

Classical and Quantum impurities in superconductors

100 years old and still dirty

Ilya Vekhter

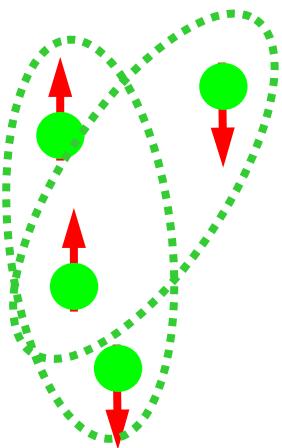
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Superconductivity review I

Simplest (well understood) correlated system:

often even when emerges from a strange normal state



pairing of electrons
 near the Fermi surfc
 +
 Bose-condensation
 of Cooper pairs

Superconductivity

Nontrivial object: *pairing amplitude*

$$\Psi(\mathbf{r}_1, \alpha; \mathbf{r}_2, \beta) \propto \langle \psi_\alpha(\mathbf{r}_1) \psi_\beta(\mathbf{r}_2) \rangle$$

Simplest case: $\alpha, \beta = \uparrow, \downarrow$

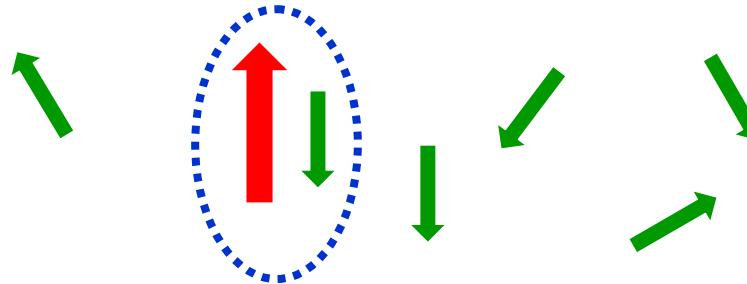
$$\Psi(\mathbf{r}_1, \alpha; \mathbf{r}_2, \beta) = \chi_{\alpha\beta} \rho(\mathbf{r}_1 - \mathbf{r}_2)$$

Cooper pairs have well-defined spin (singlet or triplet pairs)

Why impurities?

Kondo impurity:

local singlet + electrons



Simplest superconductor: no spin-orbit

singlet $S=0$

$$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

$$\chi_{s,\alpha\beta} = (i\sigma^y)_{\alpha\beta}$$

$$\Psi(\mathbf{r}_1, \alpha; \mathbf{r}_2, \beta) = \chi_{\alpha\beta} \varphi(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\chi_{s,\alpha\beta} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

triplet $S=1$

$$|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle$$

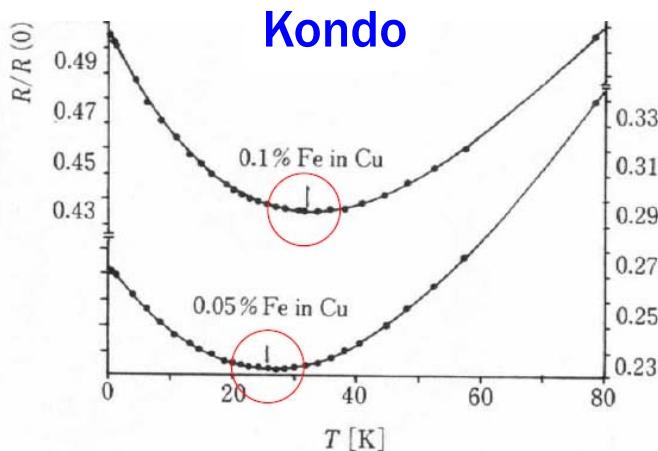
$$\chi_{t,\alpha\beta} = [(i\sigma^y)(\mathbf{d} \cdot \boldsymbol{\sigma})]_{\alpha\beta}$$

$$\chi_t = \begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix}$$

Competition of energy scales:
impurities vs pairing

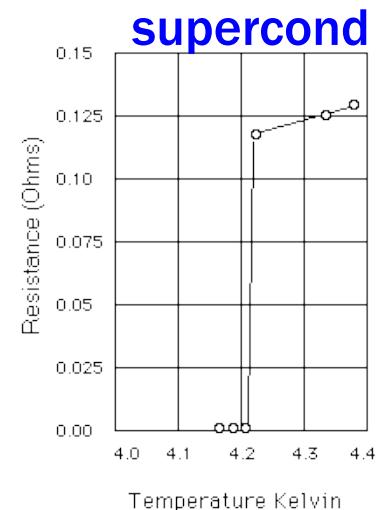


Superconductors vs Kondo metals

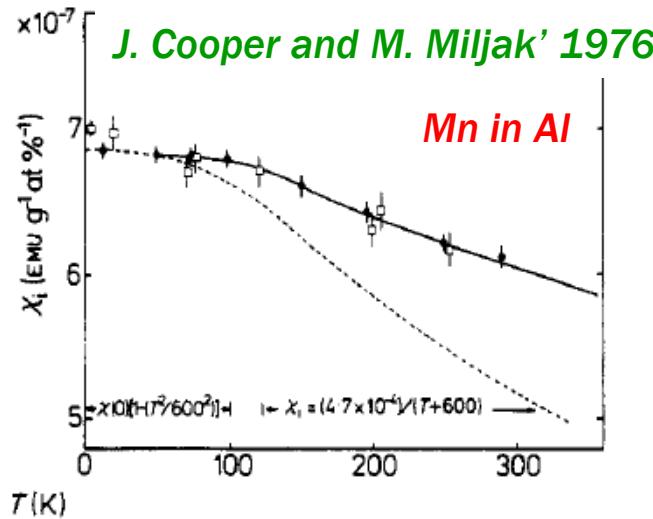


From D. MacDonald et al. 1962

No resistance minimum:
superconductivity

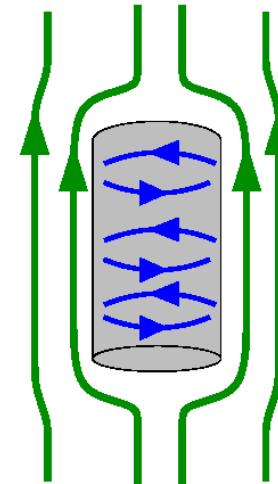


H. Kamerlingh-Onnes 1911



No susceptibility:
Meissner effect

NB: sometimes NMR



Superconductivity review II

BCS Hamiltonian:

$$H_{BCS} = \underbrace{\sum \xi_{\mathbf{k}} c_{\mathbf{k}\alpha}^+ c_{\mathbf{k}\alpha}}_{\text{band}} - \underbrace{\Delta_{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}\alpha}^+ c_{-\mathbf{k}\beta}^+}_{\text{pairing, "anomalous"}}$$

Order parameter:

$$\Delta_{\alpha\beta}(\mathbf{k}) = \sum V_{\alpha\beta,\gamma\delta}(\mathbf{k}, \mathbf{k}') \langle c_{-\mathbf{k}'\delta} c_{\mathbf{k}'\gamma} \rangle \quad \}$$

singlet/triplet;
isotropic/anisotropic;
unitary or not...

Superconductivity review II

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singlet/triplet;
isotropic/anisotropic;
unitary or not...

Matrix form:

$$H_{BCS} = \begin{pmatrix} c_{\mathbf{k}\alpha}^+ & c_{-\mathbf{k}\bar{\alpha}} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} & \Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & -\xi_{-\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\alpha} \\ c_{-\mathbf{k}\bar{\alpha}}^+ \end{pmatrix}$$

singlet

Superconductivity review II

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singlet

$$H_{BCS} = \sum E(\mathbf{k}) \gamma_{\mathbf{k}\sigma}^+ \gamma_{\mathbf{k}\sigma} \quad \text{Bogoliubov transformation}$$

Excitation energies

$$E(\mathbf{k}) = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta(\mathbf{k})|^2} \quad \text{energy gap}$$

$$\gamma_{\mathbf{k}\sigma} = u_{\mathbf{k}} c_{\mathbf{k}\sigma} - \sigma v_{\mathbf{k}}^* c_{-\mathbf{k}\bar{\sigma}}^\dagger$$

$|u_{\mathbf{k}}|^2$ electron
 $|v_{\mathbf{k}}|^2$ hole

Eigenstates

Isotropic vs anisotropic superconductors



Connection to pair wave function

$$\Delta_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2) \propto \Psi(\mathbf{r}_1, \alpha; \mathbf{r}_2, \beta) = \chi_{\alpha\beta} \varphi(\mathbf{r}_1 - \mathbf{r}_2)$$

Fermion exchange

$$\Psi(\mathbf{r}_1, \alpha; \mathbf{r}_2, \beta) = -\Psi(\mathbf{r}_2, \beta; \mathbf{r}_1, \alpha)$$

$$\Psi(\mathbf{r}_1, \alpha; \mathbf{r}_2, \beta) = \chi_{\alpha\beta} \varphi(\mathbf{r}_1 - \mathbf{r}_2)$$

Spin part: 2x2 matrix

singlet $S=0$

$$\chi_{s,\alpha\beta} = (i\sigma^y)_{\alpha\beta} = -\chi_{s,\beta\alpha}$$

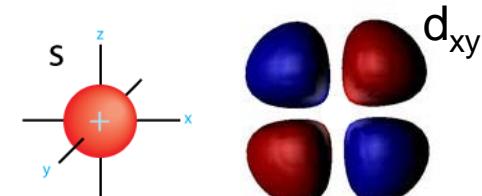
triplet $S=1$

$$\chi_{t,\alpha\beta} = [(i\sigma^y)(\mathbf{d} \cdot \boldsymbol{\sigma})]_{\alpha\beta} = \chi_{t,\beta\alpha}$$

Spatial part: angular momentum l

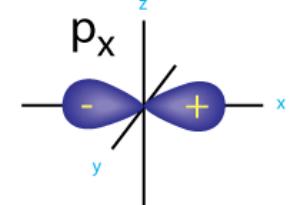
$$l = 0, 2, 4, \dots$$

s, d, \dots wave



$$l = 1, 3, 5, \dots$$

p, f, \dots wave



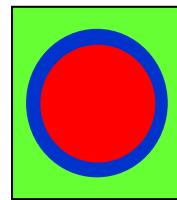
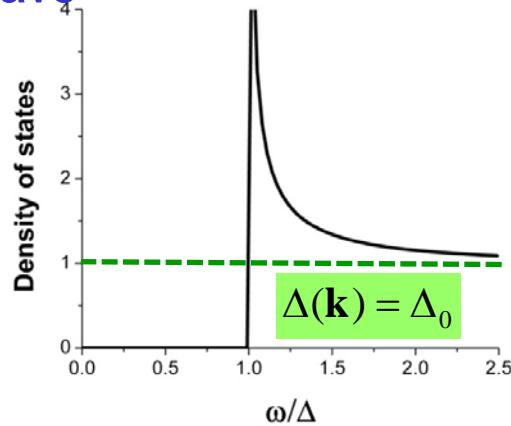
non-s-wave (anisotropic) states favored by strong Coulomb repulsion

Anisotropic superconductors

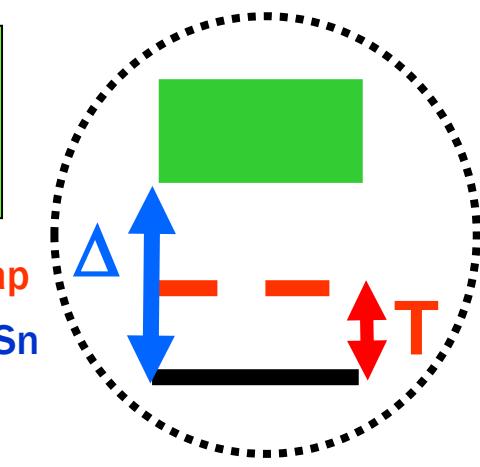


density of states

s-wave

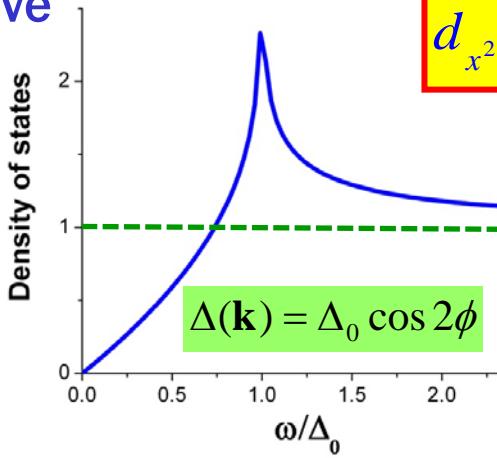


Isotropic gap
Al, Be, Nb_3Sn
< 1978

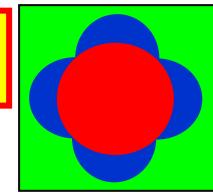


No excitations at low T
Activated behavior $e^{-\Delta/T}$

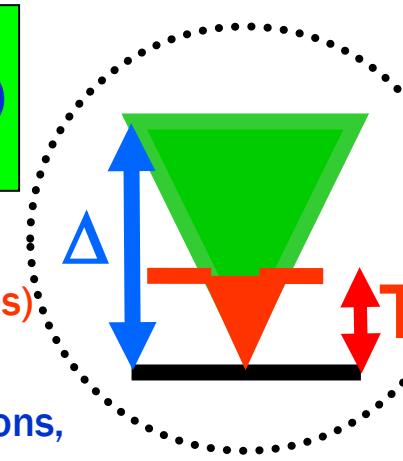
d-wave



$d_{x^2-y^2}$



Gap with zeroes (nodes)
Cuprates,
heavy fermions,
> 1979



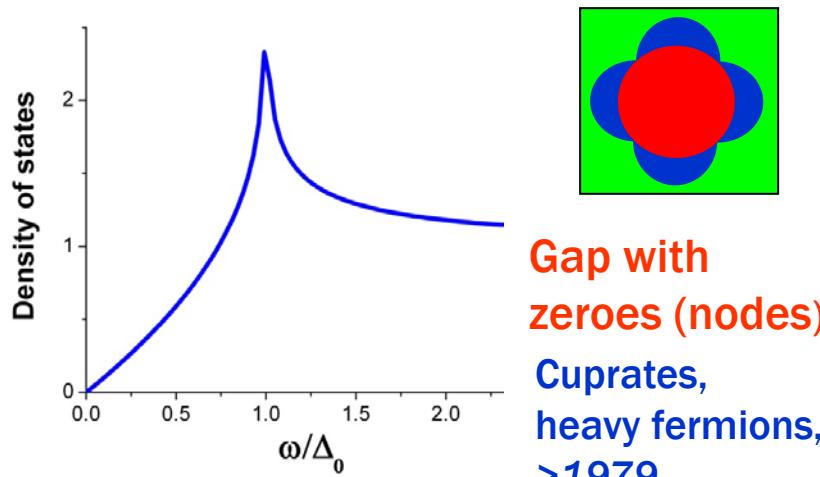
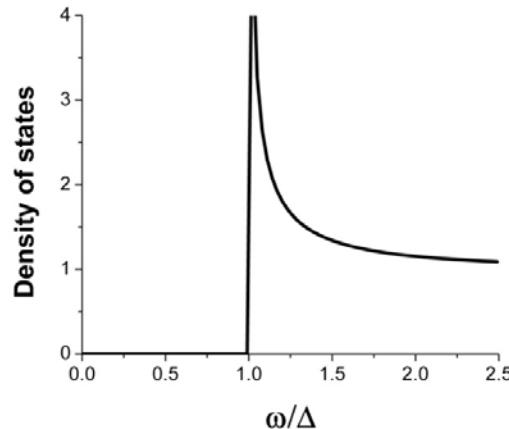
Density of qp $\propto T$
Specific heat $C(T) \propto T^2$
NMR $T_1^{-1} \propto T^3$
universal κ/T

Power laws

Pure and impure superconductors



Pure superconductor:
density of states



What is the effect of:

- 1) an isolated impurity
(STM spectra)
- 2) ensemble of impurities
(T_c, planar junctions)

How is this picture modified by impurities:

- 1) locally
- 2) globally

Classical and quantum impurities

1. Potential scatterers

$$H_{\text{imp}} = \sum_{\alpha} \int d\mathbf{r} \psi_{\alpha}^{\dagger}(\mathbf{r}) U_{\text{pot}}(\mathbf{r}) \psi_{\alpha}(\mathbf{r})$$

2. Spin scattering

$$H_{\text{imp}} = \sum_{\alpha\beta} \int d\mathbf{r} J(\mathbf{r}) \psi_{\alpha}^{\dagger}(\mathbf{r}) \mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\beta} \psi_{\beta}(\mathbf{r})$$

2a. Classical spin

$$[S_i, S_j] = 0$$

2b. Quantum spin

$$[S_i, S_j] \neq 0$$

3. Anderson impurity: interpolate between the two regimes

$$H_{\text{imp}} = E_0(n_{i\uparrow} + n_{i\downarrow}) + Un_{i\uparrow}n_{i\downarrow} + \sum_k Vd_{\sigma}^{+}c_{k\sigma} + h.c.$$

4. Single Impurity vs. many impurities

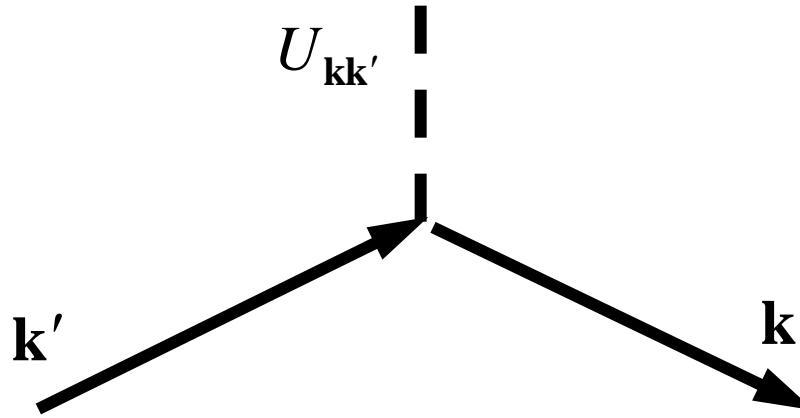
5. Conventional vs unconventional superconductors

Single Impurities

Single Impurity Problem

We are solving a scattering problem (drop spin indices)

$$\begin{aligned}
 H_{imp} &= \int U(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} = \int d\mathbf{r} U(\mathbf{r}) \Psi_\sigma^+(\mathbf{r}) \Psi_\sigma(\mathbf{r}) \\
 &= \int d\mathbf{r} U(\mathbf{r}) \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma}
 \end{aligned}$$



For classical impurities (U is a function) this can be solved exactly

Reminder: Green's functions



Prescription:

$$G_{\alpha\beta}(\mathbf{r}_1, \tau; \mathbf{r}_2, \tau') = -\left\langle T_\tau \psi_\alpha(\mathbf{r}_1, \tau) \psi_\beta^+(\mathbf{r}_2, \tau') \right\rangle \rightarrow G_{\alpha\beta}(\mathbf{r}_1, \mathbf{r}_2; \omega_n) \quad \omega_n = 2\pi T(n+1/2)$$

Matsubara

- obtain retarded Green's function
- poles=excitation energies
- density of states=Im part

$$i\omega_n \rightarrow \omega + i\delta \quad G^R(\mathbf{r}_1, \mathbf{r}_2; \omega)$$

$$\begin{aligned} N(\mathbf{r}, \omega) &= -\pi^{-1} \operatorname{Im} G^R(\mathbf{r}, \mathbf{r}; \omega) \\ &= -\pi^{-1} \int d\mathbf{k} \operatorname{Im} G^R(\mathbf{k}; \omega) \end{aligned}$$

Example: **normal metal**

$$G(\mathbf{k}, \omega_n) = [i\omega_n - \xi_{\mathbf{k}}]^{-1} \rightarrow [\omega - \xi_{\mathbf{k}} + i\delta]^{-1}$$

$$N(\omega) = \int d\mathbf{k} \delta(\omega - \xi_{\mathbf{k}})$$

Nambu formalism and matrices I

- Mix particles/holes,
spin up/down

4x4 matrix

$$\Psi^\dagger(\mathbf{r}) = (\psi_\uparrow^\dagger, \psi_\downarrow^\dagger, \psi_\uparrow, \psi_\downarrow)$$

$$\hat{G}(x, x') = -\langle T_\tau \Psi(x) \Psi^\dagger(x') \rangle$$

Nambu-Gor'kov

- BCS hamiltonian

$$\mathcal{H}_{\text{BCS}} = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) [\xi(-i\nabla) \tau_3 + \Delta \tau_1 \sigma_2] \Psi(\mathbf{r})$$

- Matrices σ_i, τ_i in spin and particle-hole space respectively

- Matrix structure of the impurity scattering:

Potential: $\hat{U}(\mathbf{r}) \Rightarrow U(\mathbf{r}) \tau_3$ e.g attracts electrons/repels holes

Magnetic: $\mathbf{S} \cdot \boldsymbol{\sigma} \Rightarrow \mathbf{S} \cdot \mathbf{a}$ $\mathbf{a} = [(1 + \tau_3) \boldsymbol{\sigma} + (1 - \tau_3) \sigma_3 \boldsymbol{\sigma} \sigma_3]/2$

- Pure BCS

$$\hat{G}_0^{-1}(\mathbf{k}, \omega) = i\omega_n - \xi(\mathbf{k}) \tau_3 - \Delta(\mathbf{k}) \sigma_2 \tau_1$$

Nambu formalism and matrices II



Green's function of
a superconductor

$$\hat{G}_0(\mathbf{k}; \omega) = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & i\omega_n + \xi_{\mathbf{k}} \end{pmatrix}^{-1}$$

“anomalous” Green’s
function, ODLRO

“normal” particle &
hole propagators

Nambu formalism and matrices II

Green's function of
a superconductor

$$\hat{G}_0(\mathbf{k}; \omega) = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & i\omega_n + \xi_{\mathbf{k}} \end{pmatrix}^{-1}$$

“anomalous” Green’s
function, ODLRO

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Density of states

$$N(\mathbf{r}, \omega) = -\pi^{-1} [\text{Im } G^R]_{11}(\mathbf{r}, \mathbf{r}; \omega)$$

“normal” part

poles: energies → energy gap

Self-consistency
condition on the
order parameter

$$\Delta_{\mathbf{k}} = T \sum_{\omega_n} \int d\mathbf{k}' V(\mathbf{k}, \mathbf{k}') G_{12}(\mathbf{k}', \omega_n)$$

“anomalous” part
highest T with sol’n →
transition temperature

Not important for single impurity

Crucial for multiple impurities

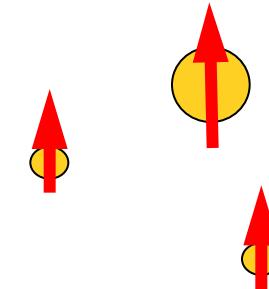
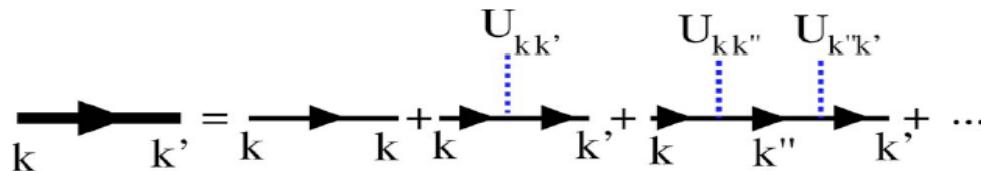
Single impurity



- Key: multiple scattering

$$H_{imp} = \sum_{\mathbf{kk}'} U_{\mathbf{kk}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma} + h.c.$$

change of momentum/spin at each scattering event



$$\begin{aligned} \hat{G}(\mathbf{k}, \mathbf{k}') &= \hat{G}_0(\mathbf{k}) + \hat{G}_0(\mathbf{k}) \hat{U}_{\mathbf{k}, \mathbf{k}'} \hat{G}_0(\mathbf{k}') \\ &\quad + \sum_{\mathbf{k}''} \hat{G}_0(\mathbf{k}) \hat{U}_{\mathbf{k}, \mathbf{k}''} \hat{G}_0(\mathbf{k}'') \hat{U}_{\mathbf{k}'', \mathbf{k}'} \hat{G}_0(\mathbf{k}') + \dots \end{aligned}$$

can include all the scattering events ... in principle

T-matrix solution



$$\xrightarrow{\quad} = \xrightarrow{k} + \xrightarrow{k} \boxed{T_{kk}},$$

$$\boxed{T_{kk}} = U_{kk'} + \xrightarrow{k''} \begin{matrix} U_{kk''} \\ U_{k''k} \end{matrix} + \dots$$

$$\hat{G}(\mathbf{k}, \mathbf{k}') = \hat{G}_0(\mathbf{k}) + \hat{G}_0(\mathbf{k}) \hat{T}_{\mathbf{k}, \mathbf{k}'} \hat{G}_0(\mathbf{k}')$$

$$\hat{T}_{\mathbf{k}, \mathbf{k}'} = \hat{U}_{\mathbf{k}, \mathbf{k}'} + \sum_{\mathbf{k}''} \hat{U}_{\mathbf{k}, \mathbf{k}''} \hat{G}_0(\mathbf{k}'') \hat{U}_{\mathbf{k}'', \mathbf{k}'} + \dots$$

$$= \hat{U}_{\mathbf{k}, \mathbf{k}'} + \sum_{\mathbf{k}''} \hat{U}_{\mathbf{k}, \mathbf{k}''} \hat{G}_0(\mathbf{k}'') \hat{T}_{\mathbf{k}'', \mathbf{k}'}$$

T-matrix solution

$$\xrightarrow{\quad} = \xrightarrow{k} + \xrightarrow{k} \boxed{T_{kk}},$$

$$\boxed{T_{kk}} = U_{kk'} + \xrightarrow{k''} \begin{matrix} U_{kk''} \\ U_{k''k} \end{matrix} + \dots$$

structure is especially simple for isotropic scatterers, $U_{\mathbf{k},\mathbf{k}'} = U$ T-matrix depends on ω only. $T_{\mathbf{k},\mathbf{k}'} = T(\omega)$

$$\hat{G}(\mathbf{k}, \mathbf{k}') = \hat{G}_0(\mathbf{k}) + \hat{G}_0(\mathbf{k}) \hat{T}_{\mathbf{k}, \mathbf{k}'} \hat{G}_0(\mathbf{k}')$$

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$$= \hat{U}_{\mathbf{k}, \mathbf{k}'} + \sum_{\mathbf{k}''} \hat{U}_{\mathbf{k}, \mathbf{k}''} \hat{G}_0(\mathbf{k}'') \hat{T}_{\mathbf{k}'', \mathbf{k}'}$$

$$\hat{T}(\omega) = \hat{U} + \hat{U} \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k}, \omega) \hat{T}(\omega)$$

$$\hat{T}(\omega) = \left[1 - \hat{U} \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k}, \omega) \right]^{-1} U$$

T-matrix includes all the effects of multiple scattering on a single impurity

T-matrix solution

$$\xrightarrow{\quad} = \xrightarrow{k} + \xrightarrow{k} \boxed{T_{kk'}},$$

$$\boxed{T_{kk'}} = U_{kk'} + \xrightarrow{k''} \begin{matrix} U_{kk''} \\ U_{k''k'} \end{matrix} + \dots$$

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$$\hat{G}(\mathbf{k}, \mathbf{k}') = \hat{G}_0(\mathbf{k}) + \hat{G}_0(\mathbf{k}) \hat{T}_{\mathbf{k}, \mathbf{k}'} \hat{G}_0(\mathbf{k}')$$

$$\hat{T}_{\mathbf{k}, \mathbf{k}'} = \hat{U}_{\mathbf{k}, \mathbf{k}'} + \sum_{\mathbf{k}''} \hat{U}_{\mathbf{k}, \mathbf{k}''} \hat{G}_0(\mathbf{k}'') \hat{U}_{\mathbf{k}'', \mathbf{k}'} + \dots$$

$$= \hat{U}_{\mathbf{k}, \mathbf{k}'} + \sum_{\mathbf{k}''} \hat{U}_{\mathbf{k}, \mathbf{k}''} \hat{G}_0(\mathbf{k}'') \hat{T}_{\mathbf{k}'', \mathbf{k}'}$$

Local G at impurity site

$$\hat{T}(\omega) = \left[1 - \hat{U} \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k}, \omega) \right]^{-1} U$$

T-matrix includes all the effects of multiple scattering on a single impurity

Scattering strength

$$\hat{T}(\omega) = \left[1 - \hat{U} \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k}, \omega) \right]^{-1} \hat{U} = \left[(UN_0)^{-1} - \tau_3 \int_{FS} d\hat{\mathbf{k}} \hat{g}(\hat{\mathbf{k}}, \omega) \right]^{-1} \tau_3$$

phase shift of scattering

integral over Fermi surface

$$\hat{g}(\hat{\mathbf{k}}, \omega) = \int_{FS} d\xi \hat{G}_0(\hat{\mathbf{k}}, \xi, \omega) = g_i \tau_i$$

$$(UN_0)^{-1} = \cot^{-1} \delta_0$$

generally depends on band structure

strong scatterers

$$(UN_0)^{-1} \ll 1$$

$$\delta_0 \approx \pi/2$$

unitarity

weak scatterers

$$(UN_0)^{-1} \gg 1$$

$$\delta_0 \approx 0$$

Born

Classical impurities: fixed phase shift

Quantum impurities: phase shift depends on energy scale

DOS and T-matrix

- Density of states
- T-matrix in real space
- With impurity
- Impurity-induced

$$N(\omega, \mathbf{r}) = -\pi^{-1} \operatorname{Im} \hat{G}_{11}(\mathbf{r}, \mathbf{r}; \omega)$$

$$G(\mathbf{r}, \mathbf{r}; \omega) = G_0(\mathbf{r}, \mathbf{r}; \omega) + G_0(\mathbf{r}, \mathbf{r}_0; \omega)T(\omega)G_0(\mathbf{r}_0, \mathbf{r}; \omega)$$

$$N(\omega, \mathbf{r}) = N_0(\omega) - \pi^{-1} \operatorname{Im}[G_0(\mathbf{r}, \mathbf{r}_0; \omega)T(\omega)G_0(\mathbf{r}_0, \mathbf{r}; \omega)]$$

$$\delta N(\omega, \mathbf{r}) \propto \operatorname{Im} T(\omega) |G_0(\omega, \mathbf{r})|^2$$

**Impurity-induced new states appear at energies
where T-matrix has imaginary part: poles of $T(\omega)$**

DOS and T-matrix

- Density of states
- T-matrix in real space
- With impurity
- If for some w
- New states

$$N(\omega, \mathbf{r}) = -\pi^{-1} \operatorname{Im} \hat{G}_{11}(\mathbf{r}, \mathbf{r}; \omega)$$

$$G(\mathbf{r}, \mathbf{r}; \omega) = G_0(\mathbf{r}, \mathbf{r}; \omega) + G_0(\mathbf{r}, \mathbf{r}_0; \omega)T(\omega)G_0(\mathbf{r}_0, \mathbf{r}; \omega)$$

$$N(\omega, \mathbf{r}) = N_0(\omega) - \pi^{-1} \operatorname{Im}[G_0(\mathbf{r}, \mathbf{r}_0; \omega)T(\omega)G_0(\mathbf{r}_0, \mathbf{r}; \omega)]$$

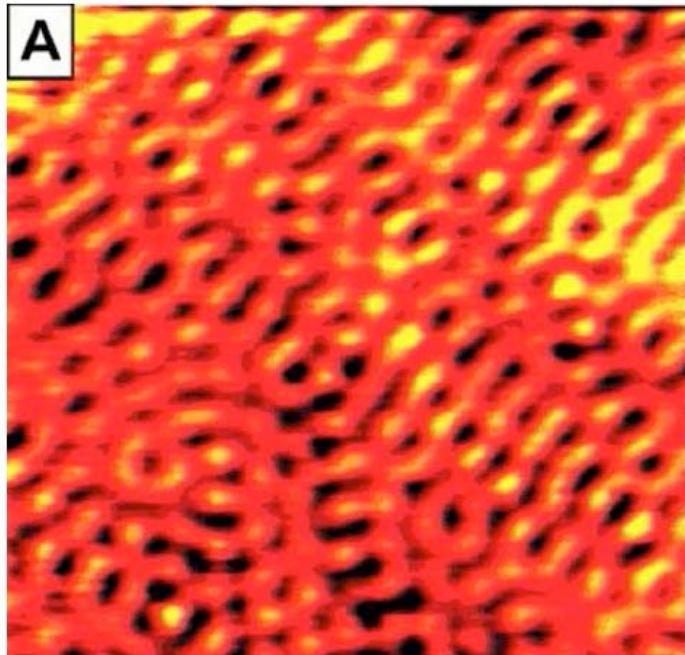
$$N_0(\omega) = -\pi^{-1} \operatorname{Im} G_0(\mathbf{r}, \mathbf{r}; \omega) = 0$$

$$\delta N(\omega, \mathbf{r}) \propto \operatorname{Im} T(\omega) |G_0(\omega, \mathbf{r})|^2$$

Friedel oscillations

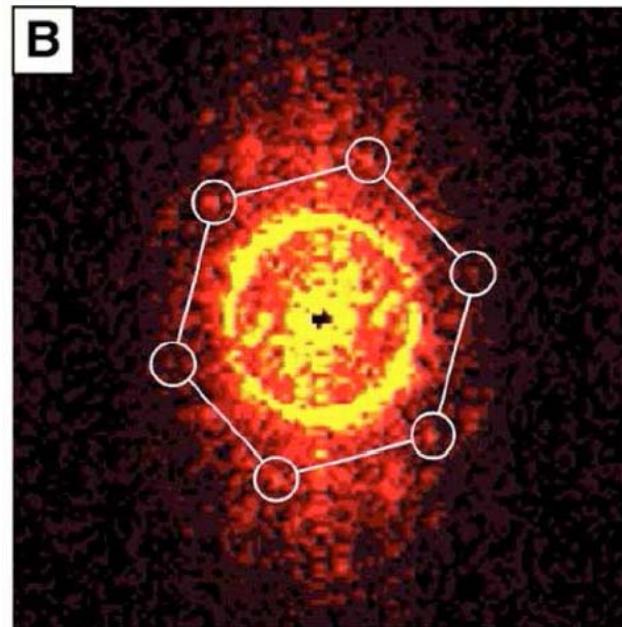
**Impurity-induced new states appear at energies
where T-matrix has imaginary part: poles of $T(\omega)$**

2D Metal: experiment



real space

Be



Fourier transform

P. Sprunger et al. 1997

Spatial oscillations with $k_F r$: Fourier transform gives image of the Fermi surface

2D superconductors

$$E(\mathbf{k}) = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta(\mathbf{k})|^2}$$

Tight binding dispersion

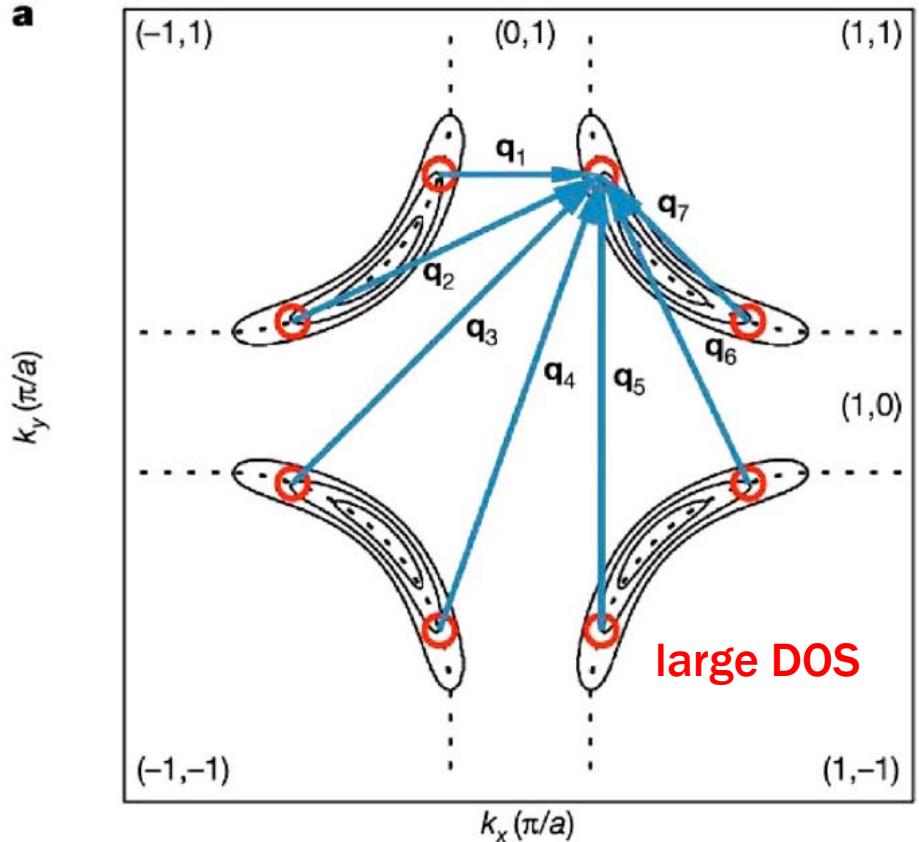
$$\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$$

d-wave gap

$$\Delta(\mathbf{k}) = \Delta_0 (\cos k_x - \cos k_y)$$

Follow dominant wave vectors
as a function of energy

a



K. McElroy et al. 2003

Simple example: potential scattering

$4 \times 4 \rightarrow 2 \times 2$

spin is not “active”

$$\hat{T}(\omega) = \frac{g_0\tau_0 - g_1\tau_1 - (UN_0)^{-1}\tau_3}{(UN_0)^{-2} - g_0^2 - g_1^2}$$

$$g_0(\omega) = - \int_{FS} d\hat{\mathbf{k}} \frac{i\omega}{\sqrt{\omega^2 - |\Delta(\hat{\mathbf{k}})|^2}}$$

$$g_1(\omega) = - \int_{FS} d\hat{\mathbf{k}} \frac{\Delta(\hat{\mathbf{k}})}{\sqrt{\omega^2 - |\Delta(\hat{\mathbf{k}})|^2}}$$

$$\sum_{\mathbf{k}} \Delta(\mathbf{k}) = 0 \Rightarrow g_1 \text{ vanishes}$$

**Different structure of T-matrix for conventional and nodal superconductors:
check for new poles**

Potential scatterer: s-wave



$$H_{imp} = \sum_{\mathbf{k}\mathbf{k}'} U c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma}$$

$$\Delta(\mathbf{k}) = const$$

$$\hat{T}(\omega) = \frac{\sum_i a_i \tau_i}{((UN_0)^{-2} + 1)}$$

no new poles

Physics: we are pairing time-reversed states:
potential impurity makes states not simply
 $|\mathbf{k}\rangle$, but does not violate time-reversal.

$$|\mathbf{k} \uparrow\rangle, |-\mathbf{k} \downarrow\rangle$$

$$|n \uparrow\rangle, T |n \uparrow\rangle$$

The only situation where impurities are not harmful to superconductivity at all: no impurity states

P. W. Anderson, 1957

Resonant impurity: s-wave

Non-magnetic
“resonant scattering”

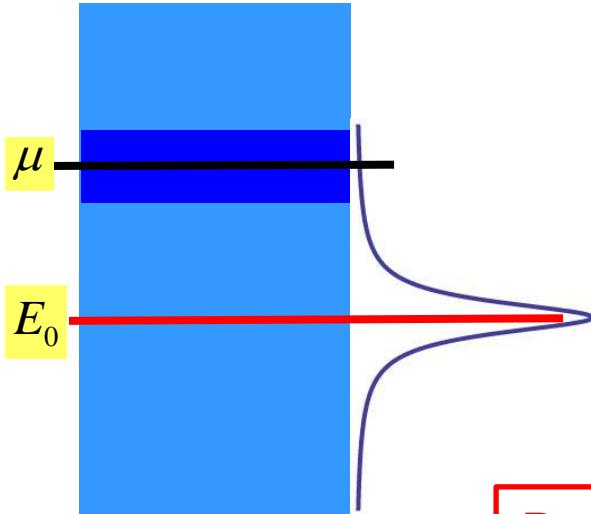
$$H_{imp} = E_0(n_{i\uparrow} + n_{i\downarrow}) + \sum_k V d_\sigma^+ c_{k\sigma} + h.c.$$

Machida & Shibata 1972, H. Shiba 1973

Hybridization with
the conduction band

$$\Gamma = \pi |V|^2 N_0 \quad \Gamma \gg \Delta$$

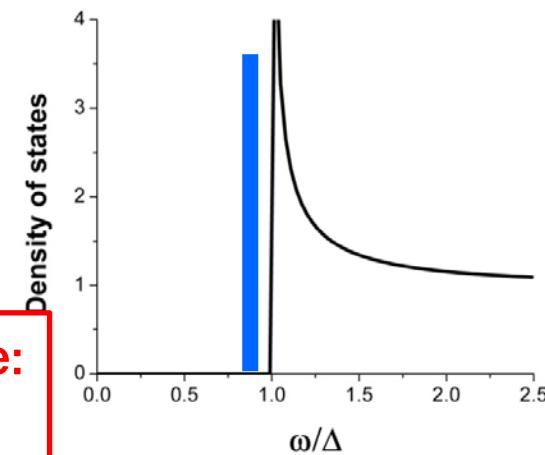
$$\hat{T}(\omega) = |V|^2 \tau_3 \left[\omega - E_0 \tau_3 - |V|^2 \tau_3 \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k}, \omega) \tau_3 \right]^{-1} \tau_3$$



$$N_d(0) = \pi^{-1} \Gamma / (\Gamma^2 + E_0^2)$$

$$\omega_0 = \pm \Delta \underbrace{\{1 - 2\pi^2 [\Delta N_d(0)]^2\}}_{\sim 10^{-3}}$$

Bound state pinned to the gap edge:
largely irrelevant



Potential scatterer: d-wave



$$H_{imp} = \sum_{\mathbf{k}\mathbf{k}'} U c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma}$$

$$\Delta(\phi) = \Delta_0 \cos 2\phi$$

$$\int_{FS} d\hat{\mathbf{k}} \Delta(\hat{\mathbf{k}}_F) = 0$$

Poles of T-matrix ? Yes

Wait, no gap!

$$\Omega_0 = \Omega_1 + i\Omega_2 = -\Delta_0 \frac{\pi c/2}{\ln 8/\pi c} \left[1 + \frac{i\pi/2}{\ln 8/\pi c} \right]$$

$$c = (UN_0)^{-1}$$

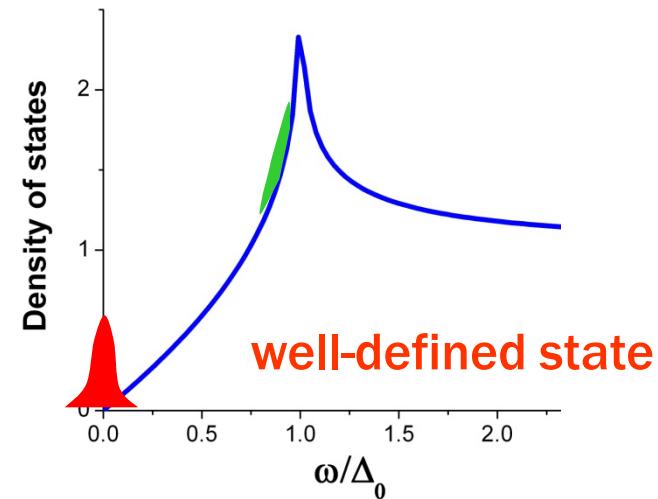
resonance

energy

lifetime

strong scatterers $\Omega_2 \ll \Omega_1$ sharp

weak scatterers $\Omega_2 \geq \Omega_1$ smeared

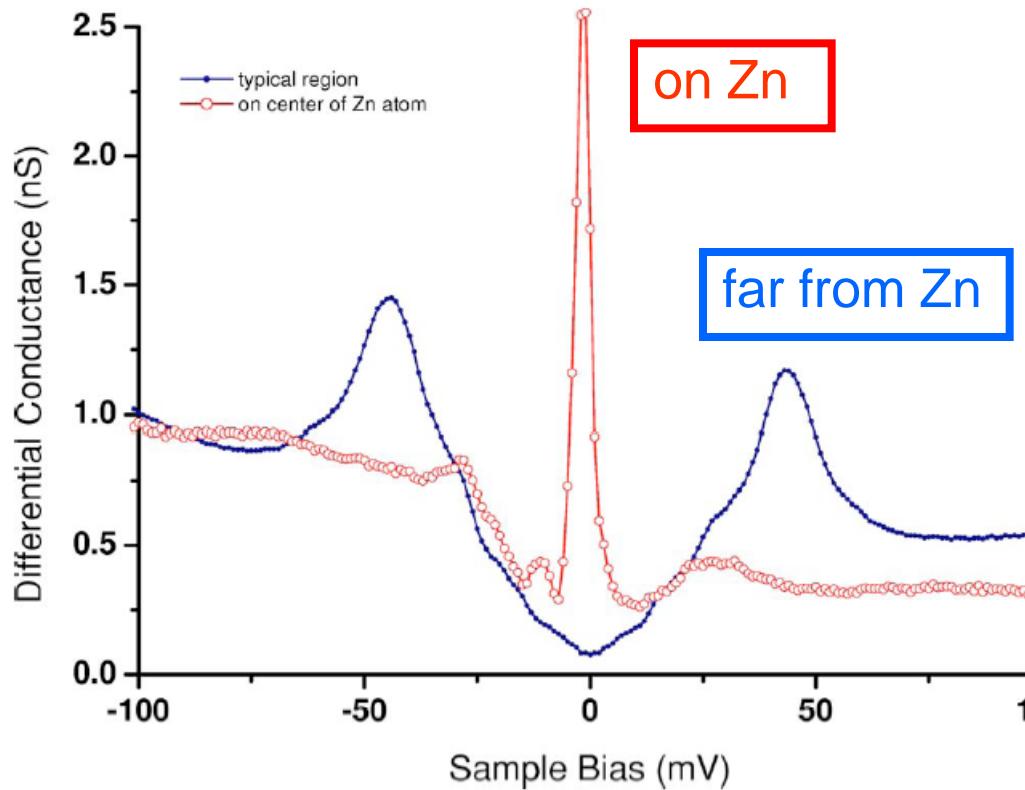


*P. Stamp 1987, J. Byers and D. Scalapino 1993,
A. V. Balatsky et al. 1995*

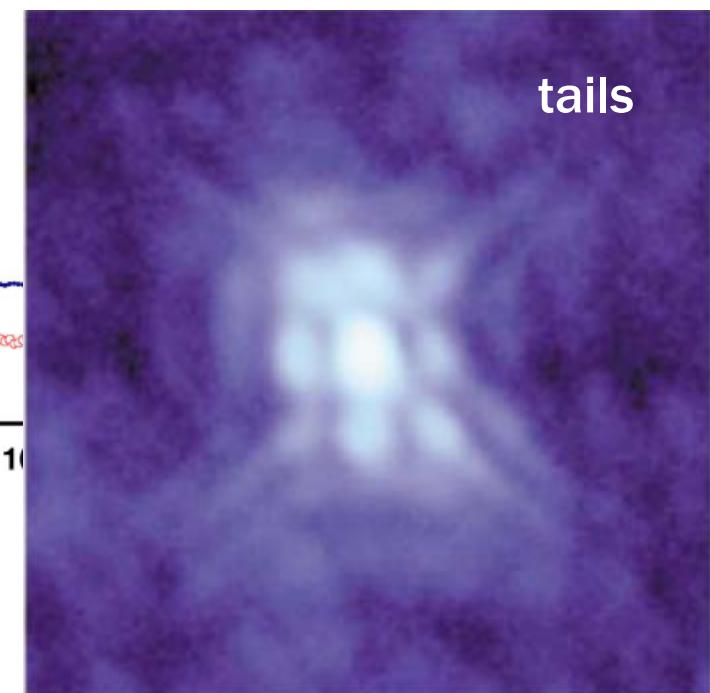
Experiment: d-wave



Zn impurity in BSCCO



Spatial dependence
is poorly understood:



S. Pan, E. Hudson et al., 2000

Message: part I

Potential (electrostatic) scattering

- Isotropic s-wave gap: normally no bound state, never states deep in the gap
- Anisotropic states with sign changing order parameter: all scattering produced bound states, these states are deep in the gap for strong scattering

Now on to spin-dependent scattering starting with classical spin

Classical spin: isotropic gap

$$H_{imp} = J \sum_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\alpha}^+ \mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}'\beta}$$

classical spin S

$$\Delta(\mathbf{k}) = \Delta$$

s -wave

$$\hat{T}(\omega) \propto \frac{(JS/2)^2 \hat{g}_0^2(\omega)}{1 - [JS\hat{g}_0(\omega)/2]^2}$$

new poles

$$\epsilon_0 = \frac{E_0}{\Delta_0} = \frac{1 - (JS\pi N_0/2)^2}{1 + (JS\pi N_0/2)^2}$$

Time-reversal violated: new states below the gap edge

$$JSN_0 \approx 1$$

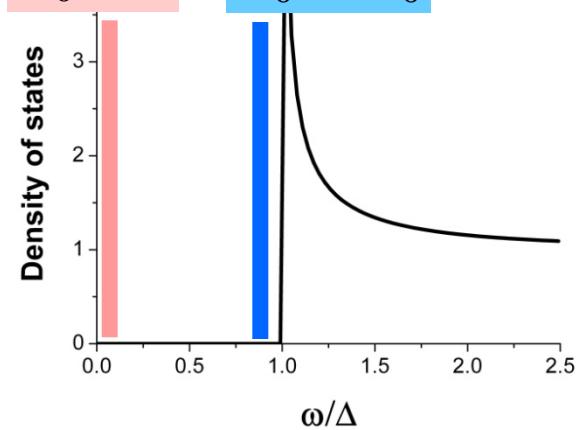
state in midgap

$$E_0 \approx 0$$

$$E_0 \approx \Delta_0$$

$$JSN_0 \ll 1$$

state near gap edge



A. Rusinov, 1968; H. Shiba, 1968, L. Yu 1965

第 21 卷 第 1 期
1965 年 1 月

物 理 学 报
ACTA PHYSICA SINICA

Vol. 21, No. 1
January, 1965

含順磁杂质超导体中的束缚态*

于 涯

提 要

本文利用广义正则变换和自治场方法, 討論了单个杂质对超导体的影响。証明在磁性杂质附近, 可能形成一个束缚态的元激发, 其能量位于能隙之中。求出了能級和波函数的解析表达式, 并計算了束缚能級所引起的附加电磁吸收。討論了与此有关的隧道和高頻吸收實驗。此外, 还討論了非磁性杂质对連續譜元激发的影响及杂质附近能隙的变化。

一、引 言

BOUND STATE IN SUPERCONDUCTORS WITH PARAMAGNETIC IMPURITIES

Yu Luh

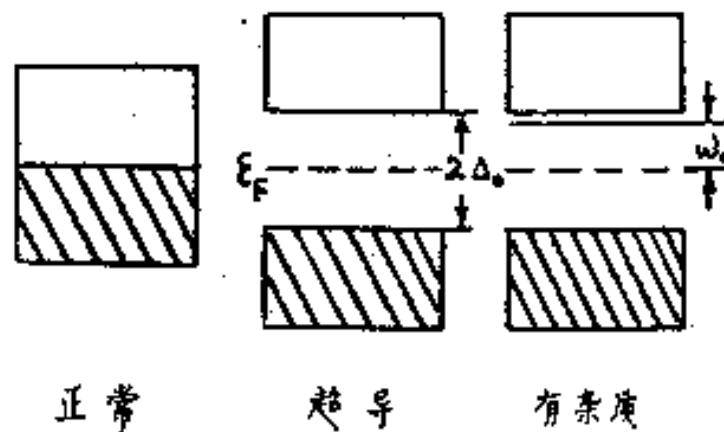


图 1

Quantum phase transition

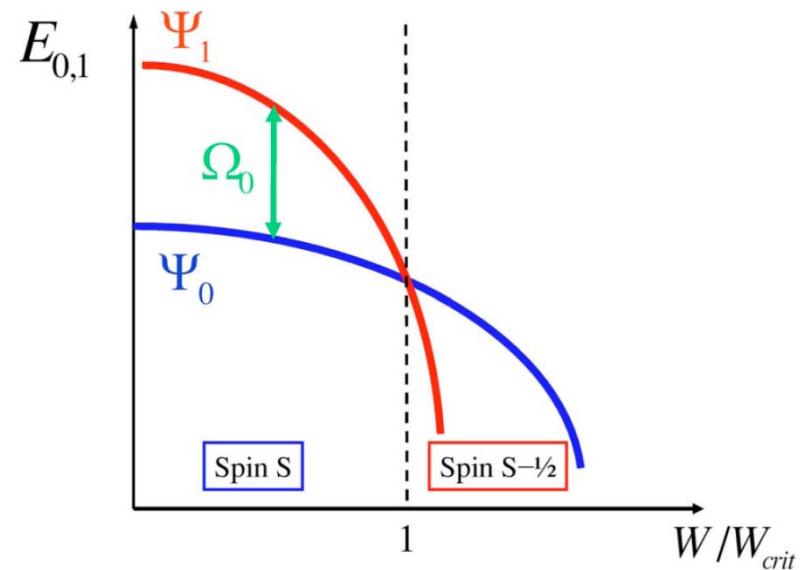
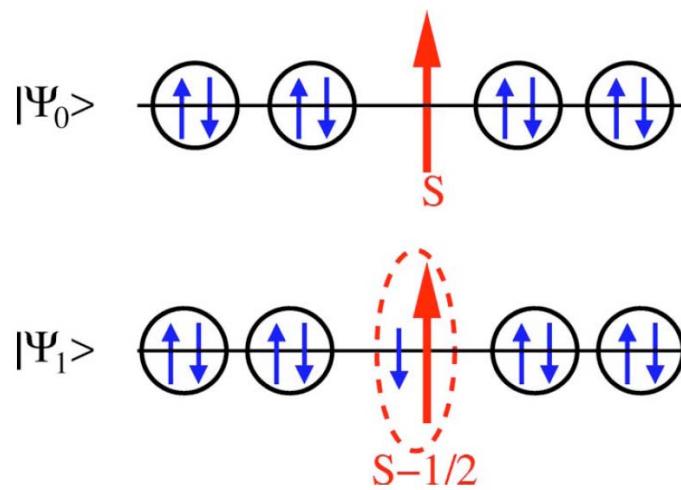
Bound state energy

$$\epsilon_0 = \frac{E_0}{\Delta_0} = \frac{1 - (JS\pi N_0/2)^2}{1 + (JS\pi N_0/2)^2}$$

Critical value

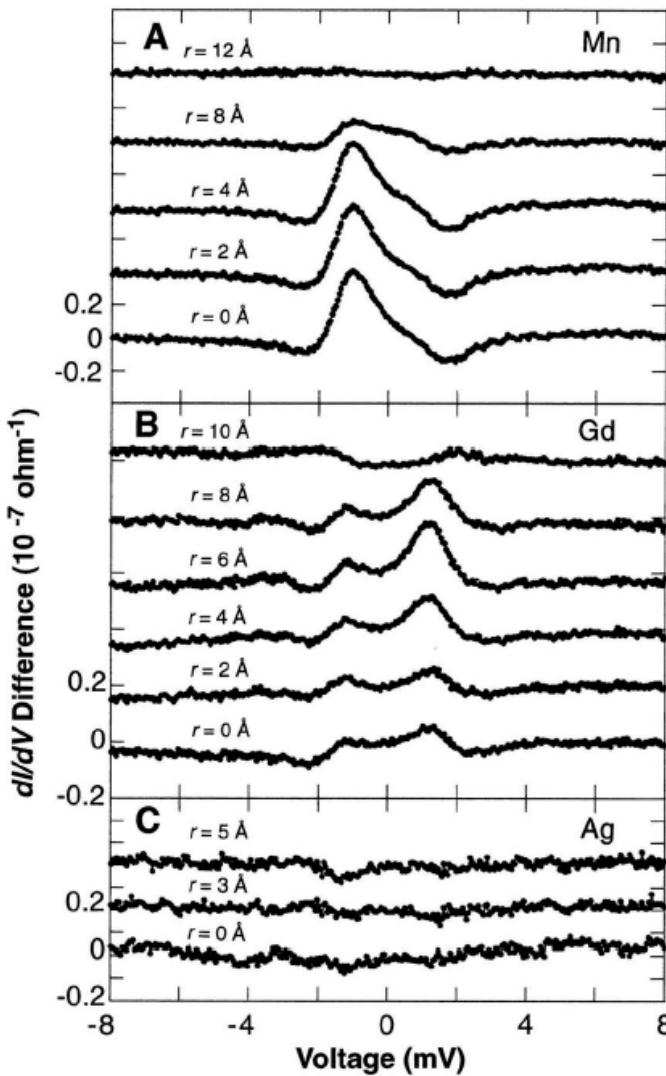
$$J_c = [\pi N_0 S / 2]^{-1}$$

Occupied to unoccupied transition



In both cases similar bound state spectra (extra Cooper pair does not count)

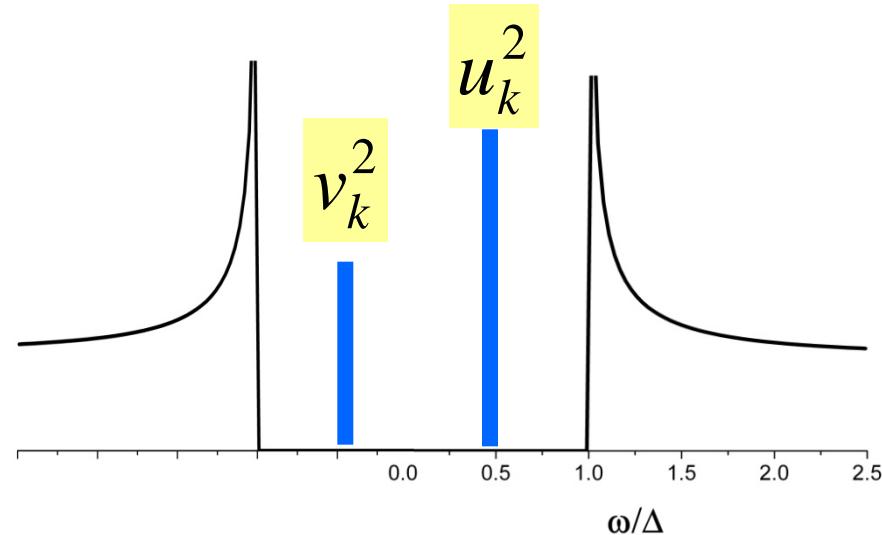
Experiment: s-wave



A. Yazdani et al, 1997

Mn & Gd magnetic, Ag non-magnetic

Asymmetric spectra: extract/inject e



Decay of the state on the scale:

$$|\psi|^2 \propto \exp(-r/r_0)$$

$$r_0 \approx \xi_0 / \sqrt{1 - (E_0/\Delta_0)^2}$$

Quantum impurities



why can't we do the same for quantum impurities?

Recall: single ion Kondo model perturbative RG

$$H_{imp} = JS \cdot \sigma(\mathbf{r}_0) = J \sum_{\mathbf{k}\mathbf{k}'} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{\mathbf{k}\alpha}^+ c_{\mathbf{k}'\beta}$$

$$\frac{dJ}{d \ln D} = -\rho(D) J^2$$

value of coupling depends on
what energy we are looking at

constant density of states:

$$\rho(E) = N_0$$

$$\bar{J} = \frac{J}{1 - JN_0 \ln D/T}$$

AFM $J > 0$

$$\bar{J} \rightarrow \infty$$

$$T_K \approx D \exp(-1/JN_0)$$

impurity
screened

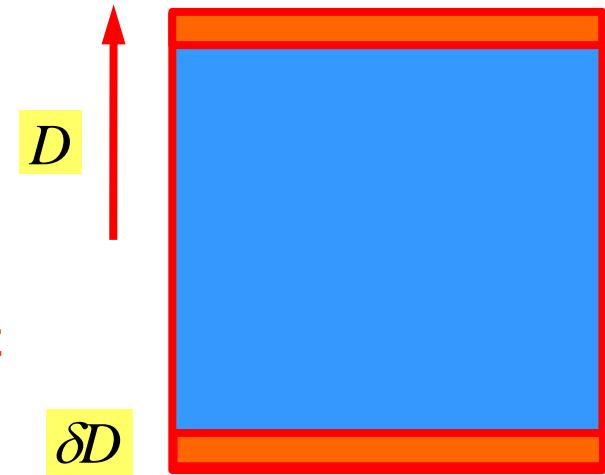
FM

$$J < 0$$

$$\bar{J} \rightarrow 0$$



Impurity
decouples



Quantum impurities



why can't we do the same for quantum impurities?

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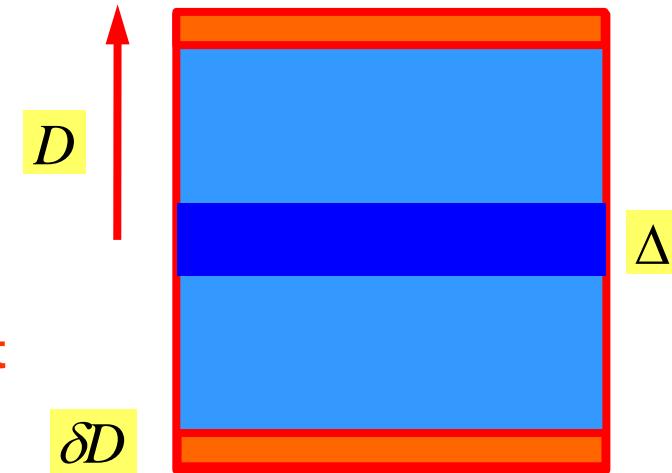
$$T_K \approx D \exp(-1/JN_0)$$

superconductor:

$$\rho(E < \Delta) \ll N_0$$

$T_K \gg \Delta$ impurity screened

$T_K \ll \Delta$ impurity not screened



Quantum character of spin

Classical spin:
T-matrix result

$$\epsilon_0 = \frac{E_0}{\Delta_0} = \frac{1 - (JS\pi N_0/2)^2}{1 + (JS\pi N_0/2)^2}$$

Does not depend on sign of
the exchange interaction

Expect: difference between AFM ($J>0$) and FM ($J<0$) exchange

Renormalizes to large J
Competition with pairing
May be Kondo screened

Renormalizes to small J
Always unscreened

Need new approaches: numerical RG etc.

K. Satori et al. 1992, O. Sakai et al 1993

Kondo S=1/2 spin: NRG

Classical spin:
T-matrix result

$$\epsilon_0 = \frac{E_0}{\Delta_0} = \frac{1 - (JS\pi N_0/2)^2}{1 + (JS\pi N_0/2)^2}$$

Ferromagnetic:

$$\frac{E_0}{\Delta} \approx 1 - \frac{\pi^2}{8} \left[\frac{J/D}{1 + (J/D) \ln[D/\Delta]} \right]^2$$

RG flow stops at Δ

bound state close to gap edge

Kondo S=1/2 spin: NRG

Classical spin:
T-matrix result

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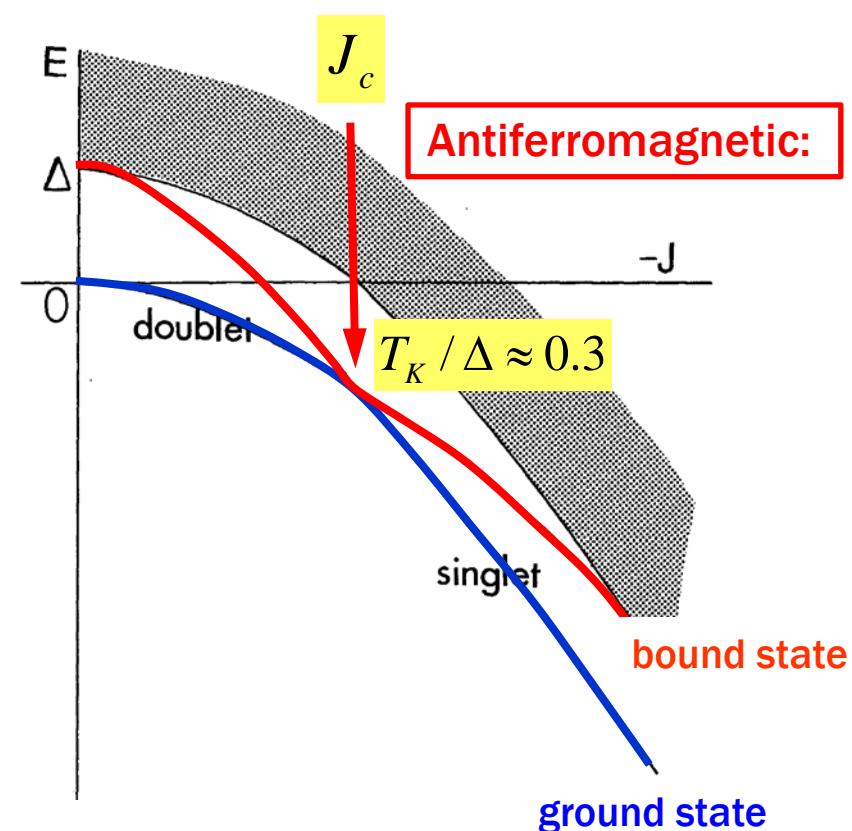
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Antiferromagnetic:

critical value of coupling



K. Satori et al. 1992, O. Sakai et al 1993

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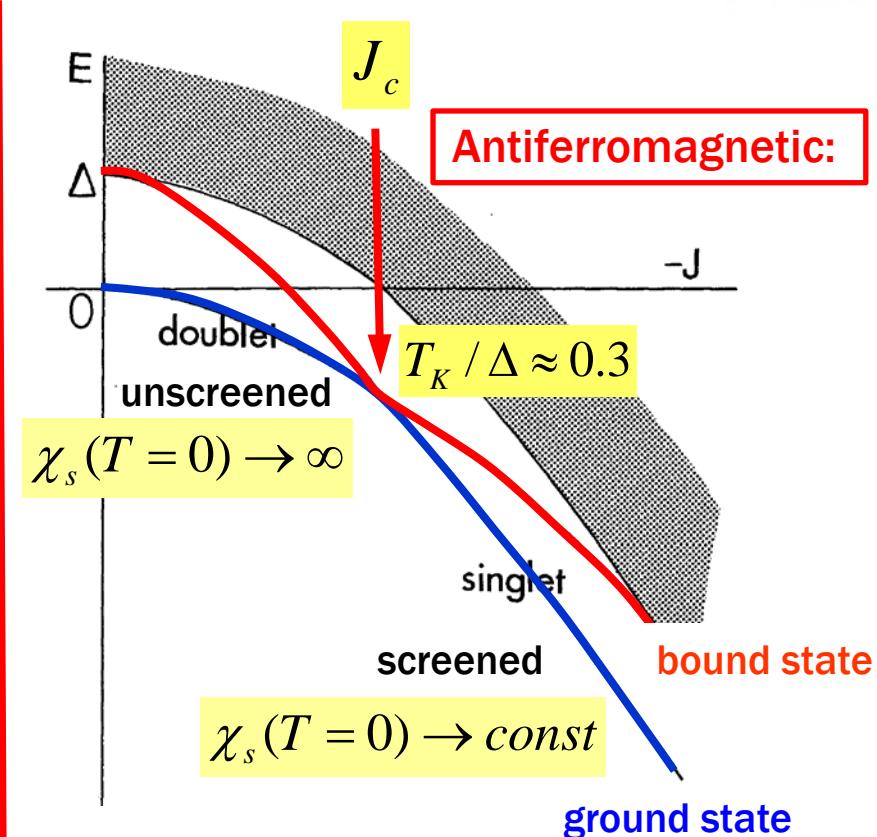
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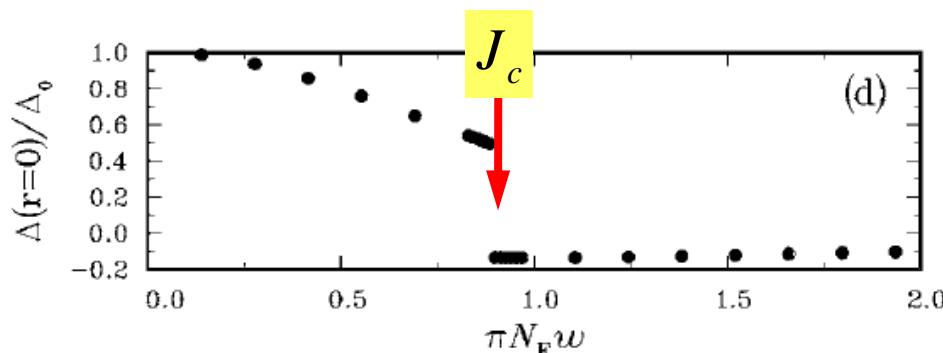
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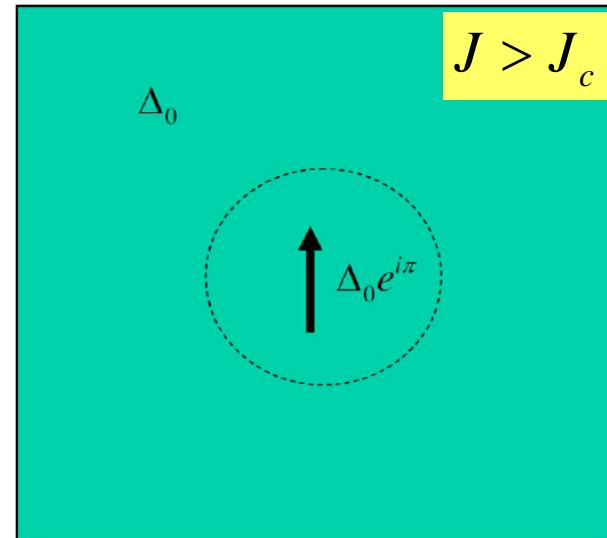
K. Satori et al. 1992, O. Sakai et al 1993

π -phase shifts

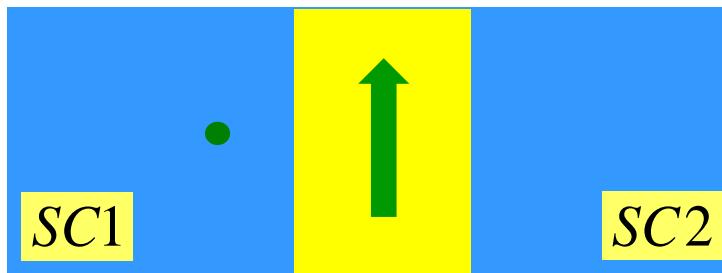


M. Salkola, A. Balatsky, J. R. Schrieffer 1997

Self-consistent calculation
including OP suppression



Cf. π -Josephson junction L. Bulaevskii et al. 1983



Ground state: order parameters
have opposite signs on both
sides of the junction

Cooper pair tunneling via the spin

Gapless superconductors I

Classical spin: potential part of scattering needed

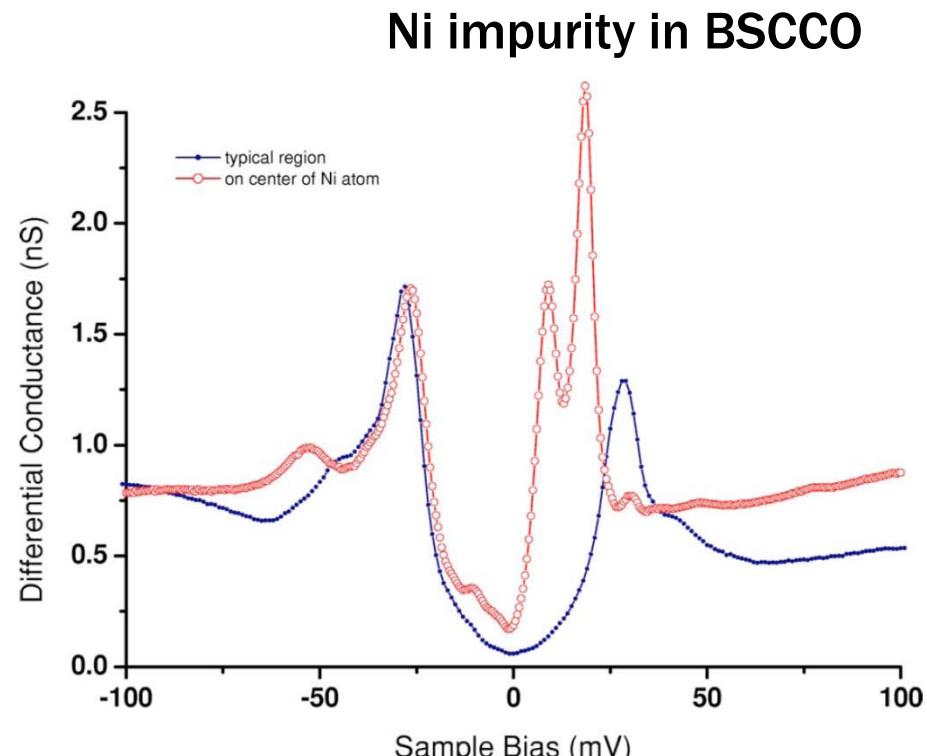
$$U_0 \geq J$$

T-matrix result:

$$\Omega_{1,2} = -\frac{\Delta_0}{2N_0(U_0 \pm J)\ln|8N_0(U_0 \pm J)|}$$

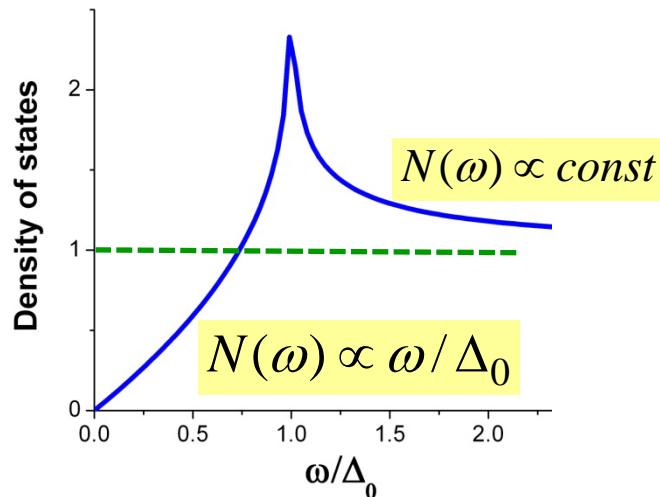
M. Salkola, et al. 1997

Splitting of the resonances (one for each spin species)



E. Hudson ,et al. 2001

Kondo effect in gapless superconductors



Pseudogap Kondo models

$r = \infty$

Hard gap

$r = 0$

Normal metal

$r = 1$

Semimetals, d-wave superconductors...

Density of states suppressed,
does not vanish: **Kondo or not?**

RG until Δ

$$\bar{J} \approx \frac{J}{1 - J N_0 \ln D / \Delta}$$

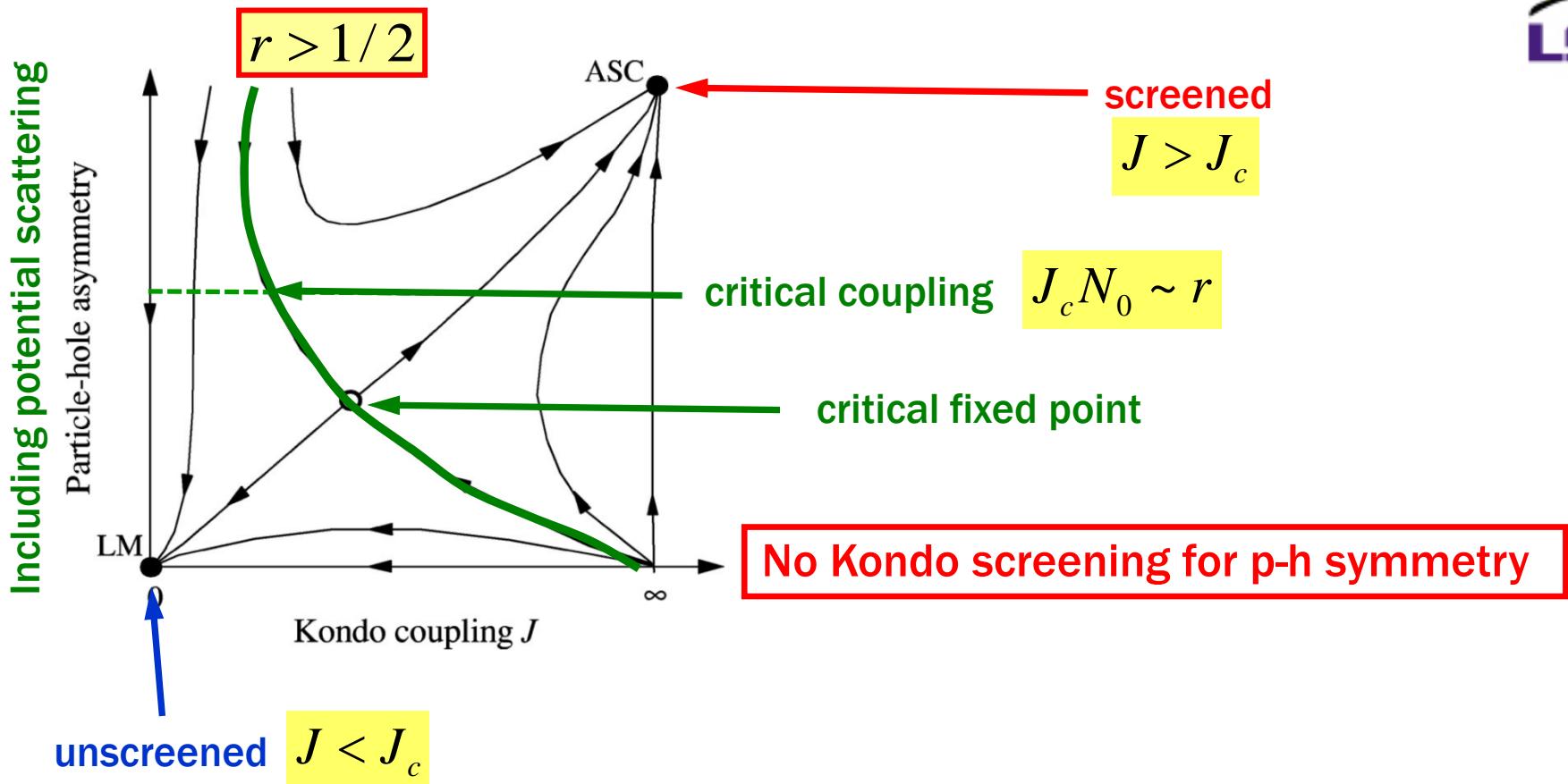
After that?

$N(\omega) \propto \omega^r$

- D. Withoff and E. Fradkin 1990*
- L. Borkowski and P. Hirschfeld 1992*
- K. Ingersent 1996*
- C. Gonzales-Buxton and K. Ingersent 1998*
- R. Bulla and M. Vojta 2001*
- L. Fritz and M. Vojta 2004*
-

Inaccessible from $r \ll 1$

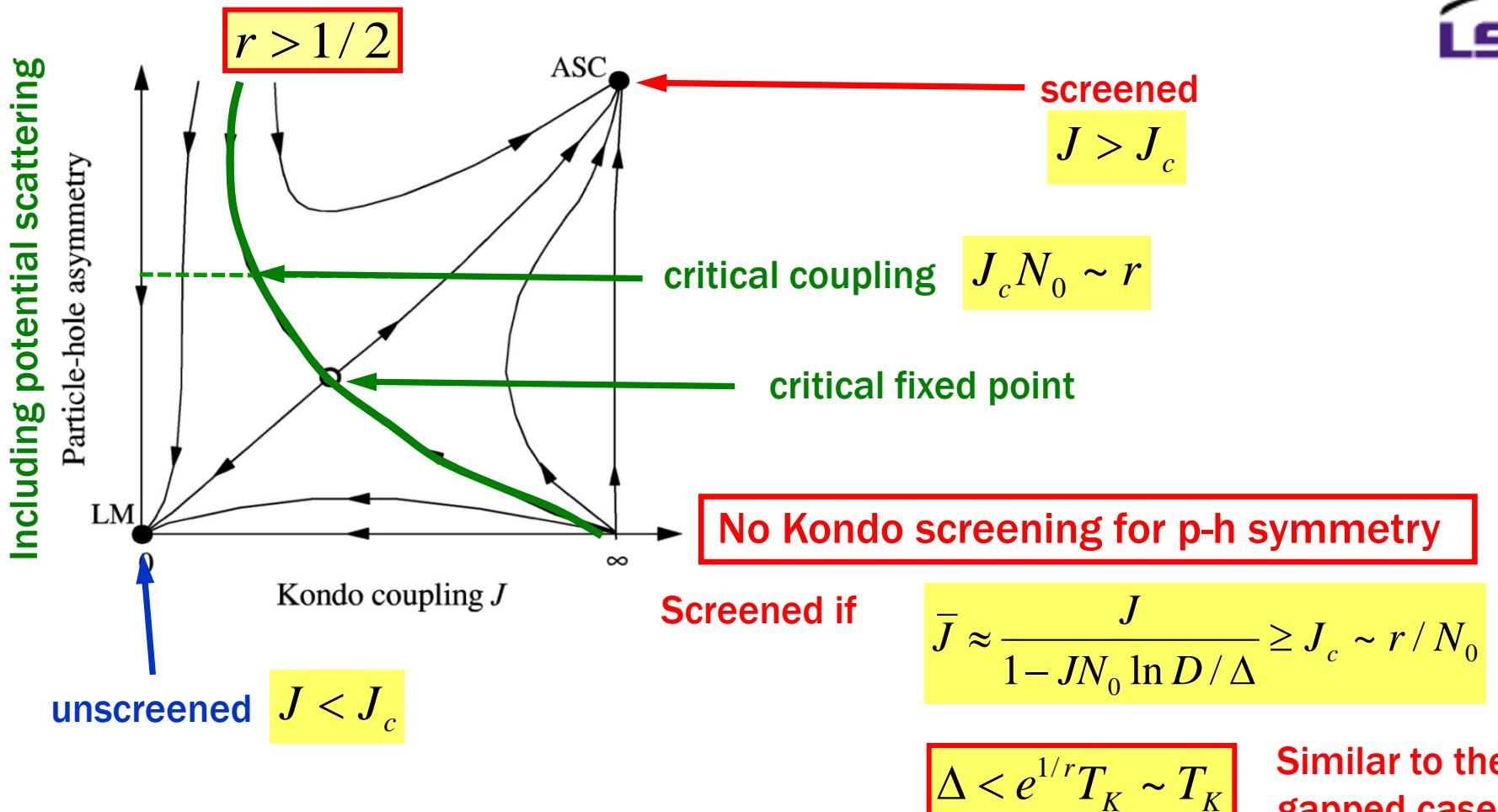
Pseudogap Kondo model



C. Gonzales-Buxton and K. Ingersent 1998

R. Bulla and M. Vojta 2001

Pseudogap Kondo model

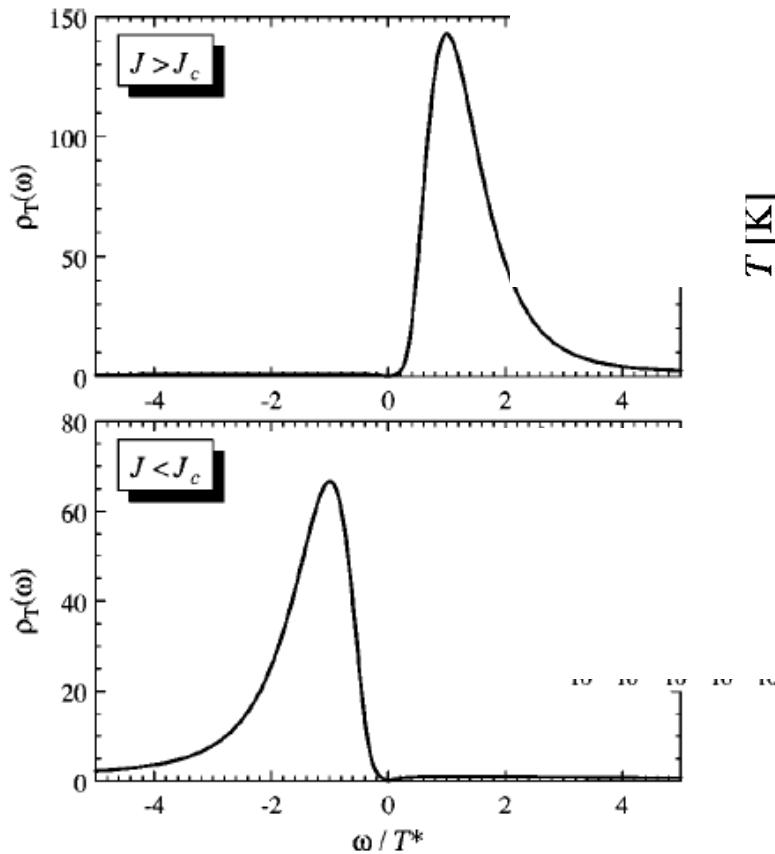


C. Gonzales-Buxton and K. Ingersent 1998

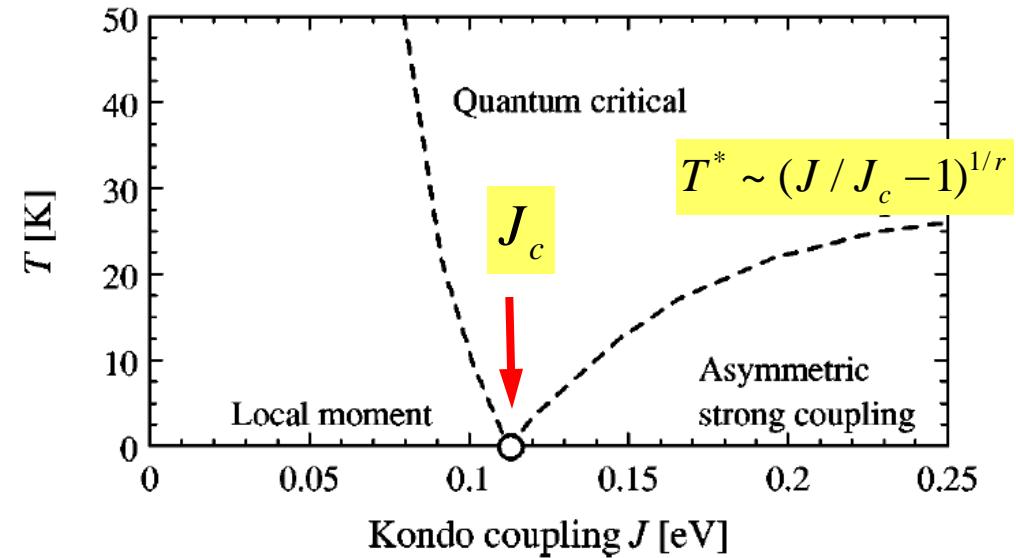
R. Bulla and M. Vojta 2001

M. Vojta and L. Fritz 2004

Impurity density of states



**Localized states
on both sides**



M. Vojta and R. Bulla 2001

Message: part II

Spin-dependent scattering

- Isotropic s-wave gap:
 - FM coupling: bound state near the gap edge
 - AFM coupling: screening requires critical Kondo coupling,
bound state deep into the gap if $T_K / \Delta \approx 0.3$
- Gap with nodes: need potential scattering, form bound states, screening requires critical Kondo coupling.

What about anomalous propagators?



$$\hat{T}(\omega) = \hat{U} + \hat{U} \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k}, \omega) \hat{T}(\omega)$$

Recall: if interaction is local,
T-matrix depends on local
Green's function

$$\hat{G}_0(\mathbf{r}, \mathbf{r}; \omega) = \sum_k \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & i\omega_n + \xi_{\mathbf{k}} \end{pmatrix}^{-1}$$

Off-diagonal part
vanishes if $\sum_{\mathbf{k}} \Delta_{\mathbf{k}} = 0$

For local coupling only density of states matters

For non-local coupling anomalous propagators are relevant

$$H_{imp} = \sum_{\mathbf{k}\mathbf{k}'} J(\mathbf{k}, \mathbf{k}') \mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}\alpha}^+ c_{\mathbf{k}'\beta}$$

M. Vojta and R. Bulla, 1998-2001
M. Vojta & L. Fritz 2004

Multichannel Kondo etc.

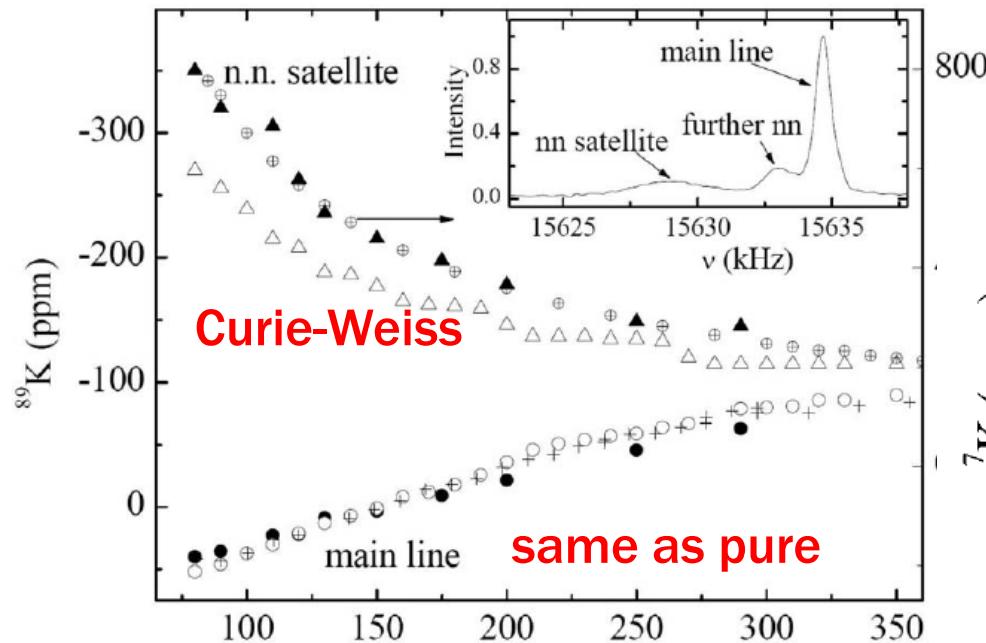
Why may this be relevant?



Question: can one get Kondo behavior from a non-magnetic impurity?

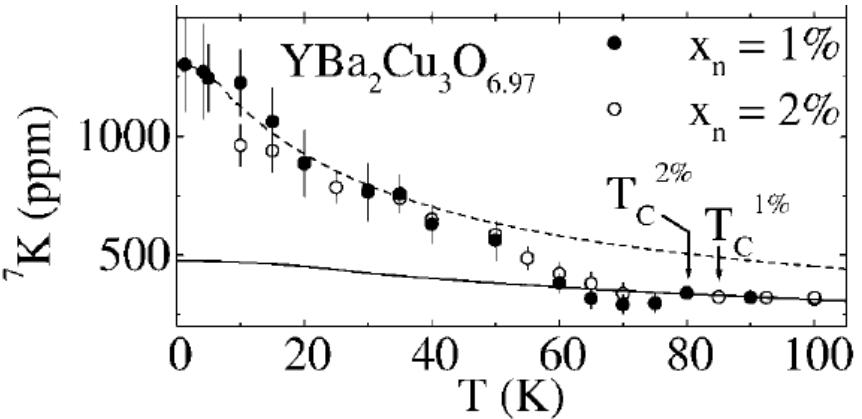
Answer: non-magnetic impurity in a correlated host can generate a magnetic moment distributed around it

Example: Li or Zn in high-temperature superconductor



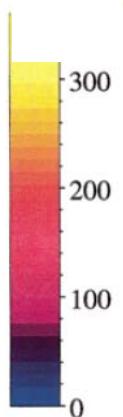
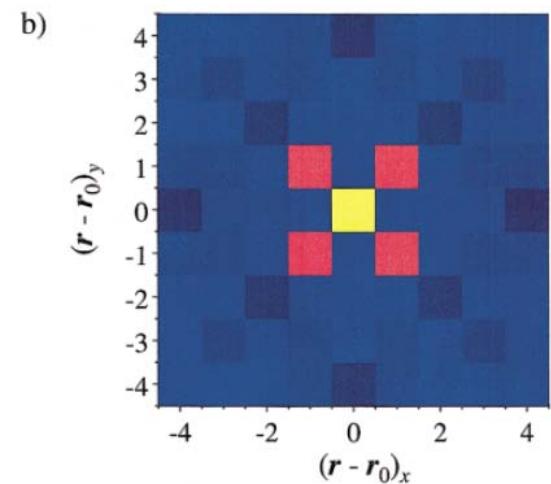
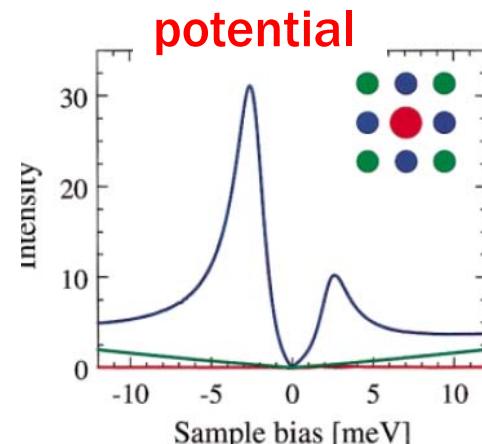
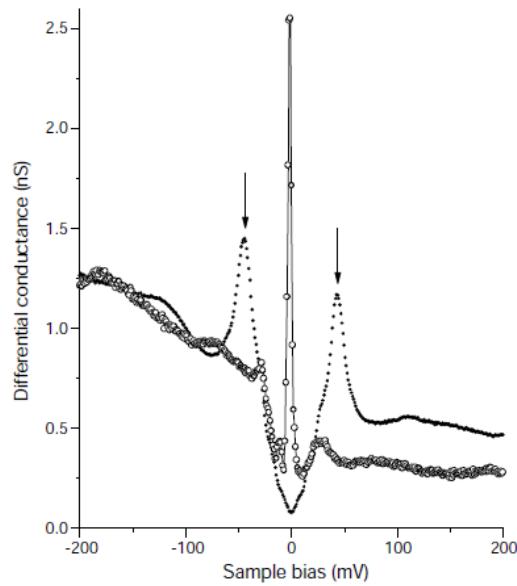
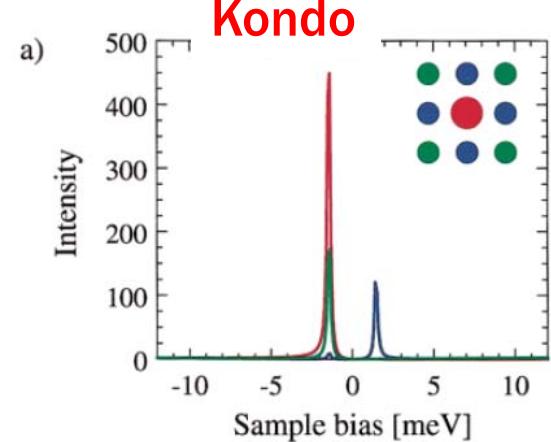
J. Bobroff et al. 1999-2001

Moment distributed over nearest neighbors

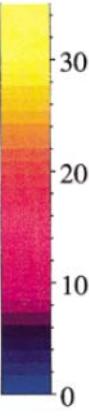
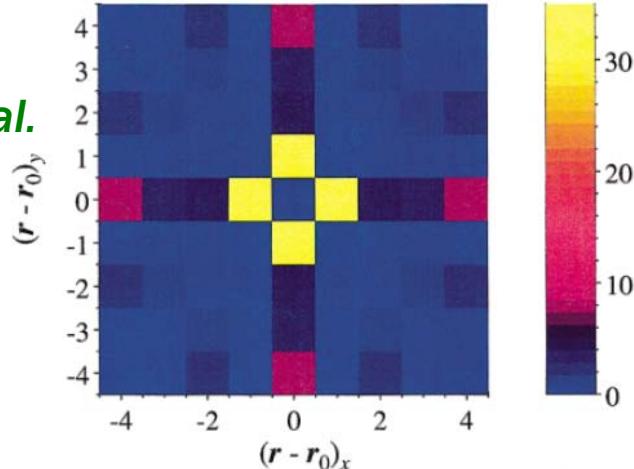


lines: scaled from Cu:Fe alloys

Kondo vs potential scattering

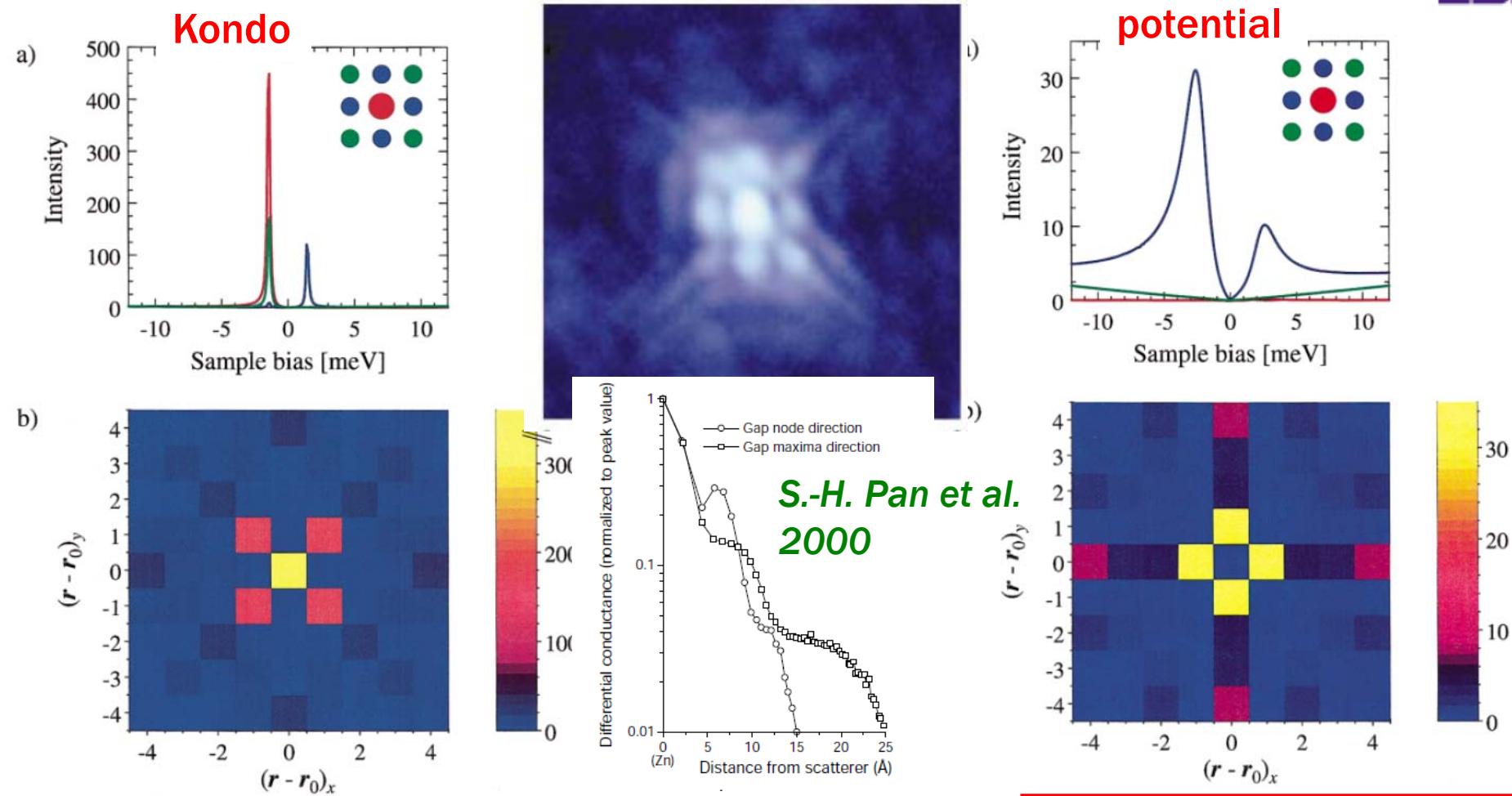


**S.-H. Pan et al.
2000**



A. Polkovnikov, M. Vojta, S. Sachdev 2001

Kondo vs potential scattering



A. Polkovnikov, M. Vojta, S. Sachdev 2001

Neither fits experiment

Message: part III

Sometimes moments appear unexpectedly in correlated systems with magnetic tendencies

**But that does not mean that
Kondo can explain everything**

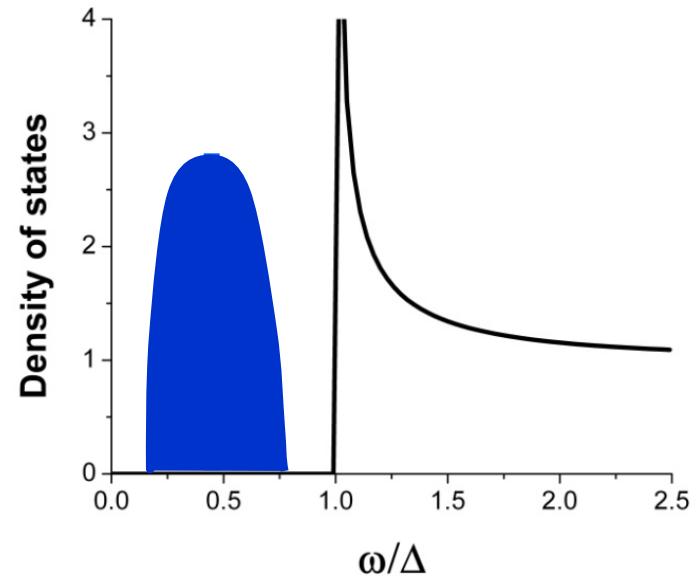
Corollary: draw conclusions about cuprates at your own risk

Many Impurities

From single to many impurities

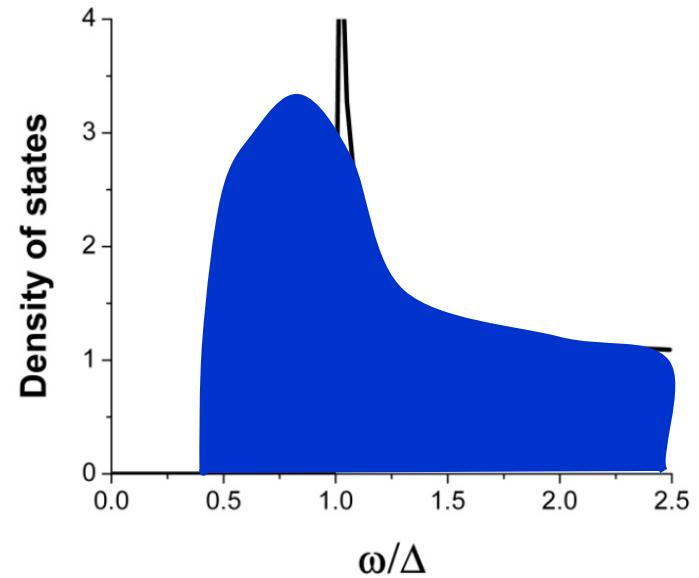
1. Individual bound states around the impurities broaden into a band

2. The bandwidth grows with the impurity concentration. Depending on the location of the single imp state:
 - either touches Fermi energy first (gapless superconductivity)
 - or mixes with continuum first



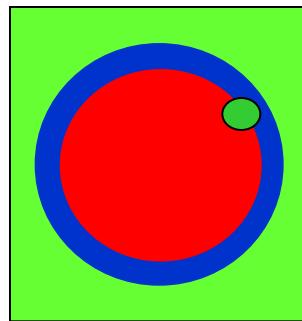
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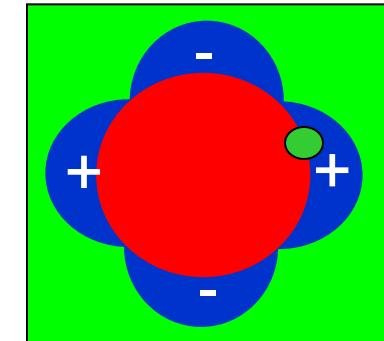


At the same time impurities affect superconductivity

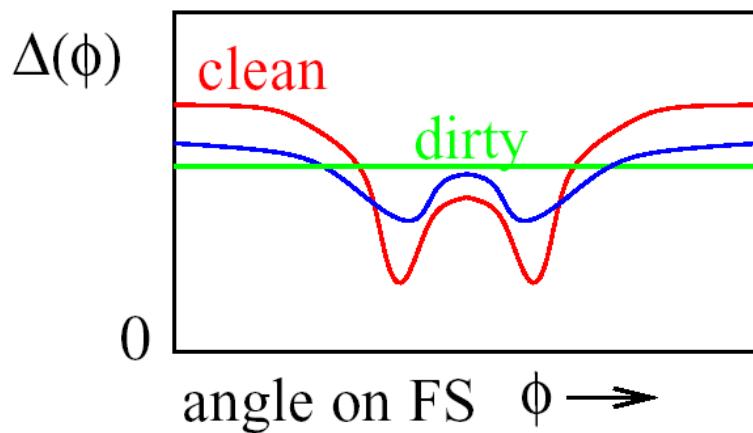
Impurities and superconductivity



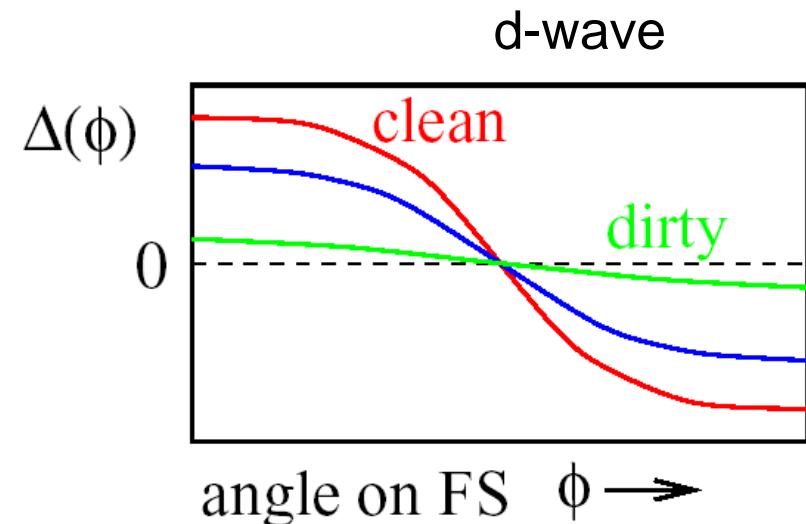
Scattering mixes gaps at different points at the FS



anisotropic s-wave



Anisotropy smeared out,
 T_c slightly suppressed



Gap and T_c suppressed

Self-consistent approximation



dilute impurities

$$n_{imp} \ll 1$$

$$\begin{aligned} \vec{r} \rightarrow \vec{r}' = & \vec{r} \rightarrow \vec{r}' + \vec{r} \xrightarrow{\hat{U}(\mathbf{r}_1)} \vec{r}' + \vec{r} \xrightarrow{\hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_1)} \vec{r}', \\ & + \vec{r} \xrightarrow{\hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_2)} \vec{r}', + \vec{r} \xrightarrow{\hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_2) \hat{U}(\mathbf{r}_2)} \vec{r}', \\ & + \vec{r} \xrightarrow{\hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_2) \hat{U}(\mathbf{r}_1)} \vec{r}', \end{aligned}$$

improbable: ignore

Then average over random positions of all impurities

Self-consistent approximation



dilute impurities

$$\vec{r} \rightarrow \vec{r}' = \vec{r} \rightarrow \vec{r}' + \dots$$

$\hat{U}(\mathbf{r}_1)$

$\hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_2)$

$\hat{U}(\mathbf{r}_1) \hat{U}(\mathbf{r}_2) \hat{U}(\mathbf{r}_2)$

Self-consistent T-matrix

$$\hat{G}^{-1}(\mathbf{k}, \omega) = i\omega_n - \xi(\mathbf{k})\tau_3 - \Delta_0\sigma_2\tau_2 - \hat{\Sigma} \equiv i\tilde{\omega} - \tilde{\varepsilon}(\mathbf{k})\tau_3 - \tilde{\Delta}\sigma_2\tau_2$$

$$\hat{\Sigma}(\mathbf{p}, \omega) = n_{\text{imp}} \hat{T}_{\mathbf{p}, \mathbf{p}}$$

$$\hat{T}_{\mathbf{p}, \mathbf{p}'} = \hat{U}_{\mathbf{p}, \mathbf{p}'} + \int d\mathbf{p}_1 \hat{U}_{\mathbf{p}, \mathbf{p}_1} \hat{G}(\mathbf{p}_1, \omega) \hat{T}_{\mathbf{p}_1, \mathbf{p}'}$$

Gap and order parameter
are not the same.

Full Green's function with
scattering on *all other impurities*:
need self-consistency

P. Hirschfeld et al., S. Schmitt-Rink et al. 1986

Abrikosov-Gorkov theory



Isotropic s-wave. Weak scatterers: Born approximation (2nd order)

Potential scattering does not affect T_c or gap: Anderson's theorem

Abrikosov-Gorkov theory



Isotropic s-wave. Weak scatterers: Born approximation (2nd order)

Potential scattering does not affect T_c or gap: Anderson's theorem

(Weak) magnetic scattering destroys superconductivity and the gap

$$\alpha_s = n_{imp} N_0 J^2 S(S+1)$$

FM coupling or small effective AFM coupling

Normal state scattering rate

single parameter: impurity concentration and strength appear together. Only in Born

Abrikosov, Gorkov, 1960

$$\ln \frac{T_c}{T_{c0}} = \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{\alpha_s}{2\pi T_{c0}}\right)$$

General equation:
needs correct definition of α

Abrikosov-Gorkov theory



Isotropic s-wave. Weak scatterers: Born approximation (2nd order)

Potential scattering does not affect T_c or gap: Anderson's theorem

(Weak) magnetic scattering destroys superconductivity and the gap

$$\alpha_s = n_{imp} N_0 J^2 S(S+1)$$

FM coupling or small effective AFM coupling

Normal state scattering rate

Gap for excitations (pole of Green's function) vanishes at

Order parameter (solution of self-consistency equation) exists up to

$$\alpha_s = \alpha_g = \Delta_0 \exp(-\pi/4)$$

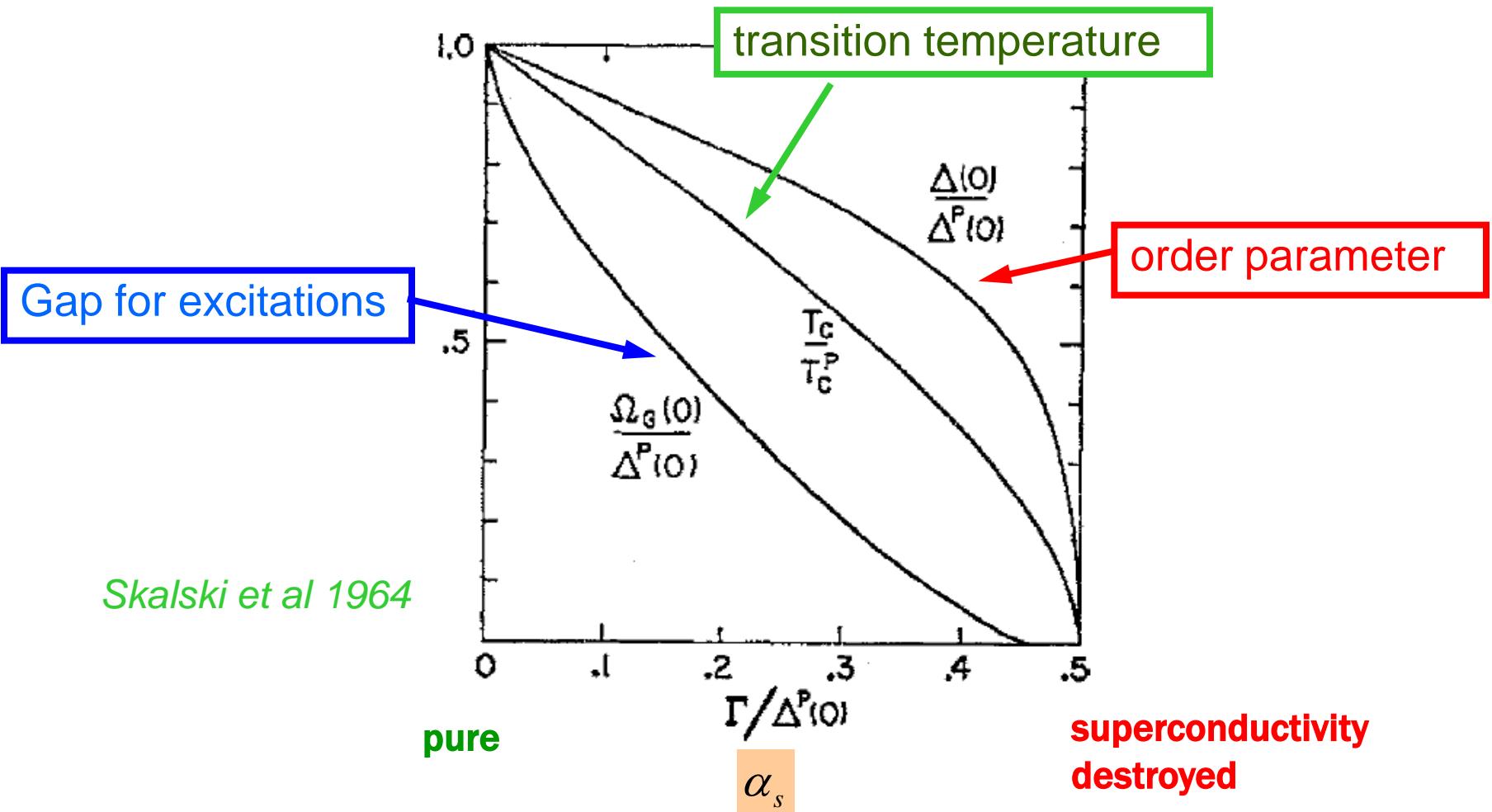
<

$$\alpha_s = \alpha_c = \Delta_0 / 2 \approx 1.1 \alpha_g$$

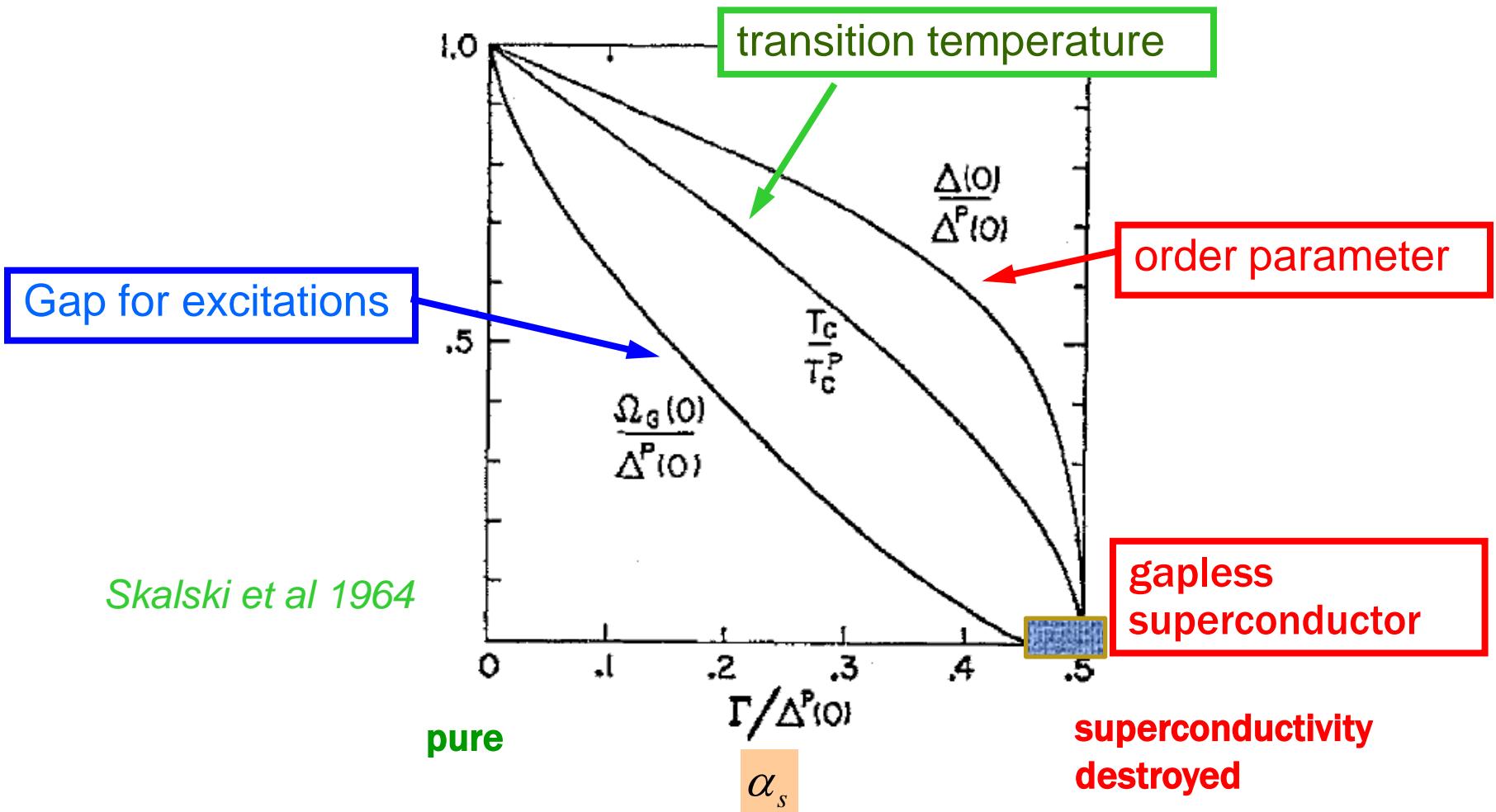
There exists a regime of gapless superconductivity!

Abrikosov, Gorkov, 1960

s-wave, weak magnetic scattering

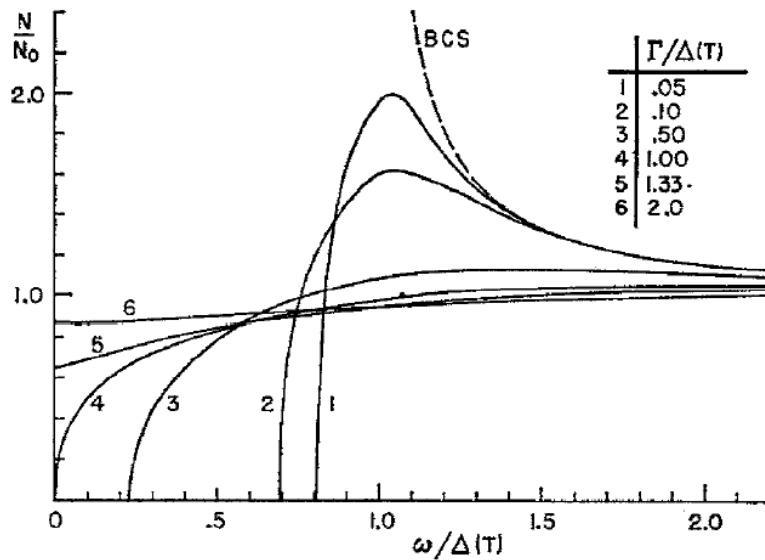


s-wave, weak magnetic scattering



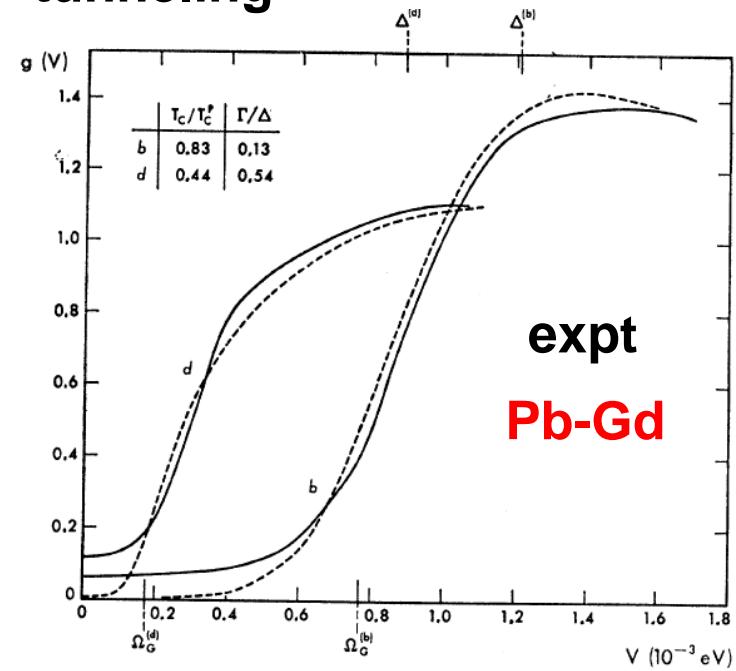
Comparison with experiment

theory



Skalski et al 1964

tunneling



M. Woolf and F. Reif, 1965

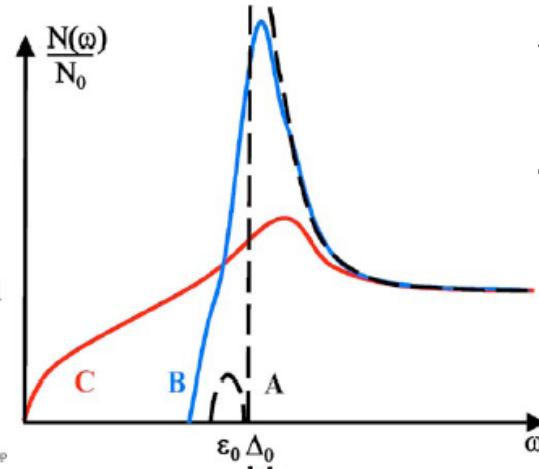
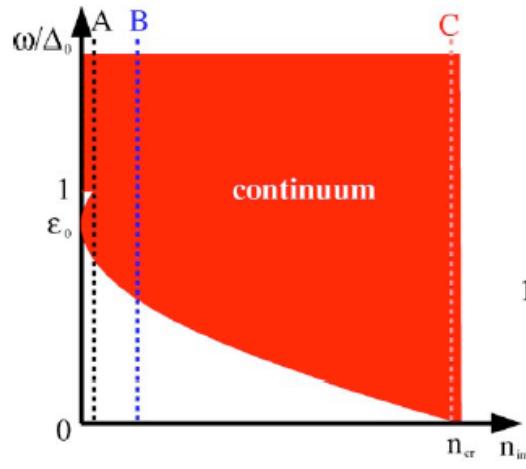
Shiba bands



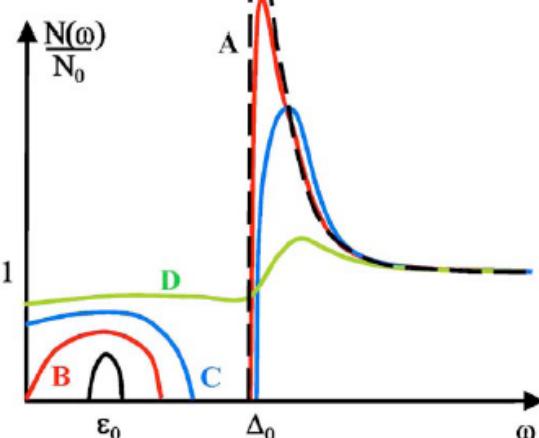
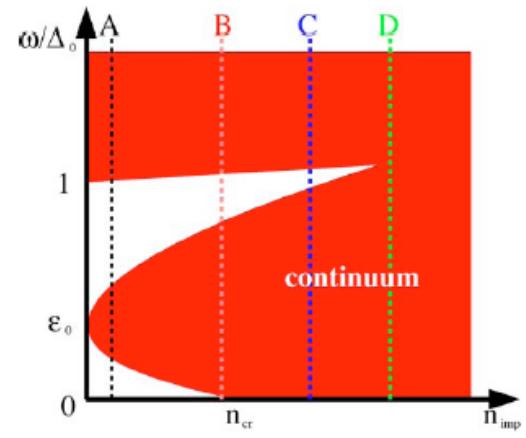
Abrikosov-Gorkov: smearing out of the gap edge

$$\alpha_s = n_{imp} N_0 J^2 S(S+1)$$

Growth of impurity band from the position of the bound state: hopping



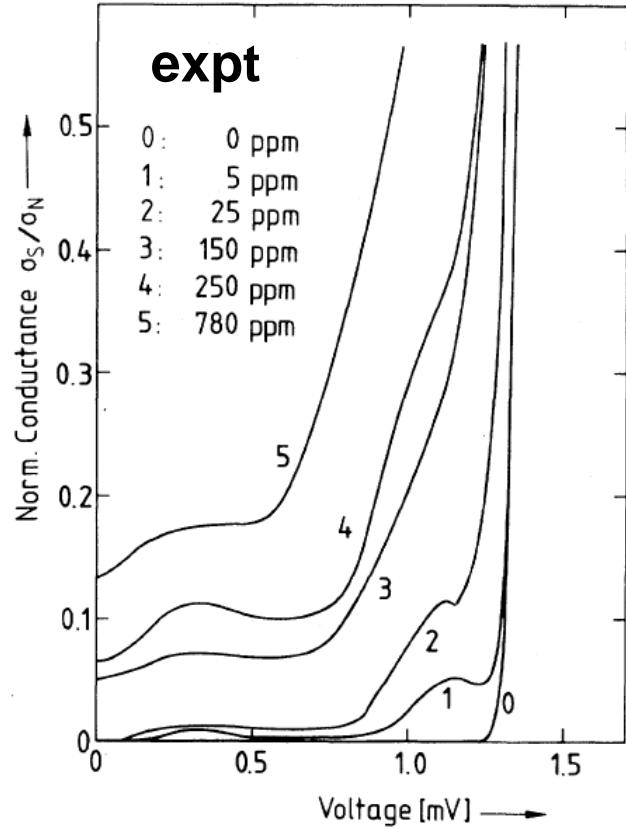
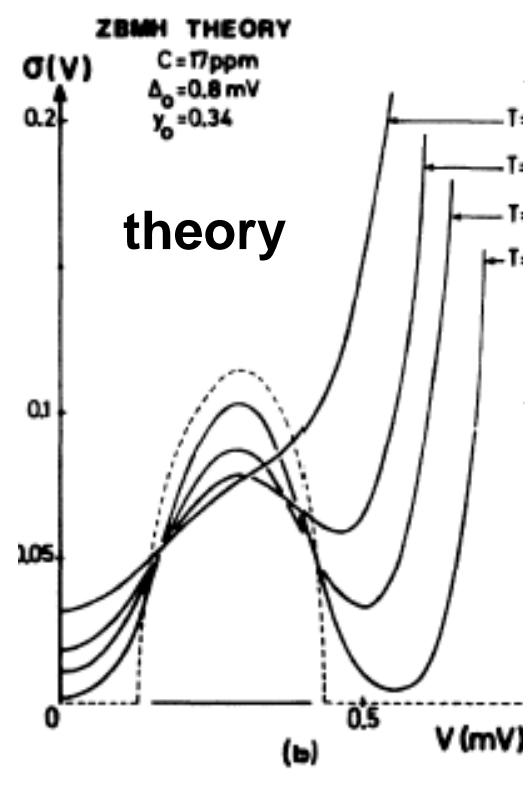
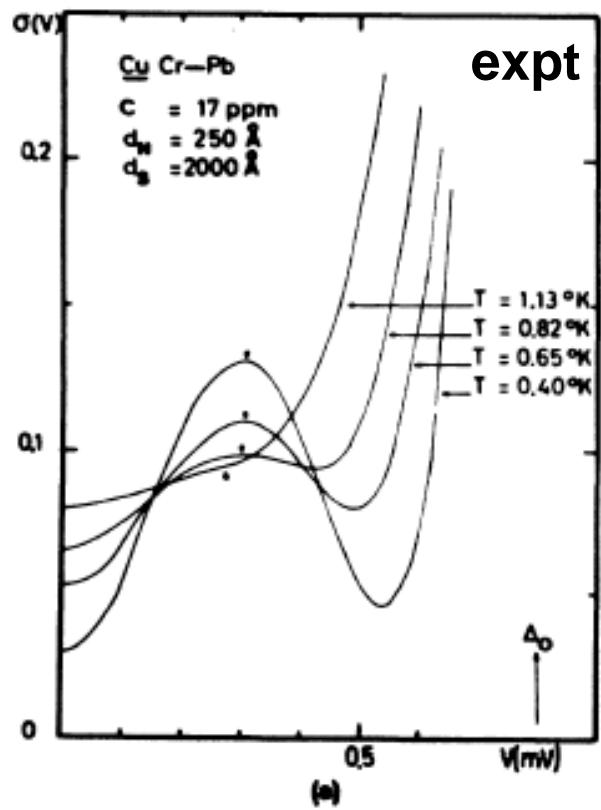
Weak scattering: bound state near the gap edge, smearing of the gap



Strong scattering: growth of impurity band from the position of the bound state in the gap

A. Balatsky, IV, J-X. Zhu 2006

Experiment



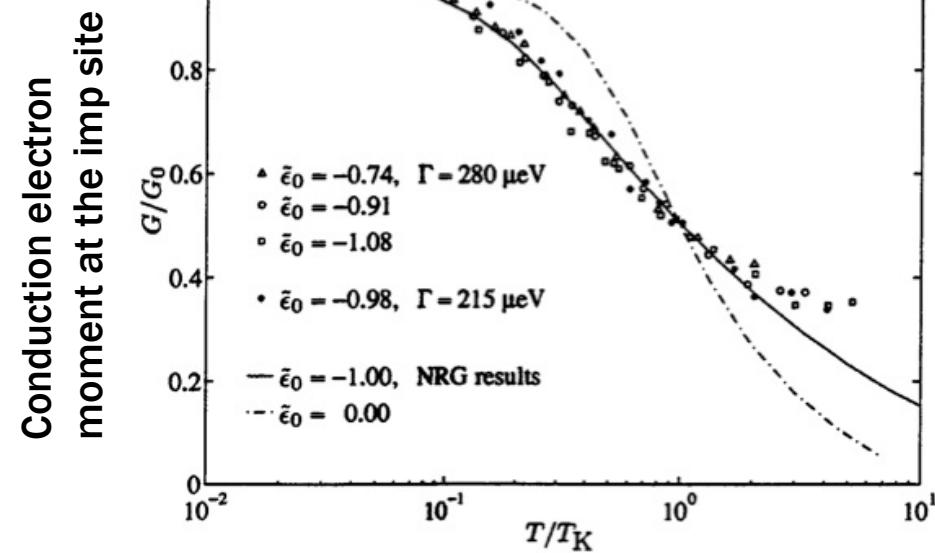
L. Dumoulin et al., 1977

W. Bauriedl et al., 1981

Many impurities: Kondo



Reminder: quantum effects mean that scattering depends on energy/temperature, is strongest for $T \sim T_K$



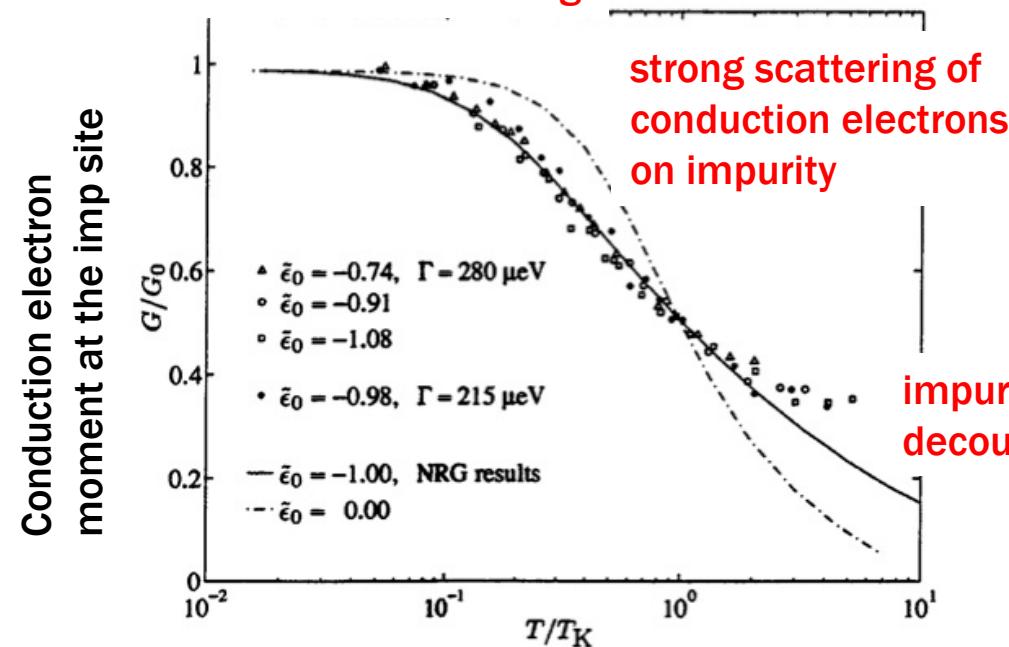
D. Goldhaber-Gordon et al 1998

Many impurities: Kondo



Reminder: quantum effects mean that scattering depends on energy/temperature, is strongest for $T \sim T_K$

impurity spin nearly screened: weak scattering



D. Goldhaber-Gordon et al 1998

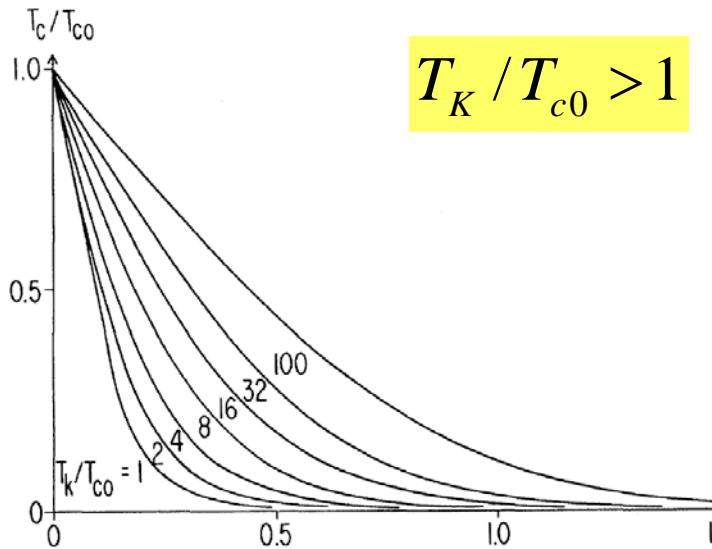
Scattering rate depends on the ratio of T_c/T_K

$$\alpha \approx n_{imp} \frac{\pi^2 S(S+1)}{\ln^2 T_c/T_K + \pi^2 S(S+1)}$$

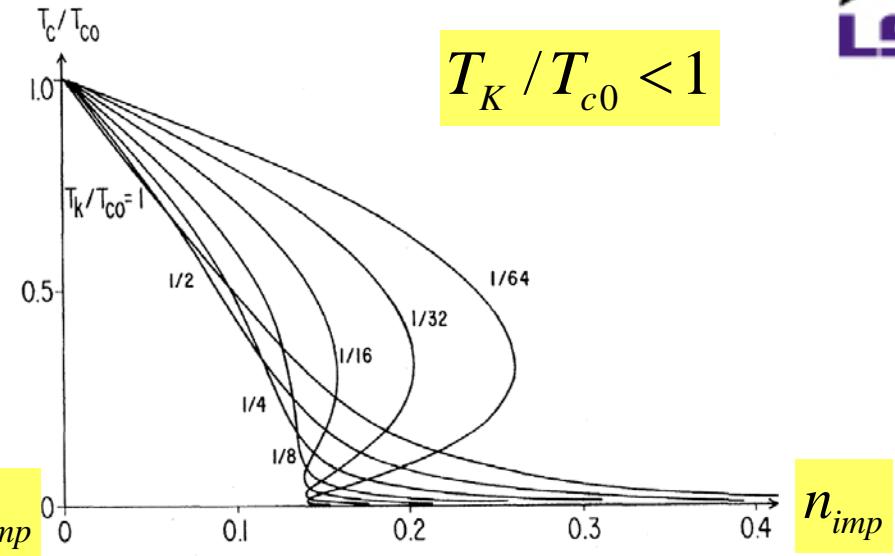
J. Zittartz and E. Müller-Hartmann 1971

Determine T_c self-consistently

Many impurities: Kondo II



$$T_K / T_{c0} > 1$$



$$T_K / T_{c0} < 1$$

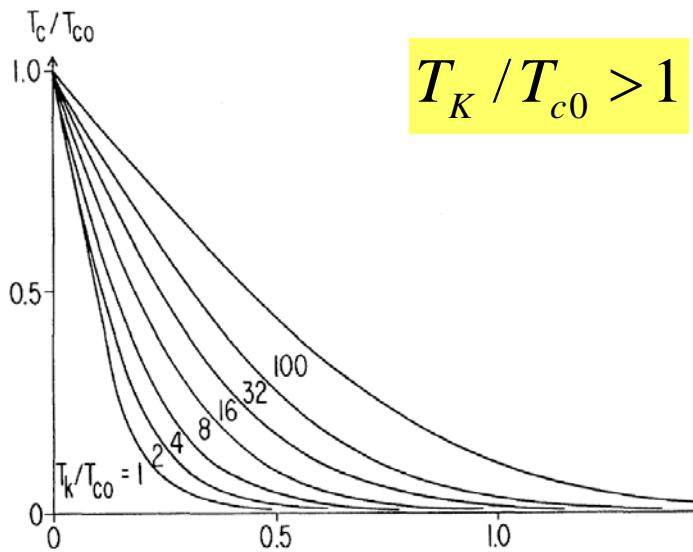
At $T=0$ fully screened impurity:
no pairbreaking

Lower T_{c0} : less efficient scattering

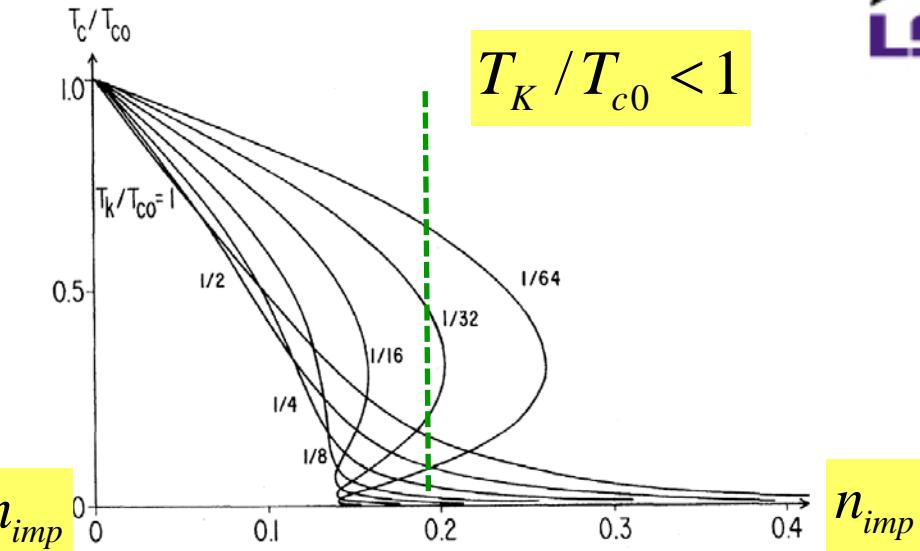
Approximation questionable

J. Zittartz and E. Müller-Hartmann 1971

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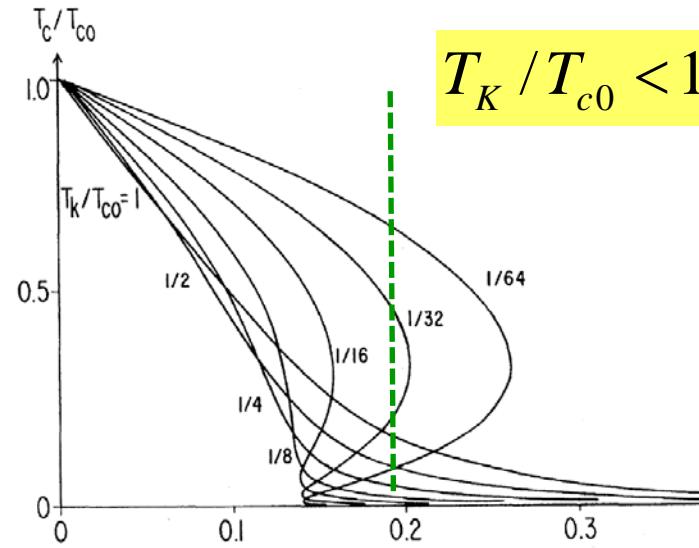
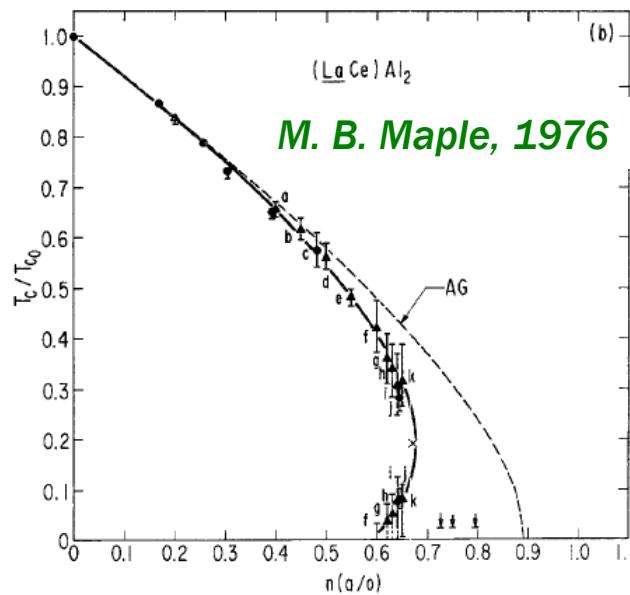
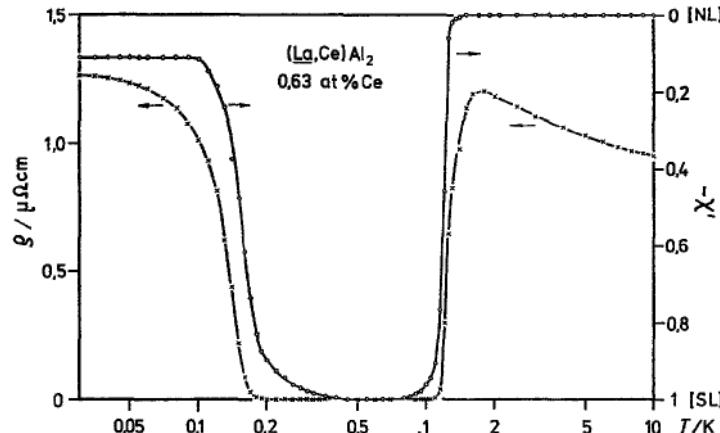
Reentrance:

- a) Superconducting at $T_c > T_K$
- b) Approach T_K : scattering increases, back to normal
- c) At $T < T_K$ screening, scattering decreases:,back to superconductor

Many impurities: Kondo II

K. Winzer, 1973

K. Winzer



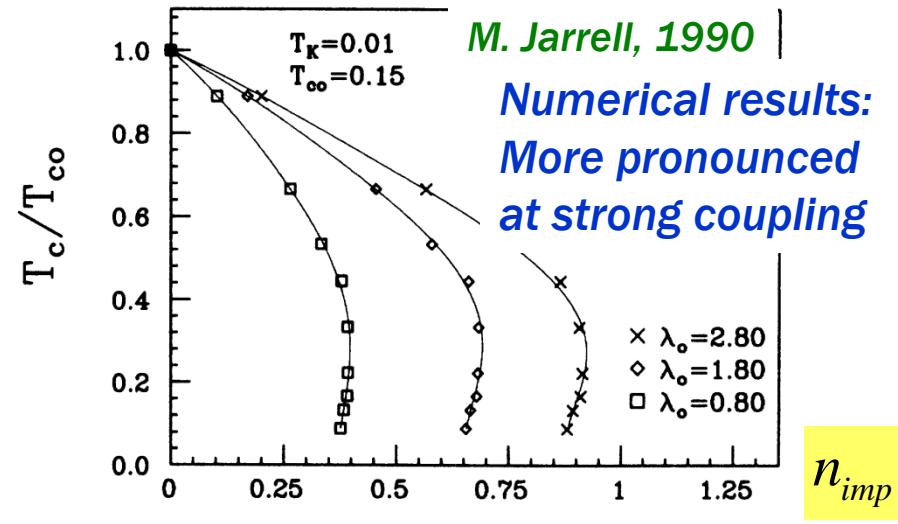
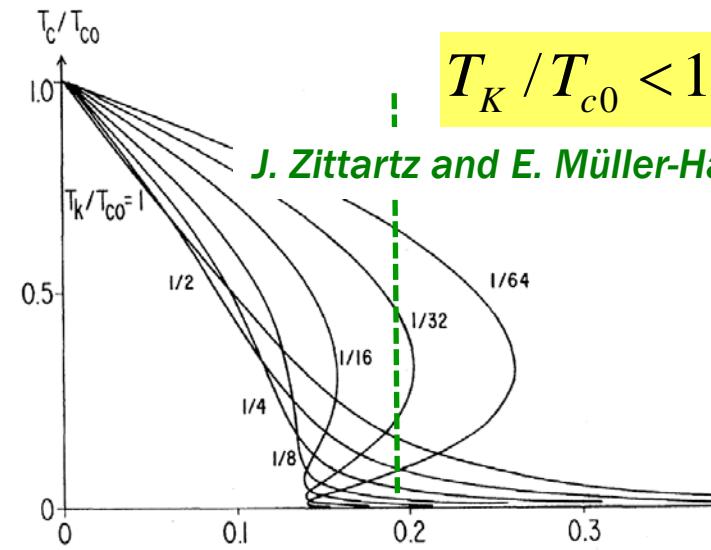
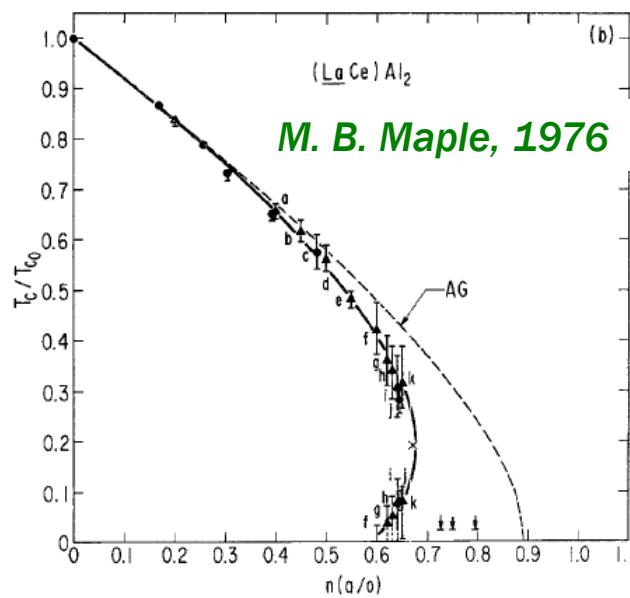
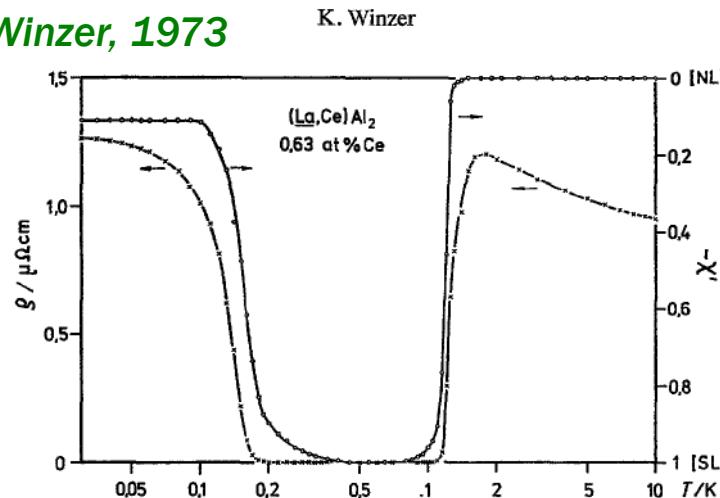
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J. Zittartz and E. Müller-Hartmann 1971

Many impurities: Kondo II

K. Winzer, 1973



Dirty superconductors with nodes



All impurities are pairbreaking

Γ scattering rate in the normal state

Always gapless (in self-consistent T-matrix)

Born limit (weak scattering)

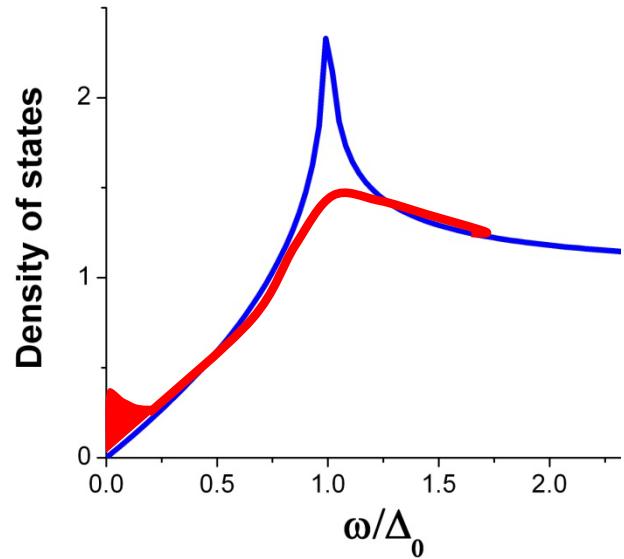
$$\frac{N_{sc}(0)}{N_0} \approx \frac{\Delta_0}{\Gamma} \exp\left[-\frac{\Delta_0}{\Gamma}\right]$$

*L. Gorkov and P. Kalugin, 1985,
T. Rice and K. Ueda, 1985*

Unitarity limit (strong scattering)

$$\frac{N_{sc}(0)}{N_0} \approx \sqrt{\frac{\Gamma}{\Delta_0}}$$

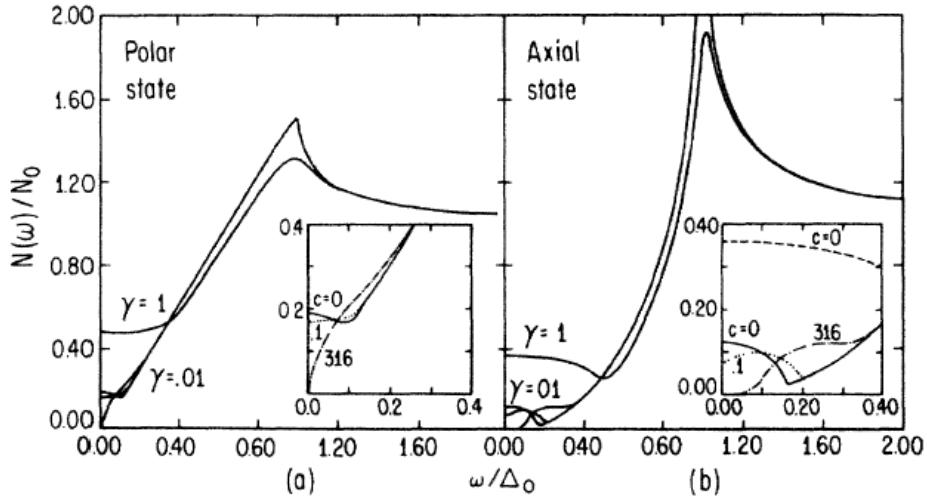
*P. Hirschfeld et al., 1986,
S. Schmitt-Rink et al., 1986*



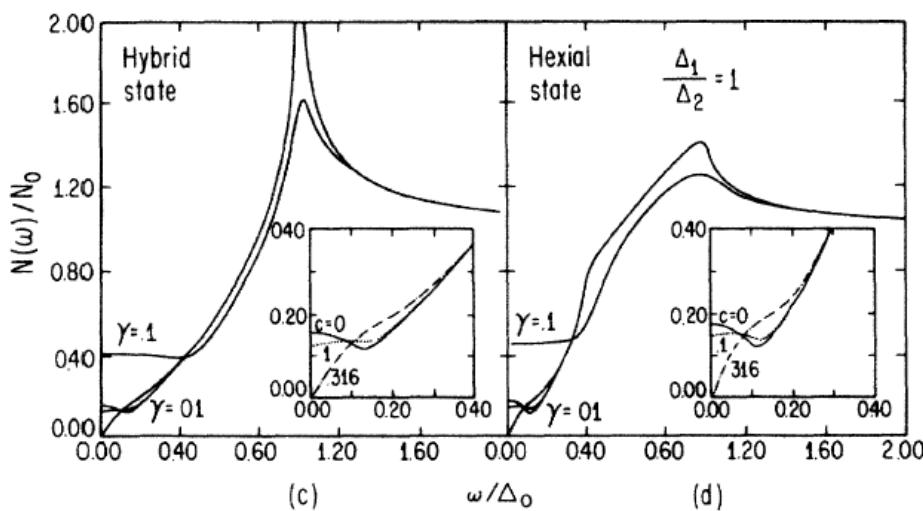
Gapless behavior in nodal SC



P. Hirschfeld et al., 1989,



Finite DOS at $\omega=0$ (gapless)



Impurity bandwidth

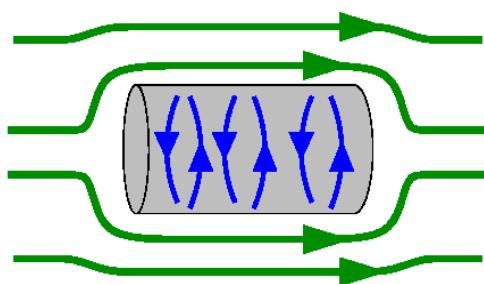
$$\frac{\gamma}{\Delta_0} \approx \frac{N_{sc}(0)}{N_0}$$

Born: small

Unitarity: large

Can be experimentally measured

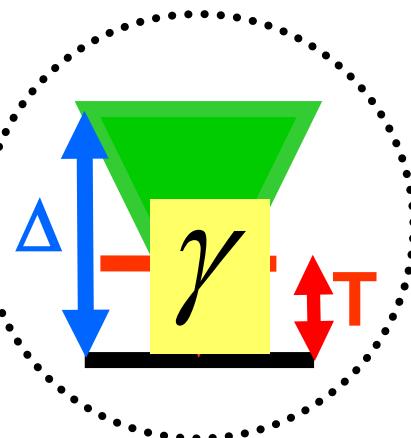
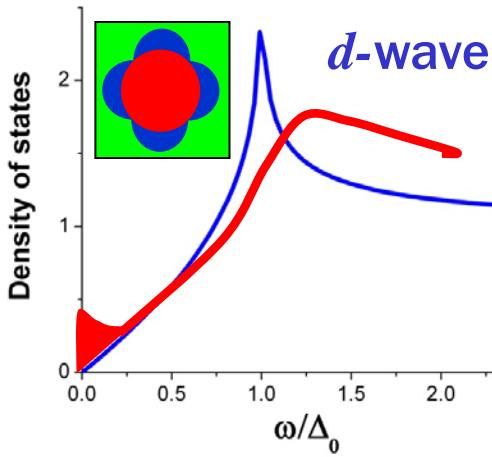
Penetration depth in superconductors



Magnetic field is screened at the length

$$\lambda_L^{-2} \propto n_s$$

density of superconducting electrons

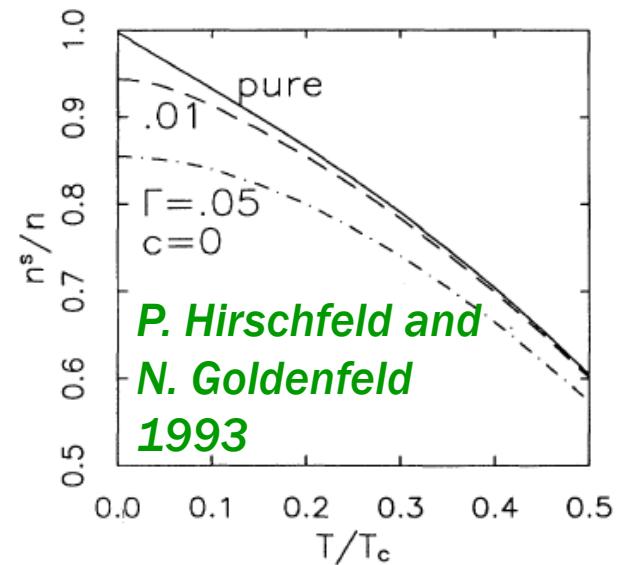


$$\Delta\lambda_L^{-2} \propto T$$

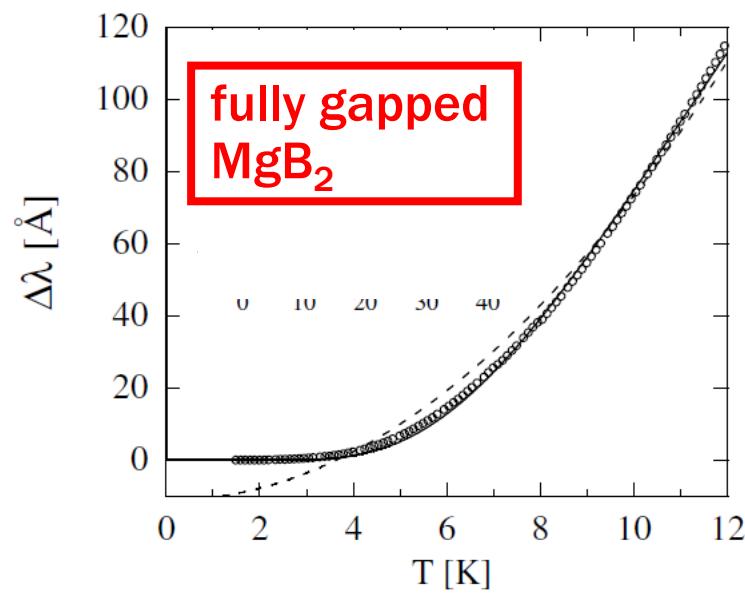
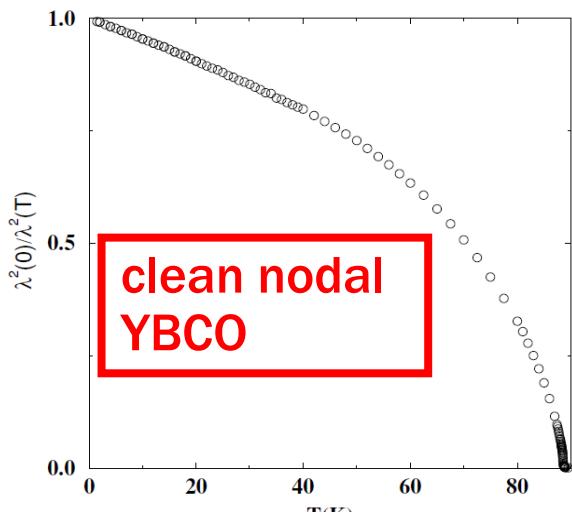
at low T

$$\Delta\lambda_L^{-2} \propto T^2 / \gamma$$

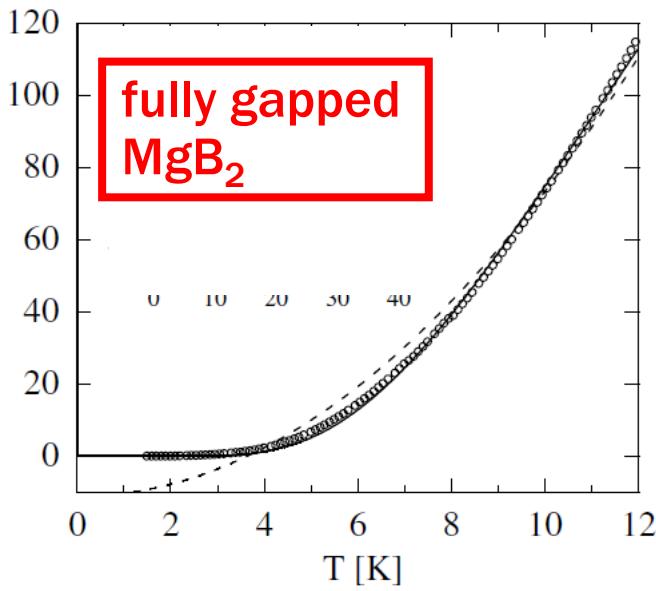
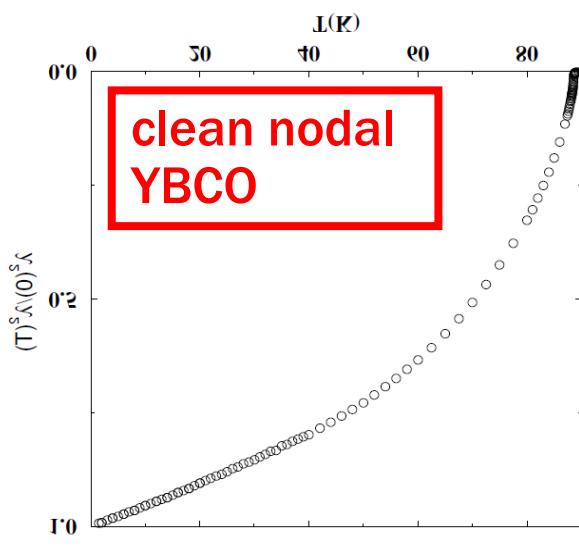
at low T



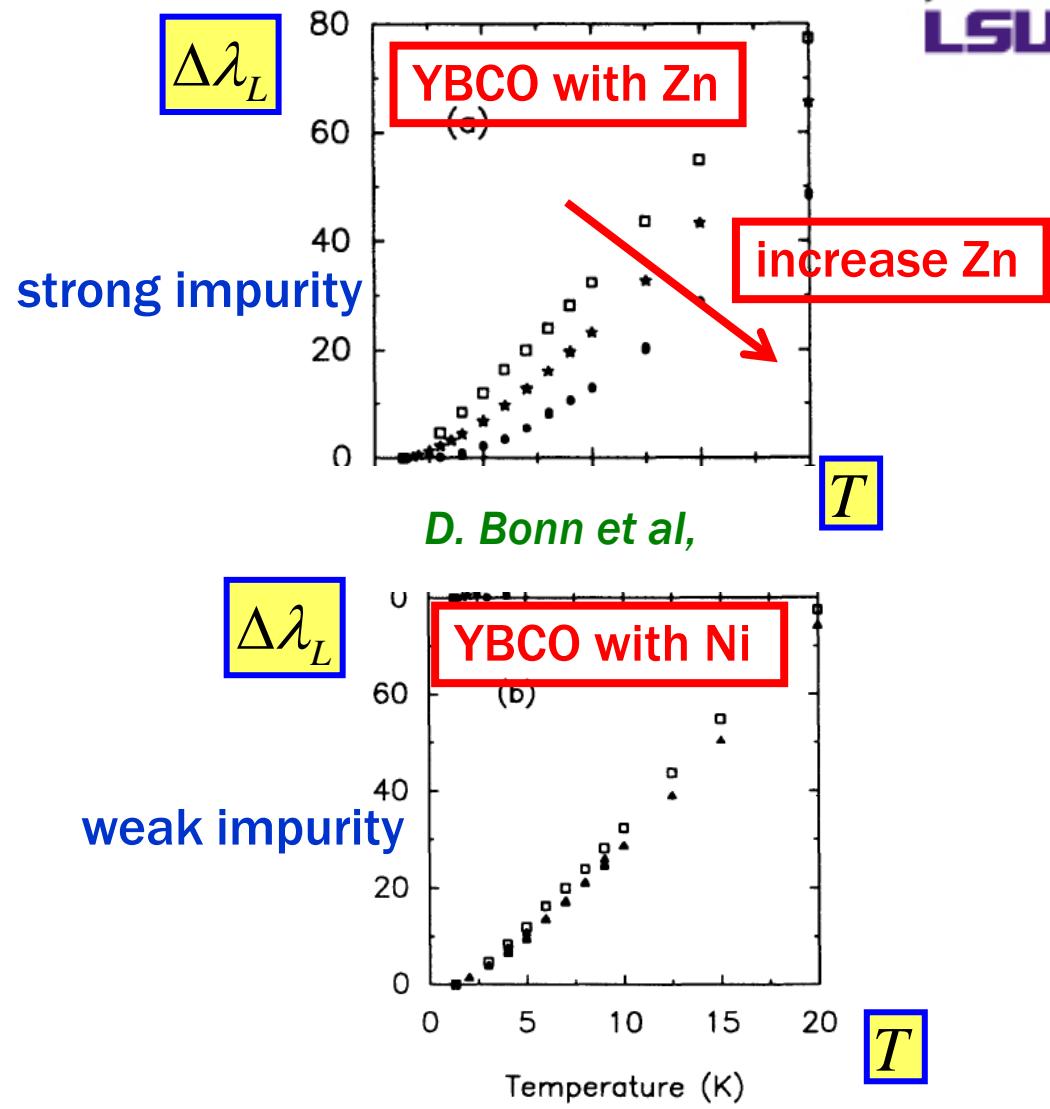
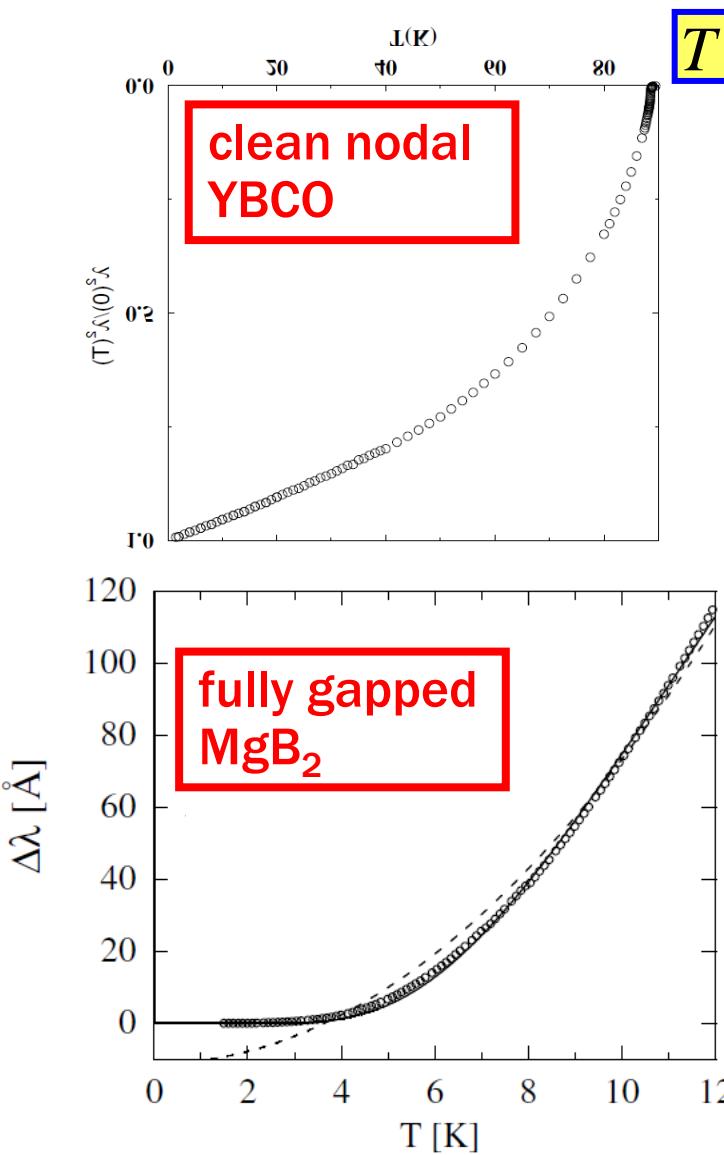
Penetration depth in superconductors



Penetration depth in superconductors



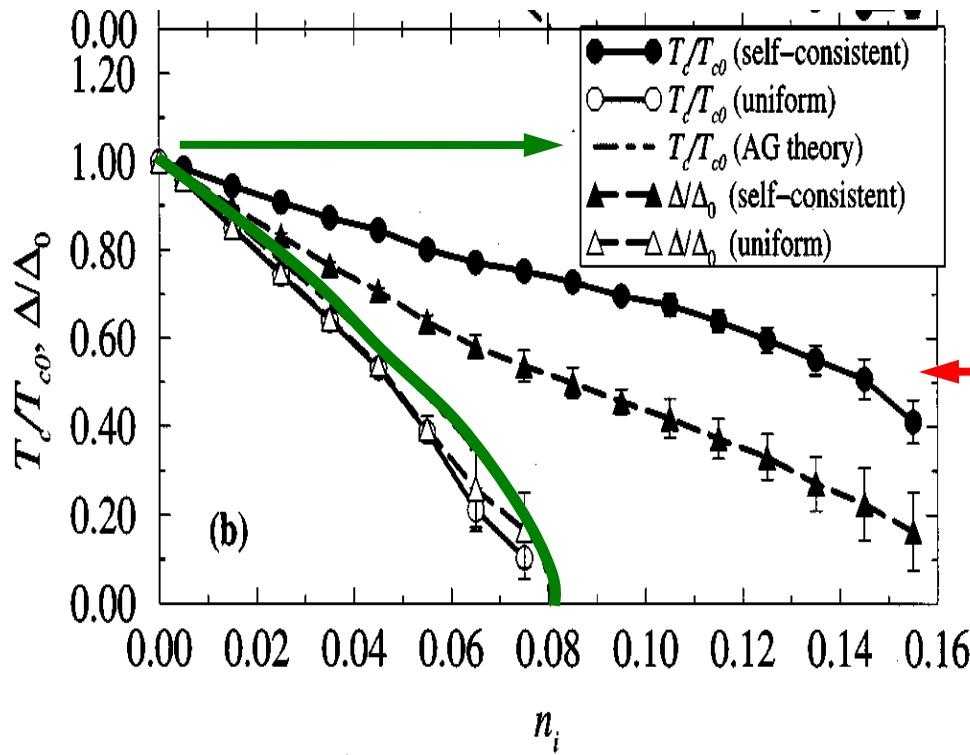
Penetration depth in superconductors



Transition temperature suppression



Non-magnetic impurities suppress unconventional superconductivity
just as magnetic impurities suppress isotropic pairing



AG theory assumes uniform suppression of the gap in the bulk

For short coherence length, a local suppression (“swiss cheese” superconductor) may be better

M. Franz et al. 1997

Message: part IV



Impurity bands in superconductors:

- s-wave: due to magnetic impurities
- d-wave: due to any impurities

Transition temperature suppressed by these impurities in a similar fashion for both cases.

Gapless superconductors:

- s-wave: above critical concentration *not counting tails*
- d-wave: at any concentration *small for Born*

Final Summary

Impurity bound/resonant states grow into impurity bands

- s-wave: due to magnetic impurities
- d-wave: due to any impurities

Screening of the local moment competes with pairing: from local moment + pairs to local singlet + unpaired electron

Understanding of single impurity Kondo in s-wave systems, open questions (pseudogap Kondo, quantum criticality) in d-wave.

Re-entrant superconductivity in Kondo s-wave superconductors

Impurity-controlled physics at low T in nodal systems

And now what happens if we have Kondo ion on each site?