{\pi}{\sqrt{3}} \left(\frac{k_B}{e}\right)$$

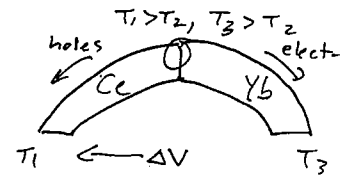
(2) FOR Ce^{3+}: $\tilde{\varepsilon}_f > 0 \Rightarrow S(T) > 0$. THE RESONANCE LIVES "ABOVE" E_F SO PARTICLES ARE SCATTERED MORE STRONGLY THAN HOLES.

(3) FOR Yb^{3+}: WE HAVE IF HOLE ($4f^{13}$) SO $\tilde{\varepsilon}_f < 0$ AND $S(T) < 0$ (HOLES SCATTERED MORE STRONGLY THAN PARTICLES).

(4) "PUDGY FERMIONS" MAY FIND USE IN THERMOELECTRIC HEATERS/COOLERS! (LATTER IS BEING APPLIED IN CAMPER/TRAILERS & US NAVY VESSELS - LESS NOISE!)



JUNCTION HEATED



JUNCTION COOLED

NEED LARGE $S(T) > 0$ FOR CE
LARGE $S(T) < 0$ FOR YB
OVER BROAD T RANGE, LARGE T_K, LARGE N
DOES THIS! [EG, $CePd_3$, $T_K \sim 700K$, $N \sim 6$
$YbAl_3$, $T_K \sim 400K$, $N \sim 8$]

FIGURE OF MERIT IS BEGINNING TO APPROACH SEMICONDUCTOR BASED DEVICES.

ELECTRON ADDITION / REMOVAL SPECTRUM

PHYSICAL ELECTRON:

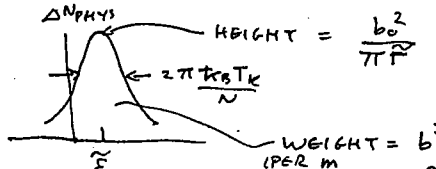
$$f_m^+ \xrightarrow[U_{ff}\to\infty]{} \tilde{f}_m^+ b$$

$$f_m \longrightarrow \tilde{f}_m b^+$$

SO TO ADD A PHYSICAL f-ELECTRON IS DIFFERENT THAN ADDING ONE "QUASIPARTICLE":

(33) $\Delta N_{PHYS} \approx b_0^2 \, \Delta N_f$

$N \gg 1$

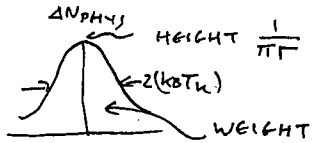


HEIGHT $= \frac{b_0^2}{\pi \tilde{\Gamma}} = \frac{1}{\pi \Gamma} \frac{\tilde{\Gamma}}{\Gamma} = \frac{1}{\pi \Gamma}$

INDEPENDENT OF $U_{ff}, |\tilde{\varepsilon}_f|$ -- GENERAL RESULT.

WEIGHT $= b_0^2$ (PER m VALUE) $= \frac{\tilde{\Gamma}}{\Gamma} \underset{N\gg 1}{\approx} \frac{\pi (k_B T_K)}{N \Gamma}$

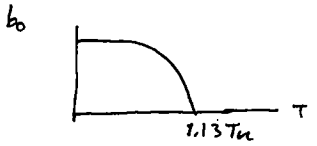
FOR $N = 2$



HEIGHT $\frac{1}{\pi \Gamma}$

WEIGHT $\left(\frac{k_B T_K}{\Gamma}\right)$ (PER SPIN)

WHAT WE HAVE NOT DISCUSSED IS THAT $b_0(T) \to 0$ AT $T \approx T_K$ ... HENCE WE EXPECT THE WEIGHT IN THE KONDO RESONANCE TO CONTINUOUSLY DIMINISH WITH T, GETTING VANISHINGLY SMALL AS $T \gg T_K$ (THE PHASE TRANSITION IS SMEARED BY FLUCTUATIONS.)



FOR YB COMPOUNDS THIS "ABRIKOSOV-SUHL-KONDO" RESONANCE APPEARS ON THE PES SIDE WHERE RESOLUTION IS GOOD -- DESPITE ONGOING CONTROVERSY ** ABOUT EXPERIMENTAL ISSUES, THIS APPEARS TO HAVE BEEN SEEN IN $YbAl_3$ AS THE FIGURES BELOW SHOW:*

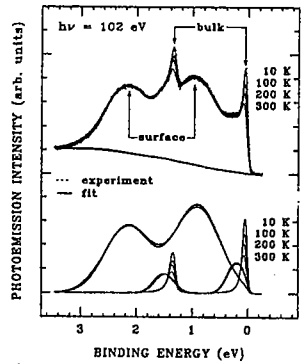
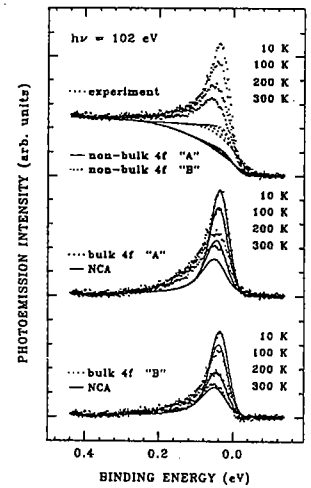


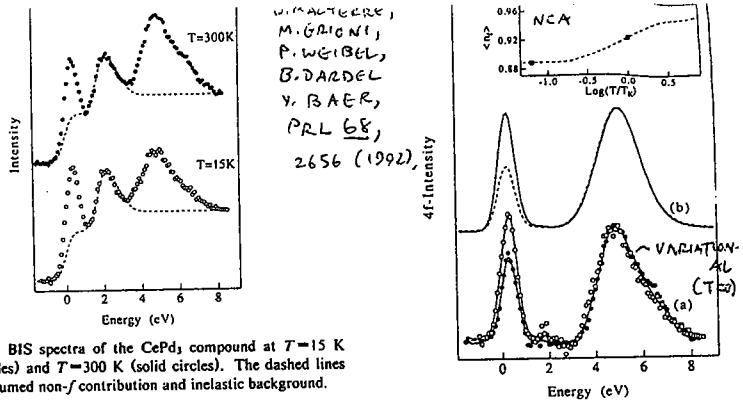
FIG. 1. Temperature dependent valence band PES spectra of $YbAl_3$. Dots are data points, and solid lines are fits as explained in the text.



FOR CE, THE RESONANCE IS ON THE IPS OR BIS SIDE, WHERE RESOLUTION IS NO BETTER THAN ~0.5 eV. STILL, SPECTRAL WEIGHT MUST BE CONSERVED -- THE NEUCHATEL GROUP HAS OBSERVED A T DEPENDENT TRANSFER FROM NEAR E_F TO THE $f^1 \to f^2$ PEAK WHICH IS FULLY CONSITENT WITH THE KONDO RESONANCE PICTURE ... SEE THE PICTURE WHICH APPEARS ON THE NEXT PAGE.

** SEE: J.J. JOYCE ET AL, PRL 68, 236 (1992);
F. PATTHEY ET AL, PRL 70, 1179 (1993);
J.W. ALLEN & O. GUNNARSSON, PRL 70, 1180 (1993);
J.J. JOYCE & A.J. ARKO, PRL 70, 1181 (1995).

* SEE L.H. TJENG ET AL, PRL 71 1419 (1993)
C. DALLGRA ET AL, PRL 88 196403 (2002).



O. GUNNARSSON, M. GRIONI, P. WEIBEL, B. DARDEL, Y. BAER, PRL 68, 2656 (1992),

FIG. 1. BIS spectra of the $CePd_3$ compound at $T=15$ K (open circles) and $T=300$ K (solid circles). The dashed lines are the assumed non-f contribution and inelastic background.

L NOTE ON SUM RULES: (IN A SLIGHTLY OVERSIMPLIFIED NEW!)

THE TOTAL # OF ELECTRONS THAT CAN BE HELD IN AN f-BAND ARE $14 = 2(2l+1)$, $l=3$. HENCE

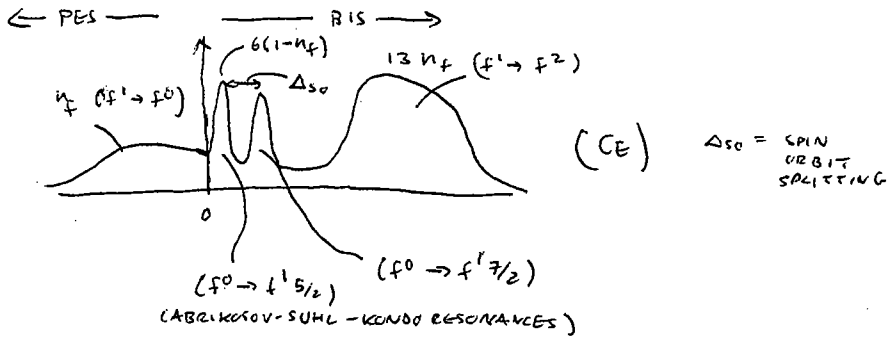
$$(34)\quad \int \frac{d\omega}{\pi}\, \underbrace{\Delta N^{TOT}_{PHYS}(\omega)}_{\text{INCLUDES DEGENERACY}} = 14$$

BELOW THE FERMI LEVEL WE MUST COUNT THE NUMBER OF f-ELECTRONS -- FOR CE

$$(35)\quad \int \frac{d\omega}{\pi}\, \Delta N^{TOT}_{PHYS}(\omega)\, f(\omega) = n_f \qquad (CE)$$

WHILE ABOVE E_F

$$(36)\quad \int \frac{d\omega}{\pi}\, \Delta N^{TOT}_{PHYS}(\omega)\,(1-f(\omega)) = 14 - n_f = \underbrace{14(1-n_f)}_{\text{KONDO}} + \underbrace{13 n_f}_{f^1\to f^2} \quad (CE)$$



(CE) Δ_{so} = SPIN ORBIT SPLITTING

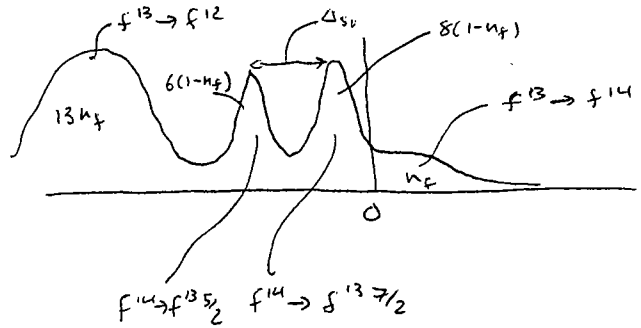
(ABRIKOSOV-SUHL-KONDO RESONANCES)

FOR YB, n_f SHOULD COUNT HOLES .... SO

$$(37)\quad \int \frac{d\omega}{\pi}\, \Delta N^{TOT}_{PHYS}(\omega)\, f(\omega) = 14 - n_f = \underbrace{14(1-n_f)}_{\text{KONDO}} + \underbrace{13 n_f}_{f^{13}\to f^{12}} \quad (YB)$$

$$(38)\quad \int \frac{d\omega}{\pi}\, \Delta N^{TOT}_{PHYS}(\omega)\, f(-\omega) = n_f \quad (f^{13}\to f^{14}) \qquad (YB)$$

(YB)



SO AS $(1-n_f)$ GOES DOWN, WEIGHT MUST INCREASE IN THE $f^1\to f^0$ AND $f^1\to f^2$ PEAKS FOR CE, $f^{13}\to f^{14}$ AND $f^{13}\to f^{12}$ PEAKS FOR YB.

BEYOND MEAN FIELD: LOCAL FERMI LIQUID THEORY

WE HAVE SEEN THAT THE SLAVE BOSON MEAN FIELD THEORY LEADS US TO A PICTURE OF AN EFFECTIVE FERMI GAS FOR THE LOW TEMPERATURE ANDERSON/KONDO MODELS WITH TEMPERATURE DEPENDENT PARAMETERS $\tilde{\varepsilon}_f$, $\tilde{V}$. THE GAS IS PARAMETRIZED ENTIRELY BY THE PHASE SHIFT δ, WHICH MEASURES HOW ENERGY LEVELS ARE SHIFTED FROM THE NONINTERACTING ($V=0$) LIMIT, AND BY THE EXTRA QUASIPARTICLE DOS PER SPIN, $\Delta N_f(\omega) = \frac{1}{\pi}\frac{d\delta}{d\omega}$ WHICH

FEEDS INTO A CALCULATION OF PHYSICAL PROPERTIES.

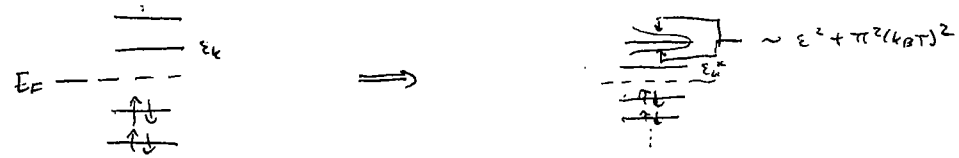
WHAT HAPPENS WHEN WE GO BEYOND MEAN FIELD? WE SHALL INDUCE INTERACTIONS BETWEEN THE FERMIONIC QUASIPARTICLES, ONE APPROACH TO THIS IS AN EXPLICIT EXPANSION IN FLUCTUATIONS ABOUT MFT, AS WAS CARRIED OUT BY READ & NEWNS. A MORE PHYSICAL AND INTUITIVE APPROACH IS TO DEVELOP A LOCAL FERMI LIQUID THEORY, PIONEERED BY NOZIÈRES. BEFORE WE CARRY THAT OUT, IT IS HELPFUL TO REVIEW LANDAU'S FERMI LIQUID CONCEPT BRIEFLY --

[SEE CH. 1. OF STATISTICAL MECHANICS, VOL 2, LIFSCHITZ + PITAEVSKII]

REVIEW OF LANDAU THEORY

FOR A HOMOGENEOUS, ISOTROPIC SYSTEM OF INTERACTING FERMIONS:

① IN THE LANDAU PICTURE, THE LOW TEMPERATURE EXCITATIONS OF AN INTERACTING FERMI SYSTEM ARE ASSUMED TO HAVE A 1:1 MAP TO THE NON INTERACTING SYSTEM --



GAS (ELECTRON GAS) LIQUID (QUASIPARTICLE GAS)

$\varepsilon_k = v_F (k - k_F)$ $\quad \varepsilon_k^* = \underbrace{v_F^*}_{k_F/m^*} (k - k_F)$

② THE ENTROPY IS

(39) $$S = -\frac{1}{N_S} \sum_{km} \left[n_{km} \ln n_{km} + (1 - n_{km}) \ln (1 - n_{km}) \right]$$

WHICH, VARIED SUBJECT TO FIXED NUMBER AND ENERGY GIVES

(40) $$n_{km} = \left(e^{\beta \tilde{\varepsilon}^*_{km}} + 1 \right)^{-1}$$

WITH $\tilde{\varepsilon}^*_{km}$ TO BE SPECIFIED.

[THAT THE VOLUME OF THE FERMI SURFACE IS PRESERVED (FOR A SPHERE, $k_F^3 = 3\pi^2 n_{el}$) IS CALLED LUTTINGER'S THEOREM. IT HOLDS SELF CONSISTENTLY GIVEN ASSUMPTION ② AND NO PHASE TRANSITION AS A FUNCTION OF INTERACTION STRENGTH.]

③ AWAY FROM $T = 0$, $\mu = \mu(T=0)$, $h = 0$ (CHEMICAL POTENTIAL) THE QUASIPARTICLE INTERACTIONS MODIFY THE QUASIPARTICLE DISPERSION -- THE TOTAL ENERGY CHANGE AWAY FROM THE GROUND STATE IS

(41) $$\delta E = \underbrace{\sum_{km} \varepsilon_k^* \, \delta n_{km}}_{\substack{\text{EXCITATIONS OF QUASIPARTICLE GAS -- MUCH MANY BODY THEORY ALREADY}}} + \frac{1}{N_S} \sum_{\substack{kk' \\ mm'}} \underbrace{f_{mm'}(k,k')}_{\substack{\text{FEEDBACK OR "MOLECULAR FIELD" FROM QUASIPARTICLE INTERACTIONS}}} \delta n_{km} \, \delta n_{k'm'}$$

$$\left[\delta n_{km} = n_{km}(k, T, \omega \ldots) - n_{km}(0) \right]$$

OR

$$\delta E = \sum_{km} \tilde{\varepsilon}^*_{km} \, \delta n_{km}$$

(42) $$\underbrace{\tilde{\varepsilon}^*_{km}}_{\substack{\text{FULL INTERACTING ENERGY DEPENDS ON DISTRIBUTION OF ALL OTHER QUASIPARTICLES}}} = \varepsilon^*_{km} + \frac{1}{N_S} \sum_{kk'} f_{mm'}(k,k') \, \underbrace{\delta n_{k'm'}}$$

④ FOR $T \to 0$, ONLY $|k| \approx |k'| \approx k_F$ MATTER, SO FOR $S = 1/2$

(43) $$\underbrace{N^*(E_F^*)}_{\frac{3}{2 v_F^* k_F}} f_{\sigma\sigma'}(k,k') = F^s(\hat{k}\cdot\hat{k}') \delta_{\sigma\sigma'} + 2\sigma\sigma' \, F^a(\hat{k}\cdot\hat{k}')$$

AND, FOR A SPHERICAL SURFACE

(44) $$F^s(\hat{k}\cdot\hat{k}') = \sum_{l=0}^{\infty} (2l+1) F_l^s \, P_l(\hat{k}\cdot\hat{k}'), \quad F^a(\hat{k}\cdot\hat{k}') = \sum_{l=0}^{\infty} (2l+1) F_l^a$$

-- THE $\{F_\ell^s, F_\ell^a\}$ ARE CALLED LANDAU PARAMETERS AND PROVIDE A WAY TO PARAMETERIZE THE LOW ENERGY PROPERTIES OF THE SYSTEM -- MUCH HIGH ENERGY PHYSICS IS FOLDED DOWN INTO THE LANDAU PARAMETERS.

(3) PHYSICAL PROPERTIES DEPEND UPON $\begin{cases} m^* = \frac{k_F}{v_F^*} = \frac{d\varepsilon_k}{d\varepsilon_k^*}\Big|_0 \\ \{F_\ell^s, F_\ell^a\} \end{cases}$

A) ENTROPY AND SPECIFIC HEAT ARE GIVEN BY

(45) $S(T) \approx C_{el}(T) \underset{T\to 0}{\approx} \frac{N\pi^2}{3} k_B^2 N^*(E_F^*) T$

B) χ IS MODIFIED BY INTERACTION EFFECTS ... IN THE PRESENCE OF A FIELD h ($S = \frac{1}{2}$ FOR SIMPLICITY)

(46) $\delta\tilde{\varepsilon}^*_{k\sigma} \equiv -\mu h\sigma = \underbrace{-\mu_0 h\sigma}_{\text{GAS}} + \frac{2}{N_s}\sum_{k'\sigma'} \sigma\sigma' \frac{F^a(\hat{k}\cdot\hat{k}')}{N^*(\varepsilon_{k'})} \delta n_{k'\sigma'}$

NOW

$$\delta n_{k'\sigma'} \approx \left(\frac{\partial n_{k'\sigma'}}{\partial \tilde{\varepsilon}^*_{k'\sigma'}}\right)\Big|_{h=0} \delta\tilde{\varepsilon}^*_{k\sigma} \approx \frac{\partial n_{k'\sigma'}}{\partial \varepsilon^*_{k'\sigma'}}\Big)_{h=0} (-\mu h\sigma')$$

$\Rightarrow$

(47) $-\mu h\sigma = -\mu_0 h\sigma - \mu h\sigma \int d\varepsilon' \underbrace{\left(\frac{\partial n(\varepsilon')}{\partial \varepsilon'}\right)}_{\approx -\delta(\varepsilon')} \int \frac{d\hat{k}'}{4\pi} F^a(\hat{k}\cdot\hat{k}')$

$\Rightarrow$ $\boxed{(48)\ \mu = \mu_0 - \mu F_0^a}$ $\overset{T\to 0}{}$

$\Rightarrow$ $\boxed{(49)\ \mu = \frac{\mu_0}{1+F_0^a}}$ } MOLECULAR FIELD ENHANCEMENT OF MAG. MOMENT.

STABILITY REQUIRES $F_0^a > -1$

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THEN

(50) $\chi = \frac{M}{h}\Big|_{h=0} = \frac{1}{h}\frac{\mu_0}{N_s}\sum_{k\sigma'} \sigma' \delta n_{k'\sigma'}\Big|_{h=0}$

$= \frac{1}{h}\frac{\mu_0\mu h}{2}\int d\varepsilon' \left(\frac{-\partial n(\varepsilon')}{\partial \varepsilon'}\right) N^*(\varepsilon')$

$= \frac{\mu_0^2}{2(1+F_0^a)} N^*(0)$

$\Rightarrow$ (51) $\frac{\pi^2 k_B^2}{\mu_0^2 S(S+1)} \left(\frac{\chi}{C/T}\right)_{T\to 0} = \frac{1}{1+F_0^a}$ } MODIFICATION BY MAGNETIC INTERACTIONS.

LOCAL FERMI LIQUID THEORY

THE THEORY OF NOZIÈRES BEGINS FROM THE QUASIPARTICLE GAS ENERGIES WE HAVE IDENTIFIED IN OUR MFT ... SPECIFICALLY

(52) $\varepsilon = \frac{v_F\pi}{L}\left[m + \frac{1}{2}\right] \Rightarrow \varepsilon^* = \frac{\pi v_F}{L}\left[m + \frac{1}{2} + \delta(\varepsilon^*)/\pi\right]$

$= \varepsilon + \frac{1}{N_0}\frac{\delta(\varepsilon^*)}{\pi}$ $\left[N_0 = \frac{1}{\Delta\varepsilon} = \frac{L}{\pi v_F}\right]$

IN THE APPROPRIATE ANGULAR MOMENTUM CHANNEL. HENCE, THE ANALOGY OF N^* IS $\Delta N_f = \frac{1}{\pi}\frac{d\delta}{d\varepsilon}$

AWAY FROM $T\to 0$, NOZIÈRES ASSUMED AN EXPANSION FOR $\tilde{\varepsilon}^*$ THROUGH THE PHASE SHIFT, SO FOR A GIVEN SPIN

(53) $\tilde{\varepsilon}^*_\sigma = \varepsilon - \mu_0 h\sigma + \frac{1}{N_0}\left[\frac{\delta(0)}{\pi} + \Delta N_f(0)\,\varepsilon + \frac{1}{\pi}\sum_{\varepsilon'<\varepsilon} \phi_{\sigma\sigma'}\delta n_{\sigma'}(\varepsilon') + \cdots\right]$

BECAUSE NO ANGULAR INTEGRATION EXISTS, $\phi_{\sigma\sigma'}$ ONLY DEPENDS UPON SPIN -- FOR $S = \frac{1}{2}$

(54) $\phi_{\sigma\sigma'} = \phi^s + 2(\sigma\sigma')\phi^a$ (CORRESPONDS TO $f_{\sigma\sigma'}(\hat{k},\hat{k}')$)

(55) $\delta\tilde{\varepsilon}^{x}_{\sigma} = -\mu_0 h\sigma + \frac{2\phi^a}{\pi N_0}\sigma m$

WITH THE POLARIZATION

(56) $m = \sum_{\varepsilon'\sigma'} \sigma' \delta n_{\sigma'}(\varepsilon') = \sum_{\varepsilon'\sigma'} \left[-\mu_0 h + \frac{2\phi^a}{\pi N_0} m\right](\sigma')^2 \left(\frac{\partial n(\varepsilon')}{\partial \varepsilon'}\right)$ $\xrightarrow{T\to 0} -\delta(\varepsilon')$

$= -\left[-\mu_0 h + \frac{2\phi^a}{\pi N_0} m\right] \frac{N_0}{2}\left[1 + \frac{\Delta N_f(0)}{N_0}\right]$

$\Rightarrow \quad m\left[1 + \frac{\phi^a}{\pi}\right] = \frac{N_0\mu_0 h}{2}\left[1 + \frac{\Delta N_f(0)}{N_0}\right]$

$\Rightarrow$ (57) $m \approx \frac{N_0\mu_0 h}{2}\left[1 + \underbrace{\frac{\Delta N_f(0)}{N_0}}_{\Delta m\ (\text{IMPURITY CONTRIBUTION})} - \frac{\phi^a}{\pi}\right] + O\left(\frac{1}{R^2}\right)$

So (58) $\Delta\chi = \frac{\mu_0 \Delta m}{h} = \frac{\mu_0^2}{2}\left[\Delta N_f(0) - \frac{N_0\phi^a}{\pi}\right]$

$= \frac{\mu_0^2 \Delta N_f(0)}{2}\left[1 - \frac{N_0\phi^a}{\pi \Delta N_f(0)}\right]$

So (59) $R = \frac{\pi^2 k_B^2}{\mu_0^2 S(S+1)}\frac{\Delta\chi}{\Delta\gamma} = 1 - \frac{N_0\phi^a}{\pi\Delta N_f(0)}$

NEXT, CONSIDER $\Delta\chi_{CHARGE}$. IN THE KONDO REGIME, CHARGE FLUCTUATIONS ARE FROZEN SO $\Delta\chi_{CHARGE} = 0$.

WE FIND (60) $\chi_{CHARGE} = \frac{\partial N}{\partial\mu}$, SO CONSIDER A SMALL CHANGE OF μ, $\delta\mu$:

(61) $\tilde{\varepsilon}_\sigma = \varepsilon - \delta\mu + \frac{\Delta N_f \varepsilon}{\pi N_0} + \frac{\delta_0}{\pi N_0} + \frac{\phi^s}{\pi N_0}\delta N$

WITH

(62) $\delta N = \sum_{\sigma\varepsilon} \delta n_\sigma(\varepsilon) = 2\sum_{\varepsilon} \delta\tilde{\varepsilon}\ \frac{\partial n(\varepsilon)}{\partial\varepsilon}\Big)_{\delta\mu=0}$

$= 2\delta\mu \sum_\varepsilon \left(\frac{-\partial n}{\partial\varepsilon}\right) - \frac{2\phi^s}{\pi N_0}\delta N \sum_\varepsilon \left(\frac{-\partial n}{\partial\varepsilon}\right)$

$= 2\delta\mu\left[1 + \frac{\Delta N_f(0)}{N_0}\right] N_0 - \frac{2\phi^s}{\pi}\delta N + O\left(\frac{1}{R}\right)$

SOLVING:

$\frac{\delta N}{\delta\mu} = \chi_{CHARGE} = N_0\left[1 + \frac{\Delta N_f(0)}{N_0} - \frac{2\phi^s}{\pi}\right]$

(63) SO

$\Delta\chi_{CHARGE} = \Delta N_f\left[1 - \frac{2\phi^s N_0}{\pi\Delta N_f(0)}\right] = 0$

$\Rightarrow$ $\boxed{1 = \frac{2\phi^s N_0}{\pi\Delta N_f(0)}}$ (64)

NOW: APPLY THE PAULI PRINCIPLE:

$\phi_{\uparrow\uparrow} = 0 = \phi^s + 2\left(\frac{1}{4}\right)\phi^a = \phi^s + \frac{1}{2}\phi^a$

$\Rightarrow$ $\boxed{2\phi^s = -\phi^a}$ (65)

HENCE: (66) $\boxed{R = 1 - \frac{N_0\phi^a}{\pi\Delta N_f(0)} = 1 + \frac{2\phi^s N_0}{\pi\Delta N_f(0)} = 2}$

THAT IS, INTERACTIONS ENHANCE $\Delta\chi(0)$ OVER $\Delta\gamma(0)$ BY A FACTOR OF 2 FOR $S = 1/2$.

FOR $N > 2$, ASSUMING SU(N) SYMMETRY SO THAT

(67) $\phi_{mm'} = \phi_0(1 - \delta_{mm'})$

ONE CAN SHOW BY SIMILAR ARGUMENTS

(68) $R = 1 + \frac{1}{N-1} \underset{N\to\infty}{\approx} 1 + \frac{1}{N}$

CLEARLY, QUASIPARTICLE FLUCTUATION/INTERACTION EFFECTS ARE DOWN BY $\sim 1/N$ AS $N\to\infty$! HENCE THE $1/N$ EXPANSION MAKES SENSE!

EXTENSION TO LATTICE

WE JUST WANT TO BRIEFLY REMARK HERE THAT SBMFT MAY BE DONE FOR THE LATTICE -- THE SLAVE BOSONIZED LATTICE MODEL IS

$$(69)\quad \sum_{\vec{k}m} \varepsilon_{\vec{k}} n_{\vec{k}m} + \varepsilon_f \sum_{m\vec{R}} \tilde{f}^\dagger_{\vec{R}m} \tilde{f}_{\vec{R}m} + \frac{V}{\sqrt{N_S}} \sum_{\vec{k}m\vec{R}} \left\{ e^{i\vec{k}\cdot\vec{R}} \tilde{f}^\dagger_{\vec{k}m} c_{\vec{k}m} b_{\vec{R}} + \text{h.c.} \right\}$$
$$- \sum_{\vec{R}} \lambda_{\vec{R}} \left[\sum_m \tilde{f}^\dagger_{\vec{R}m} \tilde{f}_{\vec{R}m} + b^\dagger_{\vec{R}} b_{\vec{R}} - 1 \right]$$

SO THE CONSTRAINT MUST BE IMPLEMENTED ON EACH SITE.

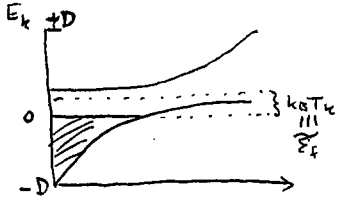
IN MEAN FIELD WE REPLACE

$$(70)\quad b_{\vec{R}} \longrightarrow b_0 + \delta b_{\vec{R}}, \qquad \lambda_{\vec{R}} \longrightarrow \lambda_0 + \delta\lambda_{\vec{R}}$$

SO, WITH $\tilde{\varepsilon}_f = \varepsilon_f - \lambda_0$, AND FOURIER TRANSFORMING ($\tilde{V} = bV$)

$$(71)\quad \tilde{H}_{MF} = \sum_{\vec{k}m} \left\{ \varepsilon_{\vec{k}} c^\dagger_{\vec{k}m} c_{\vec{k}m} + \tilde{\varepsilon}_f \tilde{f}^\dagger_{\vec{k}m} \tilde{f}_{\vec{k}m} + \tilde{V} (\tilde{f}^\dagger_{\vec{k}m} c_{\vec{k}m} + \text{h.c.}) \right\}$$
$$- N_S \lambda_0 (b_0^2 - 1)$$

IT IS EASY TO DIAGONALIZE $\tilde{H}_{MF}$ AT EACH $\vec{k}$ POINT... WE OBTAIN HYBRIDIZED BANDS ($N > 2$)



$$(72)\quad \tilde{E}^{(\pm)}_{\vec{k}} = \frac{1}{2}\left[(\varepsilon_{\vec{k}} + \tilde{\varepsilon}_f) \pm \sqrt{(\varepsilon_{\vec{k}} - \tilde{\varepsilon}_f)^2 + 4\tilde{V}^2} \right]$$

AND

$$\tilde{f}_{\vec{k}m} = u_{\vec{k}}\, \alpha_{\vec{k}+m} + v_{\vec{k}}\, \alpha^\dagger_{\vec{k}-m}$$
$$c_{\vec{k}m} = -v_{\vec{k}}\, \alpha_{\vec{k}+m} + u_{\vec{k}}\, \alpha^\dagger_{\vec{k}-m}$$

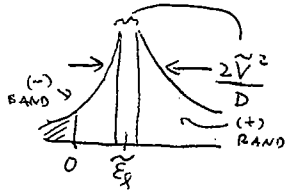
$$(73a)\quad u_{\vec{k}}^2 = \frac{(E^{(-)}_{\vec{k}} - \tilde{\varepsilon}_f)^2}{(E^{(-)}_{\vec{k}} - \tilde{\varepsilon}_f)^2 + \tilde{V}^2} = \frac{\tilde{V}^2}{(E^{(+)}_{\vec{k}} - \tilde{\varepsilon}_f)^2 + \tilde{V}^2}$$

$$(73b)\quad v_{\vec{k}}^2 = \frac{(E^{(+)}_{\vec{k}} - \tilde{\varepsilon}_f)^2}{(E^{(+)}_{\vec{k}} - \tilde{\varepsilon}_f)^2 + \tilde{V}^2} = \frac{\tilde{V}^2}{(E^{(-)}_{\vec{k}} - \tilde{\varepsilon}_f)^2 + \tilde{V}^2}$$

THE DOS IS

$$(74)\quad \tilde{N}(E_\alpha) = N(0) \left| \frac{d\varepsilon}{dE_\alpha} \right| = N(0) \left[1 + \frac{\tilde{V}^2}{(E_\alpha - \tilde{\varepsilon}_f)^2} \right]$$

(BARE + ENHANCED)



WHICH IS SHARPLY PEAKED WITH A SMALL INDIRECT GAP ABOUT $\tilde{\varepsilon}_f$ (GAP $\sim 2\tilde{V}^2/D$)

NOW WE AGAIN FIND EQUILIBRIUM VALUES BY DIFFERENTIATING THE FREE ENERGY:

$$(75)\quad \frac{F_{MF}}{N_S} = -\frac{k_B T}{N_S} \sum_{\vec{k}m\alpha \atop \alpha = \pm} \ln\left(1 + e^{-\beta \tilde{E}^\alpha_{\vec{k}}}\right) - \lambda_0 (b_0^2 - 1)$$

WITH MINOR ALGEBRA, USING (73a,b), (74) WE GET FROM $\partial F / \partial b_0 = 0$

$$(76)\quad \lambda_0 \approx \varepsilon_f = N N(0) V^2 \int_{-D}^{0} \frac{dE_-}{E_- - \tilde{\varepsilon}_f} = \frac{N\Gamma}{\pi} \ln \frac{\tilde{\varepsilon}_f}{D} \Rightarrow \tilde{\varepsilon}_f \cong D \exp\left(-\frac{\pi |\varepsilon_f|}{N\Gamma}\right), \quad = k_B T_K$$

SAME KONDO SCALE AS IMPURITY! ($N > 2$)

SO NEXT, FROM $\partial F / \partial \lambda_0 = 0$ WE GET

$$(77)\quad 1 = \frac{1}{N_S} \sum_{\vec{k}m} \langle \tilde{f}^\dagger_{\vec{k}m} \tilde{f}_{\vec{k}m} \rangle + b_0^2 = N N(0) \tilde{V}^2 \int_{-D}^{0} \frac{dE_-}{(E_- - \tilde{\varepsilon}_f)^2} + b_0^2$$
$$= \left(\frac{N\Gamma}{\pi \tilde{\varepsilon}_f} + 1 \right) b_0^2 \Rightarrow b_0^2 = \frac{1}{1 + \frac{N\Gamma}{\pi (k_B T_0)}} \approx \frac{\pi (k_B T_0)}{N\Gamma}$$

SO: GAP $= \frac{2\tilde{V}^2}{D} = \frac{2}{N} \frac{N\Gamma}{\pi N(0) D} \frac{\pi (k_B T_0)}{N\Gamma} = \frac{4}{N} (k_B T_0) \xrightarrow[N \to \infty]{} 0$

WITH (76), (77) WE OBTAIN

(78) $\chi = \frac{N\mu^2 S(S+1)}{3} N(0)\left[1 + \frac{\tilde{V}^2}{\tilde{\epsilon}_f^2}\right] = \frac{N\mu^2 S(S+1)}{3}\tilde{N}(0)$

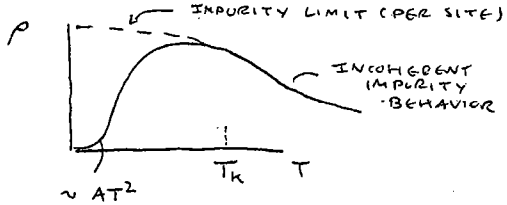
$\Rightarrow \Delta\chi = \frac{N\mu^2 S(S+1)}{3}\frac{\tilde{V}^2}{\tilde{\epsilon}_f^2} = \frac{N\mu^2 S(S+1)}{3}\frac{N\tilde{\Gamma}}{\pi(k_B T_0)^2} = \frac{N\mu^2 S(S+1)}{3k_B T_0}$

SIMILARLY

(79) $\Delta\gamma = \frac{N\pi^2}{3}\frac{k_B}{T_0}$

HENCE, AT MEAN FIELD, $R = 1$, (WILSON RATIO)
CALCULATIONS TO $O(1/N)$ REGAL $R \approx 1 + 1/N$ AS IN THE IMPURITY (SEE NOZIERES & BLANDIN, AND MILLIS & LEE).

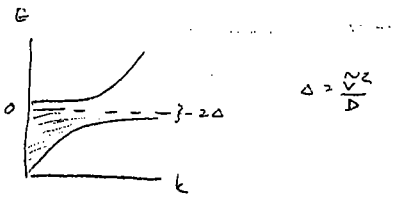
FOR THE RESISTIVITY, AT LOW T A FERMI LIQUID T^2 COEFFICIENT IS FOUND -- SO A PICTURE IS



[SEE P. COLEMAN, PRL 59, 1026 (1987) & D.L. COX & N. GREWE, Z. PHYS. B 71 321 (1988)]

THIS LOOKS A GOOD DEAL LIKE THE RESISTIVITY OF $CeAl_3$ WE SAW LAST TIME. THE REASON $\rho(T=0)$ MUST BE ZERO FOR THE LATTICE IS BLOCH'S THEOREM -- A PHASE SHIFT AT EACH SITE SIMPLY RENORMALIZES THE LATTICE POTENTIAL, AND THE ELECTRON WAVES PERFECTLY DIFFRACT -- INTERACTION DRIVEN FLUCTUATIONS IN THE PHASE SHIFT GIVE A T^2 RISE.

N=2 CASE : IF WE HAVE JUST ONE CONDUCTION BAND FOR N=2, AND HAVE 1F + 1 CONDUCTION ELECTRON PER SITE, BY COUNTING ARGUMENTS WE MUST GET AN INSULATOR. A PICTURE APPEARS ON THE NEXT PAGE.



NOW, $\partial F_{MF}/\partial b_0$, $\partial F_{MF}/\partial \lambda_0$ GIVE

(80) $\lambda_0 \approx \epsilon_f = \frac{2\Gamma}{\pi}\int_{-D}^{-\Delta}\frac{dE_-}{E_-} \Rightarrow \epsilon_f \approx \frac{2\Gamma}{\pi}\ln\frac{\Delta}{D} \Rightarrow \Delta = D\exp\left(-\frac{\pi|\epsilon_f|}{2\Gamma}\right)$

AND

(81) $1 = 2N(0)\tilde{V}^2\int_{-D}^{-\Delta}\frac{dE_-}{E_-^2} + b_0^2 \approx b_0^2\left(\frac{2\Gamma}{\pi(k_B T_0)} + 1\right)$

$\Rightarrow b_0^2 \approx \frac{\pi k_B T_0}{2\Gamma}$

THE MATERIALS Ce_3RhSb_3, $Ce_3Bi_4Pt_3$, AND SEVERAL OTHERS APPEAR TO OBEY THE CONDITION OF ONE BAND AT E_F AND N=2 -- THESE ARE ALL SMALL GAP INSULATORS -- FOR Ce_3RhSb_3 $\Delta \approx 4K$, $Ce_3Bi_4Pt_3$ $\Delta \approx 150K$. FOR EXAMPLE

AND ARE CALLED "KONDO INSULATORS." THE ABOVE DESCRIPTION SEEMS PRETTY GOOD! (THERE ARE MORE CANDIDATES

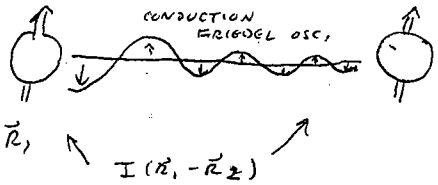
DONIACH CRITERION : MAGNETIC INTERACTIONS

TO BACK UP ON OUR $1/N$ RESULTS -- WHAT SHOULD WE DO TO GET A SENSIBLE $N \to \infty$ LIMIT? TO HAVE A WELL DEFINED KONDO SCALE, WE SHOULD HOLD NV^2 FIXED, AS $k_B T_K \sim D\exp(-\pi|\epsilon_f|/N\Gamma)$. TO SEE THIS MORE EXPLICITLY, CONSIDER A SLAVE BOSON DECAY --

THIS GIVES A FREE SUM ON m -- TO NORMALIZE

WE MUST TAKE $NV^2 \sim 1$ AS $N \to \infty$ OR ELSE THE CALCULATION IS ILL DEFINED IN THIS (UNUSUAL) THERMODYNAMIC LIMIT, (FOR COMPARISON, WE ALWAYS PUT A $1/\sqrt{N_s}$ IN FRONT TO NORMALIZE THE k SUM -- CF EQ. (1) OF THIS LECTURE).

NOW, INTERSITE INTERACTIONS WHICH PROVIDE THE POSSIBILITY FOR MAGNETIC ORDER ARE PRODUCED BY FRIEDEL OSCILLATIONS -- AS A GEDANKEN, POLARIZE ONE SITE - THIS WILL PRODUCE A CONDUCTION CLOUD



WHICH CAN POLARIZE A DISTANT SITE -- IGNORING THE CONDUCTION ELECTRON WE HAVE AN EFFECTIVE INTERACTION I BETWEEN SITES WHICH DEPENDS ON $(\vec{R}_1 - \vec{R}_2)$,

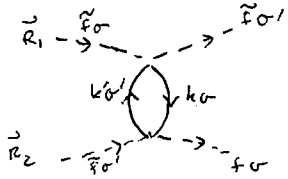
THIS IS THE SO CALLED RUDERMAN-KITTEL-KASUYA-YOSIDA OR RKKY INTERACTION.

MATHEMATICALLY

$$(P2)\quad I(\vec{R}_1 - \vec{R}_2) \sim \frac{J^2}{N_s^2} \sum_{k,k'} P \frac{f(\varepsilon_{k'})(1-f(\varepsilon_k))}{\varepsilon_k - \varepsilon_{k'}} e^{i(k-k')\cdot\vec{R}} \sim N_{IOS}^2 J^2 \frac{\cos 2k_F R}{(k_F R)^3}$$

$$\left(J \sim \frac{V^2}{|\varepsilon_f|}\right)$$

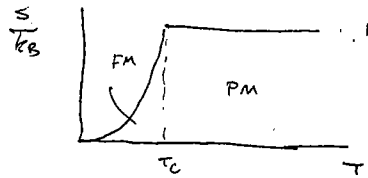
THE FEYNMAN DIAGRAM IS



BECAUSE NO FACTORS OF N ARISE IN CALCULATING THIS, THE DIAGRAM GOES AS $1/N^2$ AND HENCE VANISHES AS $N \to \infty$. SO INTERSITE MAGNETIC COUPLINGS ARE FROZEN OUT FOR $N \to \infty$!

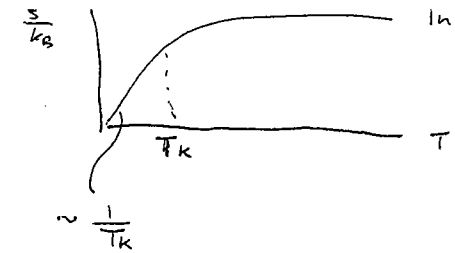
[P. COLEMAN, PRB 29 2035 (1984)]

AT ANY FINITE N, THOUGH, MAGNETIC INTERSITE COUPLINGS ARE IMPORTANT! WE CAN ENVISION THAT THESE WILL FAVOR A REDUCTION OF MAGNETIC ENTROPY THROUGH MAGNETIC ORDER (FOR EXAMPLE) IN GD METAL:



[THE 3RD LAW OF TD REQUIRES WE REMOVE RESIDUAL ENTROPY]

RKKY INTERACTIONS INDUCE FERROMAGNETISM, WHICH REMOVES THE LARGE ENTROPY ($S/k_B = \ln 8$ per site) OF THE PARAMAGNETIC PHASE. ON THE OTHER HAND, KONDO SINGLET FORMATION OFFERS A DIFFERENT WAY TO REMOVE ENTROPY:



SO KONDO REMOVAL OF ENTROPY COMPETES WITH MAGNETIC ORDERING REMOVAL OF ENTROPY

A ROUGH CRITERION DUE TO DONIACH (1976)) IS THAT WHEN THE ORDERING TEMPERATURE ($\sim T_c \sim z|I|$, z = COORD #) EXCEEDS T_K, MAGNETIC ORDER WILL WIN -- WHEN $T_c < T_K$, THE KONDO EFFECT WINS, PUT DIFFERENTLY -- THE ENERGY GAIN PER SITE DUE TO MAGNETIC ORDER IS $\sim z|I|$ -- FROM THE KONDO EFFECT IT IS $k_B T_K$ -- SO THE GROUND STATE SHOULD BE MAGNETIC IF $k_B T_K < z|I|$, NONMAGNETIC OTHERWISE.

TAKING $\cos 2k_F R \sim 1$, AND $k_F R \sim \pi$ ($k_F^{-1} \sim 1\text{Å}$)

$z \sim 6$

THEN THE DOMACH CRITERION IS

$$1 = \frac{k_B T_k}{Z I} \approx \frac{D \exp(-1/N N(0) J)}{Z N(0) J^2/(k_F R)^3}$$

$$\approx \frac{64}{12} \frac{\exp\left(\frac{-1}{N N(0) J}\right)}{(N(0)J)^2}$$

$$\approx 5 N^2 \left[\frac{\exp(-1/x)}{x^2}\right] \qquad x = N N(0) J$$

CLEARLY, LARGE N FAVORS $k_B T_k >> k_B T_c$, AS x_c DEFINED BY THIS IS SHOVED TO ZERO AS $N \to \infty$. IF WE SOLVE FOR $x_c(N)$ WE GET THE FOLLOWING

$N(0)J_c$	N	$x_c(N)$
0.073	2	0.146
0.029	4	0.115
0.017	6	0.103
0.012	8	0.096

NOTE x_c (BELOW WHICH MAGNETIC ORDER IS FAVORED) GOES DOWN SLOWLY WITH N! ($\sim 1/\log N$)

BUT $(N(0)J)_c$ GOES FASTER....

NOTE THAT EVEN CRYSTAL FIELD SPLIT CASES WITH N=2 HAVE SMALL x_c -- THE REASON IS THAT

$$k_B T_k \propto D \underbrace{\left(\frac{D}{\Delta}\right)^{\frac{N_{ex}}{N_{gnd}}}}_{\text{THIS CRYSTAL FIELD ENHANCEMENT IS A LARGE N LEGACY}} \exp\left(-\frac{1}{2N(0)J}\right)$$

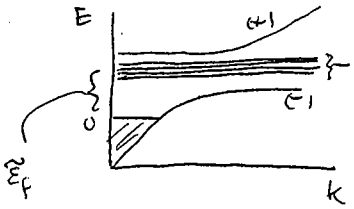
$N_{ex} \equiv$ ↕ Δ N_{gnd}

-- FOR $k_B T >> \Delta$ $N_{eff} = N_{gnd} + N_{ex}$

$k_B T << \Delta$ $N_{eff} = N_{gnd}$

[SEE HANZAWA, YAMADA, YOSIDA, J. MAG. MAG. MAT. 47, 357 (1985)]

[NOTE: IF $N > 2$ AND ONLY ONE BAND (CONDUCTION EXISTS AT E_F, THE PICTURE IS (EG, N=6, FOR Ce^{3+})



ONLY THE COMBINATION

$$\tilde{f}_{k\sigma} \sim \frac{1}{\sqrt{N_s}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \sum_m \langle \tfrac{5}{2} m \,|\, 3m-\sigma, \tfrac{1}{2}\sigma \rangle Y^*_{3m-\sigma}(\hat{k}) \hat{f}_{\vec{R}}$$

HYBRIDIZES WITH $c_{k\sigma}$.

SEE ...

Z. ZOU & P.W. ANDERSON, PHYS. REV. LETT. 57 2073 (1986)
F.C. ZHANG & T.K. LEE, " " " 58 2728 (1987)
G. AEPPLI & C.M. VARMA, " " " 58 2729 (1987)
D.L. COX, " " " 58 2730 (1987)
P.W. ANDERSON & Z. ZOU, " " " 58 2731 (1987)

MULTICHANNEL KONDO MODELS

OUTLINE

A. PURE MODELS- NOZIÈRES & BLANDIN
   i) COMPENSATED, UNDERCOMPENSATED, OVERCOMPENSATED
   ii) STABILITY OF GROUND STATES: STRONG COUPLING EXPANSION.
   iii) NON TRIVIAL PHYSICS OF OVERCOMPENSATED MODEL.

B. SOURCES OF TWO CHANNEL KONDO
   i) QUADRUPOLAR KONDO
   ii) TWO CHANNEL MAGNETIC KONDO
   iii) TWO LEVEL SYSTEM KONDO
   iv) COULOMB BLOCKADE

C. CRITICAL BEHAVIOR: NON CROSSING APPROXIMATION

D. SUMMARY OF CRITICAL BEHAVIORS, COMPARISON TO EXPERIMENT.

INTRODUCTION: THEORY OF NOZIÈRES & BLANDIN

THE MULTICHANNEL MODEL IS A GENERALIZATION OF THE ORIGINAL KONDO MODEL ALLOWING FOR MULTIPLE CONDUCTION BANDS TO COUPLE TO THE IMPURITY. THE ORIGINAL MOTIVATION WAS TO STUDY TRANSITION METAL IONS-- FOR EXAMPLE, FOR MN IN CU, BECAUSE SPIN ORBIT COUPLING IS NEGLIGIBLE, ELECTRON PARTIAL WAVES IN ALL FIVE d-ORBITALS COUPLE EQUIVALENTLY TO THE $S = 5/2$ SPIN. THE MODEL IS

(1) $$H = \sum_{k\sigma\alpha} \varepsilon_k c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha} + J \vec{S}_f \cdot \sum_{\mu\mu'\alpha\nu} \vec{S}_c)_{\mu\nu} c^\dagger_{\mu\alpha} c_{\mu'\alpha}$$

($S = 1/2$ MATRICES)

WHERE $\alpha = 1 \ldots M$ RUNS OVER THE CHANNELS OR BANDS, AND NOW $\vec{S}_f$ IS ALLOWED TO BE ARBITRARY, (CONDUCTION ELECTRONS IN EACH CHANNEL HAVE $S_I = 1/2$)

DEPENDING UPON THE VALUES OF M, S_I, A NUMBER OF GROUND STATES CAN BE REACHED-- IT IS HELPFUL TO ENVISION THESE IN THE STRONG COUPLING LIMIT, $J \to \infty$ -- IN THIS LIMIT WE ONLY CONSIDER CONDUCTION STATES AT THE IMPURITY SITE AND ALLOW FOR ARBITRARY CHARGE Q_c -- BECAUSE THE HAMILTONIAN IS A SIMPLE EXCHANGE THE ENERGIES ARE READILY GENERATED AS

(2) $$E(Q_c, S_{TOT}) = J \vec{S}_f \cdot \vec{S}_c(Q_c) = \frac{J}{2}\left[S^2_{TOT} - S^2_c(Q) - S^2_f\right]$$

THE CHARGE Q_c FIXES THE TOTAL CONDUCTION SPIN.

FOR EXAMPLE, IN THE ORIGINAL KONDO MODEL, IF WE MEASURE Q_c FROM THE SINGLET GROUND STATE, WHERE ONE ELECTRON SCREENS THE $S_f = 1/2$ IMPURITY, WE HAVE THE FOLLOWING STATES:

STATE	S_{TOT}	$S_c(Q_c)$	Q_c	E	ΔE
$\frac{1}{\sqrt{2}}[c_\uparrow^\dagger \lvert f\downarrow\rangle - c_\downarrow^\dagger \lvert f\uparrow\rangle]$	0	$1/2$	0	$-3J/4$	0
$\lvert f\uparrow\rangle, \lvert f\downarrow\rangle$	$1/2$	0	± 1	0	$3J/4$
$c_\uparrow^\dagger c_\downarrow^\dagger$ ($\lvert f\uparrow\rangle, \lvert f\downarrow\rangle$)	$1/2$	0	$+1$	0	$3J/4$
$c_\uparrow^\dagger \lvert f\uparrow\rangle$, $c_\downarrow^\dagger \lvert f\downarrow\rangle$	1	$1/2$	0	$J/4$	J
$\frac{1}{\sqrt{2}}[c_\uparrow^\dagger \lvert f\downarrow\rangle + c_\downarrow^\dagger \lvert f\uparrow\rangle]$					

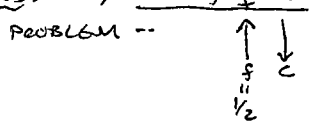
HERE $c_\sigma^\dagger$ CREATES AN UPSPIN CONDUCTION STATE AT THE IMPURITY.

NOW LET US CLASSIFY THE POSSIBLE GROUND STATES:

(1) COMPENSATED: $2S_f = M$

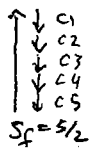
IN THIS CASE, THE CONDUCTION ELECTRONS HAVE EXACTLY ENOUGH SPIN TO "COMPENSATE" THE IMPURITY AND PRODUCE A SINGLET GROUND STATE.

EXAMPLES: a) $M=1$, $S_f = 1/2$ THIS IS THE ORIGINAL KONDO PROBLEM --



$\Rightarrow S_{TOT} = 0$

b) M_N ION = $S_f = 5/2$, $M = 5$



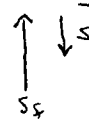
$\Rightarrow S_{TOT} = 0$

THE EXPECTATION (BORN OUT BY EXPLICIT CALCULATION) IS THAT THE $M = 2S_f$ CASE WILL ALWAYS GIVE A FERMI LIQUID GROUND STATE AS THE MOMENT IS "LOST".

(2) UNDERCOMPENSATED $2S_f > M$

IN THIS CASE, THERE IS TOO LITTLE CONDUCTION SPIN TO COMPENSATE THE IMPURITIES AND ONLY A PARTIAL COMPENSATION OCCURS.

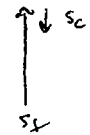
EXAMPLES: a) $S_f = 1$, $M = 1$



$\Rightarrow S_{TOT} = 1/2$

THIS CAN BE REALIZED THEORETICALLY IF TWO $S_f = 1/2$ IMPURITIES ARE BROUGHT CLOSE TOGETHER AND EXPERIENCE A LARGE FERROMAGNETIC COUPLING WITH ONE ANOTHER.

b) $S_f = 5/2$, $M = 1$

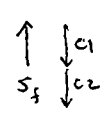


$\Rightarrow S_{TOT} = 2$

THIS COULD BE REALIZED IN CE SYSTEMS IF DIRECT COULOMB COUPLING DOMINATES

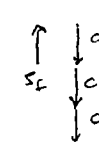
(3) OVERCOMPENSATED $2S_f < M$

IN THIS CASE, THERE ARE MORE CONDUCTION SPINS THAN NEEDED TO COMPENSATE -- THE TWO LIKELY PHYSICALLY REALIZABLE EXAMPLES ARE



$M = 2$, $S_f = 1/2$ (CE, U IMPURITIES; TWO LEVEL SYSTEMS; COULOMB BLOCKADE)

$S_{TOT} = \frac{1}{2}$



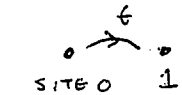
$M = 3$ $S_f = 1/2$ (CE IMPURITIES)

$S_{TOT} = 1$

STABILITY OF GROUND STATES

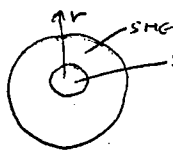
WE CAN ASK WHETHER THE ABOVE GROUND

STATES ARE STABLE WHEN COUPLING TO ELECTRONS OFF SITE — THE IDEA IS TO TURN ON HOPPING TO AN



(3) $H_t = -t\sum_{\sigma\alpha}\left(C^\dagger_{1\sigma\alpha}C_{0\sigma\alpha} + C^\dagger_{0\sigma\alpha}C_{1\sigma\alpha}\right)$

ADJACENT SITE (REALLY, THIS REPRESENTS AN ADJACENT RADIAL SHELL ABOUT THE IMPURITY)



AND DISCOVER WHAT EFFECTIVE HAMILTONIAN LIVES IN THIS SPACE ASSUMING $t \ll J$.

① COMPENSATED FOR SIMPLICITY, CONSIDER $M=1$, $S_f = 1/2$. THE RELEVANT STATES ARE

$Q_c = -1$ $(S_{TOT}=0)$

$|a,0,-1\rangle = \frac{1}{\sqrt{2}}\left[C^\dagger_{0\uparrow}|f\downarrow\rangle - C^\dagger_{0\downarrow}|f\uparrow\rangle\right]$ $(E=0)$

$|b,0,-1\rangle = \frac{1}{\sqrt{2}}\left[C^\dagger_{1\uparrow}|f\downarrow\rangle - C^\dagger_{1\downarrow}|f\uparrow\rangle\right]$ $(E=3/4\,J)$

$Q_c = +1$ $(S_{TOT}=0)$

$|a,0,+1\rangle = C^\dagger_{1\uparrow}C^\dagger_{1\downarrow}|a,0,-1\rangle$ $(E=0)$

$|b,0,+1\rangle = C^\dagger_{0\uparrow}C^\dagger_{0\downarrow}|b,0,-1\rangle$ $(E=3/4\,J)$

$Q_c = 0$ $(S_{TOT}=1/2)$

$(E=0)\rightarrow |a,\tfrac{1}{2},0\rangle = \begin{pmatrix} C^\dagger_{1\uparrow} \\ C^\dagger_{1\downarrow}\end{pmatrix}|a,0,-1\rangle$

$(E=3/4J)\begin{cases} |b1,\tfrac{1}{2},0\rangle = C^\dagger_{1\uparrow}C^\dagger_{1\downarrow}|f\uparrow\rangle,\ C^\dagger_{1\uparrow}C^\dagger_{1\downarrow}|f\downarrow\rangle \\ |b2,\tfrac{1}{2},0\rangle = C^\dagger_{0\uparrow}C^\dagger_{0\downarrow}|f\uparrow\rangle,\ C^\dagger_{0\uparrow}C^\dagger_{0\downarrow}|f\downarrow\rangle\end{cases}$

$|c\,\tfrac{1}{2}0\rangle =$
$\sqrt{\tfrac{2}{3}}C^\dagger_{1\downarrow}C^\dagger_{0\uparrow}|f\uparrow\rangle - \frac{1}{\sqrt{6}}\left(C^\dagger_{1\uparrow}(C^\dagger_{0\uparrow}|f\downarrow\rangle + C^\dagger_{0\downarrow}|f\uparrow\rangle)\right)$

$\&\ (\uparrow\leftrightarrow\downarrow)$ $(E=J)$

(NOTE: $Q_c = \sum_{R=0,1;\sigma}\left(C^\dagger_{R\sigma}C_{R\sigma} - \tfrac{1}{2}\right)$)

FOR $Q_c = \pm 1$, THE HAMILTONIAN IS JUST

(4) $H_{0,\pm1} = \begin{pmatrix} 0 & \pm t \\ \pm t & 3/4\,J\end{pmatrix}$

FOR $Q_c = 0$, $S = 1/2$ IT IS

(5) $H_{1/2,0} = \begin{pmatrix} 0 & t/\sqrt{2} & t/\sqrt{2} & 0 \\ t/\sqrt{2} & 3/4\,J & 0 & -t\sqrt{3/2} \\ t\sqrt{2} & 0 & 3/4\,J & -t\sqrt{3/2} \\ 0 & -t\sqrt{\tfrac{3}{2}} & -t\sqrt{\tfrac{3}{2}} & J\end{pmatrix}$ (rows: a, b1, b2, c; columns: a, b1, b2, c)

THE a SECTOR FORMS THE DOMINANT GROUND STATE COMPONENT IN EACH CASE. IF WE USE PERTURBATION THEORY

(6) a) $E^{(2)}_\alpha = \sum_{\beta\neq\alpha}\frac{|\langle\alpha|H_t|\beta\rangle|^2}{E^{(0)}_\alpha - E^{(0)}_\beta}$

b) $E^{(4)}_\alpha = \sum_{\substack{\gamma\neq\alpha \\ \delta\neq\alpha \\ \beta\neq\alpha}}\frac{\langle\alpha|H_t|\beta\rangle\langle\beta|H_t|\gamma\rangle\langle\gamma|H_t|\delta\rangle\langle\delta|H_t|\alpha\rangle}{(E^{(0)}_\alpha - E^{(0)}_\beta)(E^{(0)}_\alpha - E^{(0)}_\gamma)(E^{(0)}_\alpha - E^{(0)}_\delta)} - \sum_{\substack{\beta\neq\alpha \\ \gamma\neq\alpha}}\frac{|\langle\alpha|H_t|\beta\rangle|^2|\langle\alpha|H_t|\gamma\rangle|^2}{(E^{(0)}_\alpha - E^{(0)}_\beta)^2(E^{(0)}_\alpha - E^{(0)}_\gamma)}$

WE FIND

(7) a) $E_{a0-1} \approx -4t^2/3J + 64/27\ t^4/J^3 + \cdots$

b) $E_{a0+1} \approx -4t^2/3J + 64/27\ t^4/J^3 + \cdots$

c) $E_{a\frac{1}{2}0} \approx -4t^2/3J + 64/27\ t^4/J^3 - 16/3\ t^4/J^3$

$t=0$ $\qquad$ $t=0$

$Q_c=-1$ $\quad Q_c=0$ $\quad Q_c=+1$ $\Longrightarrow$ -1 $\quad 0$ $\quad +1$ } U_{eff}

WE SEE THIS GIVES NO SPIN DEPENDENCE, BUT RATHER A REPULSION BETWEEN UP & DOWN SPIN ELECTRONS ON SITE 1,

(8) $U_{eff} = E(0+1) + E(0-1) - 2E(\tfrac{1}{2}0) = \frac{32}{3}t^4/J^3$

HENCE, THE EXPECTATION FROM STRONG COUPLING IS FOR A LOCAL FERMI LIQUID, WITH A REPULSION ON THE SITE ADJACENT THE IMPURITY -- THE FIXED POINT (GROUND STATE) IS STABLE AGAINST THE HOPPING IN THAT THE PHYSICS BECOMES SIMPLE FERMION PHYSICS OUTSIDE SITE ZERO, EXACTLY AS EXPECTED BY WILSON & NOZIÈRES.

THE PHYSICAL INTERPRETATION IS EXCITATION TO A TRIPLET -- FROM THE FIRST TERM OF $\mathcal{H}(C)$ COMES U_{eff} -- THE SECOND TERM IS IDENTICAL FOR $Q_c = 0, \pm 1$. THE ONLY STATE POSSIBLE FOR $|\alpha\rangle$ GIVEN $|\alpha\rangle = |a, \tfrac{1}{2}, 0\rangle$ IS $|c, \tfrac{1}{2}; 0\rangle$, WHICH COUPLES THE TRIPLET OF SITE 0 TO THE LONE SITE 1 ELECTRON --

$$|a, \underset{\alpha}{\tfrac{1}{2}}, 0\rangle \to |b1, \underset{\beta}{\tfrac{1}{2}}, 0\rangle \to |c\ \tfrac{1}{2}0\rangle \to |b1, \underset{\delta}{\tfrac{1}{2}}, 0\rangle \to |a, \underset{\gamma}{\tfrac{1}{2}}, 0\rangle$$

"SINGLET" $|b2, \tfrac{1}{2}, 0\rangle$ (or) "TRIPLET" $|b2, \tfrac{1}{2}, 0\rangle$ (or)

THIS TERM VANISHES FOR $Q_c = \pm 1$. *

(2) UNDERCOMPENSATED CONSIDER THE SIMPLEST CASE $S_f = 1$, $M = 1$, AT SITE ZERO, THE STATES ARE

$$|\tfrac{1}{2}\tfrac{1}{2}, 0\rangle = \sqrt{\tfrac{2}{3}}\, c_{0\uparrow}^{+} |f1\rangle - \tfrac{1}{\sqrt{3}}\, c_{0\downarrow}^{+} |f0\rangle \qquad (Q_c = 0)$$
$$|\tfrac{1}{2}\,-\tfrac{1}{2}\,0\rangle = -\sqrt{\tfrac{2}{3}}\, c_{0\uparrow}^{+} |f-1\rangle + \tfrac{1}{\sqrt{3}}\, c_{0\downarrow}^{+} |f0\rangle \qquad (E = 0)$$

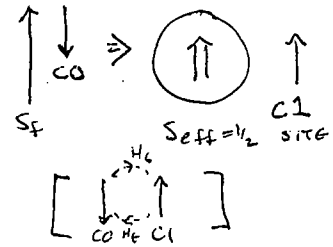
$$|\,|\alpha, -1\rangle = |f\alpha\rangle \qquad (|Q_c| = 1)$$
$$|\alpha, +1\rangle = c_{0\uparrow}^{+} c_{0\downarrow}^{+} |f\alpha\rangle \qquad (E = J)$$

$$|\tfrac{3}{2}\alpha, 0\rangle = \begin{cases} c_{0\uparrow}^{+} |f1\rangle,\ c_{0\downarrow}^{+} |f-1\rangle \\ \sqrt{\tfrac{2}{3}}\, c_{0\uparrow}^{+} |f0\rangle + \tfrac{1}{\sqrt{3}}\, c_{0\downarrow}^{+} |f1\rangle & (Q_c = 0) \\ \sqrt{\tfrac{2}{3}}\, c_{0\downarrow}^{+} |f0\rangle + \tfrac{1}{\sqrt{3}}\, c_{0\uparrow}^{+} |f-1\rangle & (E = \tfrac{3}{2} J) \end{cases}$$

---

*: NB: THE QUANTUM NUMBERS IN THE $|a\rangle$ SPACE ARE FERMIONIC: FOR $Q_c = \pm 1$, $S = 0$; FOR $Q_c = 0$, $S = \tfrac{1}{2}$ WHICH IS THE RIGHT DEFINITION FOR THIS MEASURE OF Q_c.

WHEN WE ADD SITE 1, OUR GUESS IS THAT WE WILL GENERATE A FERROMAGNETIC EXCHANGE COUPLING. WHY? BY SUPER EXCHANGE WE CAN VIRTUALLY INTERCHANGE C0, C1 -- BUT ONLY IF THEIR SPINS ARE ANTIPARALLEL. BUT IF C1 IS ANTIPARALLEL TO C0, IT IS PARALLEL TO S_{eff}.



SO IT IS ENOUGH TO EXAMINE THE SPLITTING BETWEEN THE LOCAL SINGLET AND TRIPLET FORMED FROM C1 & S_{eff} FOR $Q_c = 0$

TRIPLET

$$|a, |\alpha, 0\rangle = \begin{cases} c_{1\uparrow}^{+} |\tfrac{1}{2}\,\tfrac{1}{2}\,0\rangle \\ c_{1\downarrow}^{+} |\tfrac{1}{2}, -\tfrac{1}{2}\,0\rangle \\ \tfrac{1}{\sqrt{2}}\left(c_{1\uparrow}^{+} |\tfrac{1}{2}\,-\tfrac{1}{2}0\rangle + c_{1\downarrow}^{+} |\tfrac{1}{2}\,\tfrac{1}{2}0\rangle\right) \end{cases} \qquad E = 0$$

SINGLET

$$|a, 0, 0\rangle = \frac{1}{\sqrt{2}}\left[c_{1\uparrow}^{+} |\tfrac{1}{2}\,-\tfrac{1}{2}\,0\rangle - c_{1\downarrow}^{+} |\tfrac{1}{2}\,\tfrac{1}{2}0\rangle\right] \qquad E = 0$$

THE TRIPLET COUPLES TO THE EXCITED STATES

$$|b1, |\alpha, 0\rangle = c_{1\uparrow}^{+} c_{1\downarrow}^{+} |f\alpha\rangle \qquad \text{WITH MATRIX ELTS } \pm\sqrt{\tfrac{2}{3}}\, t$$
$$|b2, |\alpha, 0\rangle = c_{0\uparrow}^{+} c_{0\downarrow}^{+} |f\alpha\rangle$$

THE SINGLET HAS NO EXCITED STATES TO COUPLE TO.

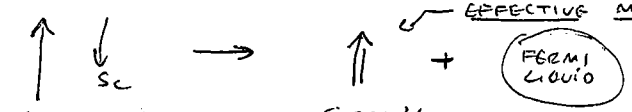
HENCE

$$E_a(|\alpha, 0) \approx -\tfrac{4}{3} t^2/J + \cdots \quad (O(t^4))$$
$$E_a(0, c) \approx 0 + \cdots \quad (O(t^4))$$

HENCE THE EFFECTIVE HAMILTONIAN IS

(9) $H_{eff} = -\left(\frac{4}{3}\frac{t^2}{J}\right) \vec{S}_{eff} \cdot \vec{S}_{c1}$ (J_{eff})

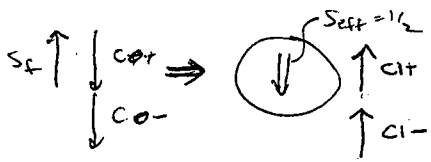
AND THIS IS STABLE: RECALL THAT FOR FERROMAGNETIC COUPLING, THE KONDO EXCHANGE SHRINKS WITH $T \to 0$. SO AS $T \to 0$ WE EXPECT



WITH WEAK DEVIATIONS FROM FERMI LIQUID THEORY DUE TO

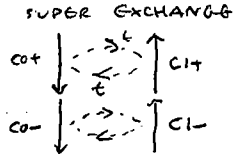
(10) $J_{eff} \sim 1/\ln\left(\frac{T_K^F}{T}\right)$ $\qquad k_B T_K^F = E_F \exp\left(-\frac{E_F}{J_{eff})_0}\right) \gg E_F$

(3) OVERCOMPENSATED WE CONSIDER THE SIMPLEST CASE, $M=2$, $S_f = 1/2$. NOW WE EXPECT AN EFFECTIVE ANTIFERROMAGNETIC COUPLING -- LABEL THE CHANNELS BY $\pm$.



NOW c_{0+} + c_{0-} DETERMINES SIGN OF S_{eff} -- SO SUPEREXCHANGE GIVES NET ANTIFERRO. COUPLING!

SUPER EXCHANGE



HOPPING ALLOWS EXCHANGE OF

NOW, PUT $Q_c = \sum_{R\alpha\sigma} (c^\dagger_{R\alpha\sigma} c_{R\alpha\sigma} - 1/2)$

SO $Q_c = \pm 1$ MEANS $1e^-$ PER SITE PER CHANNEL

ON SITE THE LOWEST STATES ARE

$|\frac{1}{2}, \frac{1}{2}, 0, 0\rangle_{\substack{S \\ Q_c}}^{\substack{T \\ \tau_c}} = \sqrt{\frac{2}{3}}\, c^\dagger_{0+\uparrow} c^\dagger_{0-\uparrow} |f\downarrow\rangle - \frac{1}{\sqrt{6}} (c^\dagger_{0+\uparrow} c^\dagger_{0-\downarrow} + c^\dagger_{0+\downarrow} c^\dagger_{0-\uparrow}) |f\uparrow\rangle$

$|\frac{1}{2}, -\frac{1}{2}, 0, 0\rangle = -\sqrt{\frac{2}{3}}\, c^\dagger_{0+\downarrow} c^\dagger_{0-\downarrow} |f\uparrow\rangle + \sqrt{\frac{1}{6}} (c^\dagger_{0+\uparrow} c^\dagger_{0-\downarrow} + c^\dagger_{0+\downarrow} c^\dagger_{0-\uparrow}) |f\downarrow\rangle$ $\quad (E=0)$

$|0, \frac{1}{2}\pm, -1\rangle = \frac{1}{\sqrt{2}} [c^\dagger_{0\pm\uparrow} |f\downarrow\rangle - c^\dagger_{0\pm\downarrow} |f\uparrow\rangle]$

$|0, \frac{1}{2}\pm, +1\rangle = \mp \frac{1}{\sqrt{2}} c^\dagger_{0\pm\uparrow} c^\dagger_{0\pm\downarrow} |0, \frac{1}{2}\mp, -1\rangle$ $\quad (E = J/4)$

WHERE τ IS THE CHANNEL SPIN:

(11) $\tau^z_{c0} = \sum_{\alpha\sigma} \left(\frac{\alpha}{2}\right) c^\dagger_{0\alpha\sigma} c_{0\alpha\sigma}$

AT THE ADJACENT SITE, TO ORDER $(\frac{t}{J})^0$, THE LOWEST STATES HAVE THE SAME FORM

$(E=0)$ $+O(t)^2$

$|a, \frac{1}{2}\frac{1}{2}, 0, 0\rangle = \sqrt{\frac{2}{3}}\, c^\dagger_{1+\uparrow} c^\dagger_{1-\uparrow} |\frac{1}{2}, -\frac{1}{2}, 0, 0\rangle - \frac{1}{\sqrt{6}} (c^\dagger_{1+\uparrow} c^\dagger_{1-\downarrow} + c^\dagger_{1+\downarrow} c^\dagger_{1-\uparrow}) \times |\frac{1}{2}\frac{1}{2} 00\rangle$

$|a, \frac{1}{2}-\frac{1}{2} 00\rangle = -\sqrt{\frac{2}{3}}\, c^\dagger_{1+\downarrow} c^\dagger_{1-\downarrow} |\frac{1}{2}\frac{1}{2} 00\rangle + \frac{1}{\sqrt{6}} (c^\dagger_{1+\uparrow} c^\dagger_{1-\downarrow} + c^\dagger_{1+\downarrow} c^\dagger_{1-\uparrow}) \wedge |\frac{1}{2} -\frac{1}{2} 00\rangle$

$(E = 0 + O(t^2))$

$|a, 0, \frac{1}{2}\pm, -1\rangle = \frac{1}{\sqrt{2}} [c^\dagger_{1\pm\uparrow} |\frac{1}{2}\frac{1}{2}, 00\rangle - c^\dagger_{1\pm\downarrow} |\frac{1}{2}\frac{1}{2} 00\rangle]$

$|a, 0, \frac{1}{2}\pm, +1\rangle = \pm\, c^\dagger_{1\pm\uparrow} c^\dagger_{1\pm\downarrow} |a, 0, \frac{1}{2}\mp, -1\rangle$

CALCULATING THE $O(t^2)$ TERMS IS QUITE INVOLVED.. IT IS SIMILAR IN SPIRIT TO THE COMPENSATED & UNDER COMPENSATED CASES.. WE JUST QUOTE HERE THAT AT SITE 1 WE HAVE AN EFFECTIVE EXCHANGE COUPLING TO THE GROUND STATE SPIN OF SITE ZERO, GIVEN BY

(12) $H_{eff} = -J_{eff}\, \underbrace{\vec{S}_{TOT}(\vec{R}=0)}_{\substack{\text{VALID FOR} \\ J \gg t}} \cdot \sum_\alpha \vec{S}_{c\alpha}(\vec{R}=1)$

WITH

(13) $J_{eff} = 4\left[E_a(0, \tfrac{1}{2}\pm, \pm 1) - E_a(\tfrac{1}{2}\pm\tfrac{1}{2}, 0, 0)\right]$

$\approx 4\left[\frac{-12t^2}{J} - \left(\frac{-18t^2}{J}\right)\right] \approx \frac{24t^2}{J} > 0$

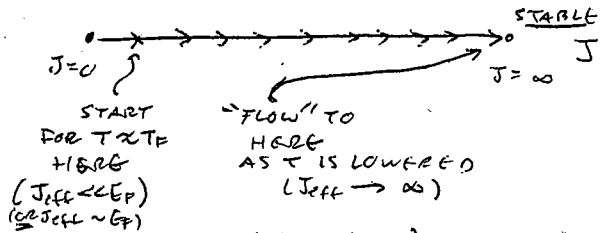
SO THE MODEL IS, LIKE THE ORIGINAL ONE, A $S_I = 1/2$ "IMPURITY (DOUBLET OF SITE 0)" COUPLED ANTIFERROMAGNETICALLY TO SITE 1 CONDUCTION SPIN.

BUT NOW $J_{eff} \sim t^2/J \ll J, t$

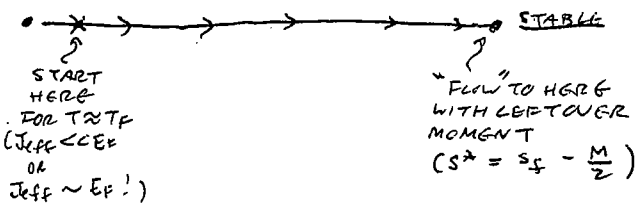
SO THE PROBLEM HAS GONE TO WEAK COUPLING AT WEAK COUPLING, AN ANTIFERRO KONDO COUPLING GROWS WITH $T \to 0$! SO THE STRONG COUPLING LIMIT IS UNSTABLE! BUT SO IS WEAK COUPLING!

LET US CONCEPTUALIZE:

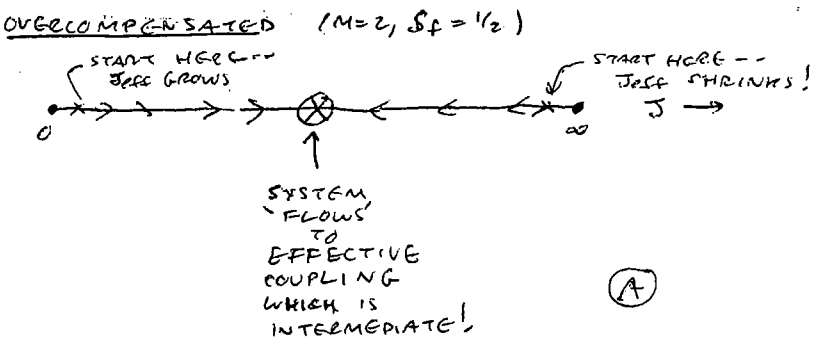
COMPENSATED $(M=1, S_f = 1/2)$



UNDER COMPENSATED $(M=1, S_f = 1)$



OVERCOMPENSATED $(M=2, S_f = 1/2)$



(A)

NOW, AS $T \to 0$, WE PROBE PROPERTIES ON LENTH SCALES OF ORDER $\hbar v_F / k_B T$.

THE TENDENCY OF THE COUPLING TO GO WITH T TO A SINGLE INTERMEDIATE VALUE IMPLIES A SELF SIMILARITY OF THE PROBLEM AS $T \to 0$ -- NAMELY A CRITICAL STATE IS FORMED, WE'LL USE ONE COMPUTATION METHOD WHICH REVEALS THIS STATE.

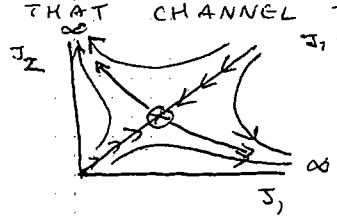
SOURCES OF TWO CHANNEL KONDO

QUADRUPOLAR KONDO

THE QUADRUPOLAR KONDO EFFECT (COX PRL 59, 1240 (1987)) DESCRIBES QUENCHING OF URANIUM ION SHAPE FLUCTUATIONS BY ORBITAL MOTION OF CONDUCTION ELECTRONS. THE SIMPLEST ANDERSON MODEL WHICH GIVES THIS IS SHOWN ON THE NEXT PAGE

(A)

WE CAN SEE INTUITIVELY THAT THE DEGENERACY OF COUPLINGS IS CRUCIAL! IF WE WOULD HAVE $J_1 \neq J_2$, THEN WHICHEVER COUPLING WAS BIGGER INITIALLY WOULD GROW MORE WITH REDUCED T AND WE WOULD 'FLOW' TO THE ORDINARY KONDO EFFECT IN THAT CHANNEL -- THE CRITICAL STATE IS ONLY STABLE TO THE EXTENT $J_1 = J_2$.



ALSO, IF WE SHOULD ADD A FIELD WHICH SPLITS THE LOCAL SPIN DEGENERACY, WE'LL STOP 'FLOWING' TO A CRITICAL STATE AND A DIFFERENT FERMI LIQUID BEHAVIOR CUTS IN.

FIRST, U^{4+} IS ASSUMED THE GROUND CONFIGURATION THIS GIVES ... $5f^2$ $J=4$ HUNDS RULE GROUND MULTIPLET -- FROM THIS ONE CAN HAVE A SO CALLED Γ_3 OR E DOUBLET GROUND STATE IN CUBIC SYMMETRY -- IN TERMS OF $J=4$ WAVE FUNCTIONS

$$|\Gamma_3+\rangle = \sqrt{\frac{5}{24}}\left[|4\rangle + |-4\rangle\right] - \sqrt{\frac{7}{12}}|0\rangle \qquad (14)$$
$$|\Gamma_3-\rangle = \frac{1}{\sqrt{2}}\left[|2\rangle + |-2\rangle\right]$$

[SEE LEA, LEASK, & WOLF, J. CHEM PHYS. SOLIDS, 23 1381 (1962)]

BY WIGNER-ECKART THEOREM, THE QUADRUPOLAR TENSOR

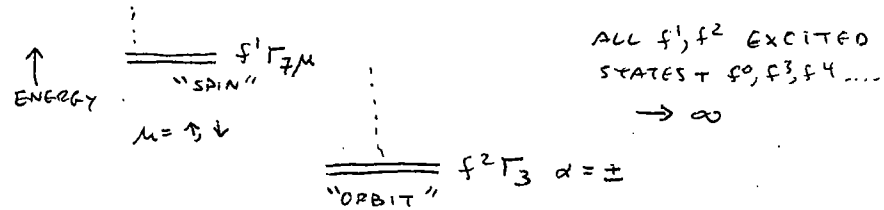
$$\hat{Q}_{00} = \int d^3r \rho_{\Gamma_3}(\vec{r})\left[2z^2 - x^2 - y^2\right] \Rightarrow \hat{Q}_{00})_{OP} \sim 3J_z^2 - J(J+1)$$
$$= 2J_z^2 - J_x^2 - J_y^2 \text{ etc}$$

WE THUS HAVE

STATE	$\mu_z = \langle\alpha\|J_z\|\alpha\rangle$	$Q_{zz} = \langle\alpha\|\hat{Q}_{00})_{OP}\|\alpha\rangle$
$\|\Gamma_3+\rangle$	0	$+\delta$ (PROLATE-STRETCHED)
$\|\Gamma_3-\rangle$	0	$-\delta$ (OBLATE-SQUASHED)

THE DOUBLET DEFINES A PSEUDOSPIN IN 'ORBITAL' OR 'SHAPE' SPACE.

NOW, AS A SIMPLE MODEL, TAKE JUST A DOUBLET FROM f^1 AND ... FROM f^2 ...



CONDUCTION ELECTRONS WHICH COUPLE TO THIS MUST HAVE BOTH SPIN AND ORBIT

LABELS -- SUCH ELECTRON PARTIAL WAVES EXIST!

$k\sigma \Rightarrow k\,3\,m_z\,\sigma \Rightarrow k\,5/2\,m \Rightarrow \begin{cases} k\,5/2\,\Gamma_7\,\mu \\ k\,5/2\,\Gamma_8\,\mu\,\alpha \end{cases}$

(PROJECTION TO f; PROJECTION TO SPIN/ORBIT BASIS; Γ_8 QUARTETS)

[GROUP THEORY: $\Gamma_8 = \Gamma_2 \otimes \Gamma_7$]

HENCE, OUR ANDERSON MODEL IS

$$H = \sum_{k\mu\alpha} \varepsilon_k c^\dagger_{k\mu\alpha} c_{k\mu\alpha} + \varepsilon_f \sum_\alpha |f^2\alpha\rangle\langle f^2\alpha| + \frac{V}{\sqrt{N_s}} \sum_{k\mu\alpha} \left(|f^2\alpha\rangle\langle f^1\mu| c^\dagger_{k\alpha-\mu} + hc \right) \quad (16)$$

APPLYING SCHRIEFFER-WOLF GIVES ($\sum$ SUM ON μ)

$$H_{eff} = \sum_{k\mu\alpha} \varepsilon_k c^\dagger_{k\mu\alpha} c_{k\mu\alpha} + J \vec{\tau}_f \cdot \sum_{k\mu k'\alpha\beta} \vec{\tau}_{c\alpha\beta} c^\dagger_{k\mu\alpha} c_{k'\mu\beta} \qquad (J = -2V^2/\varepsilon_f) \quad (17)$$

WITH $\vec{\tau}_f, \vec{\tau}_c$ SPIN 1/2 MATRICES IN ORBITAL SPACE! BECAUSE THE SPIN IS A SPECTATOR IT SERVES AS A CHANNEL INDEX -- DEGENERACY IS ASSURED IN ABSENCE OF MAGNETIC FIELD.

HOW DO WE INTERPRET THE OPERATORS?

WELL

a) $\tau_f^z = \frac{1}{2}\left[|f^2{+}\rangle\langle f^2{+}| - |f^2{-}\rangle\langle f^2{-}| \right] \sim 3J_z^2 - J(J+1)$

(18) b) $\tau_f^x = \frac{1}{2}\left[|f^2{+}\rangle\langle f^2{-}| + |f^2{-}\rangle\langle f^2{+}| \right] \sim J_x^2 - J_y^2$

c) $\tau_f^y = \frac{1}{2i}\left[|f^2{+}\rangle\langle f^2{-}| - |f^2{-}\rangle\langle f^2{+}| \right] \sim J_x J_y J_z$

(τ_f^z, τ_f^x) FORM A Γ_3 TENSOR DOUBLET (QUADRUPOLAR)

τ_f^y IS AN Γ_2 TENSOR SINGLET (OCTUPOLAR)

YOU MIGHT OBJECT TO THE GROSS OVERSIMPLIFICATION OF THE ANDERSON MODEL IN EQ. (16) -- BUT IN FACT THE ONLY SYMMETRY ALLOWED COUPLING TO THE Γ_3 DOUBLET IS OF THE FORM (17), WITH POSSIBLE ANISOTROPY ($J^y \neq J^x = J^z$). IT TURNS OUT THE GROUND STATE COUPLING IS ISOTROPIC.

SIMILAR CONSIDERATIONS HOLD FOR U^{4+} DOUBLETS IN HEXAGONAL & TETRAGONAL SYMMETRY -- A SLIGHT DIFFERENCE IS THAT THESE HAVE A FORM (ROUGHLY) LIKE

$$|\Gamma\pm\rangle \sim |\pm 1\rangle \quad (\pm \text{ to } m_J)$$

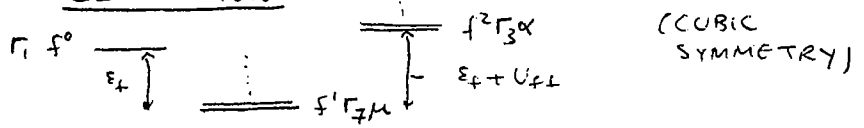
SO $\langle \Gamma\pm | J_z | \Gamma\pm \rangle \neq 0$.

BUT $\langle \Gamma\pm | J_x^2 - J_y^2 | \Gamma\mp \rangle \neq 0$

$\langle \Gamma\pm | J_x J_y + J_y J_x | \Gamma\mp \rangle \neq 0$.

OTHERWISE, A TWO CHANNEL KONDO EFFECT WILL OBTAIN,

CE^{3+} ION (COX, PHYSICA B 186-188 312 (1993); KIM & COX, PHYS REVLETT. 75, 1622 (1995))



(CUBIC SYMMETRY)

IN THIS CASE WE INCLUDE AN f^2 Γ_3 DOUBLET AND AN f^0 SINGLET -- THE CONDUCTION WAVES OF Γ_7 SYMMETRY (SPIN ONLY) MIX f^0 AND f^1 -- WAVES OF Γ_8 (SPIN + ORBIT) MIX Γ_7, Γ_3 -- THE ANDERSON MODEL IS

$$(19)\quad H = \sum_{k\mu} \varepsilon_k c^\dagger_{k7\mu} c_{k7\mu} + \sum_{k\mu\alpha} \varepsilon_k c^\dagger_{k8\mu\alpha} c_{k8\mu\alpha} + \varepsilon_f \sum_\mu |f^1\mu\rangle\langle f^1\mu| + (2\varepsilon_f + U_{ff}) \sum_\alpha |f^2\alpha\rangle\langle f^2\alpha| + \frac{V_7}{\sqrt{N_s}} \sum_{k\mu} \left(|f^1\mu\rangle\langle f^0| c_{k7\mu} + hc \right) + \frac{V_8}{\sqrt{N_s}} \sum_{k\alpha\mu} \left(|f^2\alpha\rangle\langle f^1\mu| c_{k8\mu\alpha} + h.c. \right)$$

AND THE RESULTING KONDO MODEL IS ($\Gamma << |\varepsilon_f|, \varepsilon_f + U_{ff}$)

$$H_{eff} = \sum_{k\mu} \varepsilon_k c^\dagger_{k\Gamma_7\mu} c_{k\Gamma_7\mu} + \sum_{k\mu\alpha} \varepsilon_k c^\dagger_{k\Gamma_8\mu\alpha} c_{k\Gamma_8\mu\alpha}$$
$$+ \frac{J_7}{N_s} \vec{S}_f \cdot \sum_{kk'\mu\nu} (\vec{S}_c)_{\mu\nu} c^\dagger_{k\Gamma_7\mu} c_{k'\Gamma_7\nu} \qquad (20)$$
$$+ \frac{J_8}{N_s} \vec{S}_f \cdot \sum_{kk'\mu\nu\alpha} (\vec{S}_c)_{\mu\nu} c^\dagger_{k\Gamma_8\mu\alpha} c_{k'\Gamma_8\nu\alpha}$$

$J_7 = -2V_7^2/\varepsilon_f$, $J_8 = 2V_8^2/(\varepsilon_f + U_{ff})$

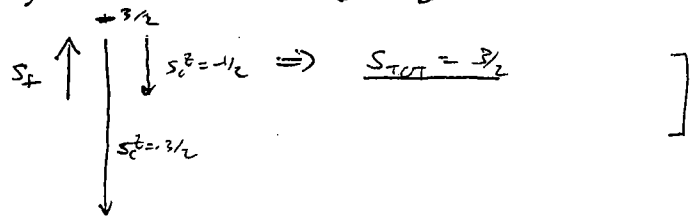
IN THIS CASE, ONE CHANNEL ($M=1$, $S_c = 1/2$) (J_7) COMPETES WITH TWO CHANNEL ($M=2$, $S_c = 1/2$ -- J_8)

FOR $J_8 > J_7$, THE GROUND STATE IS TWO CHANNEL (DOUBLET -- CRITICAL)

$J_8 < J_7$ " " " " ONE CHANNEL (SINGLET - FERMI LIQUID)

$J_8 = J_7$ THE GROUND STATE IS THREE CHANNEL! (TRIPLET - CRITICAL!)

[THIS IS NOT THE MOST GENERAL FORM OF COUPLING FOR A Ce^{3+} ION -- WHAT CAN BE SHOWN IS THAT THE STABLE ~~FIXED POINTS~~ GROUND STATES FOR THE MOST GENERAL MODEL ARE EITHER ONE CHANNEL (TWO POSSIBLE), TWO CHANNEL (ONE POSSIBLE) OR THREE CHANNEL (TWO POSSIBLE). FOR SPECIAL VALUES OF COUPLINGS, AN ∞ OF CRITICAL GROUND STATES IS POSSIBLE -- EG, $M=1$ BUT $S_c = 3/2$



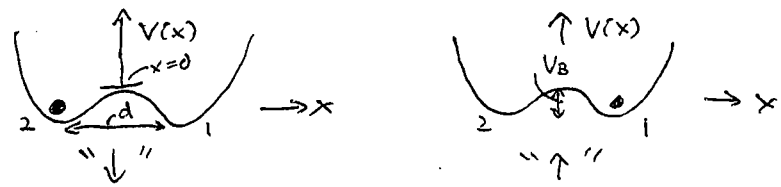
$\Rightarrow$ $S_{TOT} = 3/2$]

THE TWO CHANNEL COUPLING FOR Ce^{3+} IS ONLY POSSIBLE FOR THE Γ_7 DOUBLET IN CUBIC SYMMETRY AND THE $|\pm 3/2\rangle$ DOUBLET IN HEXAGONAL SYMMETRY, GIVEN THE ADDITIONAL $J_8 > J_7$ REQUIREMENT (WHICH ROUGHLY MEANS THE QUANTUM WEIGHT OF f^2 IN THE GROUND STATE EXCEEDS f^0 WEIGHT) IT IS MUCH LESS LIKELY TO SEE THIS THAN THE QUADRUPOLAR KONDO EFFECT.

TWO LEVEL SYSTEM KONDO EFFECT

[SEE A. ZAWADOWSKI AND K VLADÁR, QUANTUM TUNNELING IN CONDENSED MEDIA, EDS. YU. KAGAN AND A.J. LEGGETT (ELSEVIER, AMSTERDAM, 1992)]

IN THIS MODEL, AN ATOM IS CONSIDERED IN A DOUBLE WELL -- THE POSITION BECOMES THE



'SPIN' OF THE IMPURITY, SPONTANEOUS TUNNELING MAY SPLIT THE STATES BY AN AMOUNT Δ^x (A)

ELECTRONS COUPLE TO THE ATOM THROUGH THE SCREENED ION/ATOM INTERACTION U -- THE BARE COUPLING IS

$$(21)\quad H_{INT} = \frac{1}{N_s} \sum_{kk'\mu} \left[V^0_{kk'} c^\dagger_{k\sigma} c_{k'\sigma} + V^z_{kk'} \tau^z_f c^\dagger_{k\sigma} c_{k'\sigma} + V^x_{kk'} \tau^x_f c^\dagger_{k\sigma} c_{k'\sigma} \right]$$

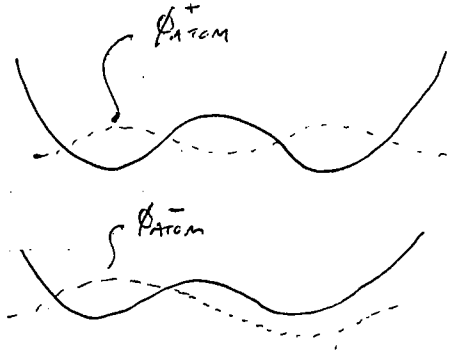
WITH

$$(22)\quad \tau^z_f = \tfrac{1}{2}[|1\rangle\langle 1| - |2\rangle\langle 2|] \qquad \tau^x_f = \tfrac{1}{2}[|1\rangle\langle 2| + |2\rangle\langle 1|]$$

$$(23)(a)\quad V^{(0)}_{kk'} = \int d^3r \left(e^{i(k-k')\cdot r} \tfrac{1}{2}[\phi_1^2(r) + \phi_2^2(r)] \right) U(k-k')$$

(ϕ: ATOMIC WAVE FUNCTIONS)

$$(b)\quad V^z_{kk'} = \int d^3r \left(e^{i(k-k')\cdot r} \tfrac{1}{2}[\phi_1^2(r) - \phi_2^2(r)] \right) U(k-k')$$



AND THE ASSISTED TUNNELING TERM

$$V^x_{kk'} \approx \Delta^x \frac{\lambda U}{24 V_B} (k_x - k'_x)^2 d^2 \quad (24)$$

WITH $\lambda \approx \frac{d\sqrt{2mV_B}}{\hbar}$ (25) THE GAMOW TUNNELING FACTOR,

AND $U(\vec{r}) \approx \frac{U}{m_e!} \delta(\vec{r})$ (26)

AT THE SAME LEVEL OF APPROXIMATION,

$$V^z_{kk'} \approx \frac{1}{2} (k_z - k'_z) d\, U \quad (27)$$

NOW, WE CAN EXPAND THE CONDUCTION STATES IN PARTIAL WAVES ABOUT THE ORIGIN --- THE AXIAL CHARACTER ENSURES THAT ONLY WAVES WITH THE SAME m_ℓ VALUE (QUANTIZED ALONG X-AXIS) WILL SURVIVE --- $V^z_{kk'}$ MUST MIX EVEN & ODD PARITY, $V^x_{kk'}$ WILL NOT FLIP PARITY -- RESTRICT TO $m_\ell = 0$, $\ell = 0, 1$ (S, P). [SUCH A RESTRICTION TO A 2 FOLD DEGENERATE SPACE CAN BE JUSTIFIED EX POST FACTO ---] THEN

S, P BASIS ($\alpha = S, P$) 1, 2 BASIS

$$\sum_{kk'} V^z_{kk'} C^+_{k\sigma} C_{k'\sigma} \Rightarrow V^z_0 \widetilde{\tau}^x_{c\alpha\beta} C^+_{k\alpha\sigma} C_{k'\beta\sigma} \Rightarrow V^z_0 \tau^z_{c\alpha\alpha} C^+_{k\alpha\sigma} C_{k'}$$

$$\widetilde{\tau}^x_{\alpha\beta} = \tfrac{1}{2}[|S\rangle\langle P| + |P\rangle\langle S|] \qquad C_{kS\sigma} = \tfrac{1}{\sqrt{2}}(C_{k1\sigma} + C_{k2\sigma})$$

$$C_{kP\sigma} = \tfrac{1}{\sqrt{2}}(-C_{k1\sigma} + C_{k2\sigma})$$

$$\sum_{kk'} V^x_{kk'} C^+_{k\alpha} C_{k'\sigma} \Rightarrow V^x_0 \widetilde{\tau}^z_{c\alpha\alpha} C^+_{k\alpha\sigma} C_{k'\alpha\sigma} \Rightarrow V^x_0 \tau^x_{c\alpha\beta} C^+_{k\alpha\sigma} C_{k'}$$

$$\widetilde{\tau}^z = \tfrac{1}{2}[|S\rangle\langle S| - |P\rangle\langle P|] \qquad \tau^z_c = \tfrac{1}{2}[|1\rangle\langle 1| - |2\rangle\langle$$

$$\tau^x_c = \tfrac{1}{2}[|1\rangle\langle 2| + |2\rangle$$

AND (NEGLECTING V^0)

$$H_{eff} = \sum_{k\alpha\sigma} \varepsilon_k C^+_{k\alpha\sigma} C_{k\alpha\sigma} + \Delta^x \tau^x_f + \frac{V^z_0}{N_S} \sum_{kk'\alpha\beta\sigma} (\tau^z_f \tau^z_c)_{\alpha\beta} C^+_{k\alpha\sigma} C_{k'\beta}$$
$$+ \frac{V^x_0}{N_S} \sum_{kk'} (\tau^x_f \tau^x_c)_{\alpha\beta} C^+_{k\alpha\sigma} C_{k'\beta\sigma} \quad (28)$$

RECENTLY, ALTSHULER & ALEINER HAVE SHOWN THAT PROPER INCLUSION OF EXCITED VIBRATIONAL STATES IN THE QUARTIC POTENTIAL LEADS TO A SITUATION WHERE $V^* << \Delta^*$, MEANING IT IS UNLIKELY THE LINEAR TLS MODEL CAN EVER REACH THE TWO CHANNEL KONDO REGIME.

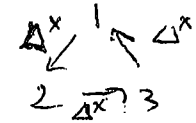
(ALEINER ETAL, PRB 63 201401 [2001]
PRL 86 2629 [2001]

)

A POTENTIAL RESOLUTION TO THIS PROBLEM IS TO CONSIDER ATOMIC MOTION WHICH IS SYMMETRY PROTECTED FROM SPONTANEOUS TUNNELING

CMOUSTAKAS & FISHER,
PRB 51 6908 [1995]
PRB 53 4300 [1996]
PRB 55 6832 [1997])

THE IDEA IS THAT AN ATOM MIGHT MOVE AMONGST 3 SITES,



THEN THE 'CHIRAL PAIR' OF ATOM ORBITALS

$$|\pm\rangle = \frac{1}{\sqrt{3}}\left[|1\rangle + e^{\pm 2\pi i/3}|2\rangle + e^{\pm 4\pi i/3}|3\rangle\right]$$

FORM THE TLS WITH ASSURED DEGENERACY PROVIDED TRIANGULAR SYMMETRY IS MAINTAINED,

HOWEVER, IT IS UNCLEAR HOW TO STABILIZE THIS DOUBLET GENERICALLY OVER THE SINGLET

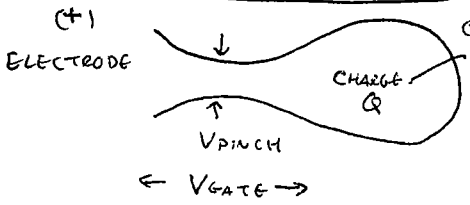
$$|0\rangle = \frac{1}{\sqrt{3}}\left[|1\rangle + |2\rangle + |3\rangle\right]$$

AT THE MOMENT, EXPERIMENTAL PHENOMENOLOGY POINTS SO STRONGLY TO AN ATOMIC TLS MODEL THAT SUCH CANDIDATES ARE WORTHY OF FURTHER EXPLORATION!

THIS HAS THE FORM OF AN ANISOTROPIC TWO CHANNEL KONDO MODEL (CHANNEL = MAG. SPIN -- A SPECTATOR AS IN THE QUADRUPOLAR KONDO MODEL--) FOR $T \to 0$ THE ANISOTROPY IS REMOVED.

COULOMB BLOCKADE

EMATUEEV, PRB 51 1943 (1995))



FOR A QUANTUM DOT THERE IS CHARGING ENERGY AND ($\alpha = \pm$)

$$(29)\quad H = \sum_{k\alpha\sigma} \varepsilon_k c^\dagger_{k\alpha\sigma} c_{k\alpha\sigma} + \frac{Q^2}{2C} + \phi Q + \sum_{kp} \left[\frac{\tau_{kp}}{N_S} c^\dagger_{k+\sigma} c_{p-\sigma} + h.c. \right]$$

WITH ϕ THE ENERGY SHIFT DUE TO V_{GATE} ($\phi \sim V_{GATE} \times$ GEOMETRY FACTOR)

CHOOSING $\phi = -\frac{e}{2C} + u$, $|u| \ll \frac{e}{C}$

BY TUNING V_{GATE} ALLOWS US TO RESTRICT TO $Q = 0, 1$ SPACE -- THEN THE PROJECTED HAMILTONIAN IS

$$(30)\quad H' = \sum_{k\alpha\sigma} \varepsilon_k c^\dagger_{k\alpha\sigma} c_{k\alpha\sigma} + eu\,|1\rangle\langle 1| + \sum_{kp} \left[\frac{\tau_{kp}}{N_S} c^\dagger_{k+\sigma} c_{k-\sigma} |0\rangle\langle 1| + h.c. \right]$$

PUT $I^z_f = \frac{1}{2}[|1\rangle\langle 1| - |0\rangle\langle 0|]$ SO $|1\rangle\langle 1| = \frac{1}{2} + I^z$

$I^+_f = |0\rangle\langle 0|$ $\qquad I^-_f = |0\rangle\langle 1|$

$I^z_{c(0)} = \frac{1}{N_S} \sum_{kk'\sigma} c^\dagger_{k+\sigma} c_{k'-\sigma} = \left(I^-_{c(0)}\right)^+$

AND TAKE $\tau_{kp} \approx \tau$ = CONSTANT

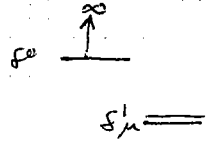
THEN

$$(31)\quad H' \approx \sum_{k\alpha\sigma} \varepsilon_k c^\dagger_{k\alpha\sigma} c_{k\alpha\sigma} + eu\left(\tfrac{1}{2} + I^z_f\right) + \frac{\tau}{N_S}\left(I^+_f \sum_{kk'\sigma} c^\dagger_{k-\sigma} c_{k'+\sigma} + h.c.\right)$$

THIS IS A PLANAR TWO CHANNEL KONDO MODEL.

CRITICAL BEHAVIOR

TO GET A FLAVOR OF THE CRITICAL BEHAVIOR WE'LL GO TO OUR Ce^{3+} MODEL BUT TAKE (ARTIFICIALLY) $f^0 \to \infty$. THEN



WE HAVE A MAGNETIC TWO CHANNEL KONDO MODEL FOR $k_B T \ll \Gamma$ --

PUT $V_\ell = V$, $\Gamma = \pi N(0) V^2$ -- WE PERTURB IN V AND GENERALIZE FROM OUR EARLIER KONDO THEORY ... INTRODUCE "GREEN'S FUNCTIONS"

$$(32a)\quad G_1(\omega) = \frac{1}{\omega - \tilde{\varepsilon}_f - \quad} \quad (V=0) \Rightarrow \frac{1}{\omega - \tilde{\varepsilon}_f - \Sigma_1(\omega)} \quad (V \neq 0)$$

Σ: RE PART: LEVEL SHIFT; IM PART: BROADENING

$$(32b)\quad G_2(\omega) = \frac{1}{-\omega} \Rightarrow \frac{1}{\omega - \Sigma_2(\omega)}$$

"SELF ENERGIES"

PERTURBATIVE $\qquad$ SELF CONSISTENT

$$(33a)\quad \Delta E_1 = \sum_\alpha 2V^2 \int d\varepsilon N(\varepsilon) f(\varepsilon) \frac{1}{\omega + \varepsilon} \Rightarrow \Sigma(\omega) = 2V^2 \int d\varepsilon f(\varepsilon) \frac{N(\varepsilon)}{\omega + \varepsilon - \Sigma_2(\omega)}$$

$\omega = \tilde{\varepsilon}_f$ INTERMEDIATE ENERGY

$$= 2V^2 \int d\varepsilon f(\varepsilon) N(\varepsilon)\, G_2(\omega + \varepsilon)$$

PERTURBATIVE

$$\Delta E_2 = 2V^2 \int d\varepsilon \frac{(1-f(\varepsilon))N(\varepsilon)}{\omega - (\tilde{\varepsilon}_f + \varepsilon)}$$

Σ_μ ; $\omega = 0$; $\tilde{\varepsilon}_f + \varepsilon$ = INTERMEDIATE ENERGIES

SELF-CONSISTENT

$$\Rightarrow \Sigma_2(\omega) = 2V^2 \int d\varepsilon \frac{N(\varepsilon)(1-f(\varepsilon))}{\omega - (\tilde{\varepsilon}_f + \varepsilon + \Sigma_1(\omega-\varepsilon))}$$

$$= 2V^2 \int d\varepsilon N(\varepsilon)(1-f(\varepsilon)) G_1(\omega-\varepsilon) \quad (33b)$$

THE SELF CONSISTENT EQUATIONS (INTEGRAL) (33a,b) ARE CALLED THE NON CROSSING APPROXIMATION (NCA), WE WANT TO SHOW

i) THESE HAVE POWER LAW SOLUTIONS
ii) THE MAGNETIC SUSCEPTIBILITY IS LOG DIVERGENT.

i) POWER LAWS

LET US TRY AS ANSATZ (E_0 = GROUND STATE ENERGY RELATIVE TO FERMI SEA)

$$(34a)\ \Sigma_1(\omega) \approx E_0 - \tilde{\varepsilon}_f + g_1 (E_0-\omega)^{\alpha_1} \qquad \omega \to E_0,\ T=0$$

$$(34b)\ \Sigma_2(\omega) \approx E_0 + g_2 (E_0-\omega)^{\alpha_2} \qquad \omega \to E_0,\ T=0$$

FOR $\omega < E_0$ Σ_1, Σ_2 ARE REAL -- FOR $\omega > E_0$

$$\left.\begin{aligned} \Sigma_1(\omega) &\to E_0 - \tilde{\varepsilon}_f + g_1 e^{-i\pi\alpha_1} |E_0-\omega|^{\alpha_1} \\ \Sigma_2(\omega) &\to E_0 + g_2 e^{-i\pi\alpha_2} |E_0-\omega|^{\alpha_2} \end{aligned}\right\} \quad \omega \to E_0,\ T=0$$

WITH THIS CHOICE

$$(35a)\quad G_1(\omega) \underset{\omega \to E_0}{\approx} -\frac{1}{g_1}(E_0-\omega)^{-\alpha_1}$$

$$(35b)\quad G_2(\omega) \underset{\omega \to E_0}{\approx} -\frac{1}{g_2}(E_0-\omega)^{-\alpha_2}$$

NOW FOR $\omega > E_0$

$$(36)\ -\mathrm{Im}\,\Sigma_1(\omega) = -\mathrm{Im}\,2V^2 \int_{-D}^{0} d\varepsilon\, N(\varepsilon)\, G_2(\omega+\varepsilon))$$

$$= \frac{2\Gamma}{\pi} \int_{E_0-\omega}^{0} d\varepsilon \frac{\sin\pi\alpha_2}{g_2} |\omega+\varepsilon-E_0|^{-\alpha_2}$$

$$= \frac{2\Gamma}{\pi} \frac{\sin\pi\alpha_2}{g_2(1-\alpha_2)} |\omega-E_0|^{1-\alpha_2} \theta(\omega-E_0)$$

$$\text{SO} \quad g_1 = \frac{\frac{2\Gamma}{\pi}\frac{\sin\pi\alpha_2}{g_2(1-\alpha_2)}}{\sin\pi\alpha_1} = \frac{2\Gamma}{\pi}\frac{1}{g_2(1-\alpha_2)} \quad (37)$$

SINCE $\boxed{\alpha_1 = 1-\alpha_2}$ (EF)

NEXT:

$$(39)\ -\mathrm{Im}\,\Sigma_2(\omega) = \frac{2\Gamma}{\pi} \int_0^{\omega-E_0} d\varepsilon \frac{\sin\pi\alpha_1}{g_1} |\omega-\varepsilon-E_0|^{-\alpha_1}$$

$$= \frac{2\Gamma}{\pi}\cdot\frac{\pi}{2\Gamma}\cdot\frac{g_2(1-\alpha_2)}{\sin\pi\alpha_1}\frac{\sin\pi\alpha_1}{1-\alpha_1}|\omega-E_0|^{1-\alpha_1}\theta(\omega-E_0)$$

BUT THIS IMPLIES, SINCE $-\mathrm{Im}\,\Sigma_2 = \sin\pi\alpha_2\, g_2 |\omega-E_0|^{\alpha_2} \times\theta(\omega-E_0)$

THAT

$$1 = \frac{1-\alpha_2}{1-\alpha_1} = \frac{1-\alpha_2}{\alpha_2} \Rightarrow \boxed{\alpha_2 = 1/2 = \alpha_1} \quad (40)$$

HENCE

$$G_1(\omega) \approx \frac{1}{g_1}(E_0-\omega)^{-1/2} \qquad G_2(\omega) \approx \frac{1}{g_2}(E_0-\omega)^{-1/2}$$

IT CAN BE SHOWN

$$g_1 = 2k_B T_K / [\#\, k_B T_K]^{1/2} \qquad g_2 = \frac{2\Gamma}{\pi} / [\#\, k_B T_K]^{1/2}$$

SO

$$G_1(\omega) \approx \frac{1}{2k_B T_K}\left[\frac{E_0-\omega}{k_B T_K}\right]^{-1/2} \qquad G_2(\omega) \approx \frac{\pi}{2\Gamma}\left[\frac{E_0-\omega}{k_B T_K}\right]^{-1/2}$$

ii) THE BOLTZMANN WEIGHTS FOR f^1, f^2 ARE

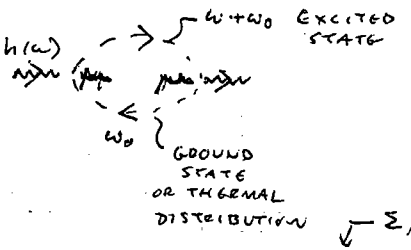
$$\frac{1}{Z_f}\int \frac{d\varepsilon}{\pi} e^{-\beta\varepsilon} \underbrace{(-\mathrm{Im}\,G_1(\varepsilon))}_{A_1(\varepsilon)} \qquad \frac{1}{Z_f}\int \frac{d\varepsilon}{\pi} \underbrace{(-\mathrm{Im}\,G_2(\varepsilon))}_{A_2(\varepsilon)} e^{-\beta}$$

$$\left(\begin{array}{c} V=0 \\ \frac{e^{-\beta\tilde{\varepsilon}_f}}{2e^{-\beta\tilde{\varepsilon}_f}+2} \end{array}\right) \qquad \left(\begin{array}{c} V=0 \\ \frac{1}{2e^{-\beta\tilde{\varepsilon}_f}+2} \end{array}\right)$$

$[A_1(\varepsilon) = \pi\delta(\varepsilon-\tilde{\varepsilon}_f)]$ $\qquad$ $[A_2(\varepsilon) = \pi\,\delta(\varepsilon)]$

$$Z_f = 2\int \frac{d\varepsilon}{\pi} e^{-\beta\varepsilon}\left[A_1(\varepsilon) + A_2(\varepsilon)\right]$$

IN LINEAR RESPONSE TO AN APPLIED AC MAGNETIC FIELD $h(\omega) = h_0 e^{-i\omega t}$, THE Ce^{3+} ION WILL HAVE A SUSCEPTIBILITY GIVEN BY THE POLARIZATION "BUBBLE"



$$\text{SO}\quad \chi_f(\omega) \sim -\frac{2\mu^2}{Z_f}\int \frac{d\varepsilon}{\pi} e^{-\beta\varepsilon} A_1(\varepsilon)\left[G_1(\omega+\varepsilon) + G_1(\varepsilon-\omega)\right]$$

($\Sigma\mu^2$: "CLOSED LOOP"; $G_1(\omega+\varepsilon)$: ABSORB FIELD QUANTA; $G_1(\varepsilon-\omega)$: EMIT QUANTA)

IM χ_f: ABSORPTION OF FIELD ENERGY
RE χ_f: REACTIVE RESPONSE TO FIELD.

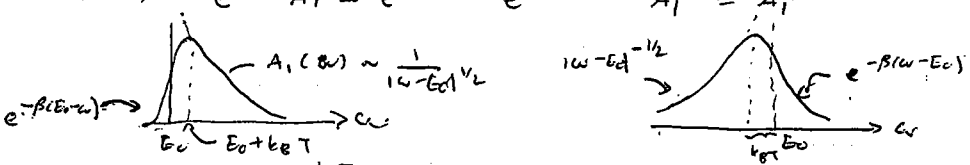
$\omega \to 0$: RESPONSE TO STATIC FIELD

SO

$$\chi_f(0,T) \approx -\frac{1}{Z_f}\int \frac{d\varepsilon}{\pi} e^{-\beta\varepsilon} A_1(\varepsilon)\, \mathrm{Re}\, G_1(\varepsilon)$$

NOW, THE $|E_0-\omega|^{-1/2}$ SINGULARITY WILL HOLD ONLY FOR $k_BT \gtrsim |E_0-\omega| \gtrsim k_BT$

ALSO: $e^{-\beta\varepsilon} A_1 \approx e^{-\beta E_0}\, e^{-\beta(\varepsilon-E_0)} A_1 = A_1^{(-)}$



$$\text{SO}\quad \chi_f \sim \frac{1}{T_K}\int_{-k_BT_K}^{-k_BT} \frac{d\varepsilon}{|\omega-E_0|^{1/2}}\,\frac{1}{|\omega-E_0|^{1/2}} \sim \frac{1}{T_K}\ln\left(\frac{T_K}{T}\right)$$

($|\omega-E_0|^{-1/2}$: A_1; $\frac{1}{|\omega-E_0|^{1/2}}$: $\mathrm{Re}\, G_1$)

ONE CAN ALSO SHOW:

$$C_f \sim \frac{T}{T_K}\ln\frac{T_K}{T} \qquad \left[\frac{\pi^2 k_B^2}{\mu_{eff}^2 S(S+1)}\frac{\chi_f}{C_f/T} = \frac{8}{3}\right]$$

$$\rho_f(T) \sim \frac{1}{\kappa\pi N(0)}\left[1 - a\sqrt{\frac{T}{T_K}} + \cdots\right]\frac{m}{ne^2}$$

$$\Delta S(0) = \frac{k_B}{2}\ln 2$$

NOTE: THE $\ln T$ IN χ_f, C_f HOLD BELOW $\sim T_K/2$ -- THE $\sqrt{T}$ IN $\rho_f(T)$ HOLDS BELOW $\sim T_K/20$.

EXPERIMENT

$Y_{0.8}U_{.2}Pd_3$ -- QUAD KONDO CANDIDATE (CUBIC)

(C. SEAMAN ET AL, PRL 67 2882 (1991))

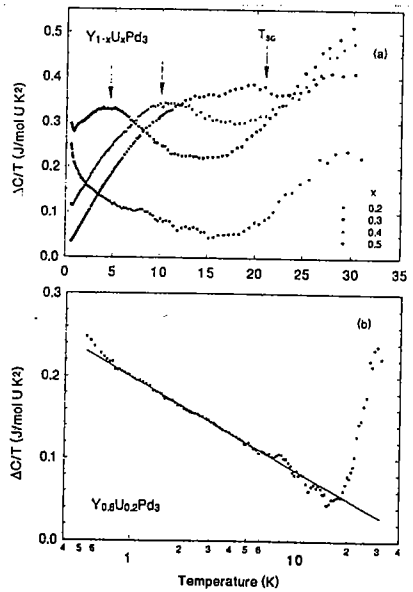


FIG. 2. (a) Temperature dependence of the electronic specific heat per U, $\Delta C(T)/T$ vs T, for $Y_{1-x}U_xPd_3$, $0.2 \le x \le 0.5$. T_{SG} is the peak position of $\Delta C(T)/T$ associated with apparent spin-glass freezing; $\chi(T)$ shows an onset to irreversibility at the same temperature. Note (i) the lack of a peak for $x = 0.2$, and (ii) the upturn near 20 K due to an apparent excited-state Schottky anomaly. (b) $\Delta C(T)/T$ vs $\ln T$ for $Y_{0.8}U_{0.2}Pd_3$. The solid line represents a least-squares fit of the data by the form $-(0.25/T_K)\ln(T/0.41T_K)+b$ [9]. From the slope we obtain $T_K = 42$ K, and the background coefficient b is 61 mJ/mol K^2, which likely arises from an excited-state Schottky anomaly.

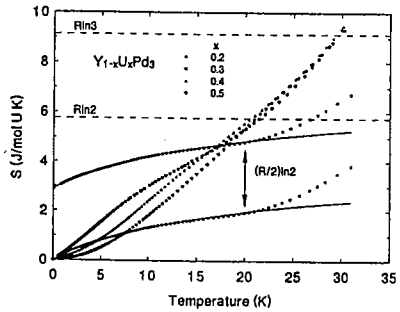


FIG. 3. Temperature dependence of the added electronic entropy per U, $\Delta S(T) - \Delta S(0)$, vs T for $Y_{1-x}U_xPd_3$ derived from the data of Fig. 2. While $\Delta S(T)$ for $0.3 \le x \le 0.5$ converges to $-R\ln(2)$ near -20 K, suggestive of freezing out of a doublet ground state, $\Delta S(T) - \Delta S(0)$ is greatly reduced for $x = 0.2$ with apparent saturation to $(R/2)\ln(2)$, suggestive of a ground-state entropy of the same value (offset curve). The upturn above 20 K is likely due to an excited-state Schottky anomaly. The solid line through the $x = 0.2$ data is obtained from the fit of Fig. 2(b).

BUT: SPIN GLASS NEARBY!

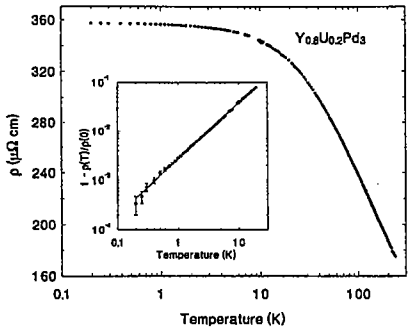


FIG. 1. Temperature dependence of the electrical resistivity $\rho(T)$ of $Y_{0.8}U_{0.2}Pd_3$. The data follow $-\ln T$ behavior, indicative of the Kondo effect, above about 80 K and saturate below ~20 K (inset) with power-law behavior $\rho/\rho(0) = 1 - (T/T_0)^n$, with best fit using $\rho(0) = 357.7\ \mu\Omega$ cm, $n = 1.13$, and $T_0 = 180$ K.

$\rho(T) \sim$ LINEAR -- EXPECT $\sqrt{T}$!

$Th_{1-x}U_xRu_2Si_2$ -- QUAD KONDO CANDIDATE (TETRAGONAL)

(K. AMITSUKA ET AL PHYSICA B 186-188, 336 (1993)).

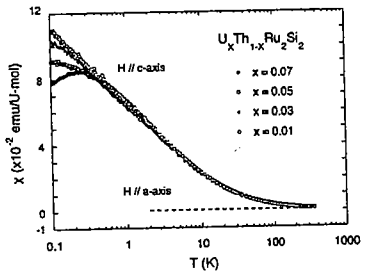


Fig. 1. Logarithmic temperature dependence of the magnetic susceptibility of $U_xTh_{1-x}Ru_2Si_2$ single crystals for $x \leq 0.07$.

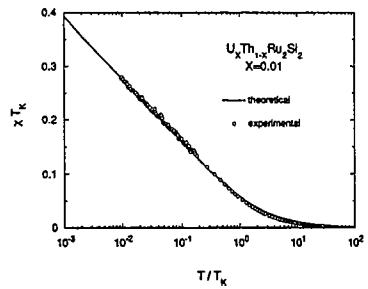


Fig. 5. Comparison between the magnetic susceptibility for $U_xTh_{1-x}Ru_2Si_2$ ($x = 0.01$), scaled by using $\mu = 1.7\mu_B$ and $T_K = 11.1$ K, and the calculations based on the two-channel Kondo model (solid line) [10].

SINGLE ION EFFECT ($T \gtrsim 0.5$K)

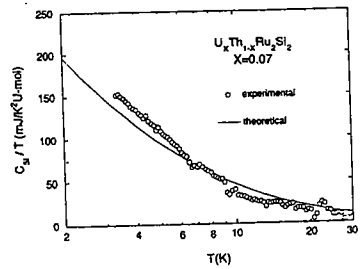


Fig. 2. Logarithmic temperature dependence of the 5f-electronic specific heat for $U_xTh_{1-x}Ru_2Si_2$ ($x = 0.07$), and the theoretical calculations (solid line) based on the two-channel Kondo model [10] with $T_K = 11.1$ K.

@ ZERO PARAMETER FIT!

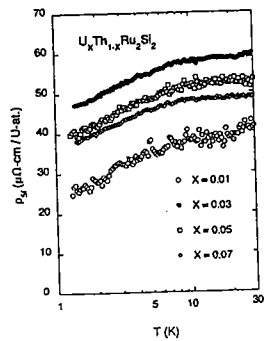


Fig. 4. Logarithmic temperature dependence of the 5f-electronic contribution to the resistivity for the $U_xTh_{1-x}Ru_2Si_2$ single crystals for $x \leq 0.07$.

BUT: WEIRD RESISTIVITY!

$La_{1-x}Ce_xCu_2Si_2$ MAGNETIC CANDIDATE (PSEUDOCUBIC)
CANDRAKA, PHYS REV B 42, 3591 (1992))

* $R = \frac{2.7}{R_{exp}}$ $R_{THEORY} = \frac{8}{3}$! (CX = 0.1)

* $\frac{C}{T}$ ↑ VS IN APPLIED FIELD (REMOVAL OF RESIDUAL ENTROPY)

PARTIAL SUMMARY -- HEAVY FERMION NFL

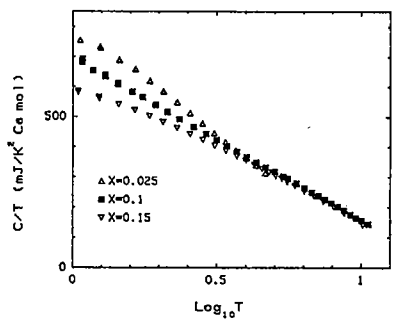


FIG. 1. C/T vs $\log_{10}T$ for $Ce_xLa_{1-x}Cu_{2.2}Si_2$; x=0.025, 0.1, and 0.15.

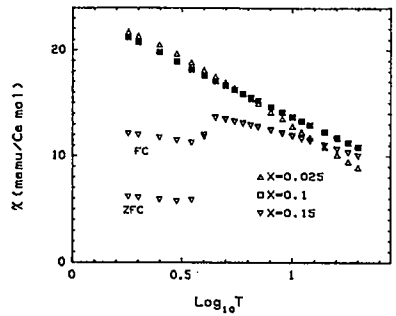


FIG. 2. χ vs $\log_{10}T$ for $Ce_xLa_{1-x}Cu_{2.2}Si_2$; x=0.025, 0.1, and 0.15. Measurements were performed at H=1 kG for x=0.025 and x=0.1, and at H=100 G for x=0.15. Points labeled ZFC (FC) correspond to the zero-field-cooled (field-cooled) χ.

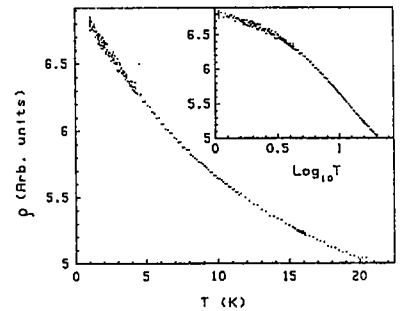


FIG. 3. Resistance (ρ) vs temperature for $Ce_{0.1}La_{0.9}Cu_{2.2}Si_2$. The inset shows ρ vs $\log_{10}T$.

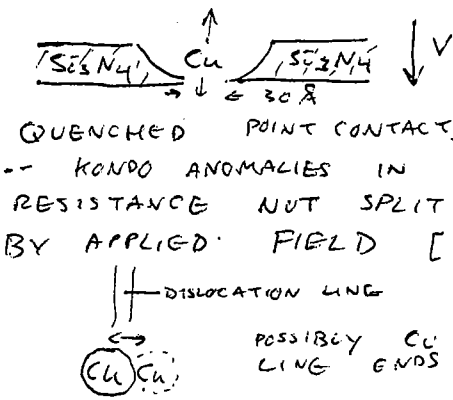
BUT: * $S(T\to 0) > 0$ (EXPECT < 0)
* SPIN GLASS NEARBY!

Table 2. Examples of f-electron systems which exhibit characteristic non Fermi liquid behavior in the low temperature electrical resistivity $\rho \sim 1 - aT/T_K$, specific heat $C/T \sim (-1/T_K)\ln(T/aT_K)$, and magnetic susceptibility $\chi \sim 1 - a(T/T_K)^{1/2}$.

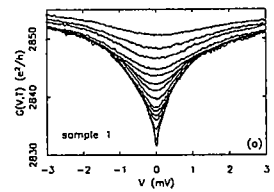
System	ρ	C/T	χ	T_K
$La_{0.9}Ce_{0.1}Cu_2Si_2$	yes	yes	— $\ln T$	9 K
$M_{1-x}U_xPd_3$	yes	yes	yes	40-220 K
$UCu_{3.5}Pd_{1.5}$	yes	yes	yes	28 K
$Th_{1-x}U_xPd_2Al_3$	yes	yes	yes	40 K
$Th_{1-x}U_xRu_2Si_2$	(a<0)	yes	$-\ln(T/aT_K)$	11 K
$Th_{0.1}U_{0.9}Be_{13}$	(a<0)	yes	yes	8 K
$CeCu_{5.9}Au_{0.1}$	(a<0)	yes	yes	3.5 K

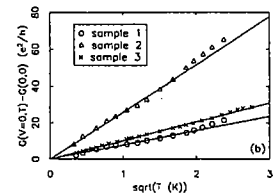
*Deduced from the slope $A = d(C/T)/d\ln T$ of the logarithmic divergence in the specific heat: $T_K = -0.251R/A$

TWO LEVEL SYSTEM KONDO



[DC RALPH & RBUHRMAN(1), RALPH ETAL(2)
(1) PRL 69 2118 (1992)
(2) PRL 72 1064 (1994)]





V=0
← ρCONTACT
~ ρ(0)[1-A√T]

FIG. 1. (a) Differential conductance of sample 1 at various T, from 0.4 K (bottom) to 5.6 K (top). (Specific values are listed in Fig. 2.) (b) Zero-bias conductance for 3 samples. Extrapolated values of $G(0,0)$ are for sample 1: $2830e^2/h$, sample 2: $3970e^2/h$, and sample 3: $30.8e^2/h$.

DYNAMICAL MEAN FIELD THEORY:

SELF CONSISTENT QUANTUM IMPURITIES

HUBBARD MODEL LIMIT OF LARGE SPATIAL DIMENSION

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

$U=0$, HYPERCUBIC LATTICE

WHAT'S THE DOS?

$$\varepsilon_k = -2t \sum_{i=1}^{D} \cos(k_i a) = -t \sum_{\vec{k} \in \text{N.N.}} e^{i \vec{k} \cdot \vec{\ell}}$$

$\sum$ SAMPLES

SUM OF D RANDOM VARIABLES DISTRIBUTED BETWEEN $-1, 1$.

$\therefore$ BY CENTRAL LIMIT THEOREM, WE EXPECT

$$N_0(\varepsilon) = \frac{1}{N_s} \sum_k \delta(\varepsilon - \varepsilon_k) \approx \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\varepsilon^2/2\sigma^2}$$

WHAT'S σ?

DIRECT CALCULATION:

$$N_0(\varepsilon) = \left(\prod_{i=1}^{D} \int_{-\pi}^{\pi} \frac{dx_i}{2\pi} \right) \delta\left(\varepsilon + 2t \sum_{i=1}^{D} \cos x_i\right)$$

$$= \int_{-\infty}^{\infty} \frac{dz}{2\pi} e^{iz\varepsilon} \left(\prod_{i=1}^{D} \int_{-\pi}^{\pi} \frac{dx_i}{2\pi} e^{2izt\cos x_i} \right)$$

$$= \int_{-\infty}^{\infty} \frac{dz}{2\pi} e^{iz\varepsilon} \left(J_0(2tz)\right)^D$$

$$= \int_{-\infty}^{\infty} \frac{dz}{2\pi} \exp\left[iz\varepsilon + D \ln\left[J_0(2zt)\right]\right)$$

APPLY STEEPEST DESCENTS:

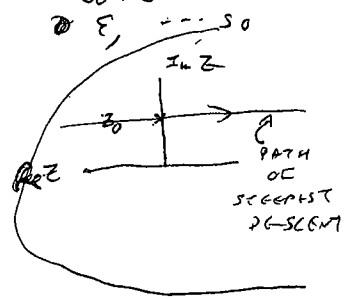
$$\frac{d}{dz}\left[iz\varepsilon + D \ln J_0(2zt)\right] = 0$$

$$i\varepsilon + \frac{D J_0'(2z_0 t)}{J_0(2z_0 t)} = 0 \qquad \text{AT} \quad z_0.$$

LARGE D WILL CESTRICT J_0'/J TO BE SMALL FOR FIXED ε, SO WE CAN USE

$$J_0(x) \approx 1 - x^2/4$$

$$J_0'(x) \approx -x/2$$



AND

$$z_0 \approx \frac{i\varepsilon}{2t^2 D} + \mathcal{O}\left(\frac{1}{D^3}\right)$$

AND

$$\left[iz\varepsilon + D \ln J_0(2tz)\right]\Big|_{z_0} \approx -\frac{\varepsilon^2}{4t^2 D}$$

HENCE $\boxed{\sigma^2 = 2t^2 D = (t^*)^2}$

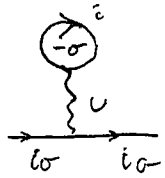
AND WE HOLD $t^2 D$ FIXED TO GET A SENSIBLE LARGE D LIMIT. NORMALIZING FOR DOING FLUCTUATION INTEGRAL) GIVES

$$N_0(\varepsilon) \approx \frac{1}{\sqrt{2\pi}\,t^*} \exp\left(-\frac{\varepsilon^2}{2t^{*2}}\right)$$

$U \neq 0$: WHAT CAN WE EXPECT?

DIAGRAMMATICS: $\overset{\sigma}{\uparrow}$ t $\sim$ U $\quad i \rightarrow j$ $\quad G^0_{ij}$ (NONINTERACTING)

HARTREE :

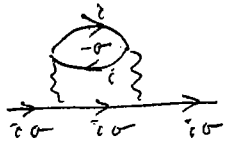


$\Theta(1/D)^0$

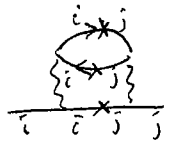
$\Theta(1/D)^0$: $t^2 \times \sum_j$ ($\sim D$) $\sim \frac{1}{D}$

$\therefore$ ALL HARTREE ARE $\Theta(1/D)^0$.

2ND ORDER :



$\Theta(1/D)^0$



$\sim t^{3|i-j|} \sim D^{-\frac{3}{2}|i-j|}$

SELF ENERGY IS LOCAL! (OFFSITE $\sim \frac{1}{D^{n/2}}$)

[NB: FOR NONLOCAL INTERACTIONS SELF ENERGY IS LOCALIZED TO A "CLUSTER" -- EC, A, SCHILLER]

(RELATIVELY FEW TERMS × SIMPLE FORM FACTORS IN $\vec{k}$)

THIS HOLDS UP TO ALL ORDERS IN U.
HENCE, FOR $D \to \infty$

$$\Sigma(\vec{k}, \omega) \longrightarrow \Sigma(\omega)$$

HOW TO FIND $\Sigma(\omega)$? LOCALITY $\Rightarrow$ SELF CONSISTENT IMPURITY.

(1) LOCAL GREEN'S FUNCTION

$$G_{00}(\omega) = G_{ii}(\omega) = \int dt\, e^{i\omega t}\left(-i\langle T c_{i\sigma}(t) c^{+}_{i\sigma}(0)\rangle\right)$$

$$= \frac{1}{N_s}\sum_{\vec{k}} G(\vec{k}, \omega)$$

$$= \frac{1}{N_s}\sum_{\vec{k}} \frac{1}{\omega - \{\vec{k} - \mu - \Sigma(\omega)}$$

$$= \int d\varepsilon\, N_0(\varepsilon)\, \frac{1}{\omega - \varepsilon + \mu - \Sigma(\omega)}$$

HOW TO COMPUTE Σ?

(2) PICK A SITE i -- CALL IT ORIGIN

$$G_{00}^{-1}(\omega) = \underbrace{\mathcal{G}^{-1}(\omega)}_{\text{GREEN'S FUNCTION WITH ONE SITE (i) OUT. "WEISS FUNCTION"}} - \Sigma(\omega)$$

PROOF: $\mathcal{G}^{-1}(\omega)$ = GREEN'S FUNCTION OF SYSTEM WITH ONE SITE CONEY ADDED BACK, BUT $U = 0$.

$$\mathcal{G}^{-1}(\omega) = \omega + \mu - t^2 \sum_{ij} \underbrace{\tilde{G}_{ij}(\omega)}_{\text{INTERACTING PROPAGATOR FOR SYSTEM WITH } i \text{ OUT!}}$$

GRAPHICALLY:

$$\tilde{G}_{ij} = \underbrace{G_{ij}}_{\text{FULL LATTICE}} - \underbrace{\frac{G_{i0}\,G_{0j}}{G_{00}}}_{\text{SUBTRACT THOSE GOING FROM } i \to j \text{ VIA } 0.}$$

NOW: $t^2 \sum_{ij} \tilde{G}_{ij}(\omega)$

$$= t^2 \sum_{ij} G_{ij}(\omega) - t^2 \sum_{i} G_{i0} \sum_{j} G_{j0} / G_{00}$$

NOTE: $G_{ij}(\omega) = \frac{1}{N_s} \sum_{k} e^{ik\cdot(\vec{R}_i - \vec{R}_j)} G(k,\omega)$

$$t \sum_{k} e^{ik\cdot\vec{R}_i} = -\varepsilon_k$$

SO $$t^2 \sum_{ij} \tilde{G}_{ij}(\omega) = \int d\varepsilon N_0(\varepsilon) \frac{\varepsilon^2}{\mathcal{G} - \varepsilon} - \frac{\left(\int d\varepsilon N_0(\varepsilon) \frac{\varepsilon}{\mathcal{G}-\varepsilon}\right)^2}{\int d\varepsilon \frac{N_0(\varepsilon)}{\mathcal{G}-\varepsilon}}$$

$$\mathcal{G} = i\omega + \mu - \Sigma(\omega)$$

NOTICE: $$\int d\varepsilon N_0(\varepsilon) \frac{\varepsilon^2}{\mathcal{G}-\varepsilon} = \mathcal{G} \int d\varepsilon \frac{N_0(\varepsilon)\,\varepsilon}{\mathcal{G}-\varepsilon}$$

$$\int d\varepsilon N_0(\varepsilon) \frac{\varepsilon}{\mathcal{G}-\varepsilon} = -1 + \mathcal{G} \int d\varepsilon \frac{N_0(\varepsilon)}{\mathcal{G}-\varepsilon}$$

USING $$\int d\varepsilon N_0(\varepsilon)\,\varepsilon = 0$$

SO $$t^2 \sum_{ij} \tilde{G}_{ij}(\omega) = \mathcal{G}(-1 + \mathcal{G}G_{00}) - \frac{(-1+\mathcal{G}G_{00})^2}{G_{00}}$$

$$= G_{00}^{-1}(-1+\mathcal{G}G_{00})\left(\cancel{\mathcal{G}G_{00}} - (-1+\cancel{\mathcal{G}G_{00}})\right)$$

$$= G_{00}^{-1}(-1+\mathcal{G}G_{00}) = \mathcal{G} - G_{00}^{-1}$$

HENCE

$$\mathcal{G}^{-1}(\omega) = \omega + \mu - (\mathcal{G} - G_{00}^{-1})$$

$$= G_{00}^{-1}(\omega) + \omega + \mu - (\omega + \mu - \Sigma(\omega))$$

$$= G_{00}^{-1}(\omega) + \Sigma(\omega)$$

AND $$\mathcal{G}^{-1}(\omega) - \Sigma(\omega) = G_{00}^{-1}(\omega)$$

(3) ALGORITHM:

A) INITIATE $\mathcal{G}^{-1}(\omega)\big|_{(0)} \approx (G^0_{00}(\omega))^{-1}$ ← NONINTERACTING LOCAL G_0

B) USE AN "ANDERSON IMPURITY ALGORITHM" TO FIND $\Sigma_{(1)}(\omega)$ FOR THIS $\mathcal{G}^{-1}|_{(0)}$.

C) CONSTRUCT

$$G_{00}(\omega)\big|_{(1)} = \frac{1}{N_s} \sum_{k} \frac{1}{\omega + \mu - \varepsilon_k - \Sigma_{(1)}(\omega)}$$

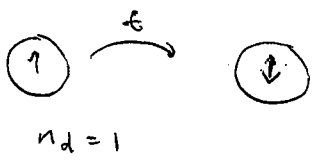
D) CONSTRUCT $\mathcal{G}^{-1}(\omega)\big|_{(1)} = \left(G_{00}(\omega)|_{(1)}\right)^{-1} + \Sigma_{(1)}(\omega)$

E) REPEAT A) – D) FOR INCREMENT 1 $\to$ (1) $\to$ (2) $\to$ ... UNTIL SELF CONSISTENCY IS ACHIEVED.

PURELY AT THE MODEL HAMILTONIAN LEVEL, THIS APPROACH HAS DISPLAYED MANY TRIUMPHS:

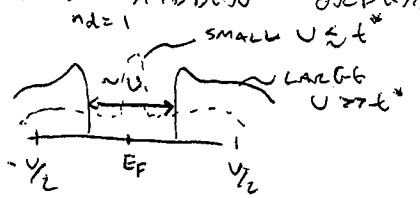
* ACCURATE CAPTURE OF THE MOTT METAL-INSULATOR TRANSITION

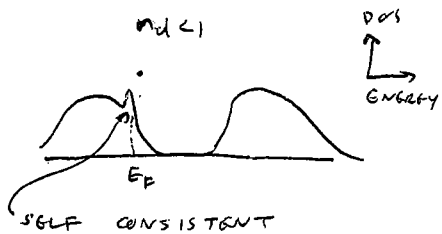
FOR HALF FILLING, THANKS TO LONG AGO ARGUMENTS BY MOTT, WE UNDERSTAND THAT THE CORRELATION ENERGY CAN ABROGATE THE ONE ELECTRON PICTURE OF METALS VS. INSULATORS, (ODD # ELS PER CELL → METAL, EVEN # → INSULATOR) THE MOST FAMOUS MATERIAL VIOLATOR HERE IS La_2CuO_4, WHICH BAND THEORY PREDICTS TO BE A METAL, (EVEN DFT), BUT IS AN INSULATOR WITH A GAP OF ~ 1.5 eV.



THE PROBLEM IS THAT IF U IS TOO LARGE, ($U \gg t$) IT COSTS TOO MUCH ENERGY TO DELOCALIZE

DMFT CAPTURES THIS TRANSITION IN DETAIL, AND AFTER CONSIDERABLE CONTROVERSY, IT APPEARS LIKELY THAT THE TRANSITION IS 1ST ORDER, THIS IS SIGNIFICANT - FOR IT TO BE 2ND ORDER WOULD REQUIRE IDENTIFICATION OF SOME HIDDEN ORDER.





SELF CONSISTENT ABRIKOSOV-SUHL-KONDO

(REFERENCES ON 1ST ORDER NATURE OF MOTT TRANSITION --

R. BULLA ETAL PRB 64 045103 [2001])
J. JOU ETAL PRB 64 193102 [2001]
ROSENBERG ET AL. PRB 83 3498 [1999]
BULLA PRL 83 136 [1999]
SCHLIPF ET AL PRL 82 4890 [1999])

$D = \infty$ ONE BAND HUBBARD (HYPERCUBE)
CFRM PRUSCHKE ET AL, PRB 47 3553 [1993])

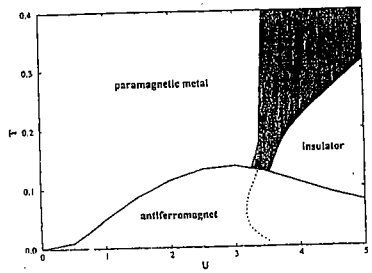


FIG. 1. Phase diagram of the infinite-dimensional Hubbard model at half filling. The shaded region is a rough estimate of the crossover region where the physics of the system resembles that of semimetal with thermally induced DOS at μ. Beyond this region it essentially behaves like an insulator.

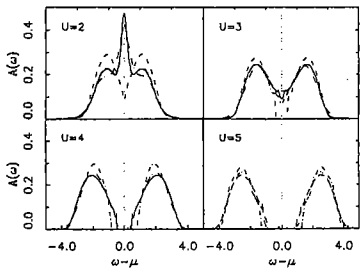


FIG. 2. DOS for the Hubbard model at half filling and $\beta = 7.2$ for some values of U. The full line represents the QMC result, the dashed line the NCA, the dashed-dotted line the LNCA, and the results obtained from perturbation theory are given by the dotted-dashed-dotted line. No QMC results are available for $U = 5$.

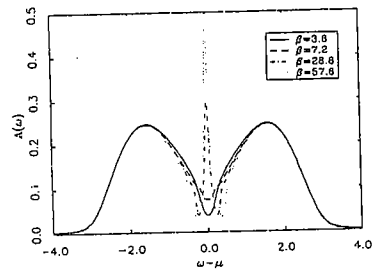


FIG. 7. Temperature dependence of the DOS for $U = 3$. Although there clearly is no gap in the spectrum, the overall temperature dependence is similar to the one expected for larger values of U: The dip in the DOS at μ for high T is replaced by a resonance at low T.

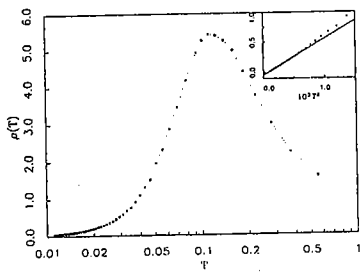


FIG. 9. Resistivity for the half-filled Hubbard model with $U = 3$ in units of $\left[\pi e^2 a t^{*2}/(2\hbar)\right]^{-1} \approx 100\ \mu\Omega$cm. The inset shows the low-temperature data plotted vs T^2 together with a fit $\rho(T) = \rho_0 + a(T/T_0)^2$, where $a = O(1)$ and $T_0 \approx 0.05$.

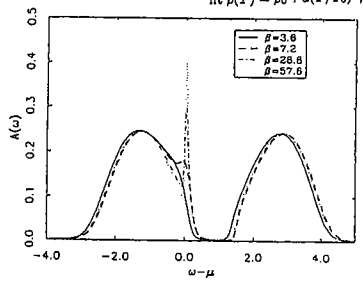


FIG. 12. Temperature dependence of the DOS for $U = 4$ and $n_e = 0.97$. Note that the increase of $A(0;T)$ with decreasing temperature is slower than for $U = 3$ and $n_e = 1$, indicating a smaller low-temperature scale T_0. From $A(0;T = 1/28.8) \approx 1/2\sqrt{\pi}$ we deduce a $T_0 \approx 1/30$ here.

THE DMFT REVEALED A NEW QUALITATIVE FEATURE, LONG SUSPECTED: THE SELF CONSISTENT KONDO EFFECT GENERATES A QUASIPARTICLE RESONANCE WHICH VANISHES AT THE U_c OF THE TRANSITION.

WHEN GENERALIZED TO MULTIPLE BANDS ($\sim N_B$) DMFT CORRECTLY INDICATES THAT U_c IS PUSHED UP BY $\sim \sqrt{N_B}$. THE ROUGH IPRA IS THAT WITH MORE ORBITALS YOU CAN AVOID THE BLOCKAGE TO SOME EXTENT IMPOSED BY A SINGLE ORBITAL. THIS AGAIN HAS MATERIAL SIGNIFICANCE: $A_3 C_{60}$, WITH $A = Na$ OR K, IS METALLIC EVEN THOUGH THE ESTIMATED U OF C_{60} ($\sim 1eV$) SIGNIFICANTLY EXCEEDS THE BANDWIDTH OF THE TRIPLET ORBITALS, HALF FILLED, THE MULTIBAND EFFECT SAVES THE DAY!

CNB: STRICTLY SPEAKING FOR THE GAUSSIAN DOS, THE GAP FOR LARGE U IS A PSEUDOGAP, EXPONENTIALLY SMALL. NONETHELESS, THE ENORMOUS RESULTING RESISTIVITY PRACTICALLY GIVES AN INSULATOR.)

* PROGRESS IN UNDERSTANDING OF BAND FERROMAGNETISM

UNTIL RECENT TIMES, IT IS FAIR TO SAY THAT FERROMAGNETISM IN THE HUBBARD MODEL WAS ASSOCIATED WITH TWO HOARY RESULTS:

→ STONER-WOHLFARTH THEORY IN HARTREE-FOCK MEAN FIELD THEORY, FERROMAGNETISM IN THE ONE BAND MODEL RESULTS IF

$$U N(E_F) > 1$$

AND $\chi(T=0) \propto (1 - N(E_F)U)^{-1}$

WITH MULTIPLE BANDS AND HUNDS' RULE EXCHANGE THE CRITERION WILL BE MODIFIED -- FOR ONE BAND IT STANDS AS AN INCORRECT BUT CONCEPTUALLY USEFUL IDEA: SUFFICIENTLY LARGE U WILL FAVOR MOMENT FORMATION AND ORDER IN PRACTICE, AT $n_d = 1$, HARTREE-FOCK THEORY WITH STAGGERED ORDER CORRECTLY PREDICTS, FOR SMALL U, ANTIFERROMAGNETIC ORDER.

→ NAGAOKAS THEOREM THIS REMARKABLE FACT RESULT OF THE MID '60S PROVED RIGOROUSLY THAT FOR MANY LATTICE STRUCTURES, ADDITION OF A SINGLE HOLE / ELECTRON AWAY FROM HALF FILLING FOR $U = \infty$ DRIVES THE SYSTEM FERROMAGNETIC. THE IDEA (AT T=0)

IS THAT THE HOLE CAN GAIN SUBSTANTIALLY IN KE AS ESSENTIALLY A VACANCY IN A SINGLE SPIN STATE FERMION SYSTEM BY MOVING IN A FULLY POLARIZED BACKGROUND.

↑↑↑ o ↑↑↑ →

WHAT WAS NOT KNOWN ABOUT NAGAOKA'S REMARKABLE THEOREM IS

1) DOES IT EXTEND TO $U < \infty$?
2) DOES IT EXTEND TO FINITE VALUES OF $n_H = 1 - n_d$?

DMFT THEORY HAS WEIGHED IN ON BOTH THESE ISSUES. FIRST, WITH FOCUS ON THE $D \to \infty$ GENERALIZATION OF THE FCC LATTICE, BOTH BECAUSE MANY ITINERANT FERROMAGNETS ARE FCC, AND BECAUSE IT PROVIDES THE (NEAREST + NEXT NEAREST NEIGHBOR)

THE TWO CHANNEL MODELS MAY ALSO HAVE WEIRD SUPERCONDUCTIVITY. FOR THE KONDO CASE, TENUOUS EVIDENCE WAS FOUND FOR A SPIN SINGLET, CHANNEL SINGLET, ODD FREQUENCY INSTABILITY GENERATED BY A RATHER EXOTIC 1ST ORDER TRANSITION.(*) FOR THE ANDERSON CASE IN A MIXED VALENT REGIME, EVIDENCE WAS FOUND FOR SECOND ORDER SPIN TRIPLET PAIRS BOUND TO LOCAL MOMENTS
CANDERS, E J PHYS B 28 9 [2002])
THE JURY IS OUT ON THE RELEVANCE OF THESE FINDINGS TO HEAVY FERMION SUPERCONDUCTIVITY.

(*) JARRELL ET AL, PRL 78 1997 [1997])

MARRYING DMFT AND ELECTRONIC STRUCTURE THEORY: LDA++ OR DFT++

SOME BIG GROWTH DIRECTIONS AND VERY IMPORTANT DEVELOPMENTS ARE FOUND IN NOW MANIFOLD EFFORTS TO JOIN AB INITIO ELECTRONIC STRUCTURE THEORY WITH DMFT.

THE ESSENTIAL IDEA IS TO USE DENSITY FUNCTIONAL THEORY (DFT) TO PROVIDE AN APPROXIMATION FOR THE ONE PARTICLE PROPERTIES THROUGH HARTREE-FOCK LEVEL, AND THE DMFT TO PROVIDE THE DYNAMIC SELF ENERGY CONTRIBUTIONS. HENCE, WITHIN

A PARTICULAR LOCAL ORBITAL BASIS,

$$\hat{G}_{00}(\omega) = \frac{1}{N_S} \sum_{\vec{k}} \frac{'}{(\omega+\mu)\hat{I} - \hat{H}_{DFT}(\vec{k}) - \hat{\Sigma}(\omega)}$$

WHERE $\hat{H}_{DFT}(\vec{k})$ IS THE EFFECTIVE ONE PARTICLE HAMILTONIAN OF DFT, INCLUDING ALL HOPPING, HARTREE-FOCK, AND $\hat{\Sigma}(\omega)$ IS THE INTERACTION SELF ENERGY FOUND WITHIN DMFT. FOR EXAMPLE, FOR UBe_{13}, WE MIGHT LEAVE "U" ON ONLY FOR U 5f ORBITALS, AND ALL OTHER VALENCE ORBITALS WOULD BE 'UNCORRELATED.'

WHAT IS NEGLECTED OR NOT QUITE RIGHT IN THIS APPROACH:

→ DOUBLE COUNTING DFT IS NOT HARTREE FOCK AND HAS NO DIAGRAMMATIC BASIS. HENCE, SOME CORRELATION ENERGY IS INCLUDED IN $\hat{H}_{DFT}$. AT THE MOMENT, WE ARE STUCK WITH THIS, AND AT THE LEAST SUBTRACT OFF HARTREE-FOCK TERMS FROM $\Sigma(\omega)$.

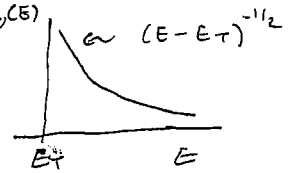
→ ASSUMPTION OF LOCAL INTERACTIONS THE ASSUMPTION OF SITE DIAGONAL INTERACTIONS IS AN APPROXIMATION WHICH CAN BE REMEDIED PARTLY BY NEW CLUSTER METHODS WE'LL DISCUSS A BIT LATER

→ MODIFICATION OF ~~DENSITY IN DMFT~~ DFT IS BASED UPON THE HOHENBERG-KOHN THEOREM STATING $E = E[\rho(r)]$ WHERE ρ IS THE ELECTRON DENSITY, ALTHOUGH MOST EFFORTS TO DATE HAVE GONE ONCE THROUGH (DFT → DMFT) IT

MOST FAVORABLE LATTICE FOR NAGAOKA'S THEOREM, A SUMMARY:

→ HYPERCUBIC LATTICE, ONE BAND, NEAREST NEIGHBOR t FM FOR FINITE REGION OF Nd, BUT $U/t^* \gtrsim 20$ OR MORE -- NOT PLAUSIBLE. (OBERMAIER ET AL, PRB 56 R9479 [1997])

→ GENERALIZED FCC -- NEAREST NEIGHBOR (⊗), ONE BAND: FM FOR FINITE U, FINITE REGION OF Nd.



THE SINGULAR DOS ENHANCES FM TENDENCIES, REDUCING U VALUES TO PLAUSIBLE LIMITS ($\frac{U}{t^*} \sim 4$-8 AT FINITE DOPING)

(WAHLE ET AL, PRB 58 12749 [1998])

→ MULTIORBITAL MODEL WITH HUNDS RULE EXCHANGE BROAD RANGE OF FM ORDER DOWN TO $J/t^* \sim 1$ (HELD & VOLLHARDT, EUR PHYS J B 5 473 [1998])

* LATTICE STUDIES OF ANDERSON AND KONDO MODELS

DMFT HAS BEEN APPLIED TO MANY DIFFERENT VERSIONS OF THE ANDERSON AND KONDO MODELS. AMONG THE KEY FINDINGS WHICH ARE NEW FROM DMFT:

→

KEY REFERENCES:

JARRELL PRB 51 7429 [1995]
PRL 70 1670 [1993]

TAHVILDAR-ZADEH ET AL PRL 80 5168 [1998]
PRB 55 R3332 [1997]

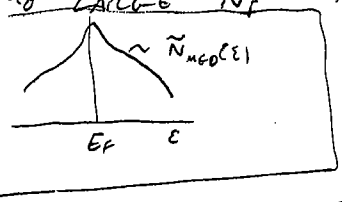
EXPT: CORNELIUS ET AL PRL 88 117201 [2002]
LAWRENCE ET AL PRB 63 054427 [2001]

→ ANDERSON LATTICE, $S = 1/2$

JARRELL EXAMINED THE $S = 1/2$ ANDERSON LATTICE, FINDING, UNSURPRISINGLY, A METAL FOR $n_c < 1$ OR $n_c > 1$ ($n_f = 1$) AND AN INSULATOR FOR $n_c = 1$ ("KONDO INSULATOR"). HOWEVER, HE FOUND TWO UNEXPECTED RESULTS

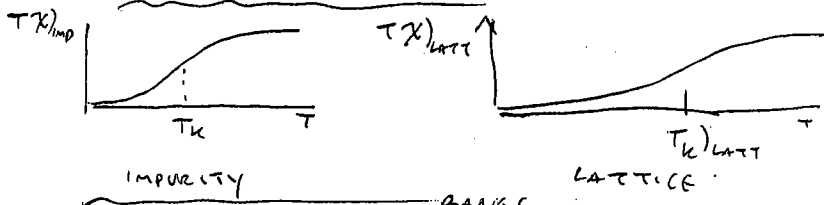
1) COLLECTIVE ENHANCEMENT OF T_K

FOR $n_c = 1$, $n_f = 1$, JARRELL FOUND $T_K)_{LATTICE} > T_K)_{IMPURITY}$, IN CONTRAST TO LARGE N_f THEORY. THE REASON IS THAT IN THE VICINITY OF THE GAP, THE MEDIUM DOS WITH THE "IMPURITY" SITE REMOVED, IS ENHANCED AT E_F. (THE FULL DOS IS GAPPED.) SIMILAR RESULTS HAD BEEN FOUND IN CRUDER VARIATIONAL TREATMENTS BUT NEVER FULLY BELIEVED.



2) EXTENDED SCREENING

FOR LOW CARRIER DENSITY,

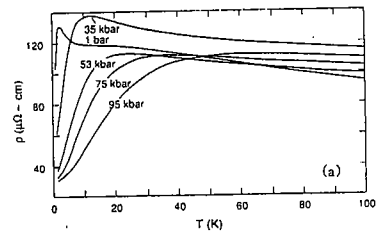


IMPURITY — LATTICE

THE TEMPERATURE RANGE OVER WHICH SCREENING OF LOCAL MOMENTS IS FOUND IS VASTLY 'STRETCHED' WITH RESPECT TO THE IMPURITY LIMIT, BASED UPON COMBINED HALL EFFECT (MEASURING n_c), $T\chi$, AND X-RAY ABSORPTION (MEASURING $n_f(T)$) DATA. EVIDENCE FOR THIS PHENOMENON HAS BEEN FOUND IN YbM$_{12}$ (M = ...) COMPOUNDS.

→ TWO CHANNEL KONDO & ANDERSON LATTICES

THE MULTICHANNEL KONDO EFFECT HAS BEEN PROPOSED TO DESCRIBE A NUMBER OF SYSTEMS AS DESCRIBED EARLIER. NOTABLY, IN THE LATTICE CONTEXT, UBe_{13}, $PrFe_4P_{12}$, $PrOs_4Sb_{12}$ ARE PROMISING QUADRUPOLAR KONDO LATTICE CANDIDATES.



UBe_{13}

CARNSON ET AL, PRL 63 2311 [1989]

THE GROUND STATES OF U, Pr IONS ARE VERY LIKELY E_g/Γ_3 DOUBLETS.

(SATO ET AL PRB62 15125 [2000])

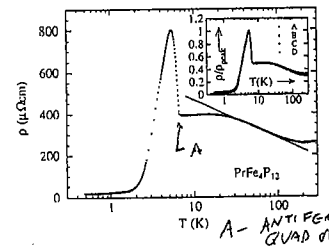
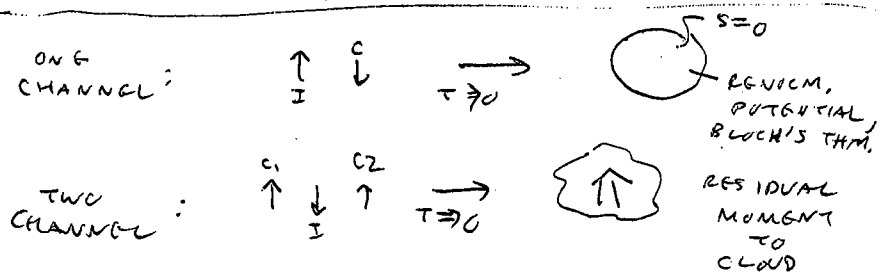


FIG. 1. Temperature dependence of the electrical resistivity for $PrFe_4P_{12}$. The inset shows the $\rho(T)$'s on four different samples normalized at the peak, where the difference is only barely discernible.

THE RESISTIVITIES OF UBe_{13}, $PrFe_4P_{12}$ IN PARTICULARLY STRIKING: WITHOUT INTERVENING ORDER, $\rho(T \to 0)$ EXTRAPOLATES TO VALUES $\sim 100\ \mu\Omega$-cm IN UBe_{13}, $\rho(0)$ APPEARS TO BE REPRODUCIBLE AND DRAMATICALLY SUPPRESSED BY PRESSURE (IT IS REVERSIBLY SUPPRESSED). IN $PrFe_4P_{12}$, THE QUADRUPOLAR ORDERING LEADS ULTIMATELY TO $\rho(0) \approx 0$. UBe_{13} IS A SUPERCONDUCTOR! IT IS REMARKABLE THAT SUPERCONDUCTIVITY CAN EMERGE FROM SUCH A HIGH RESISTIVITY STATE!

($PrOs_4Sb_{12}$, AND $PrAg\,In_2$ HAVE LOW RESISTANCES HOWEVER, AND THE FORMER IS A SUPERCONDUCTOR. ONE POSSIBILITY REQUIRING EXPLORATION IS FERMI SURFACE SHORT CIRCUITING BY CONDUCTING, 'NON HEAVY' SHEETS.)

A HEURISTIC IDEA TO EXPLAIN THE $\rho(T)$ FOR UBe_{13}, $PrFe_4P_{12}$ IS AS FOLLOWS: THE RESIDUAL DEGENERACY OF TWO CHANNEL KONDO SCREENING: UNLIKE THE SINGLET



OF THE SINGLE CHANNEL MODEL WHICH SIMPLY RENORMALIZES THE CRYSTALLINE POTENTIAL AND GIVES BACH BLOCHS' THEOREM, THE RESIDUAL DEGENERACY OF THE TWO CHANNEL CLOUDS PRESENTS A DISORDERED SPIN BACKGROUND IN THE ABSENCE OF INTERVENING ORDER.

DMFT STUDIES OF TWO CHANNEL KONDO & ANDERSON LATTICES CONFIRMED THIS PICTURE, DEMONSTRATING (IN THE ANDERSON CASE) THAT MAGNETIC FIELD WILL LIFT THE DEGENERACY AND RESTORE FERMI LIQUID PHYSICS

TWO CHANNEL KONDO

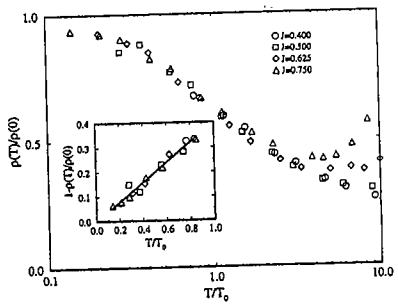


FIG. 3. Resistivity of the two-channel Kondo lattice. $\rho(T)/\rho(0)$ is plotted vs T/T_0 for various values of J. In the inset, the lowest temperature data (for $T/T_0 < 1$, shown as open circles) was fit by $\rho(T)/\rho(0) = 1 + B(T/T_0)^{\alpha}$, with $B = -0.4$ and $\alpha = 1.03$.

(JARRELL ET AL, PRL 77 1614 [1996])

TWO CHANNEL ANDERSON IN APPLIED FIELD

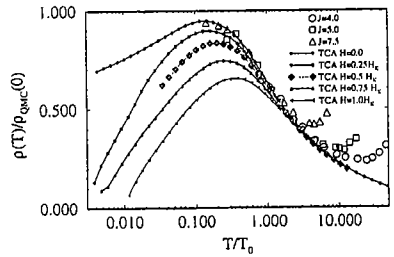


FIG. 1. Resistivity for the TCA vs temperature for different magnetic fields. We have normalized to the estimated $\rho(T = 0)$ values of the QMC data, temperature for the same parameters. The open symbols are the QMC results for different J in the two-channel Kondo lattice model.

(ANDERS ET AL., PRL 78, 2000 [1997])

IS POSSIBLE TO ITERATE SELF CONSISTENTLY

DFT → DMFT

↖ CALCULATE MODIFICATIONS TO $\rho(r)$ FROM DMFT.

THIS HAS BEEN DONE FOR A DMFT TREATMENT OF Pu AND THE CORRECTIONS ARE SIGNIFICANT.

* SUCCESSES OF DFT++

DFT++ HAS NOW BEEN APPLIED TO MANY SYSTEMS WHERE CONVENTIONAL BAND THEORY IS UNABLE TO DO THE JOB -- HERE ARE SOME EXAMPLES:

→ METALLIC PLUTONIUM Pu UNDERGOES NUMEROUS CHANGES OF PHASE IN THE PRESSURE-TEMPERATURE PLANE. FOR WEAPONS APPLICATIONS, IT IS IMPORTANT TO STABILIZE THE δ-PHASE (ACCOMPLISHED BY THE ADDITION OF Ga IMPURITIES). THE ONLY 'CONVENTIONAL' ELECTRONIC STRUCTURE APPROACH WHICH HAS GOTTEN CLOSE ON THE VOLUME OF THE δ-PHASE REQUIRES AN AD HOC DIVISION OF Pu 5f STATES INTO ITINERANT AND LOCALIZED. THE DMFT APPROACH HAS NAILED THE CORRECT VOLUME.

→ MOTT TRANSITION IN V_2O_3

IN V_2O_3, THE MIT CAN BE DRIVEN BY SLIGHT DOPING. DFT++ HAS BEEN APPLIED TO STUDY THE PHOTOEMISSION SPECTRUM AND ORBITAL/SPIN STATES -- AGREEMENT WITH EXPERIMENT IS GOOD.

→ KONDO VOLUME COLLAPSE IN Ce

ELEMENTAL Ce AT ~7KB AND ROOM TEMPERATURE UNDERGOES AN ISOSTRUCTURAL

DFT++ RESULTS

V_2O_3 (HELD ET AL., PRL 86 5345 [2001])

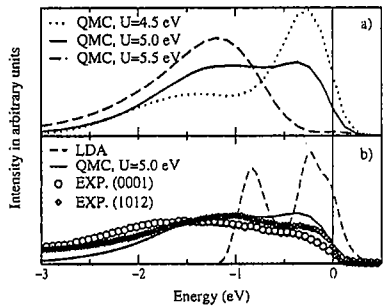


FIG. 3. (a) LDA+DMFT(QMC) spectrum for $U = 4.5$, 5, and 5.5 eV at $T \approx 0.1$ eV $\approx$ 1000 K; (b) comparison with the LDA spectrum and the photoemission experiment by Schramme *et al.* [25] for two different V_2O_3 single-crystal surfaces at $T =$ 300 K. Note that the (10$\bar{1}$2) surface has the same coordination number as the bulk.

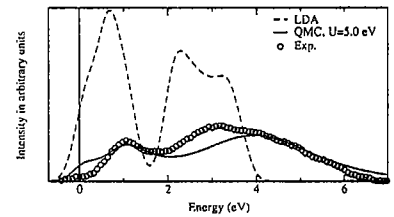


FIG. 4. Comparison of the LDA and LDA+DMFT(QMC) spectra at $T \approx 0.1$ eV (Gaussian broadened with 0.2 eV) with the x-ray absorption data of Müller *et al.* [26]. The LDA and QMC curves are normalized differently since the e_g^σ states, which are shifted towards higher energies if the Coulomb interaction is included, are neglected in our calculation.

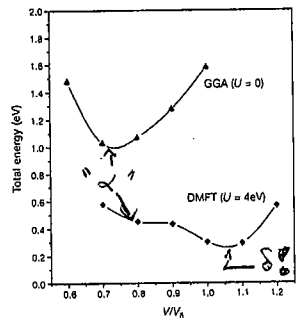


Figure 1 Calculated total energy for plutonium as a function of volume using dynamical mean-field theory (DMFT). The result of a density-functional GGA (generalized gradient approximation) calculation is also shown for comparison. Calculations were performed for the temperature 600 K, at which the δ-phase is stable. *U* denotes average Coulomb energy among f-electrons.

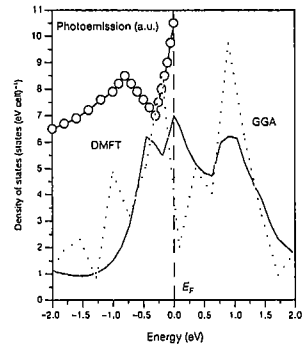


Figure 2 Comparison between calculated density of states for δ-plutonium using dynamical mean-field theory (DMFT; solid line) and recent photoemission experiments[29] (circles). The result of a density-functional GGA calculation is also shown for comparison (dotted line). Calculations are performed for the temperature 600 K at which the δ-phase is stable. EF denotes the position of the Fermi level.

(δ PHASE OF Pu (SAVROSOV ET AL, NATURE 410 793 [2001])

(SEE ALSO X. DAI ET AL, SCIENCE 300 953 [2003])

VOLUME COLLAPSE*, FROM A "LOCAL MOMENT" γ PHASE (HIGH VOLUME) TO "ENHANCED PAULI" α PHASE (LOW VOLUME), THE VOLUME CHANGE IS $\approx 15\%$.

CRUDELY, WE CAN UNDERSTAND THIS FROM THE KONDO PICTURE NOTING

$$J \approx \frac{V^2}{\varepsilon_f}$$

AND V IS A STRONG FUNCTION OF VOLUME (FOR Ce, ε_f IS NOT...)

THEN

$$F \approx \underbrace{-k_B T_K(v_\alpha) + \tfrac{1}{2}B(v_\alpha - v_\beta)^2}_{\text{LOW T, LOW VOL } v} \approx \underbrace{-k_B T \ln N_f}_{\text{HIGH T, HIGH VOL } v}$$

(T_K: KONDO FORMATION; elastic term; N_f: LOCAL MOMENT ENTROPY, $T_K \approx 0$)

NEGLECTING THE ELASTIC ENERGY AND TAKING $N_f \sim 14 \sim e^{2.5}$

GIVES $\Delta F = 0$ AT $T \approx \frac{T_K}{\ln(14)}$

$$\rightarrow T_K \approx 1000\text{K}.$$

THIS IS PRETTY CLOSE -- 1500K IS MORE ACCURATE!

TWO GROUPS APPLYING DFT++ OBTAINED SPECTRA + ENERGETICS OF THE TRANSITION IN GOOD AGREEMENT WITH EXPERIMENT - THEY USED QUANTUM MONTE CARLO AND NCA AS IMPURITY SOLVERS.

* ALLEN + MARTIN, PRL 49 1106 [1982]
LAVAGNA ET AL, PHYS LETT 90A 210 [1982]

MORE DFT++ RESULTS

KONDO VOLUME COLLAPSE

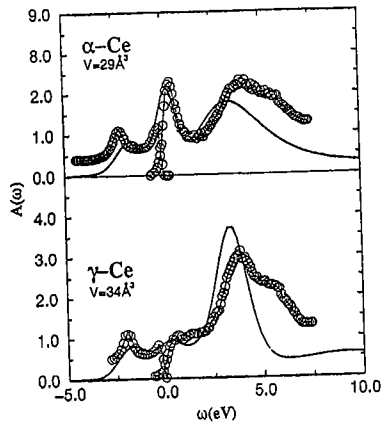


FIG. 11. Comparison of the LDA+DMFT(QMC) spectra with experiment (circles).[5] Although there are no free parameters in the calculated spectrum, the agreement is very good, in particular at the Fermi energy ($\omega=0$). The additional structure in the upper Hubbard band which is seen in the experiment is likely due to the exchange interaction that was neglected in our calculation.

(MCMAHON ET AL, PRB 67 075108 [2003])

(SEE ALSO ZÖLFL ET AL, PRL 87 276403 [2001]).

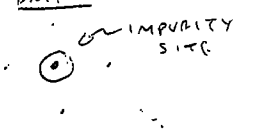
ORIGINAL DFT++: J PHYS COND MATT, 11 1037-[1999]
MI KATSNELSON + AI LICHTENSTEIN)

DYNAMICAL CLUSTER APPROXIMATIONS

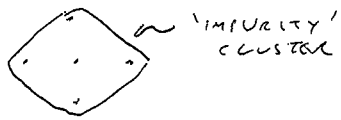
DMFT HAS THE DRAWBACK THAT INTERSITE CORRELATIONS ARE NEGLECTED -- EG, MEAN FIELD MAGNETISM ARISES BUT NOT SPIN WAVES. FOR A MODEL WITH LOCAL PHONONS, S-WAVE SUPERCONDUCTIVITY ARISES, BUT THE 'VERTEX CORRECTIONS' NEEDED FOR D-WAVE ARE $O(1/D)$ [SIMILARLY, ONLY UNVERTEX CORRECTED BUBBLES CONTRIBUTE TO $\Sigma(\omega, T)$].

ONE WAY TO SYSTEMATICALLY INCLUDE INTERSITE CORRELATIONS IS VIA A CLUSTER EMBEDDING. THE IDEA IS TO ENLARGE THE 'IMPURITY' TO A PERIODICALLY REPEATED 'MOLECULE'. FOR EXAMPLE,

DMFT



5 SITE CLUSTER



THE 5 SITE CLUSTER SHOWN AT RIGHT IS PERIODICALLY REPEATABLE AND SUFFICIENT FOR CONSIDERING D-WAVE PAIRING. (YOU NEGLECT INTERACTIONS AT THE BOUNDARY.)

CLEARLY, BY ENLARGING THE CLUSTER, YOU SELF CONSISTENTLY AND SYSTEMATICALLY MOVE TO EXACTITUDE.

YOU HAVE YOUR CHOICE IN CARRYING THIS OUT BY EITHER SOLVING IN REAL SPACE,

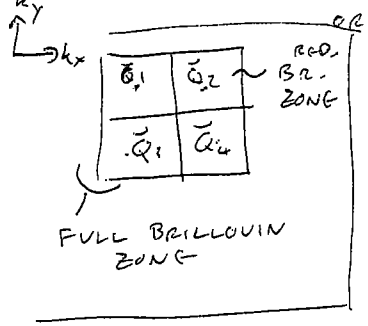
$$\hat{G}_{00}(\omega) = \frac{1}{N_s}\sum_{\vec{k}} \frac{1}{(\omega+\mu)\hat{I} - \underbrace{\hat{\mathcal{H}}_{sp}(\vec{k})}_{\text{SINGLE PART.}} - \hat{\Sigma}(\omega)}$$

WHERE $\hat{\Sigma}$, $\hat{G}$ ARE MATRICES IN THE SPACE OF 'IMPURITY' ORBITALS OF THE CLUSTER, (THIS FORMULATION IS OBVIOUSLY PARALLEL TO THE DEGENERATE DMFT CASE)

OR BY WORKING IN 'MOMENTUM' SPACE

$$\hat{G}(\vec{Q},\omega) = \frac{1}{N_{sc}}\sum_{\vec{k}}{}' \frac{1}{(\omega+\mu)\hat{I} - \hat{\mathcal{H}}_{sp}(\vec{k},\vec{Q}) - \hat{\Sigma}(\vec{Q},\omega)}$$

WHERE $\hat{G}$, $\hat{\Sigma}$ ARE MATRICES IN ONSITE ORBITALS, AND N_{sc} = # "SUPERCELLS"



Σ': RESTRICT SUM TO REDUCED BZ OF SUPERCELL LATTICE

$\vec{Q}_i$: RECIPROCAL LATTICE VECTORS OF SUPERCELL LATTICE WITHIN 1ST BZ OF ORIGINAL LATTICE.

IN PRINCIPLE, EITHER METHOD SHOULD WORK, AND SUCCESS HAS BEEN REALIZED FOR EXAMPLE FOR THE 2D HUBBARD MODEL PHASE DIAGRAM & SPECTRA (GOOD AGREEMENT WITH CUPRATES) AND FOR AB INITIO ESTIMATES OF FERROMAGNETIC SPIN WAVE SPECTRA.

FOR THE MOMENTUM SPACE APPROACH, SEE

METTLER ET AL, PRB 58 7475 (1998)
" " PRB 61 12739 (2000)
ARANYOSI ET AL, PRB 67 085101 (2003)
MAIER & JARRELL PRB 65 041104 (2002)
" " PRB 65 249904 (2002)

FOR THE REAL SPACE APPROACH, SEE

G. KOTLIAR ET AL PRL 87 186401 (2001)

CONNECTIONS TO 2D HUBBARD & D-WAVE SC.

MAIER ET AL PRL 85 1524 (2000) (*)
LICHTENSTEIN & KATSNELSON PRL

SPIN WAVES IN FERROMAGNETS (+)

KATSNELSON & LICHTENSTEIN EUR PHYS J B 30 9 (2002)

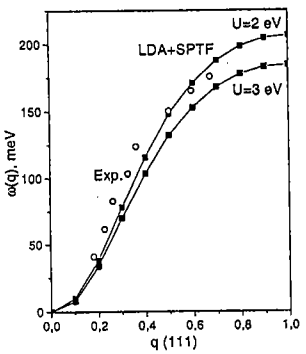


Fig. 2. Spin-wave spectrum for ferromagnetic nickel in LDA+SPTF scheme with different U and $J = 1$ eV in comparison with experimental magnon spectrum (Ref. [36]) in $\Gamma - L$ direction.

REF (+) ABOVE

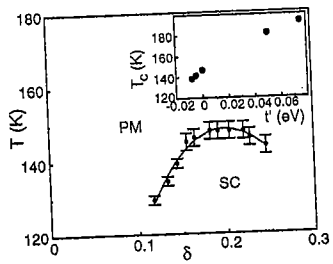


FIG. 4. Temperature-doping phase diagram for the 2D Hubbard model via DCA for a $N_c = 4$ cluster. The nearest neighbor hopping $t = 0.25$ eV, next nearest neighbor hopping $t' = 0$, and the Coulomb repulsion $U = 3$ eV. The error bars result from the finite resolution in temperature. Inset: Transition temperature $T_c(t')$ for fixed doping $\delta = 0.18$ as a function of the next nearest neighbor hopping amplitude t'.

REF (*) ABOVE

* SOME BULLET BODIES

→ WHAT IS U? FOR MIDROW 3ds (Fe, eg!) WE HAVE NO GOOD AB INITIO ESTIMATES OF U. AB INITIO THEORY BASED, EG, UPON CONSTRAINED OCCUPANCY DFT, OR SUPERCELL, TEND TO UNDERESTIMATE U.

→ NO UNIVERSAL IMPURITY SOLVER AT PRESENT, NO SINGLE IMPURITY SOLVER HAS YIELDED SATISFACTORY RESULTS FOR ALL MODELS. A KEY PROBLEM IS THE NEED TO ACCURATELY DESCRIBE HIGH & LOW ENERGY SPECTRA (THE LATTICE SELF CONSISTENCY SAMPLES HIGH ENERGY)

A SUMMARY OF SOME APPROACHES:

METHOD	+	−
QUANTUM MONTE CARLO (GOLD STANDARD, WHEN APPLICABLE!)	+ ESSENTIALLY EXACT + 'EASY' TWO PART. PROPS.	− TIME EXPENSIVE − HARD TO GO LOW IN T − HARD TO INCLUDE REALISTIC EFFECTS (SPIN ORBIT, CRYSTAL FIELD, HUNDS RULES)
NUMERICAL RENORM GROUP	+ ESSENTIALLY EXACT + GREAT AT LOW T, LOW EN.	− HARD TO GET HIGH ENERGY SPECTRA RIGHT − LIMITED TO MODELS WITH LOW DEG. − HARD 2 PART. PROPS
EXACT DIAG.	+ CAN BE FAST	− BAD AT LOW ENERGIES − DISCRETE SAMPLING OF HIGH ENERGIES
NCA + EXTENSIONS	+ FAST (COMP. TO QMC) + 'EASILY' HANDLES MULTIPLETS, ETC + GOOD AT HIGH T, ENERGY, RATHER LOW T	− BREAKDOWN AT LOW T INEVITABLE FOR FERMI LIQUID MODELS − 2 PART. PROPS. HARDER

FLEX	+ SKELETON DIAGRAM APPROACH (2 PART. PROPS) + GOOD FOR SMALL U	− FAILS TO CAPTURE MOMENT FORMATION, MOTT TRANSITION
ITERATED PERT. THEORY	+ VERY FAST! + EASY TO PROGRAM + CAPTURES MOTT TRANSITION WELL	− NON SKELETON APPROACH --- 2 PART PROPS ALL PUT IMPOSSIBLE (EXCEPT σ-!)
SLAVE BOSON INTERPOLATION (HIGH FREQ. PERT THEORY MATCHED TO LOW FREQ. SLAVE-BOSONS)	+ FAST! + GREAT JOB ON Pu!	− NON SKELETON (SEE ABOVE)