Impurity states and marginal stability of unconventional superconductors

A.V.Balatsky(LANL)

- local =atomic or coherence length scale
- impurity or defect
- Impurity states inconventional supercondcutors
- Impurity states in unconventional superconductors
- Impurity states in pseudogap state

http://theory.lanl.gov

Rev Mod Phys, v 78, p 373 (2006)

See also Peter Hischfeld lectures

REVIEWS OF MODERN PHYSICS, VOLUME 81, JANUARY–MARCH 2009

Defects in correlated metals and superconductors

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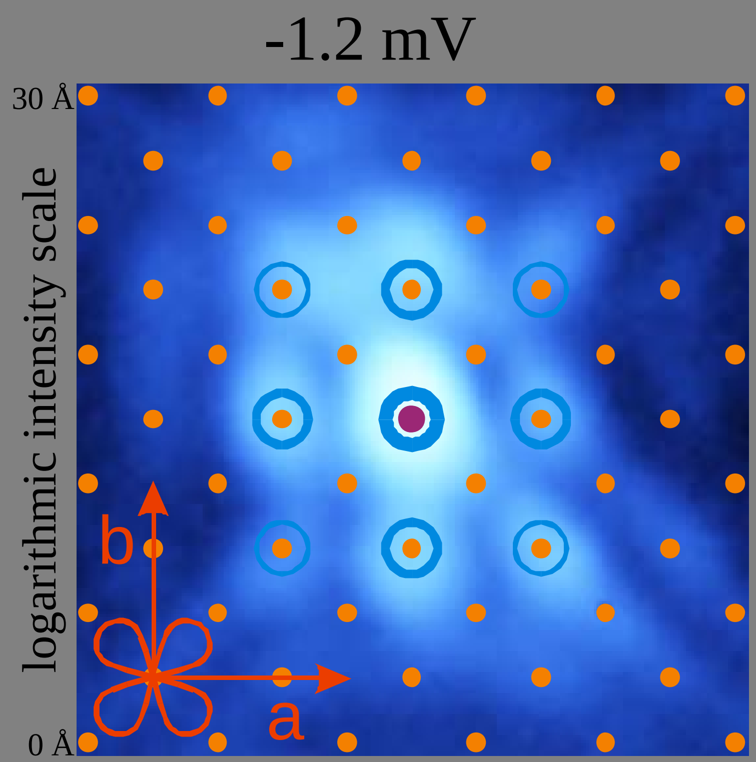
(Published 8 January 2009)

Motivation 1

Impurities as a local probe of the symmetry of the superconducting order parameter:



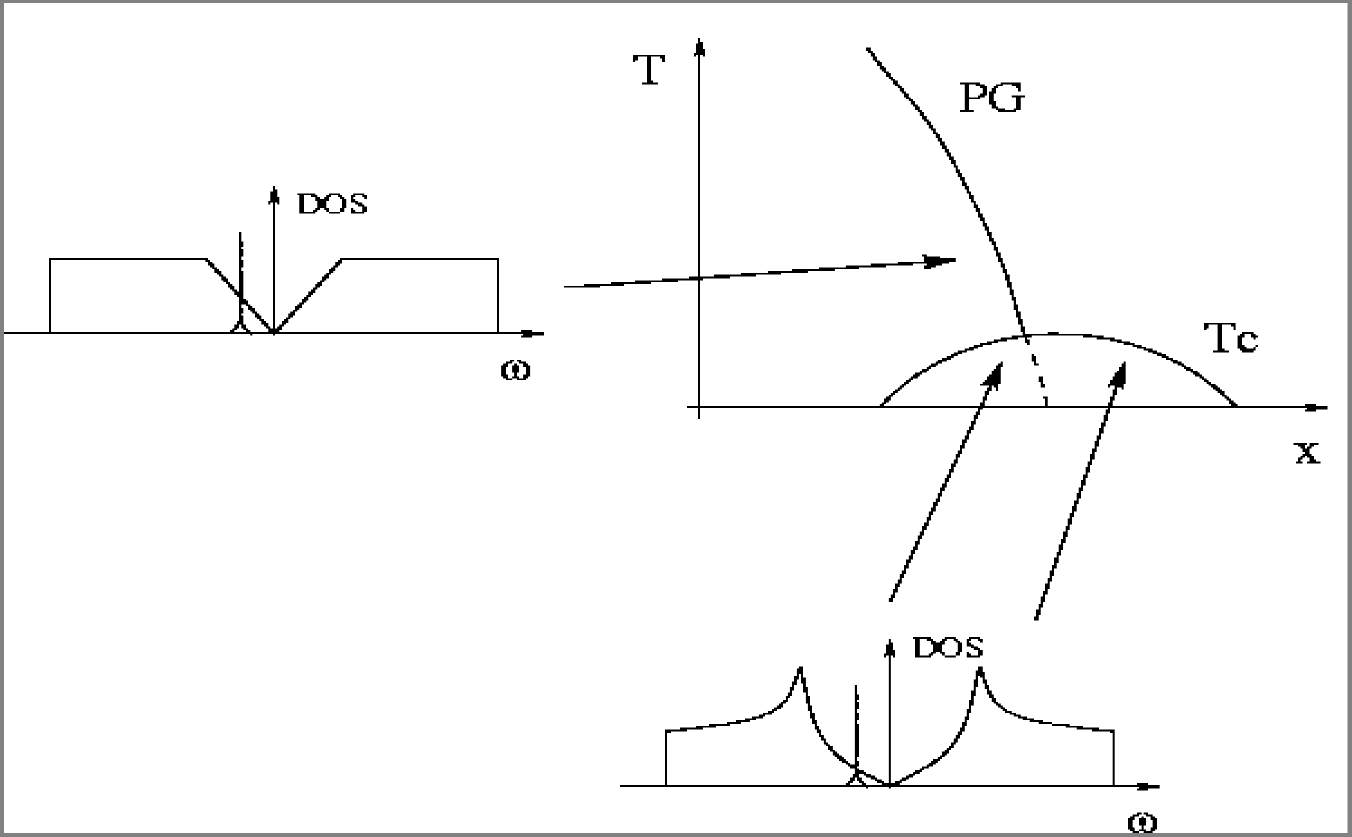
Zn atoms in $Bi_2Sr_2Ca(Cu_{1-x}Ni_x)_2O_{8+\delta}$

Four-fold symmetry,
aligned with the gap nodes

S.H. Pan et al, Nature (2000)

Motivation 2

Impurities as a probe of the Pseudogap state of high-Tc superconductors



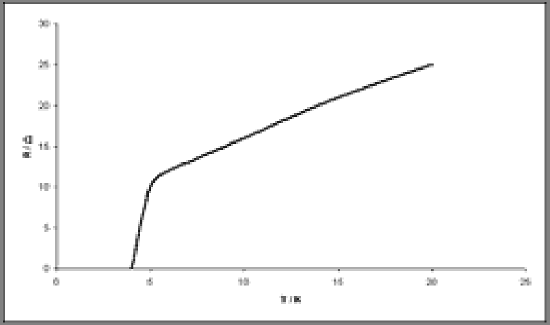
Motivation 3

Most of the theory and experiment on
conventional superconductors was done *before*
Local probes, like Scanning Tunneling Microscopy were
Invented.

A lot of views have had “calcified” into standard
Textbook wisdom.

I will show some examples where local probes bring in
New and unexpected perspective, sometime new results.

Brief history



1911 – H. Kamerlingh-Onnes: superconductivity in mercury, Tc = 4K

1933 – Meissner effect: expulsion of magnetic field

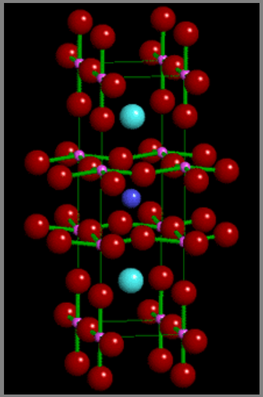
1957 – Bardeen-Cooper-Schrieffer (BCS) theory

1962 – Josephson effect

1986 – first high-Tc superconductor, LBCO Tc = 35K

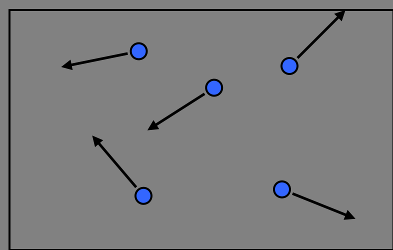
1987 – YBCO, Tc = 93K – warmer than liquid N

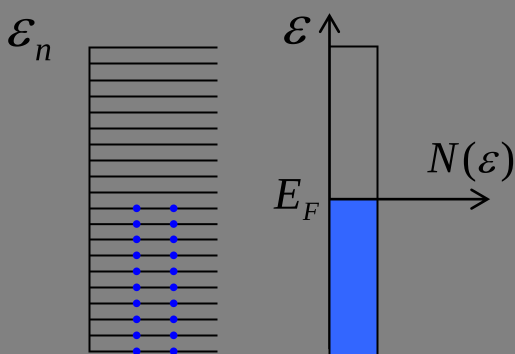
1995 – $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.33}$ Tc = 138K



Superconductivity primer

Metal



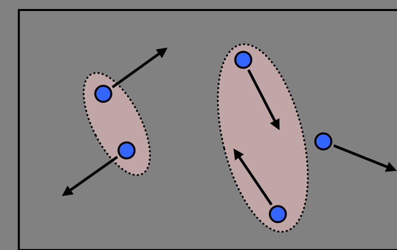


$$\varepsilon_k = \frac{k^2}{2m} - E_F$$

Electrons:

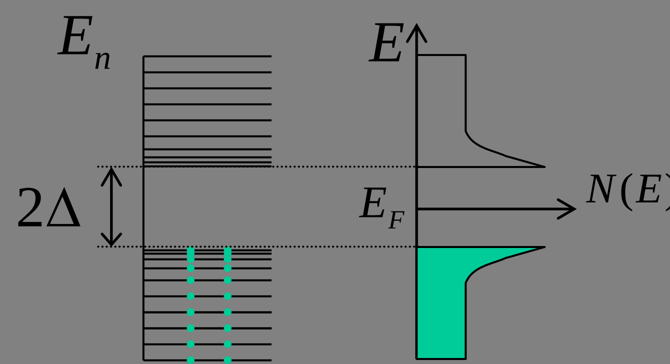
$c_{k\uparrow}, c_{k\downarrow}$

Superconductor



Cooper pairs

(k & -k)

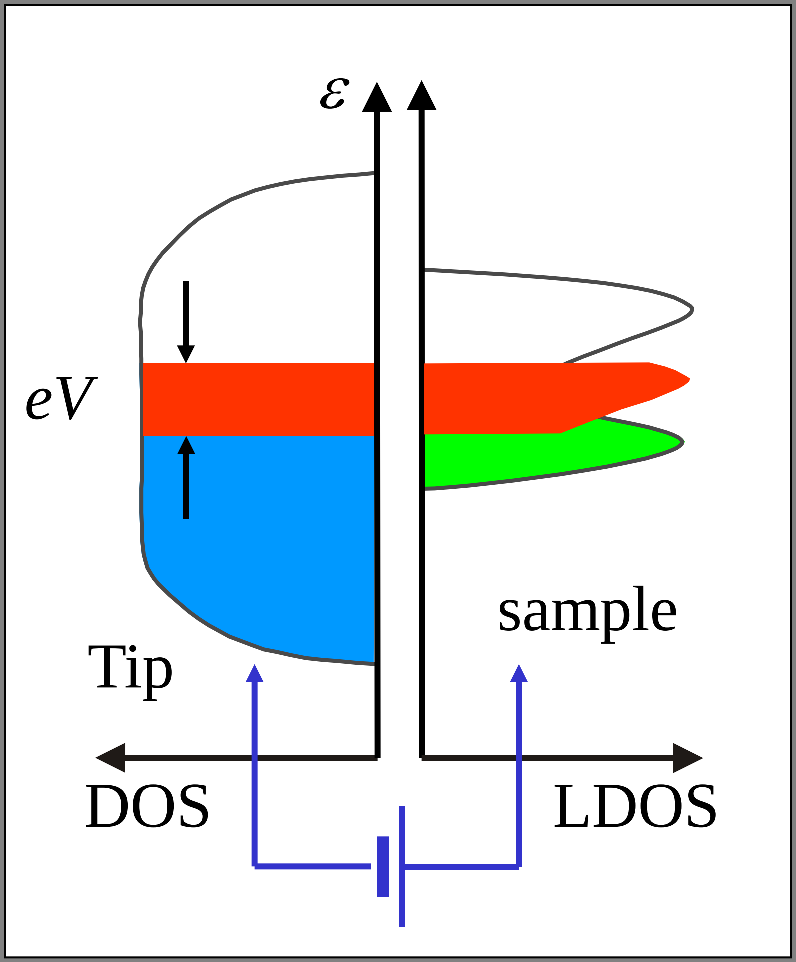


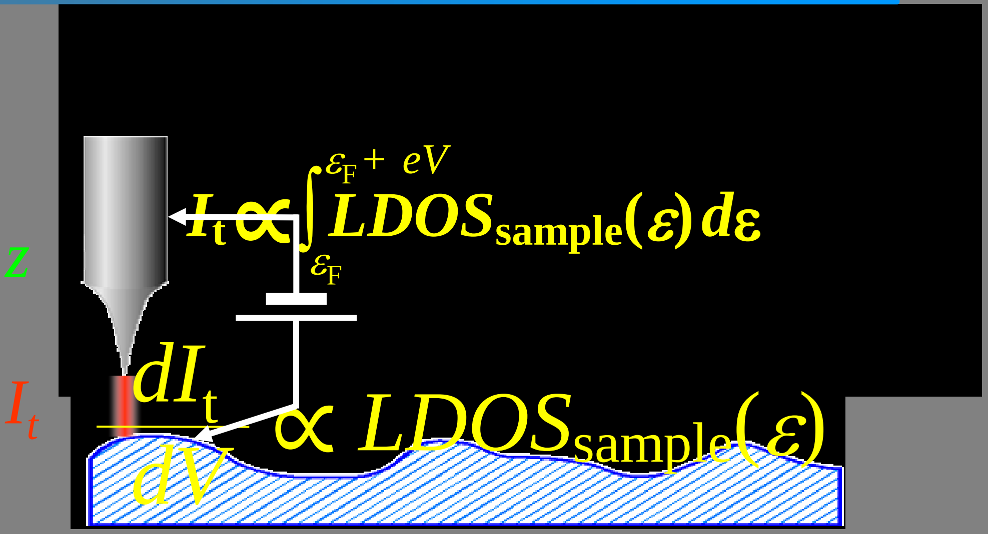
$$E_k = \pm\sqrt{\varepsilon_k^{\,2} + \Delta^2}$$

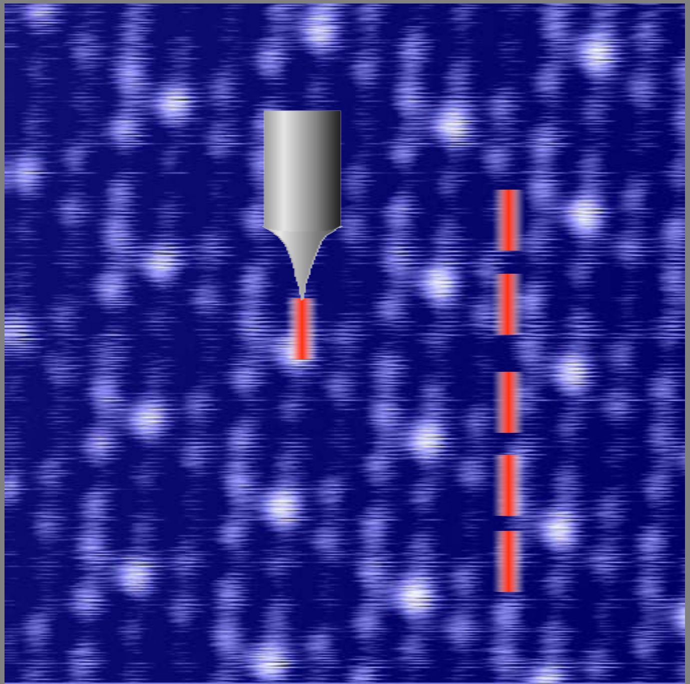
Bogoliubov q.particles:

$\gamma_{k\uparrow}, \gamma_{k\downarrow} (\gamma_{k\uparrow} = u_k c_{k\uparrow} + v_k c^{+}_{-k\downarrow})$

Local Probes:Scanning tunneling microscopy/spectroscopy







Spectroscopic map (LDOS map) can be obtained.

Bogoliubov-Nambu Hamiltonian background

Bogoliubov angle measures the relative weight between particle
And hole component in Bogoliubov deGennes quasiparticle

$$H = \varepsilon(k) c_{ks}{}^{\dagger} c_{ks} + (\Delta_k c_{ks}{}^{\dagger} c^{\dagger}{}_{-k-s} + h\ )$$

$$\gamma^{*}_{k\uparrow} = u_k c_{k\uparrow} + v_k c^{*}_{-k\downarrow}$$

True excitations in SC state
That are quantum mechanica
Mixture of particle and hole

$$\gamma_k \left| \Psi_0 \right\rangle = 0;$$
$$\gamma^{\dagger}{}_k \left| \Psi_0 \right\rangle = \left| \Psi_1 \right\rangle$$

$$|u(k)|^2 = 1/2\ 1(-\varepsilon(k)/E(k))$$
$$|v(k)|^2 = 1/2\ 1(+\varepsilon(k)/E(k))$$

Important! Dual nature of qp inSC

$$\gamma^{\dagger}{}_{\uparrow k} \left| \Psi_0 \right\rangle = \left| \Psi_1 \right\rangle \propto c^{\dagger}{}_{\uparrow}(k) \,|\, \Psi_1 \ \ \rangle$$

and at the same time $\propto \mathrm{c}_{\downarrow}(-k) \,|\, \Psi_1 \ \ \rangle$

Bogoliubov Quasiparticles

$$\gamma_{i\uparrow} = u_i \psi_{i\uparrow} - v_i \psi^{+}_{-i\downarrow}$$ mixing particles and holes

$$\gamma^{+}_{-i\downarrow} = u_i \psi^{+}_{-i\downarrow} + v_i \psi_{i\uparrow}$$

$$u_i^{\,2} + v_i^{\,2} = 1$$

GS: $$\left|\Psi_0\right\rangle = \prod_{i>0} (u_i + v_i \psi^{+}_{i\uparrow} \psi^{+}_{-i\downarrow}) \left|0\right\rangle$$

Excited State:

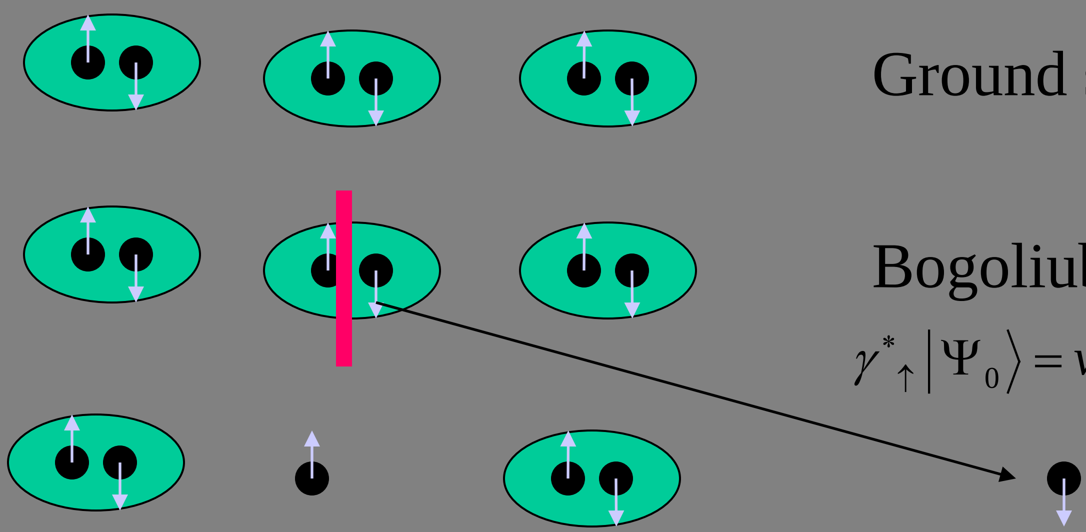
$$\left|\Psi_{-1\downarrow}\right\rangle = \gamma^{+}_{-1\downarrow}\left|\Psi_0\right\rangle = \psi^{+}_{-1\downarrow} \prod_{i>1} (u_i + v_i \psi^{+}_{i\uparrow} \psi^{+}_{-i\downarrow}) \left|0\right\rangle$$

$$\psi_{1\uparrow}\left|\Psi_0\right\rangle = v_1 \left|\Psi_{-1\downarrow}\right\rangle,$$ Negative bias

$$\psi^{+}_{-1\downarrow}\left|\Psi_0\right\rangle = u_1 \left|\Psi_{-1\downarrow}\right\rangle$$ Positive bias

Tunneling into SC

- Particle and hole component in tunneling sample the same Bogoliubov Nambu quasiparticle. The only difference is relative weight of these two processes.



Ground state $\left|\Psi_0\right\rangle$

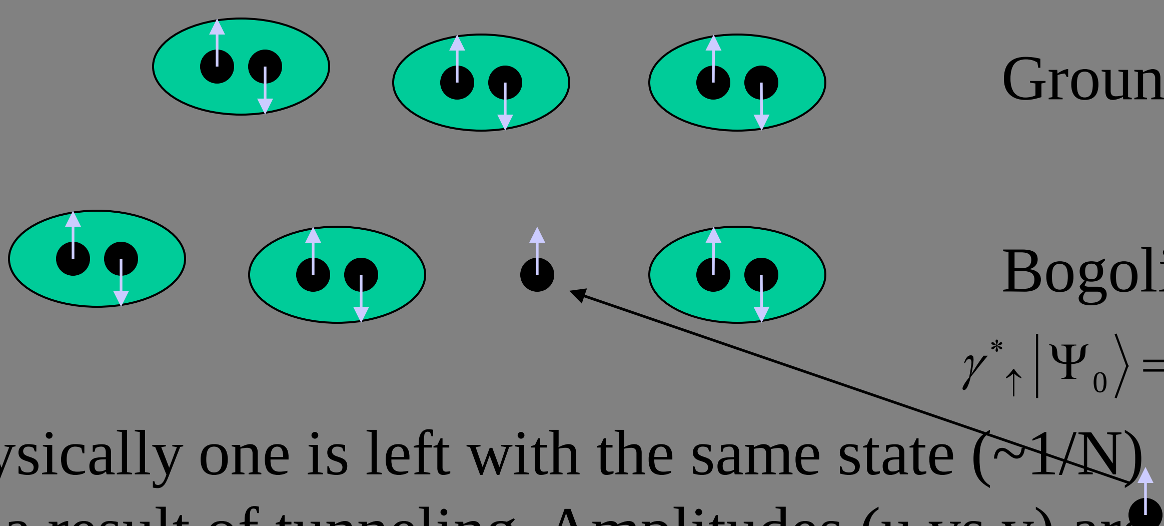
Bogoliubov excitation

$$\gamma^*_{\uparrow}\left|\Psi_0\right\rangle = v_n c_{n\downarrow} \prod_i (u_i + v_i c_i^{\,*} c_{-i}^{\,*}) \left|0\right\rangle$$

Electron spin down
Tunneling out

Tunneling into SC

- Particle and hole component in tunneling sample the same Bogoliubov Nambu quasiparticle. The only difference is relative weight of these two processes.



Ground state $|\Psi_0\rangle$

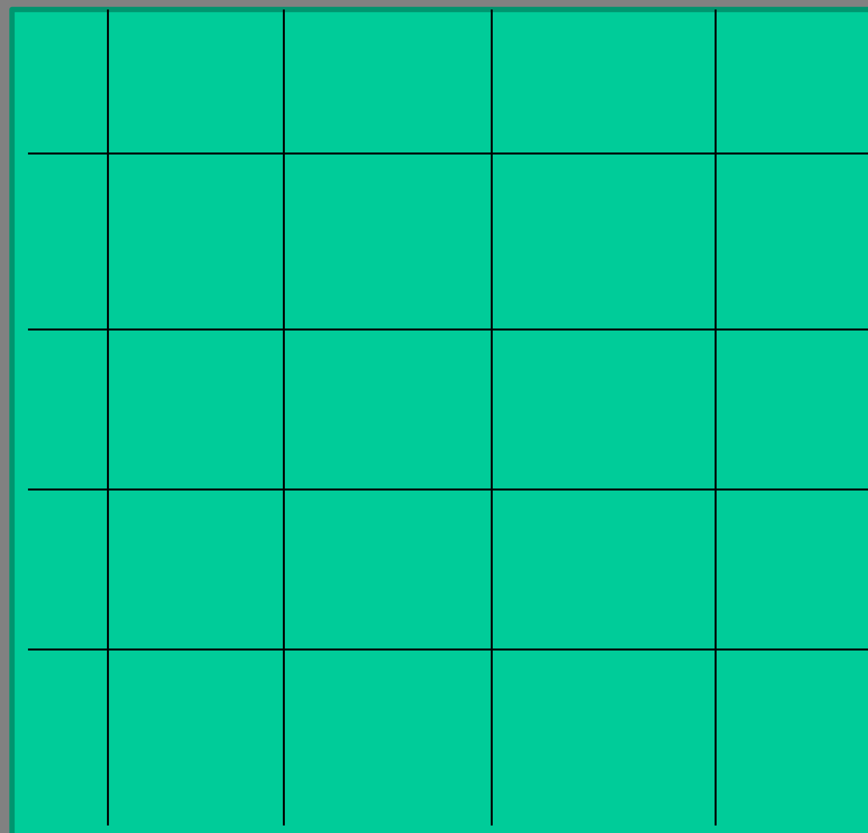
Bogoliubov excitation

$$\gamma^*_{\uparrow}|\Psi_0\rangle = u_n c*_{n\uparrow}\prod_{i\neq n}(u_i + v_i c_i^{\ *} c_{-i}^{\ *})|0\rangle$$

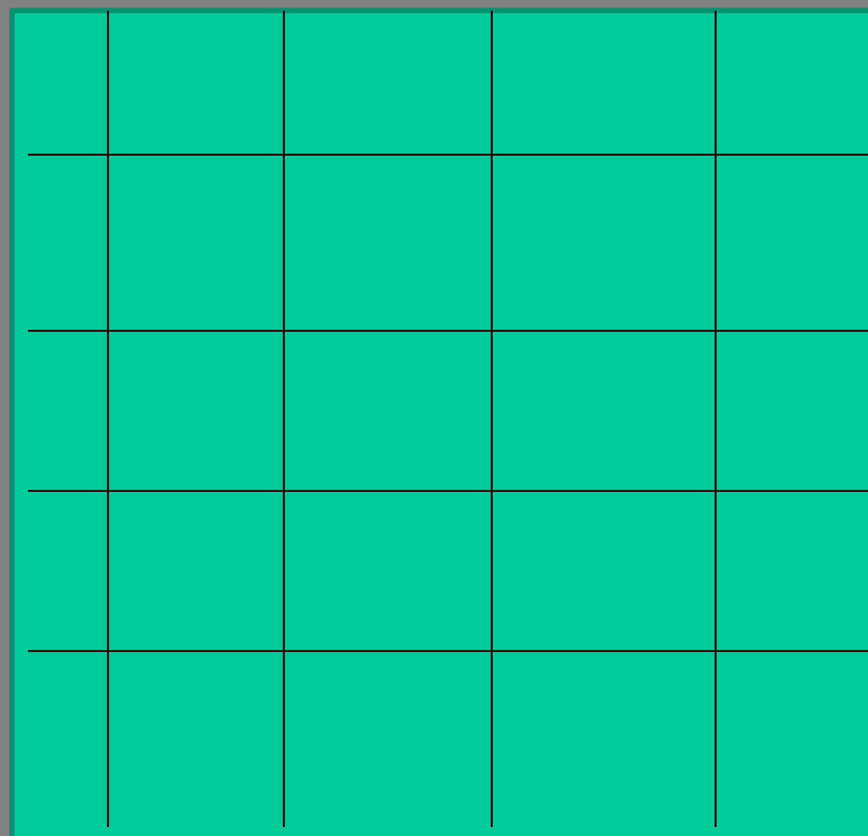
Physically one is left with the same state (~1/N)
As a result of tunneling. Amplitudes (u vs v) are different

Electron spin up
Tunneling in

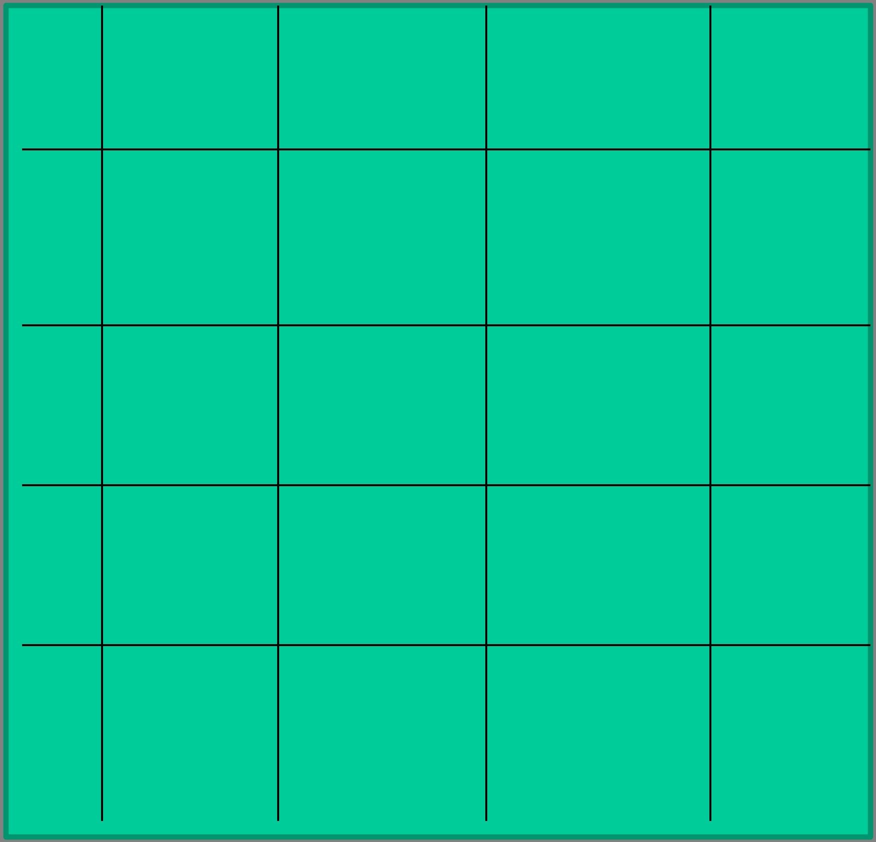
Mind trick



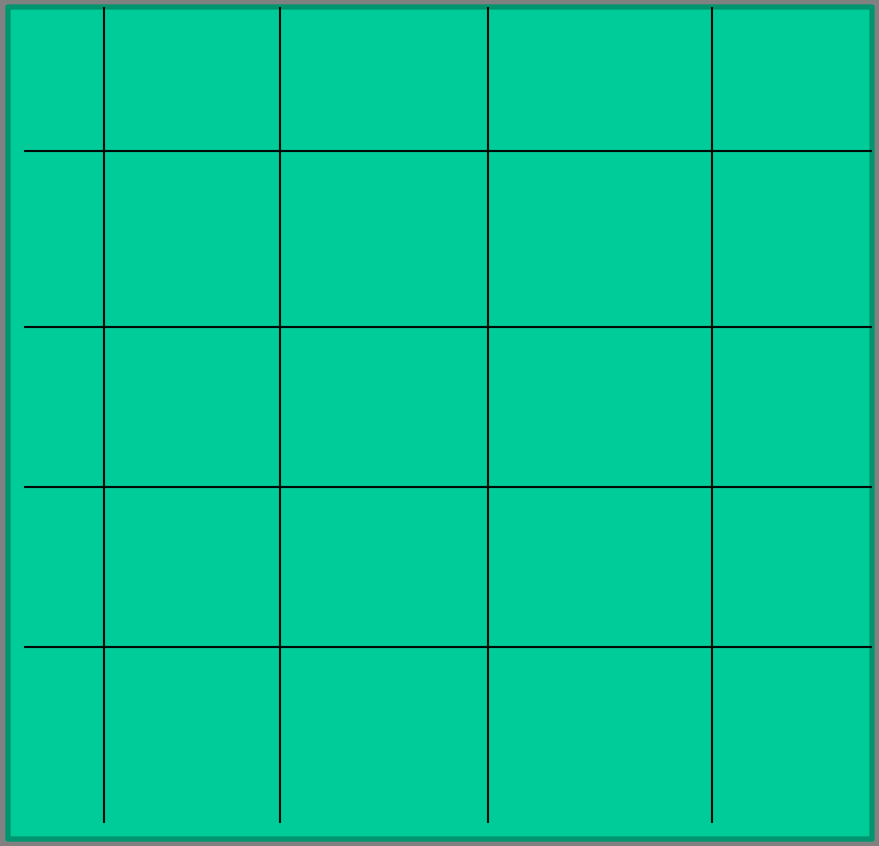
Mind trick



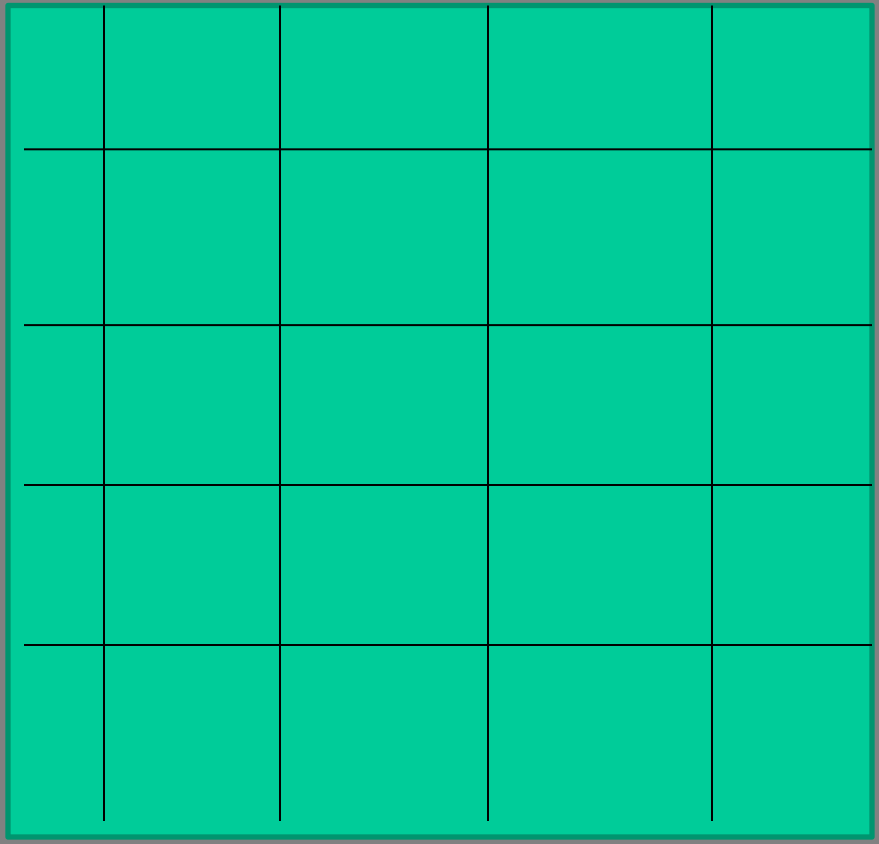
Mind trick



Mind trick



Lets do it again



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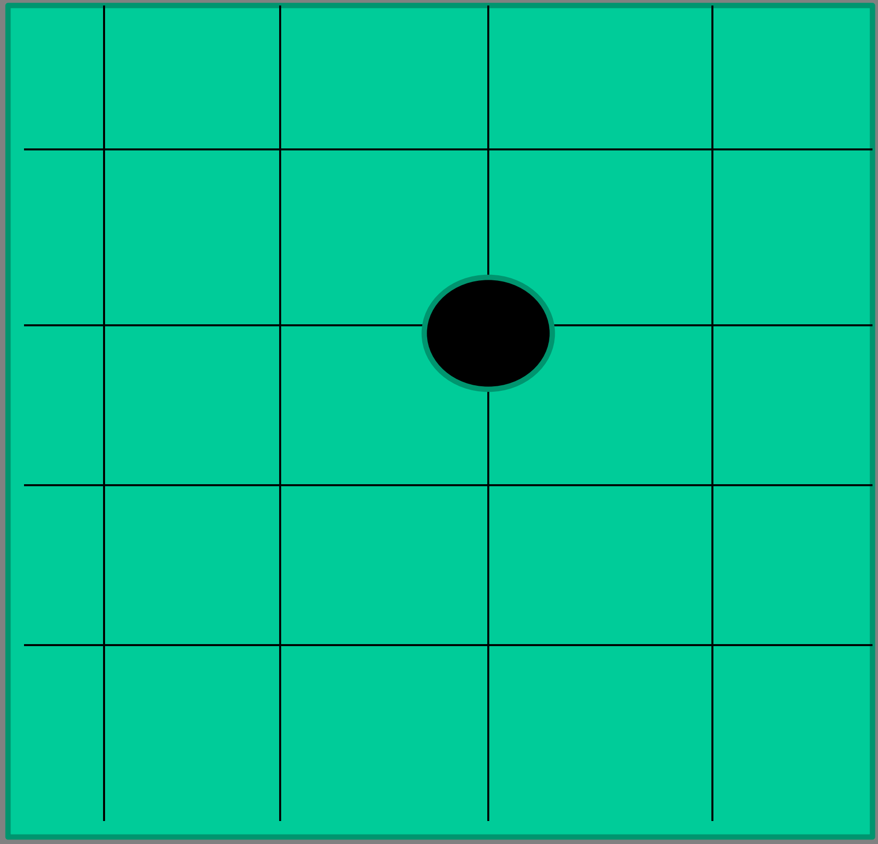

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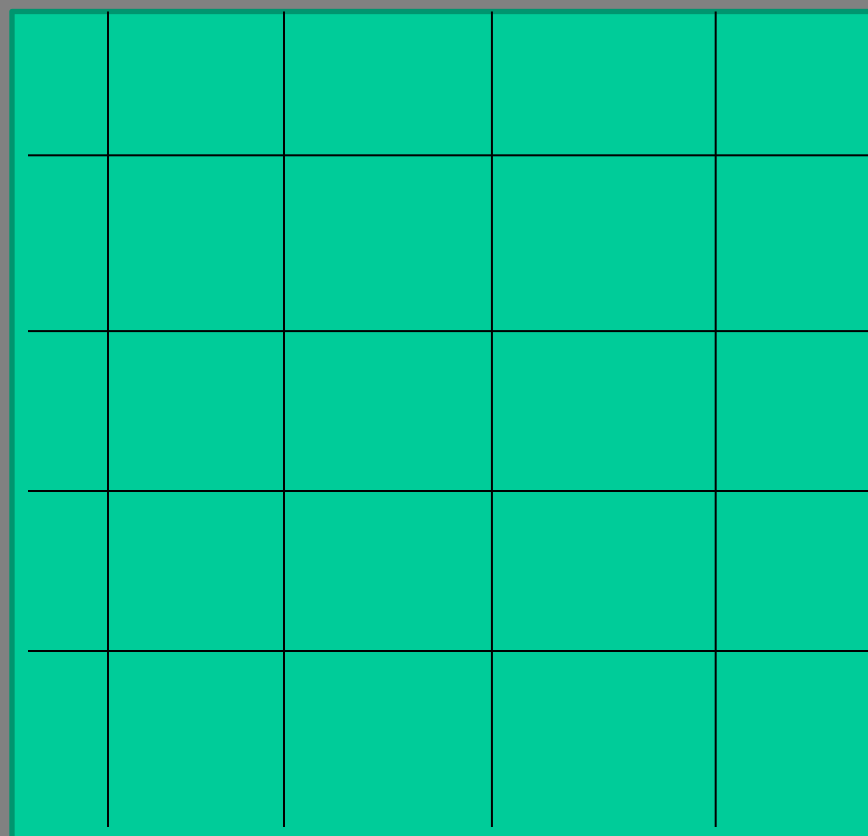
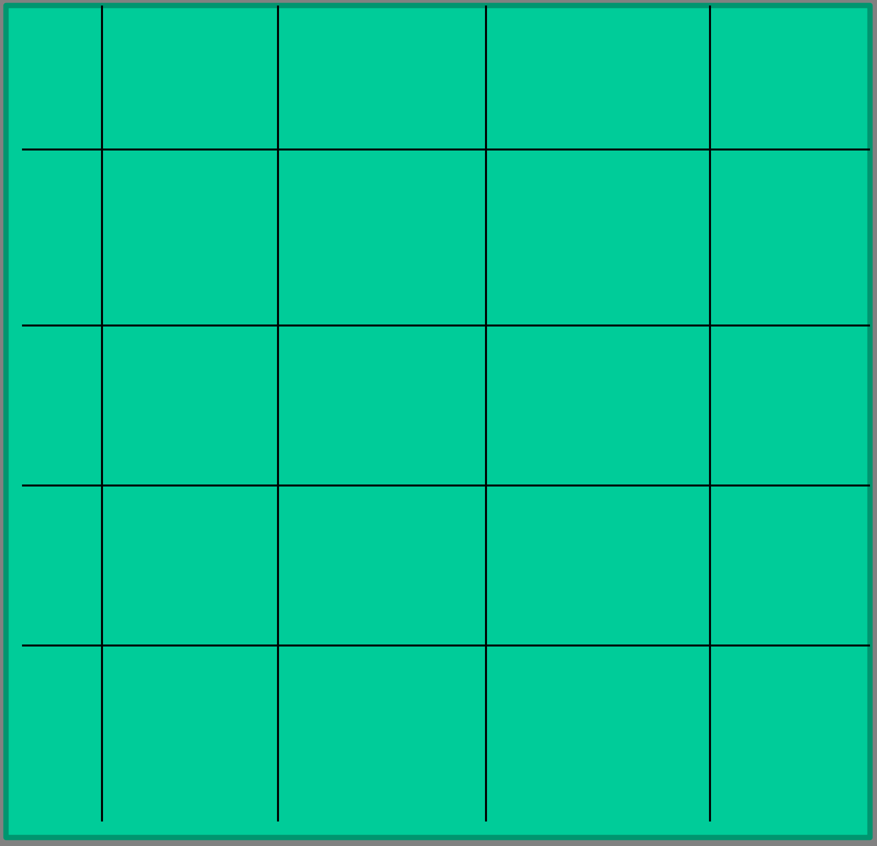


Lets do it again



You noticed!

- Few points on overall approach in this lecture:

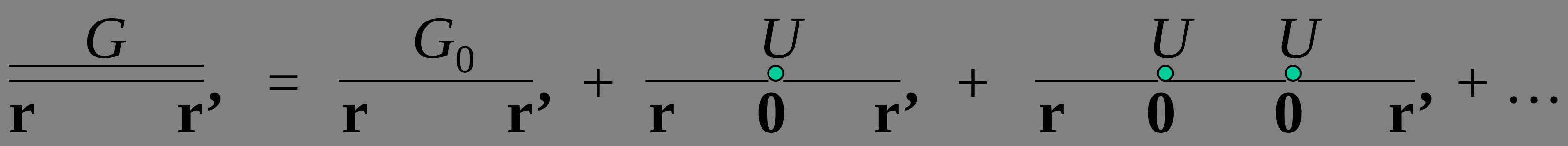
- Impurities and defects are interesting.
- They are telling us a story about host
- They can be useful as a markers of new physics
- Controlled impurity physics is at the core of multibillion $ semiconducting industry
- Impurity states enable the new functionality
, that is used in devices. Case; my computer that allows me to project this lecture.
- Impurities can be placed deliberately to destroy the state we are trying to understand
- From response of unknown state to impurities we can infer what "it is made of"
- Not average description but one at a time. Averaged quantities can be useful. But they can be misleading.

Conventional, s-wave superconductors (BCS)

T-matrix approximation

Single impurity of strength V at $\mathbf{r}$ = 0 (Yu Lu, Shiba, …):

$$G(\mathbf{r},\mathbf{r}';\omega) = G_0(\mathbf{r}-\mathbf{r}';\omega) + G_0(\mathbf{r};\omega)T(\omega)G_0(\mathbf{r}';\omega)$$



$$T(\omega) = U + U^2 G_0(0,\omega) + U^3 G_0(0,\omega)^2 + \ldots = \frac{1}{1/U - G_0(0,\omega)}$$

Impurity-induced resonance:

$$\boxed{1/U = G_0(\mathbf{r}=0,\omega) = \frac{1}{N}\sum_{\mathbf{k}} G_0(\mathbf{k},\omega)}$$

Bound state in 2D metal due to weak attarctive potential

$$\mathcal{H}=\sum_{\mathbf{k}}[\epsilon(\mathbf{k})-\mu]c^{\dagger}_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}+\sum_{\mathbf{k},\mathbf{k}'}U_0 c^{\dagger}_{\mathbf{k},\sigma}c_{\mathbf{k}',\sigma}.$$

$$U_0\delta(\mathbf{r})$$

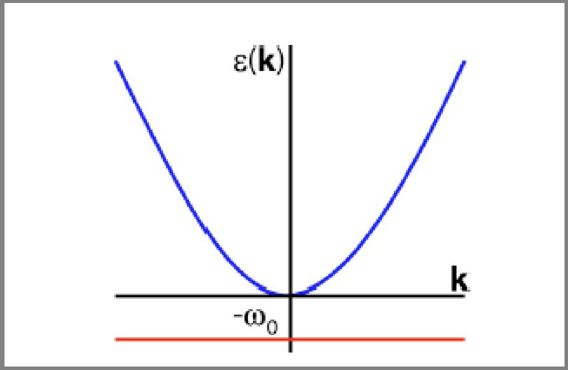
$$G_0(\omega,\mathbf{k})=[\omega-\epsilon(\mathbf{k})]^{-1}.$$

$$\omega_0 = W\exp\left(-\frac{1}{g_2}\right)\quad \text{if } d=2,$$ energy

$$T(\omega)=U_0+U_0\sum_{\mathbf{k}}G_0(\omega,\mathbf{k})T(\omega),$$

$$l_0=(\hbar^2/2m\omega_0)^{1/2}\gg a.$$ size

$$T(\omega)=\frac{U_0}{1-U_0\sum_{\mathbf{k}}G_0(\omega,\mathbf{k})}.$$



$$g_0(\omega)=\frac{1}{N}\sum_{\mathbf{k}}G_0(\omega,\mathbf{k}) = \int_0^W \frac{d\epsilon N(\epsilon)}{\omega-\epsilon}$$

$$g_d(\omega)=-\Gamma_2\ln[|W/\omega-1|].$$

$$\delta N(\mathbf{r},\omega)=|G_0(\mathbf{r},\omega_0)|^2\delta(\omega-\omega_0),$$ Local DOS

$$G_0(\mathbf{r},\omega)=N_0J_0(k_Fr)\ln[W/\omega]$$

Same prcedure is applied to SC case, except Green's functions are now matrices

$$\mathcal{H}_0 = \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} c_{\mathbf{k}\alpha} + \Delta_0 \sum_{\mathbf{k}} \{ c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \}.$$

$$H_{\mathrm{ex}} = \frac{1}{2N} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \alpha\beta}} J(\mathbf{k}-\mathbf{k}') c^{\dagger}_{\mathbf{k},\alpha} \boldsymbol{\sigma}_{\alpha\beta} \cdot \mathbf{S} c_{\mathbf{k}'\beta}.$$

$$Eu_{\alpha}(\mathbf{r}) = \varepsilon(\mathbf{k}) u_{\alpha}(\mathbf{r}) + i\Delta \sigma^{y}_{\alpha\beta} v_{\beta}(\mathbf{r}) + U_{\alpha\beta}(\mathbf{r}) u_{\beta}(\mathbf{r}),$$

$$Ev_{\alpha}(\mathbf{r}) = -\varepsilon(\mathbf{k}) v_{\alpha}(\mathbf{r}) - i\Delta \sigma^{y}_{\alpha\beta} u_{\beta}(\mathbf{r}) - U_{\alpha\beta}(\mathbf{r}) v_{\beta}(\mathbf{r}).$$

$$\hat{T}_l(\omega) = \hat{U}_l + \hat{U}_l \int d\varepsilon \hat{G}_0(\mathbf{k},\omega) \hat{T}_l(\omega).$$

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

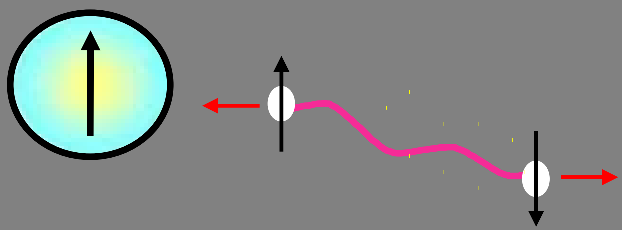
$$T^{(1)}(\omega) = \frac{1}{N} \frac{(JS/2)^2 \hat{g}_0(\omega)}{I - [JS\hat{g}_0(\omega)/2]^2}.$$

$$\frac{\sin(p_F r - \delta_0^{\pm})}{p_F r} \exp[-r|\sin(\delta_0^{+} - \delta_0^{-})|/\xi_0],$$

$$\hat{g}_0(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \hat{G}_0(\mathbf{k},\omega) = -\pi N_0 \frac{\omega + \Delta_0 \sigma_2 \tau_2}{\sqrt{\Delta_0^2 - \omega^2}}.$$

Theory of impurity states in s-wave SC

Yu Lu(65), Shiba(68)

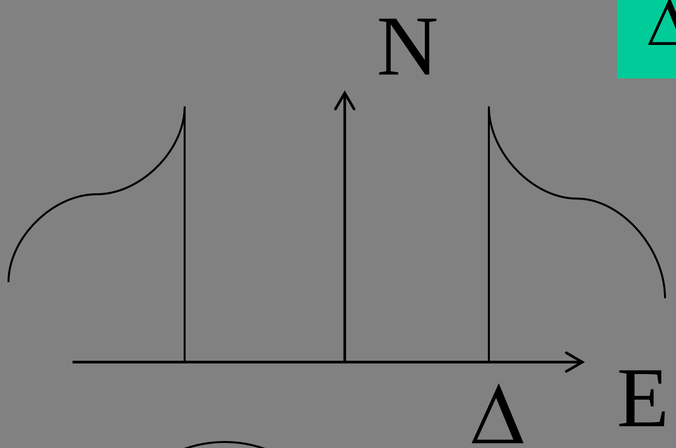


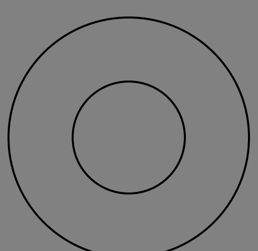
$$H = H_{BCS} + JS_{imp} \cdot \sigma$$

$$\Psi(r) = \frac{1}{\sqrt{r}} \exp(-r/\xi_{\omega_0})$$

$$\frac{\omega_0}{\Delta} = \pm \frac{1-(JN_0S)^2}{1+(JN_0S)^2}$$

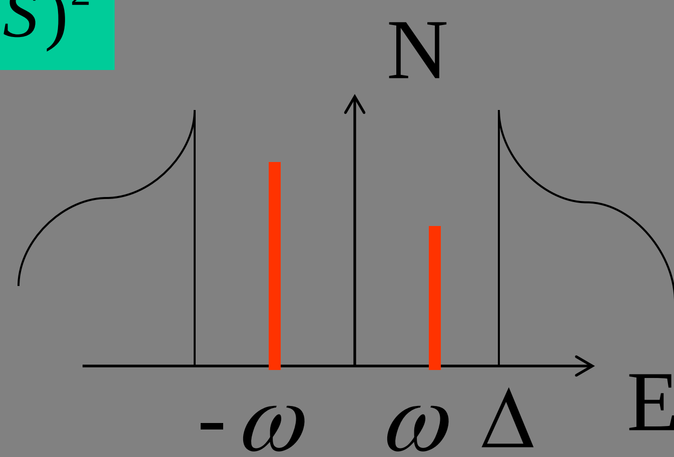
$$\xi_{\omega_0} = \xi \frac{\xi}{\sqrt{1-(\omega_0/\Delta)^2}}$$

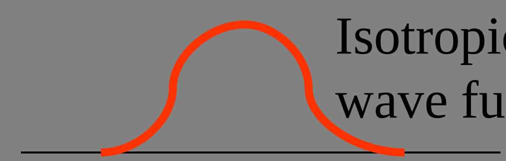




isotropic gap

Magn imp

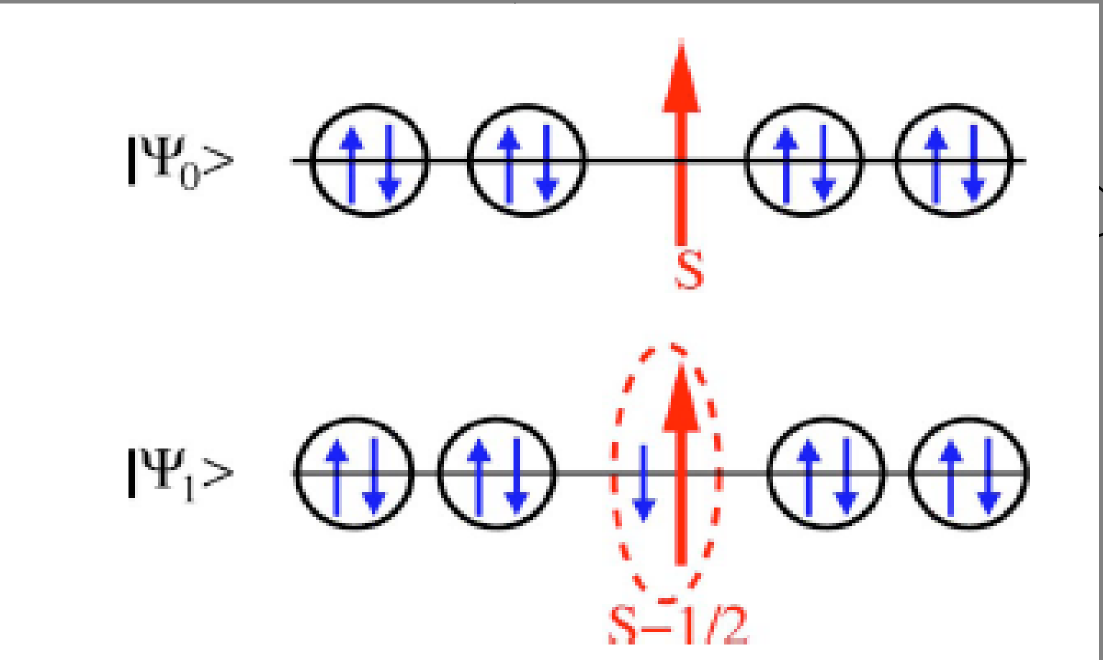


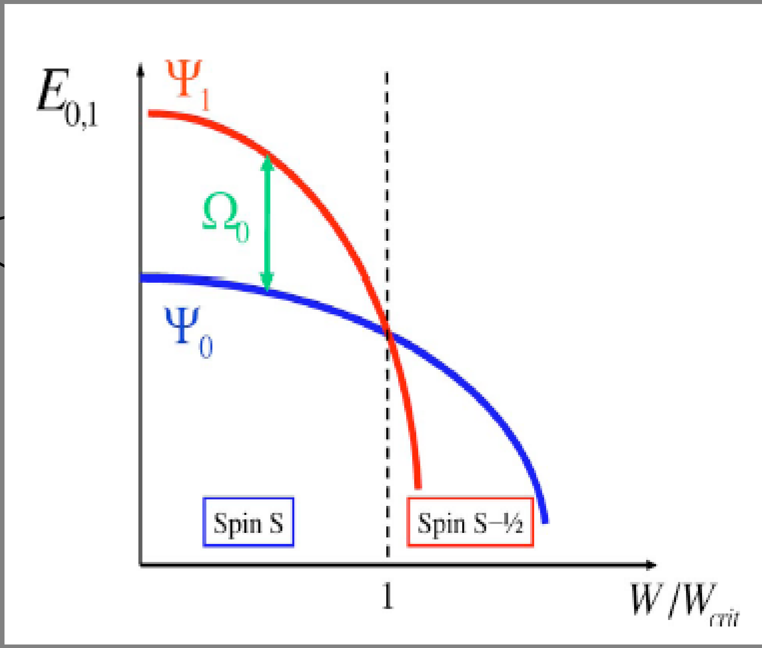


Isotropic wave function

Imp S + Cooper pairs

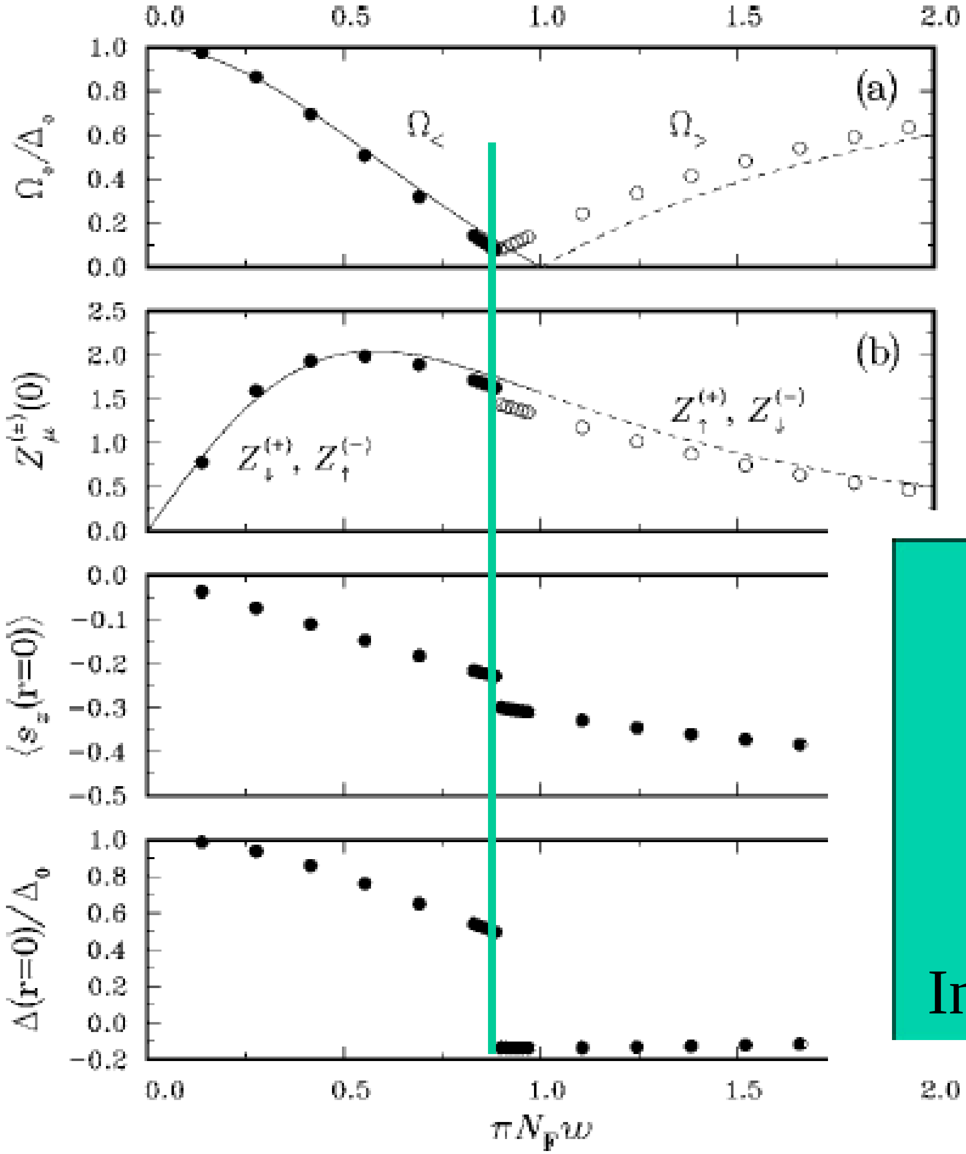
continuum

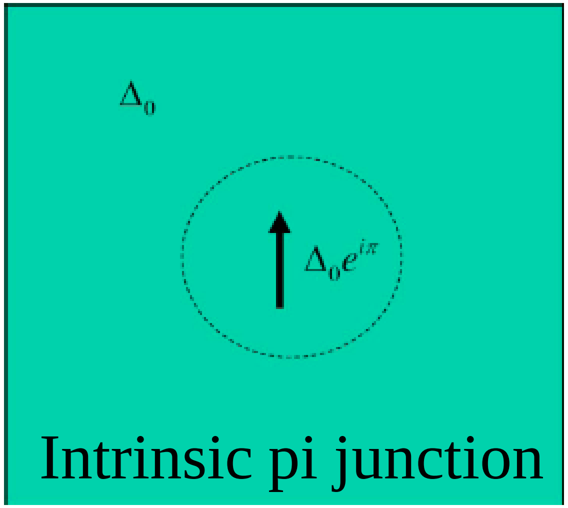




Bound state formed due to magnetic gain

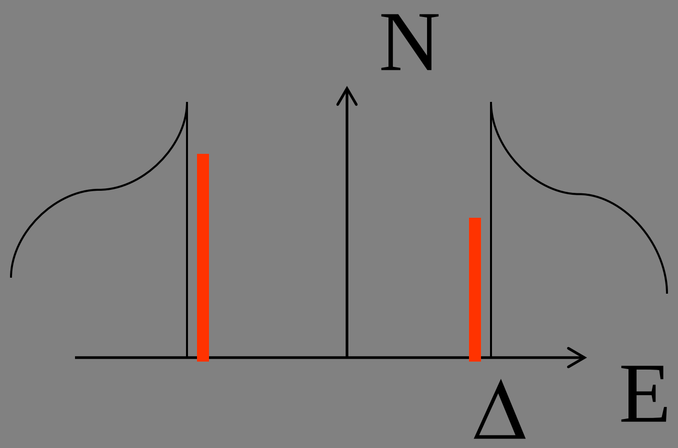
Bound state is FULLY spin polarized !



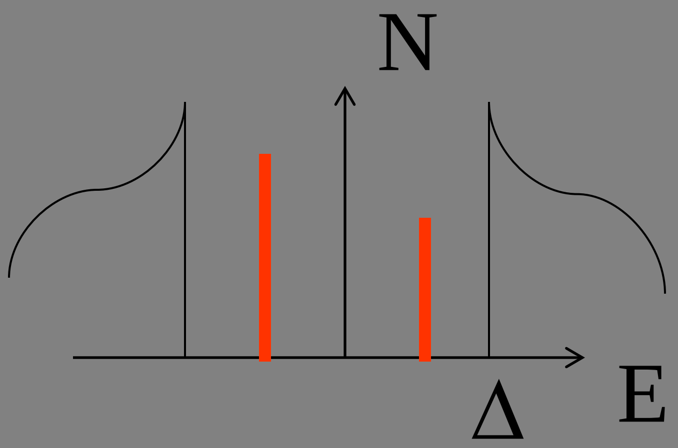


Intrinsic pi junction

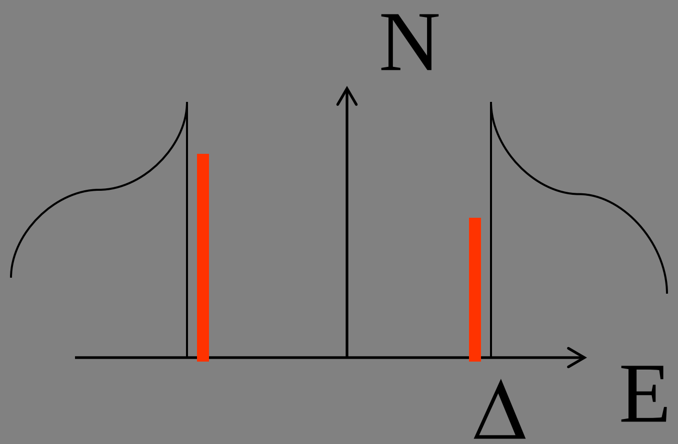
Remark about Abrikosov-Gorkov theory



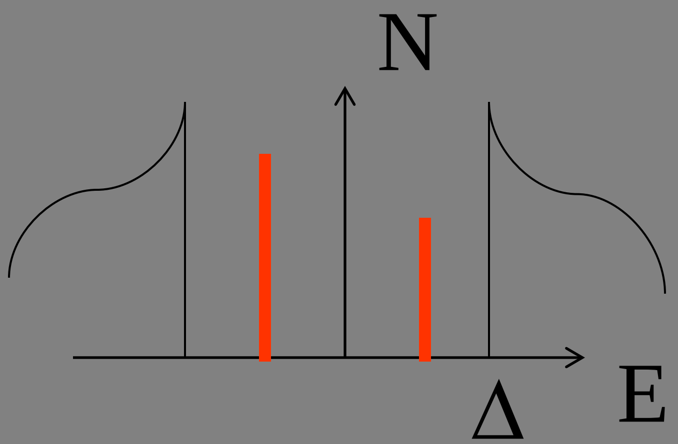
Weak impurity



Strong impurity

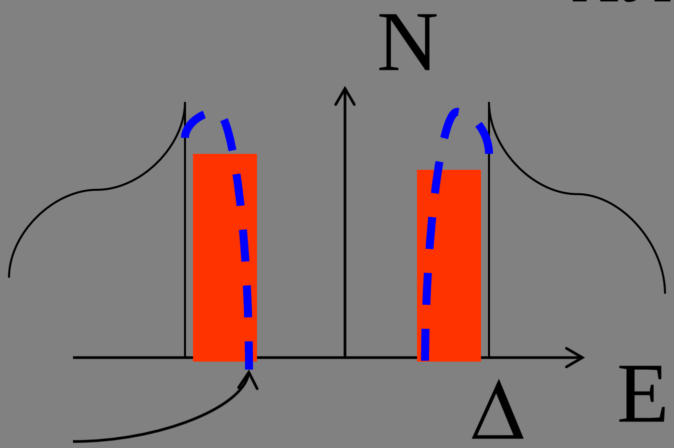


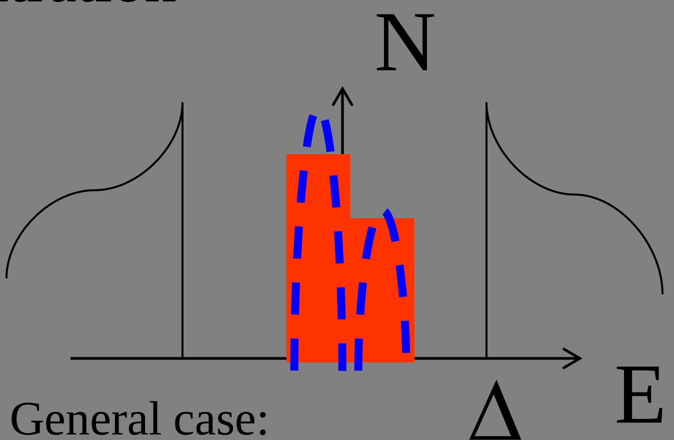
Weak impurity



Strong impurity

At finite imp concentration

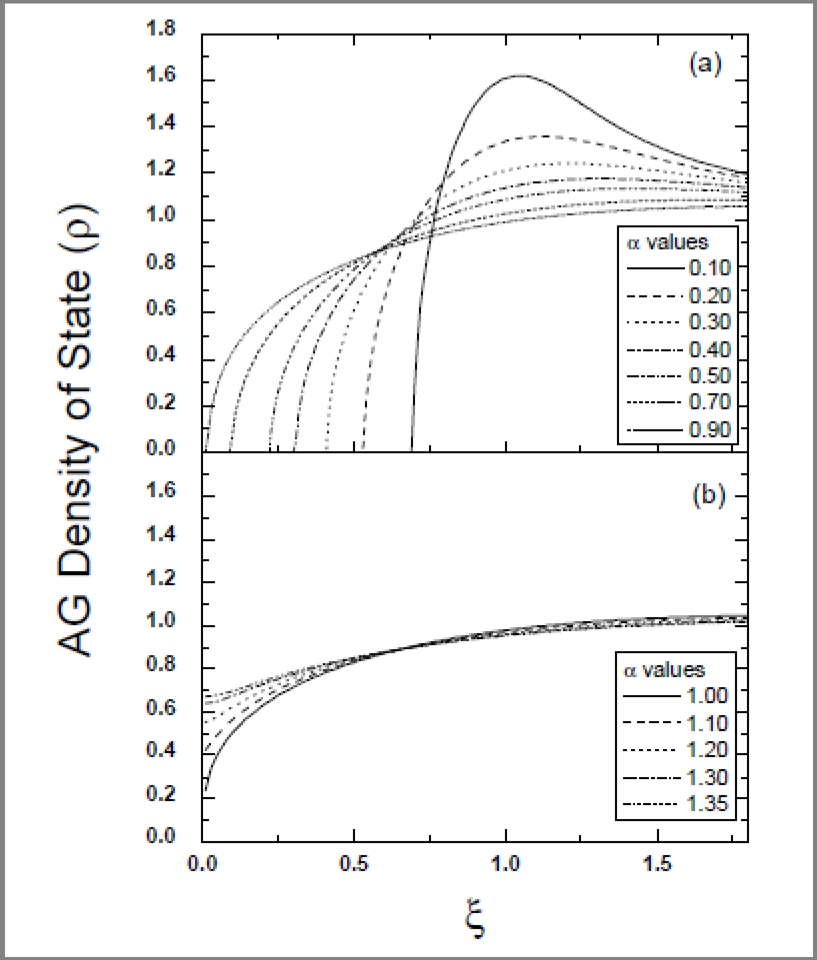


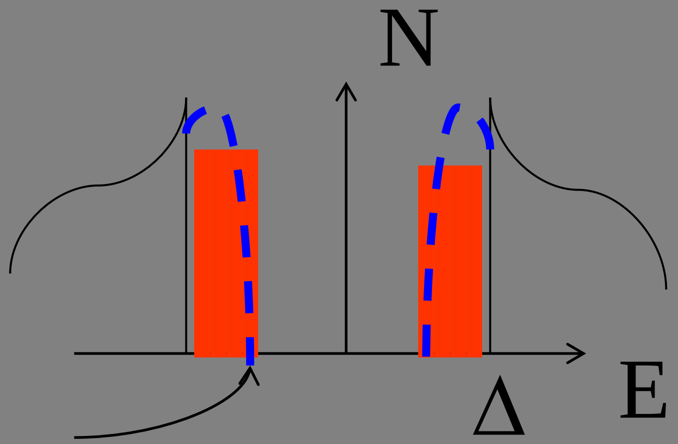


Imp band growth in Abrikosov-Gorkov theory; one parameter: Nimp N(0) J S(S+1)

General case:
Gapless SC much sooner
Lifshitz tails and gapless
Balatsky, Trugman, PRL, 97

Predicted behavior only occurs for weak impurities:





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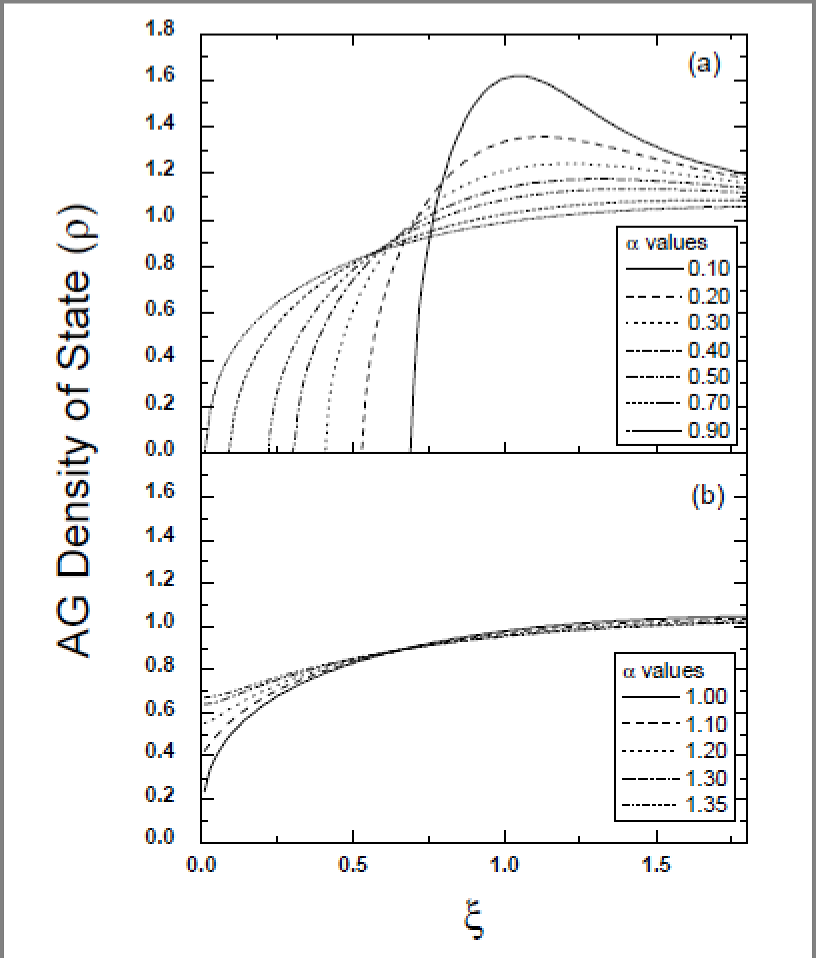

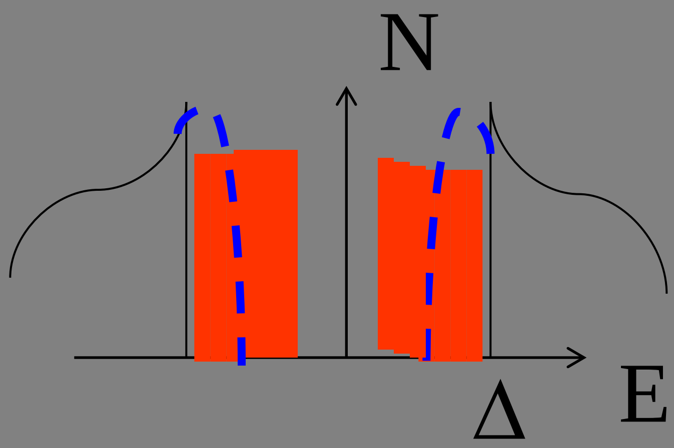

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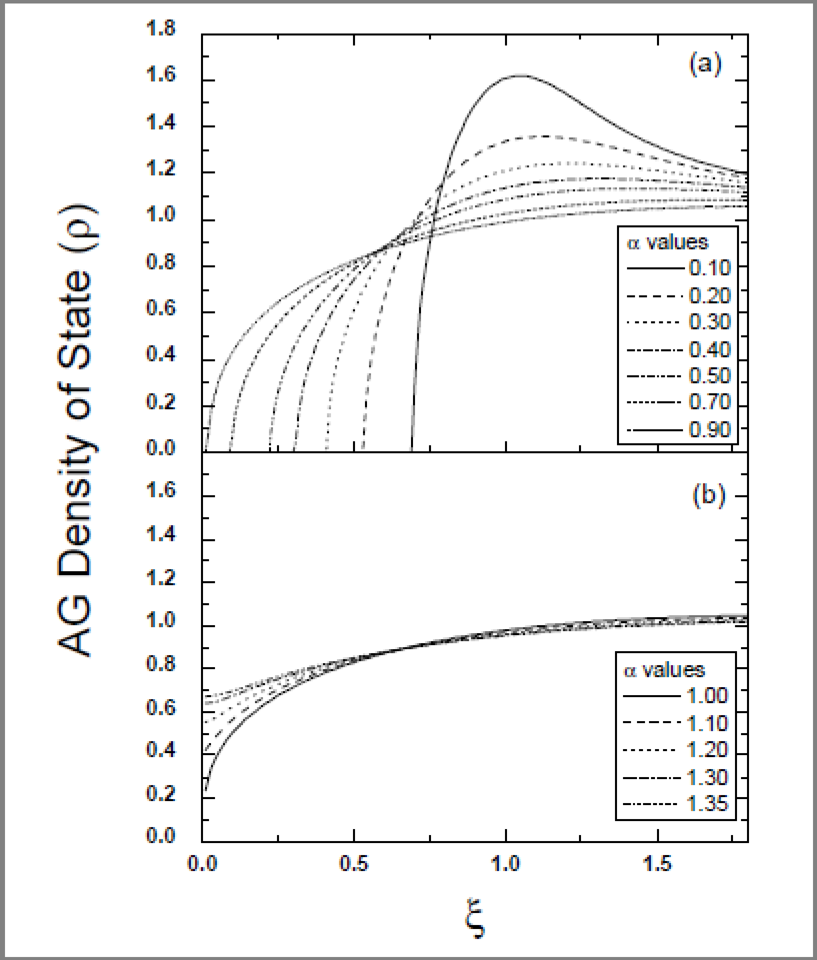
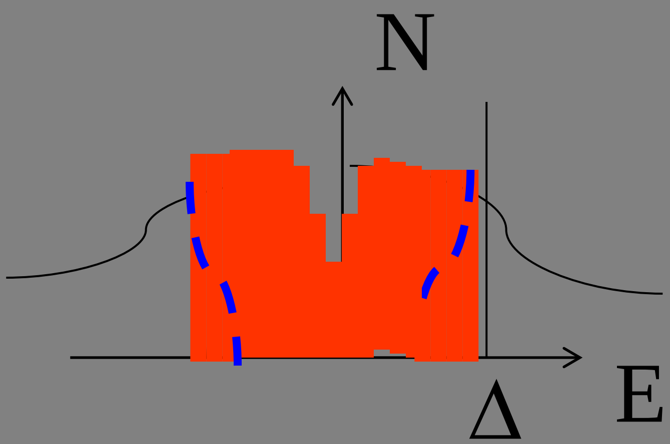
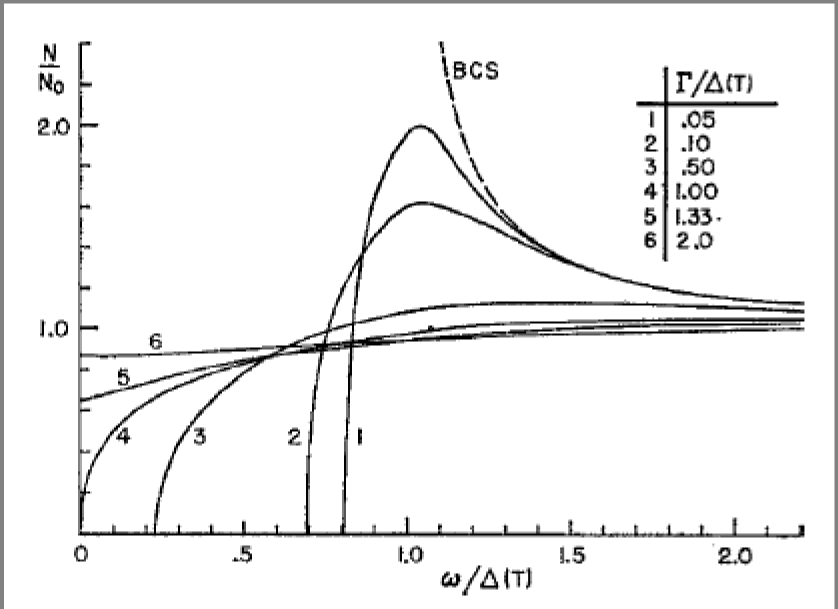
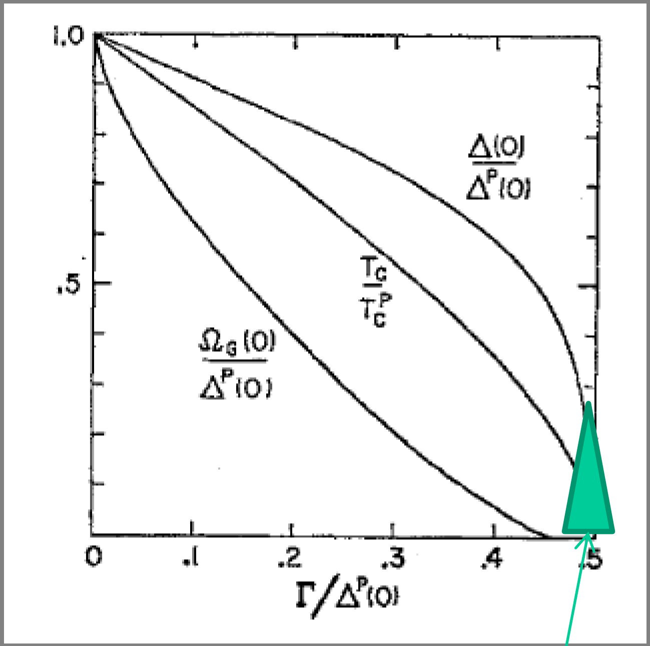


Gapless
After a large concentration is added



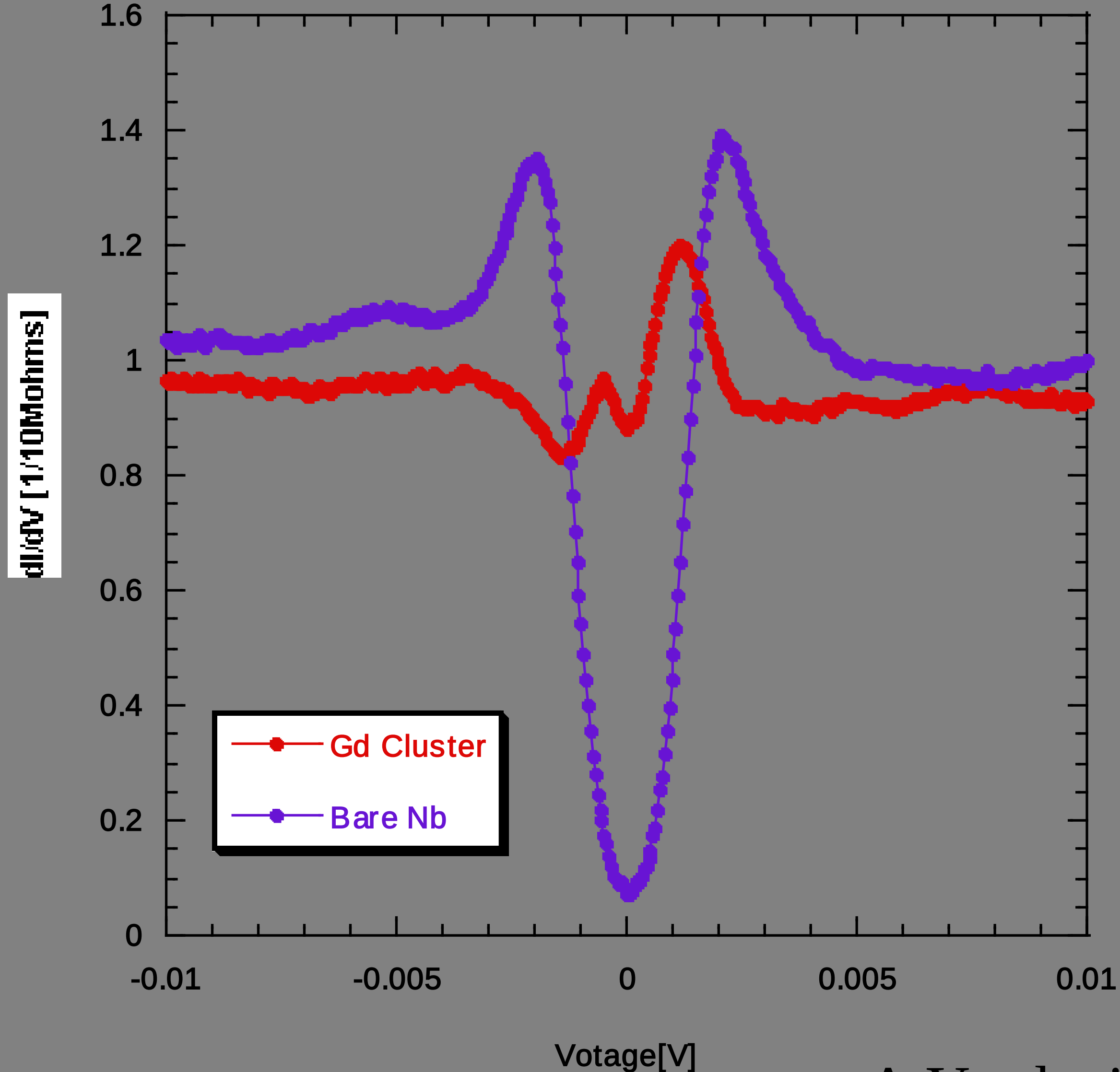




Gapless SC region

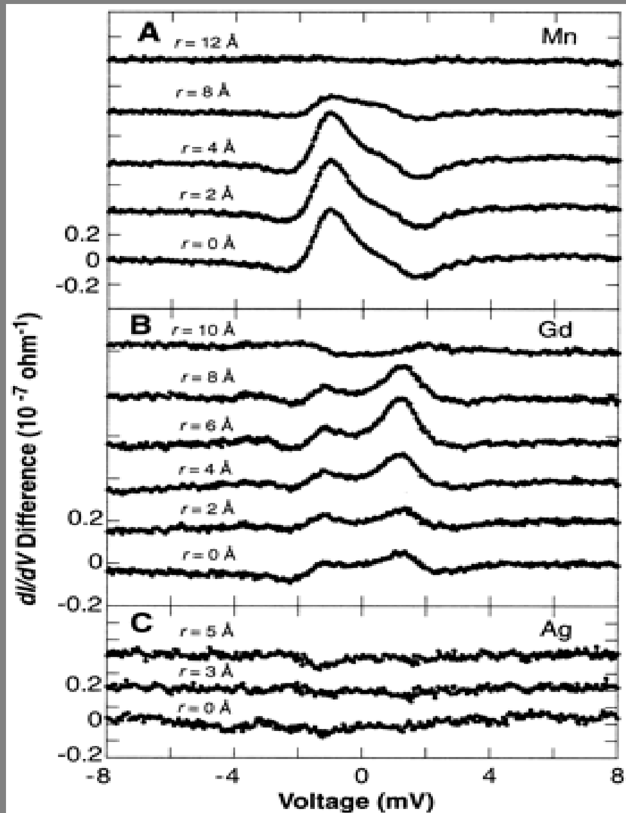
In Reality Imurity states can be at any energy

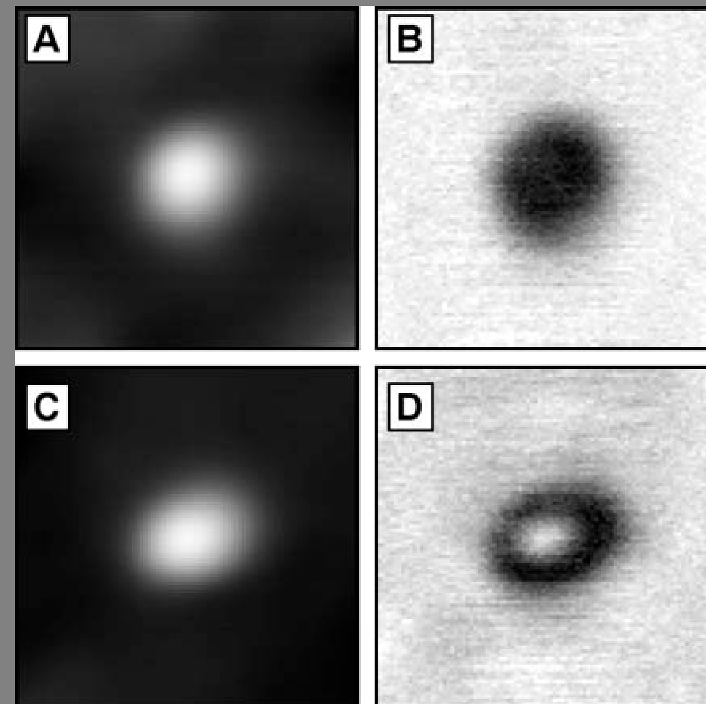
Energy of a single impurity state is a center of impurity band



A.Yazdani, Science,97

A.Yazdani et al, Science(1997)





Impurity intragap
States on Nb
Superconductor.
Gold has no effect on SC state

Wave function of imp state
Gd, Mn atoms on Nb surface
(Tc = 7K)

Lifshitz Tails and gapless supercoductivity in s-wave Case.

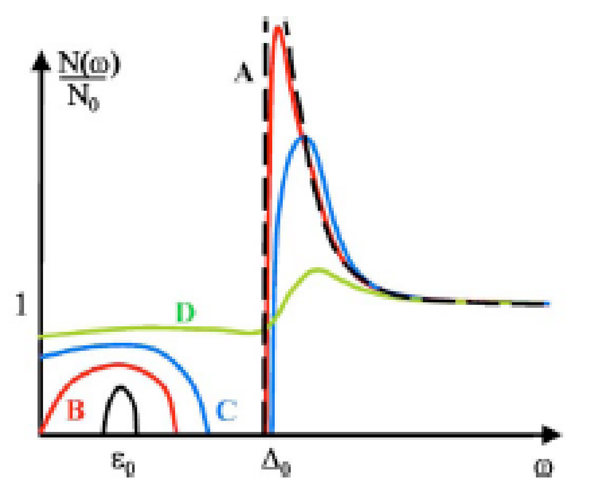
Rare fluctuations are the ones that are nominally very unlikely. However is the mean exectation of some observable is zero and Fluctuaion will render this expectation nonzero then no matter how low probability is this fluctuation is important (hugely important in fact) = 0.0001/0-> infty

Rare fluctuations in the impurity distribution will make any s-wave superconductor gapless, regardless how low impurity Concentration is. It is gapless albeit with exponentially small Density of States.

Rev Mod Phys, v 78, p 373 (2006)

Average theory of impurity scattering depend on
Only scattering rate $\Gamma = n_{imp} J^2 S^2$

Band in case of strong impurity scattering, J~1



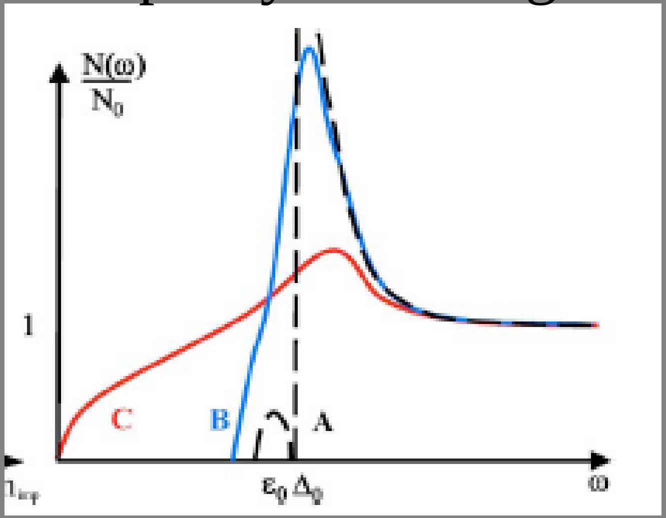
$\Gamma = const$

$n_{imp} small$

$JS >> 1$

$(unitary)$

Band in case of weak impurity scattering J <<1



$\Gamma = const$

n_{imp} large

$JS << 1$

$(Born)$

Averaged theory
From textbooks does
not capture this
ditsinction

Lifshits tails or rare fluctuations

$$P[U] \propto \exp\left[-\frac{1}{2U_0}\int d^d\mathbf{r}\, U^2(\mathbf{r})\right].$$

$$N(E) = \int \mathcal{D}U P[U]\delta(E - \mathcal{E}[U]),$$

$$\ln\frac{N(E)}{N_0} \approx -\mathcal{S}[U_{\text{opt}}], \tag{14.3}$$

where the optimal fluctuation is obtained by minimizing the functional

$$\mathcal{S}[U] = \frac{1}{2U_0^2}\int d^d\mathbf{r}\, U^2(\mathbf{r}) + \lambda(\mathcal{E}[U] - E) \tag{14.4}$$

$$E \sim U \sim L^{-2}$$

$$\mathcal{S}[U] \approx L^d U^2 / U_0^2, \text{ or } \ln[N(E)/N_0] \approx -|E|^{2-d/2}/U_0^2$$

$$\mathcal{E}[U] = \langle \hat{H} \rangle = \langle \psi | \frac{\mathbf{p}^2}{2m^*} + U | \psi \rangle = E. \tag{14.5}$$

Minimization in Eq. (14.4) with respect to U dictates that

$$U(x) = -\lambda U_0^2 \langle \psi | \frac{\delta \hat{H}}{\delta U} | \psi \rangle = -\lambda U_0^2 \psi^2(x), \tag{14.6}$$

while minimization with respect to λ requires that the bound state is at energy E, i.e. (setting $m^* = 1$),

$$\left[-\tfrac{1}{2}\nabla^2 - \lambda U_0^2 \psi^2(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{14.7}$$

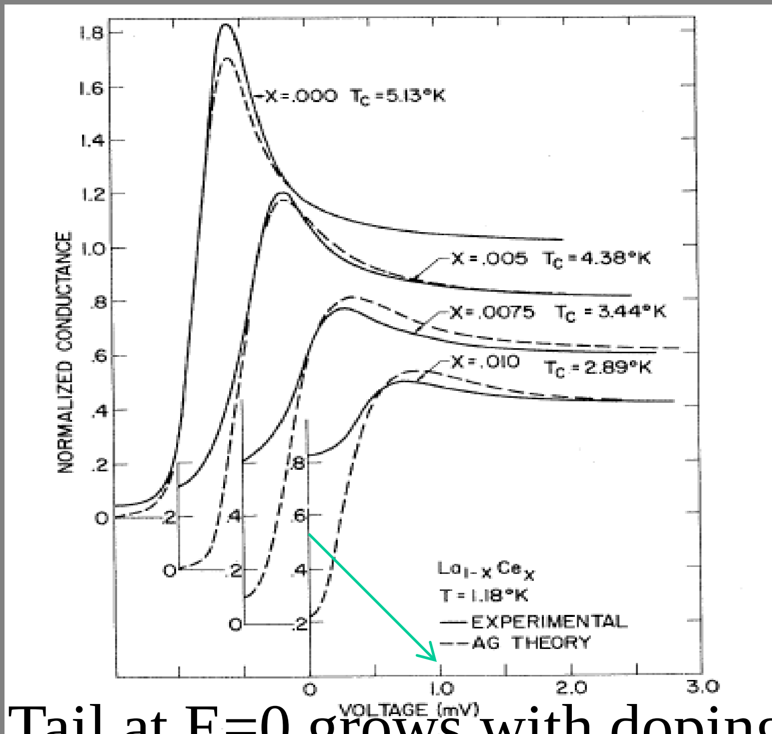
In one dimension this equation is exactly solved to give (Halperin and Lax, 1966)

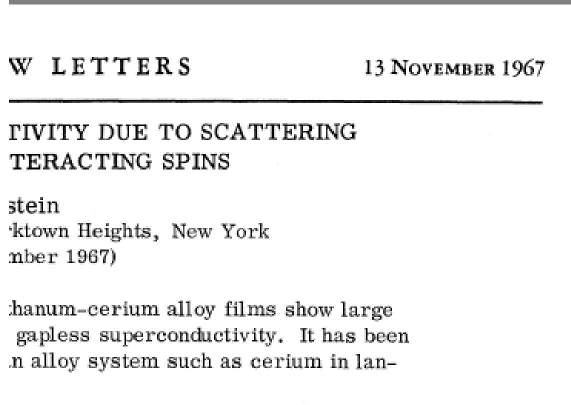
$$\psi(x) = \sqrt{\frac{\kappa}{2}}\,\text{sech}\,\kappa x, \tag{14.8}$$

$$\lambda U_0^2 = 8\kappa, \tag{14.9}$$

with $E = -\kappa^2/2$. Therefore the "optimal action" is $\mathcal{S}(U_{\text{opt}}) \simeq \kappa^2/U_0^2 \sim |E|^{3/2}$ as expected.

Lifshitz tails in SC make it gapless s wave





W LETTERS 13 NOVEMBER 1967

TIVITY DUE TO SCATTERING
TERACTING SPINS

stein
ktown Heights, New York
mber 1967)

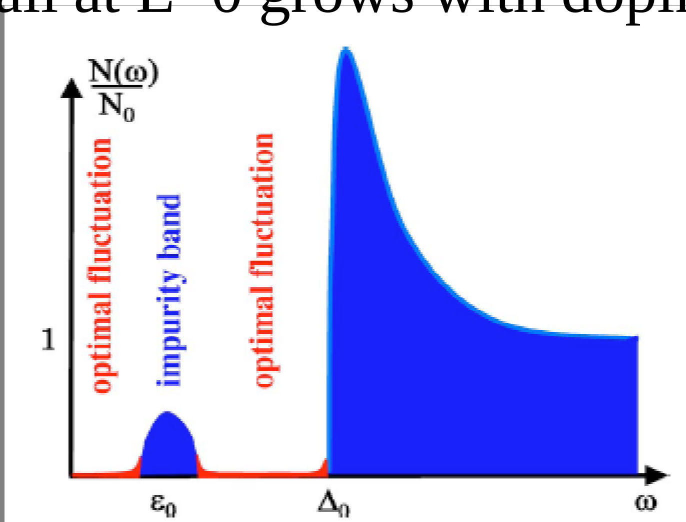
hanum-cerium alloy films show large
gapless superconductivity. It has been
n alloy system such as cerium in lan-

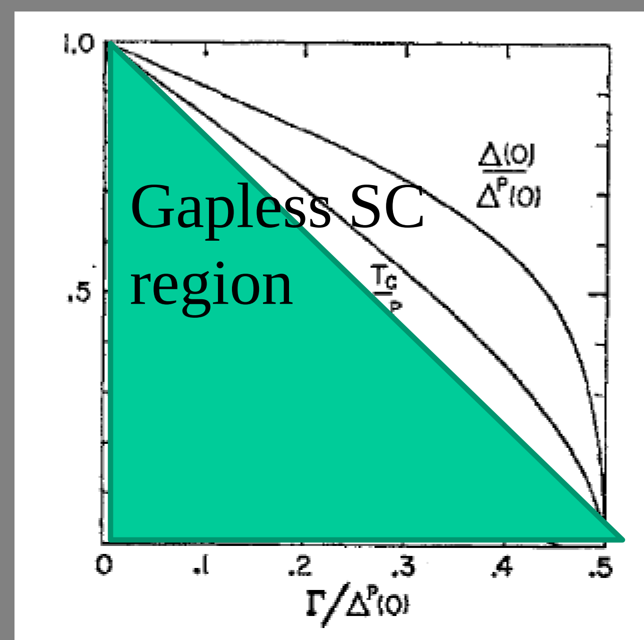
e

nd

nall

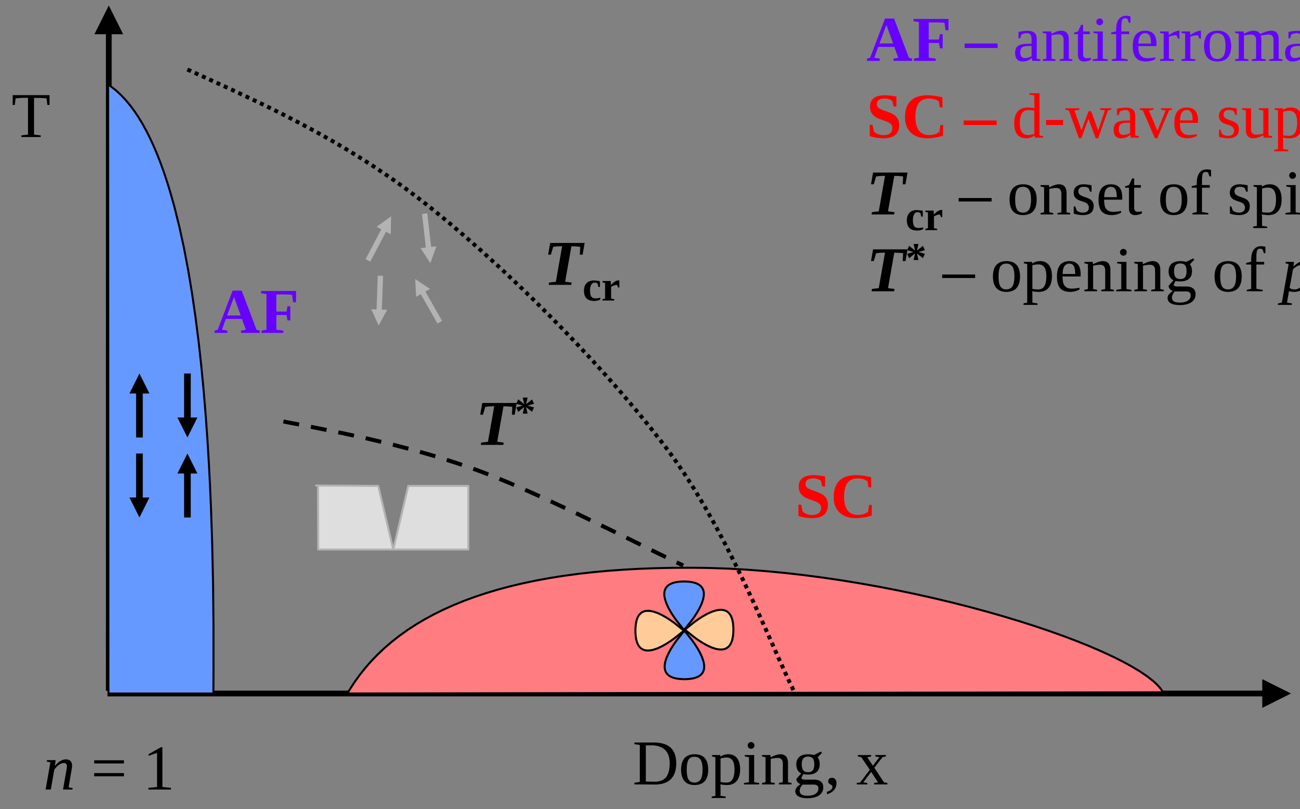
Tail at E=0 grows with doping





Unconventional Superconductors: d-wave (High Tc supercondcutors)

Experimental Phase Diagram of HTSC

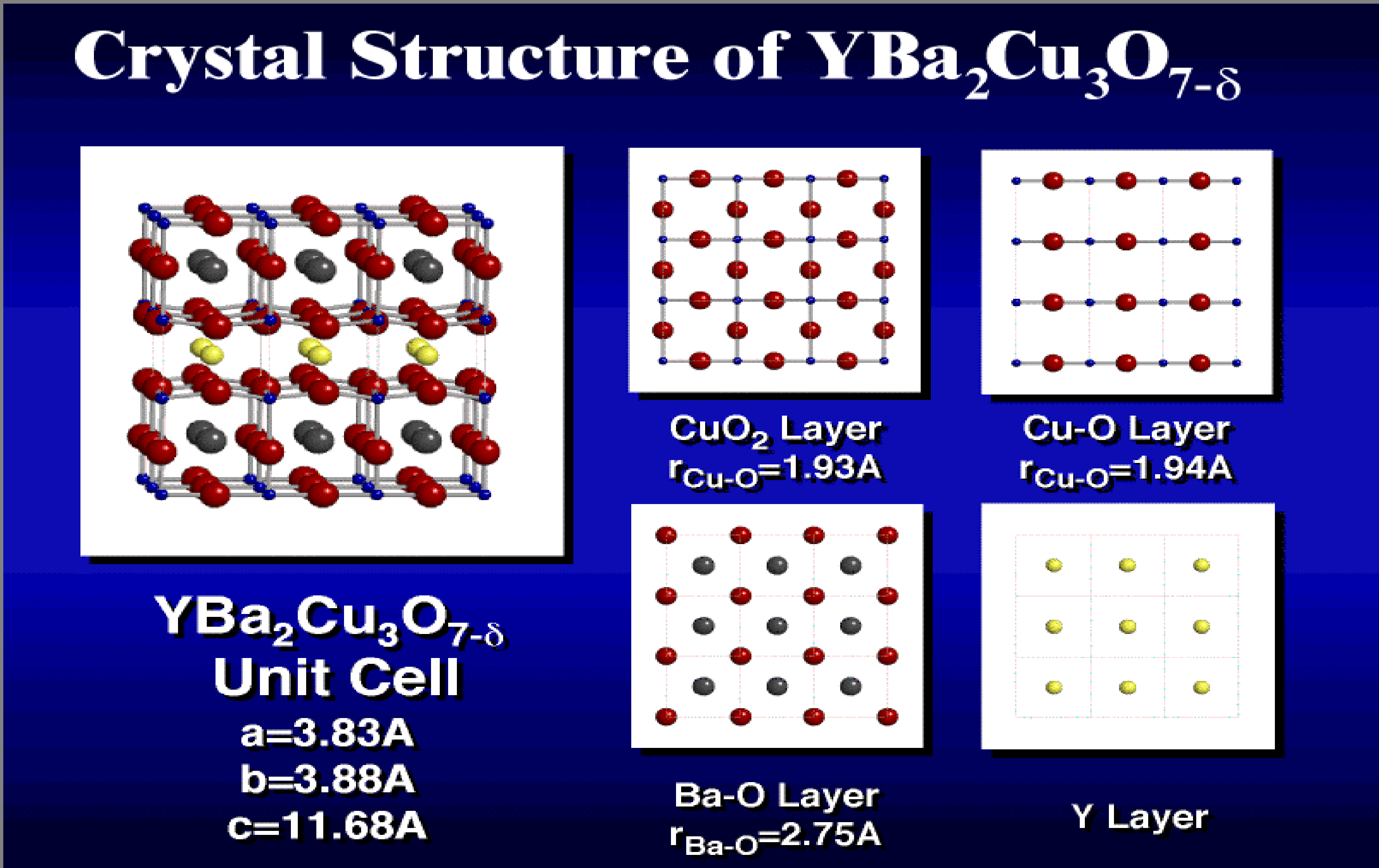


AF – antiferromagnet

SC – d-wave superconductor

T_{cr} – onset of spin fluctuations

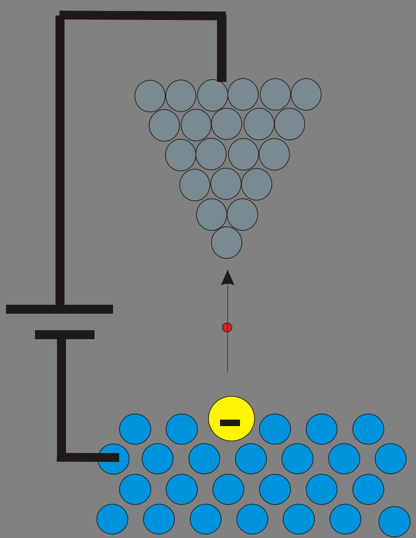
T^* – opening of *pseudo*gap



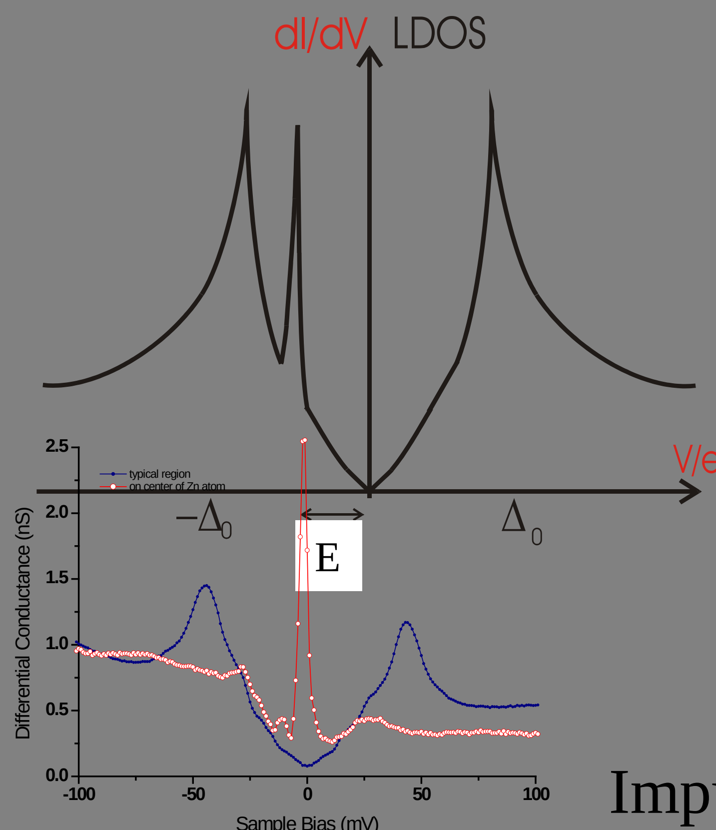
YBCO structure

Earlier work: d-SC Impurity Resonances

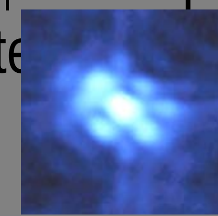
On-site potential
U>0

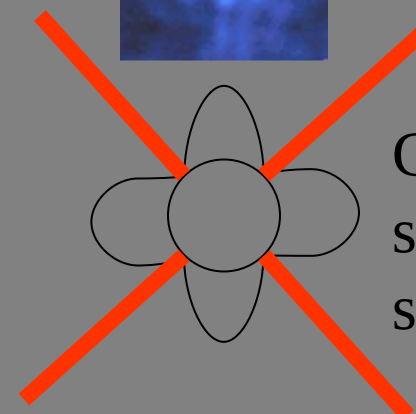


On-site LDOS



LDOS Image at Ω
$|\Psi|^2$ for impurity-state





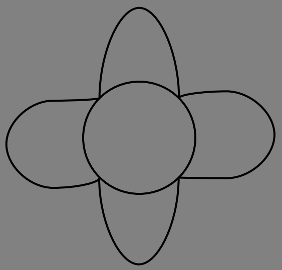
Cross
shaped
state

$$\frac{E}{\Delta_0} = \frac{-1}{2N_F U}\left(\frac{1}{\ln(8N_F U)}\right)$$

Impurities can be a useful tool
to investigate
the nature of an unknown state

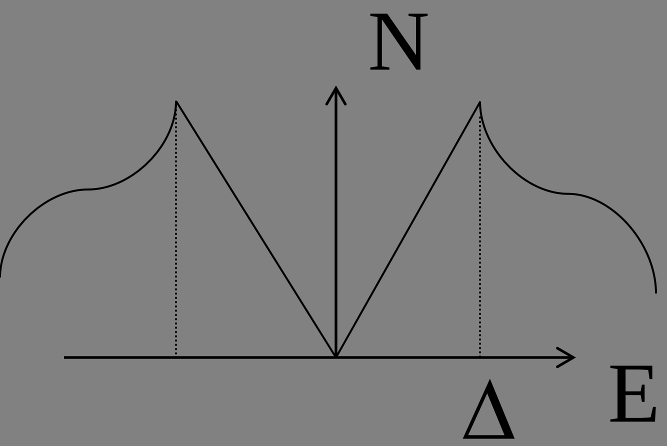
Rev. Mod Phys, **78**, p 373, (2006)

Theory of impurity resonance in d-wave SC



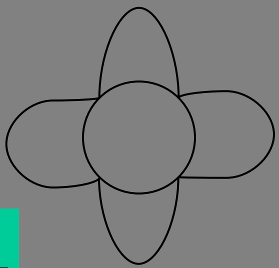
Balatsky, Salkola, Rosengren (95)

Hint = U n(0)



Nonmagnetic
And magnetic imp

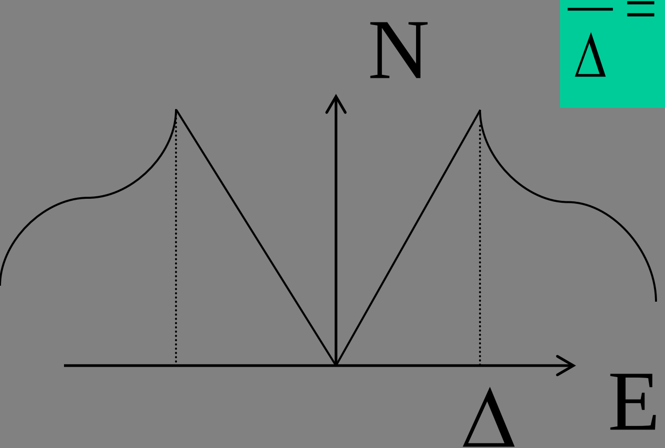
Theory of impurity resonance in d-wave SC

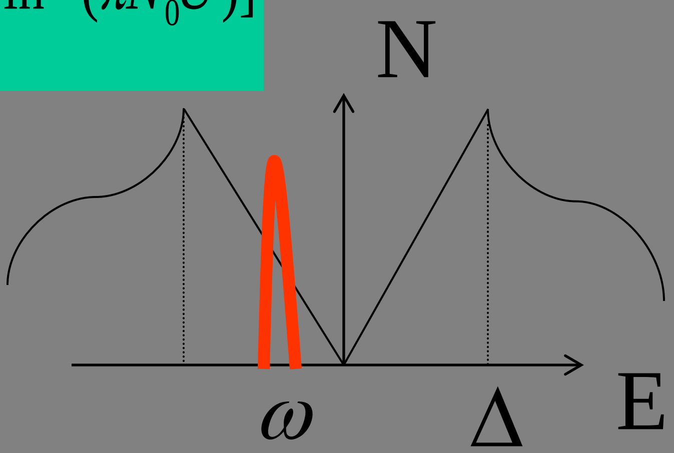


Balatsky, Salkola, Rosengren (PRB,95)

Hint = U n(0)

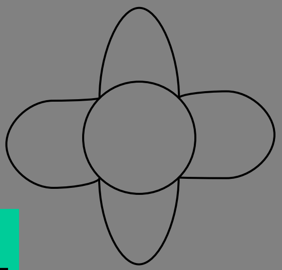
$$\frac{\omega}{\Delta} = \frac{1}{\pi N_0 U}\ln^{-1}(\pi N_0 U)[1 + i\pi \ln^{-1}(\pi N_0 U)]$$





Nonmagnetic
And magnetic imp

Theory of impurity resonance in d-wave SC



Balatsky, Salkola, Rosengren (PRB,95)

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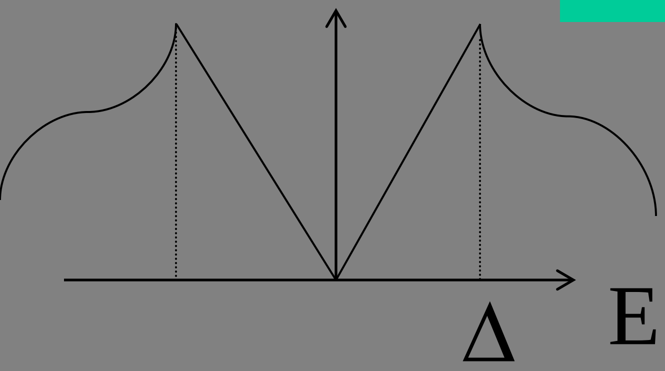
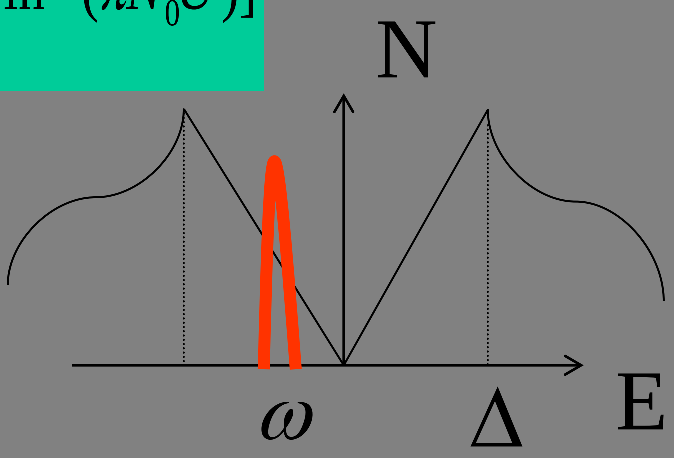
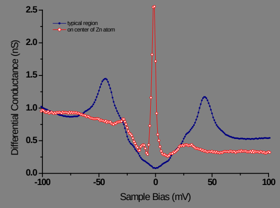
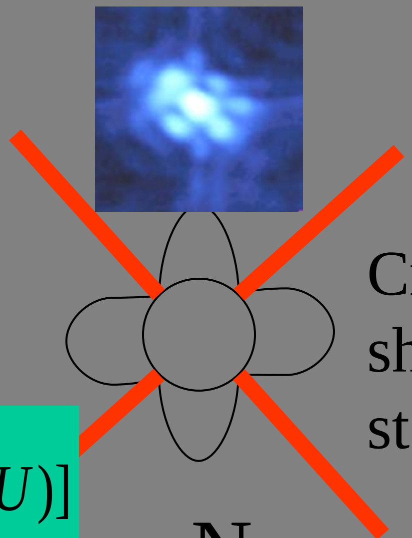




Nonmagnetic
And magnetic imp



Theory of impurity resonance in d-wave SC



Balatsky, Salkola, Rosengren (95)

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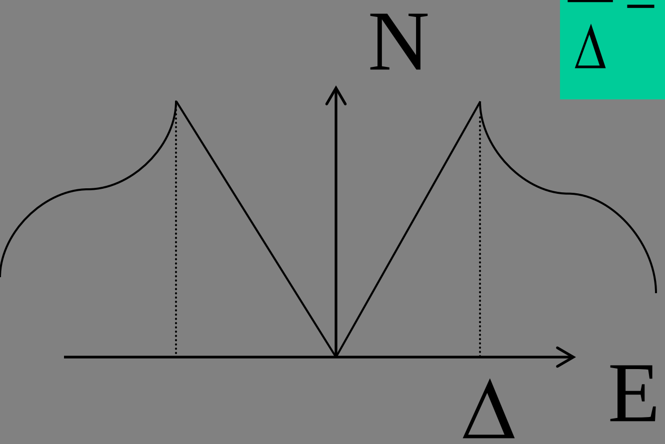
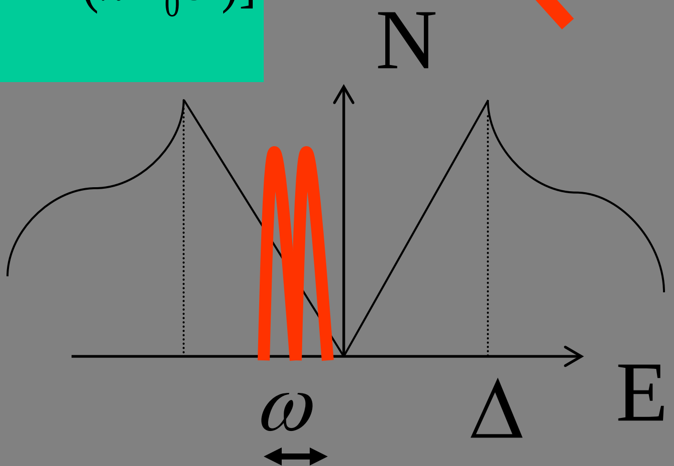
$$\frac{\omega}{\Delta} = \frac{1}{\pi N_0 U}\ln^{-1}(\pi N_0 U)[1 + i\pi \ln^{-1}(\pi N_0 U)]$$



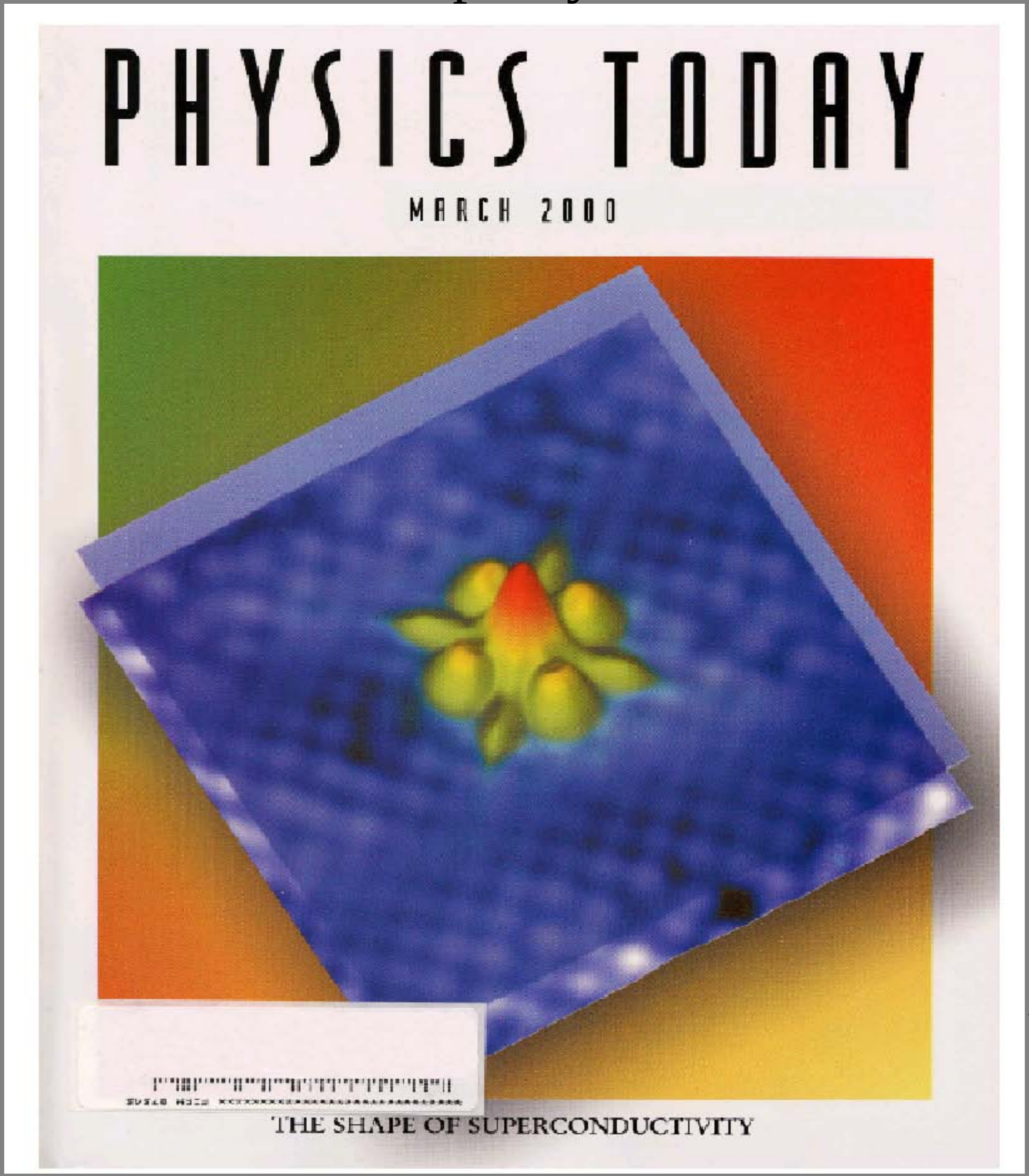


Nonmagnetic
And magnetic imp

Splitting due
to exchange J

Universal:Similar states will be created
in p,f,g…states with gap nodes.

Zn Impurity-State

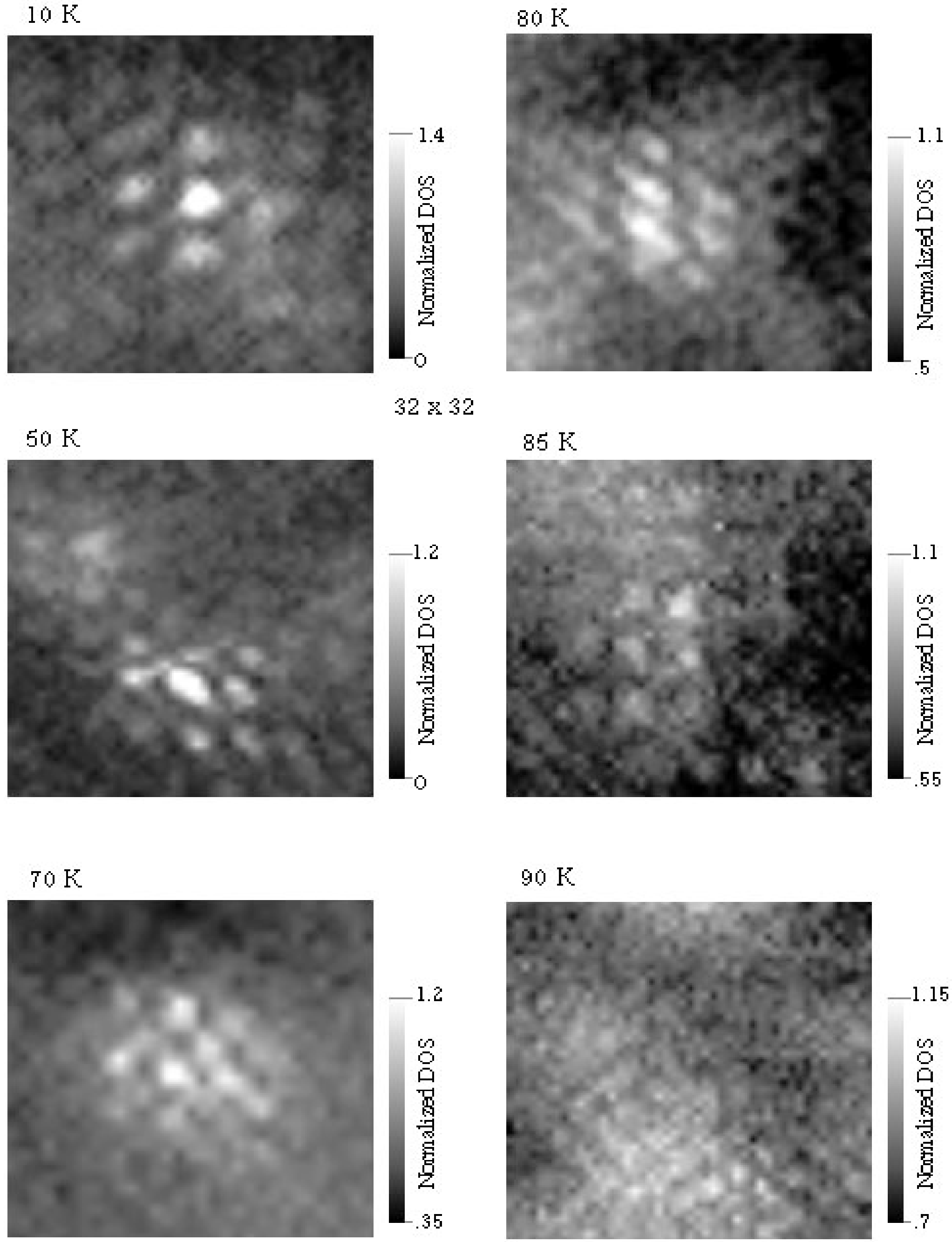


~20
Zn atoms

Cross shaped
Impurity state
(due to 4 fold ga

Å

***Nature* 403,** 746 (2000).



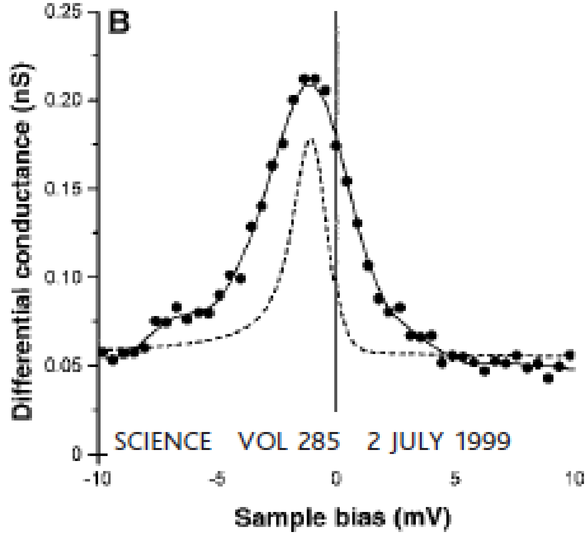
Data by A. Matsuda
NTT Research, Japan

Atomic-Scale Quasi-Particle Scattering Resonances in $Bi_2Sr_2CaCu_2O_{8+\delta}$

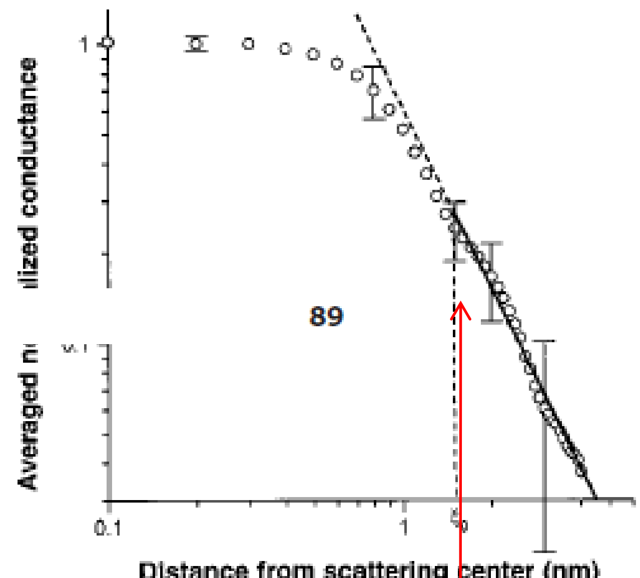
E. W. Hudson,[1] S. H. Pan,[1*] A. K. Gupta,[2] K.-W. Ng,[2] J. C. Davis[1]†

SCIENCE VOL 285 2 JULY 1999 89

This result is in excellent agreement with predictions (6, 8) that $G(r) \propto 1/r^2$ for $r > \xi_o$.



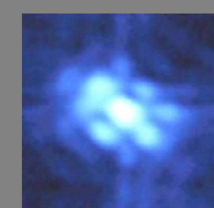
SCIENCE VOL 285 2 JULY 1999



89

Fig. 3. (A) Tunneling conductance versus sample bias taken at two different locations on the BSCCO crystal. The dashed line is taken on a "good" superconducting region, where QPSRs are absent. The solid line is a typical spectrum

$$\Omega_0 \approx \Delta_0 (2U \ln|8U|)^{-1}$$

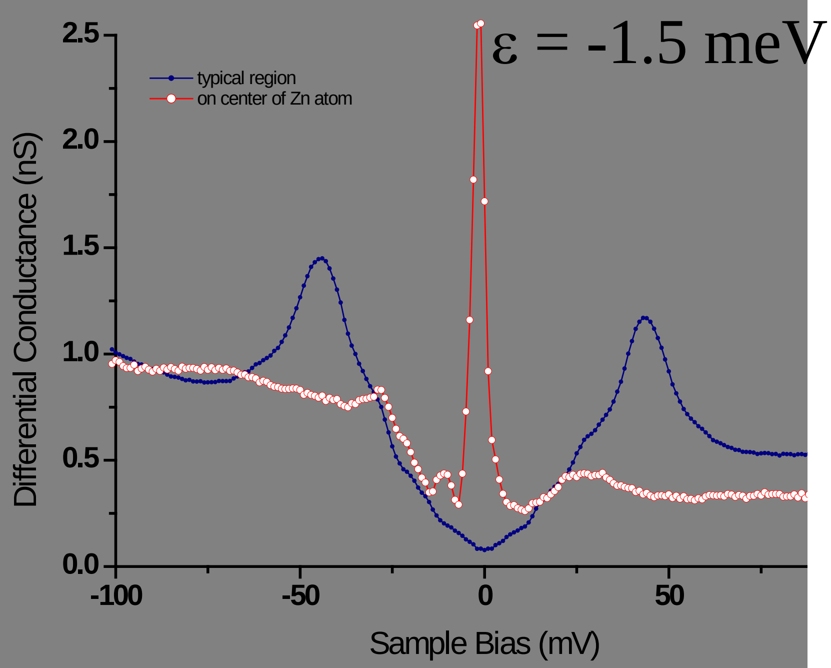


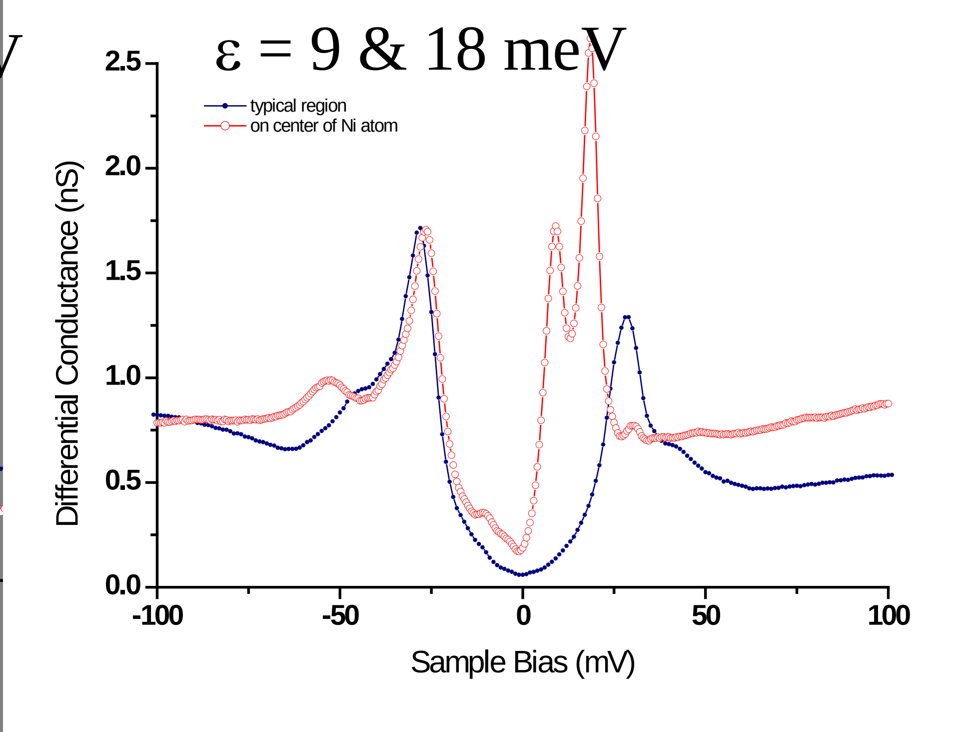
N(r) ~$1/r^2$

Remains to be seen experimentally if this is true in graphene

Motivation 2: magnetic vs nonmagnetic impurities

Impurities as a probe of the high-Tc mechanism





Zn, non-magnetic, S = 0 suppresses superconductivity

Ni, magnetic, S = 1, does not suppress superconductivity

Impurity states in ANY Dirac point materials

Impurity states in ANY Dirac point materials

Impurity states in ANY Dirac point materials

Impurity states in ANY Dirac point materials

Local Density of states in Dirac Materials:

Nonmagnetic impurity in d-wave SC and in graphene will have similar r dependence

$$N(r,\omega) \sim \mathrm{Im}\, G(r,r,\omega) \sim$$

$$\mathrm{Re}[G_0(r,r_{imp},\omega)G(r_{imp},r,\omega)]\,\mathrm{Im}\,T(\omega)$$

$$G(r,r,\omega) = G_0(r,r,\omega) + G_0(r,r_{imp},\omega)T(\omega)G_0(r_{imp},r,\omega)$$

$$= |\Psi(r,r_{imp})|^2 Z_{imp}\delta(\omega - E_{imp})$$

$$T(\omega) = U/(1 - G_0(\omega)U)$$

$$E_{imp} = \frac{1}{U\,|LogU/W|}$$

$$\text{pole } \; 1/\mathrm{U} = \mathrm{G}_0(\omega)$$

$$\Psi(r,\omega) \sim \mathrm{Re}\;\; \mathrm{G}_0(r,\omega) \sim \frac{\sin(k_F r + \delta)}{r}$$

$$G_0(\omega) = \omega[Log(\omega/W) + i\;\mathrm{sign}(\omega)]$$

$LDOS$ $\mathrm{N(r)} \sim 1/r^2$ for all Dirac propagators

nature of local scattering center is not important:

Kondo, potential scattering site, spin orbit impurity etc.

regardless being d-wave SC or graphene or anythng else

result of power counting

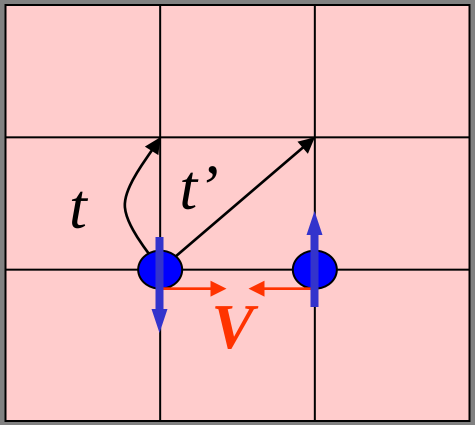
$$G(\mathbf{r},\omega \to 0) \sim \int d^2k \, \exp(i\mathbf{k}\cdot\mathbf{r})G(\mathbf{k},\omega \to 0)$$

$$\sim \int kdk \, \exp(i\mathbf{k}\cdot\mathbf{r})\frac{v_F k}{k^2} \sim 1/r.$$

T. Wehling, PRB, 75, 125425 (2007)
C. Bena, *PRL* **100**, 076601 (2008)
T. Pereg-Barnea, A. H. MacDonald, *PRB* **78**, 014201 (2008)

Model

P.J. Stamp (1987)
Byers, Flatte, Scalapino (1993)
Balatsky, Salkola, Rosengren (1995)
Salkola, Balatsky, Schrieffer (1997)



$$H = H_0 + H_{imp}$$

$$H_0 = -\sum_{i,j,\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + V \sum_{\langle i,j\rangle,\sigma} c_{i\downarrow} c_{j\uparrow} \left\langle c^+_{j\uparrow} c^+_{i\downarrow} \right\rangle + \mathrm{h.c.}$$

$$H_{\mathrm{imp}} = V_{\mathrm{imp}} (n_{0\uparrow} + n_{0\downarrow}) - S_{\mathrm{imp}} (n_{0\uparrow} - n_{0\downarrow})$$

Hopping: nn: t = 400 meV

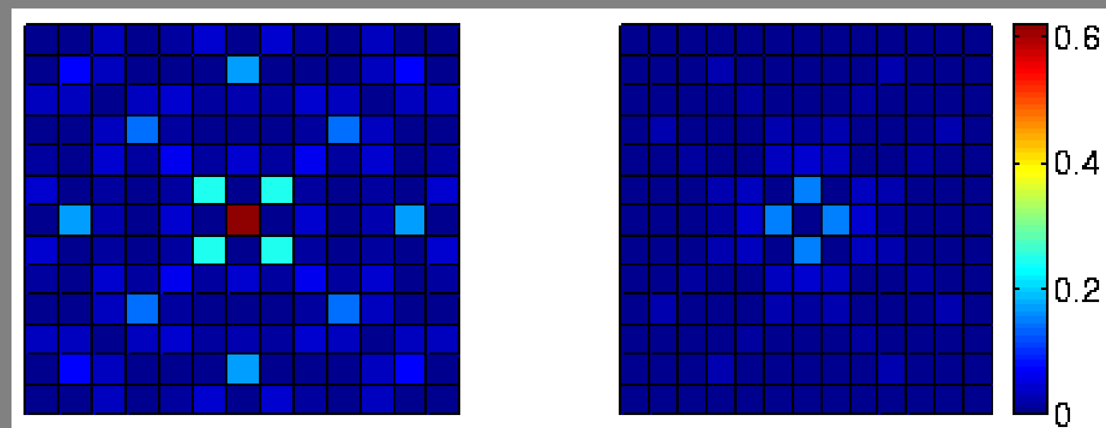
nnn: t' = 0.3 t = 120 meV

Attraction: nn: V = -0.525 t = - 210 meV

Ni,Theory vs. Expt – Images

Theory:

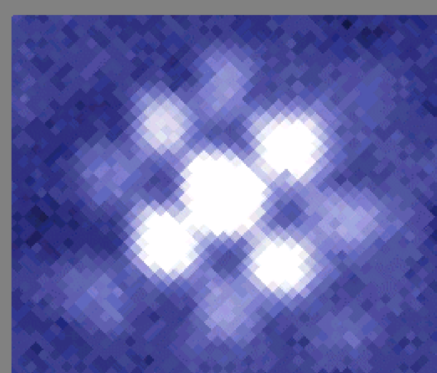
$V_{imp} = t$; $S_{imp} = 0.4\ t$;
doping 16%

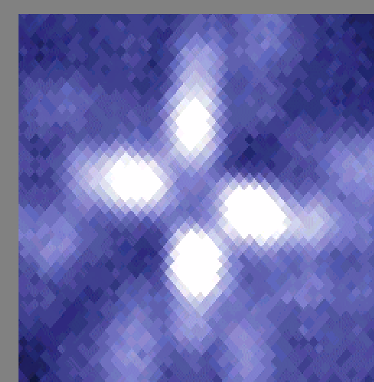


9 mV   - 9 mV

Experiment:

E.W. Hudson , *et.al.*



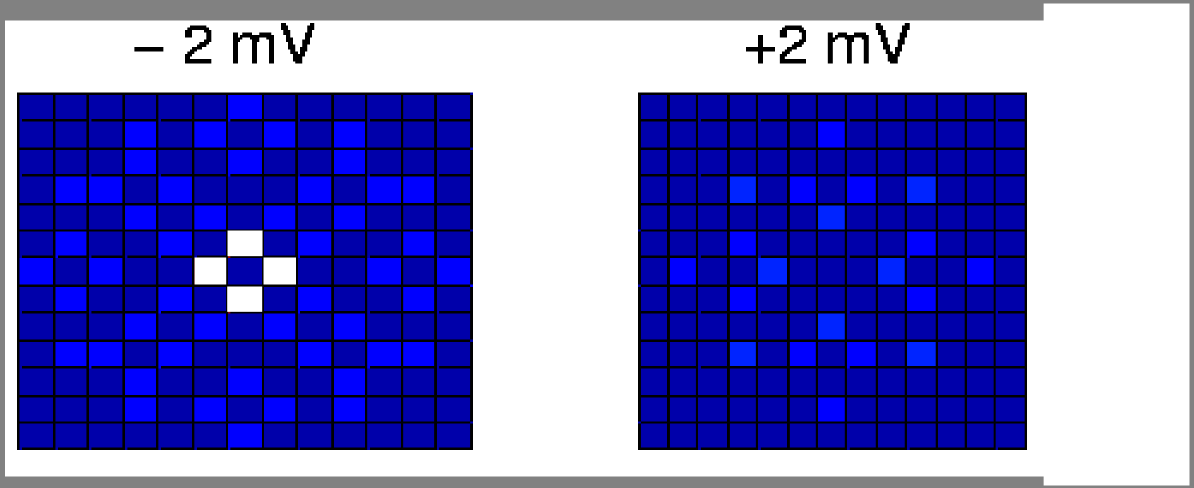


Zn: Strong potential imp

Theory

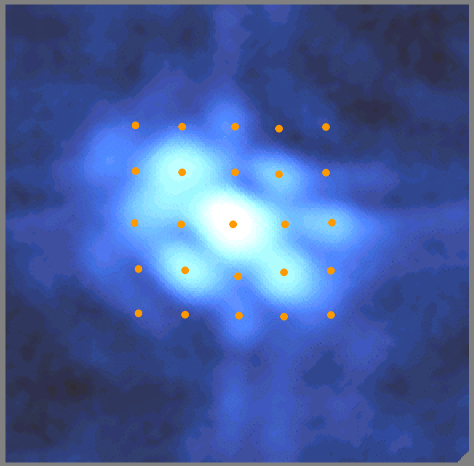
V_{imp}= -10 t = -4 eV

doping 16%



Experiment

S.H. Pan et al



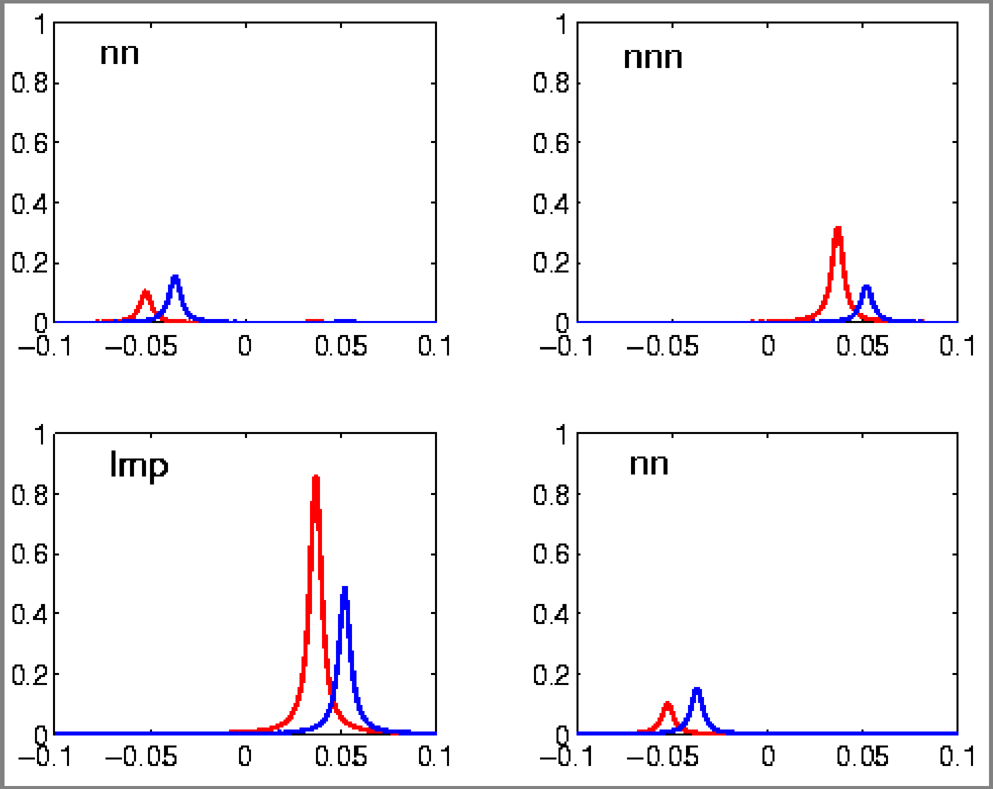
Impurity site has to be bright!!!

Ni, weak potential + spin imp

Theory:

$V_{\text{imp}} = t$; $S_{\text{imp}} = 0.4\ t$;

doping 16%

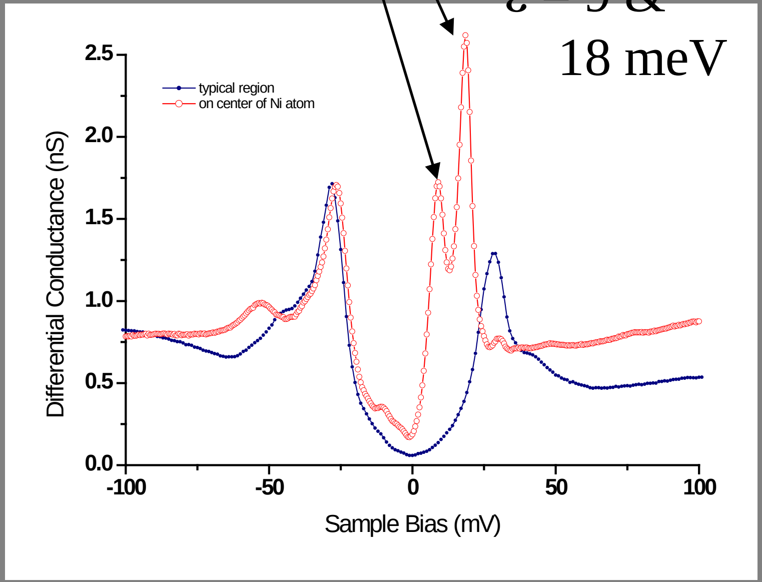


$\varepsilon_1 = 0.052\ t$ (21 mV), $\varepsilon_2 = 0.037\ t$ (15 mV)

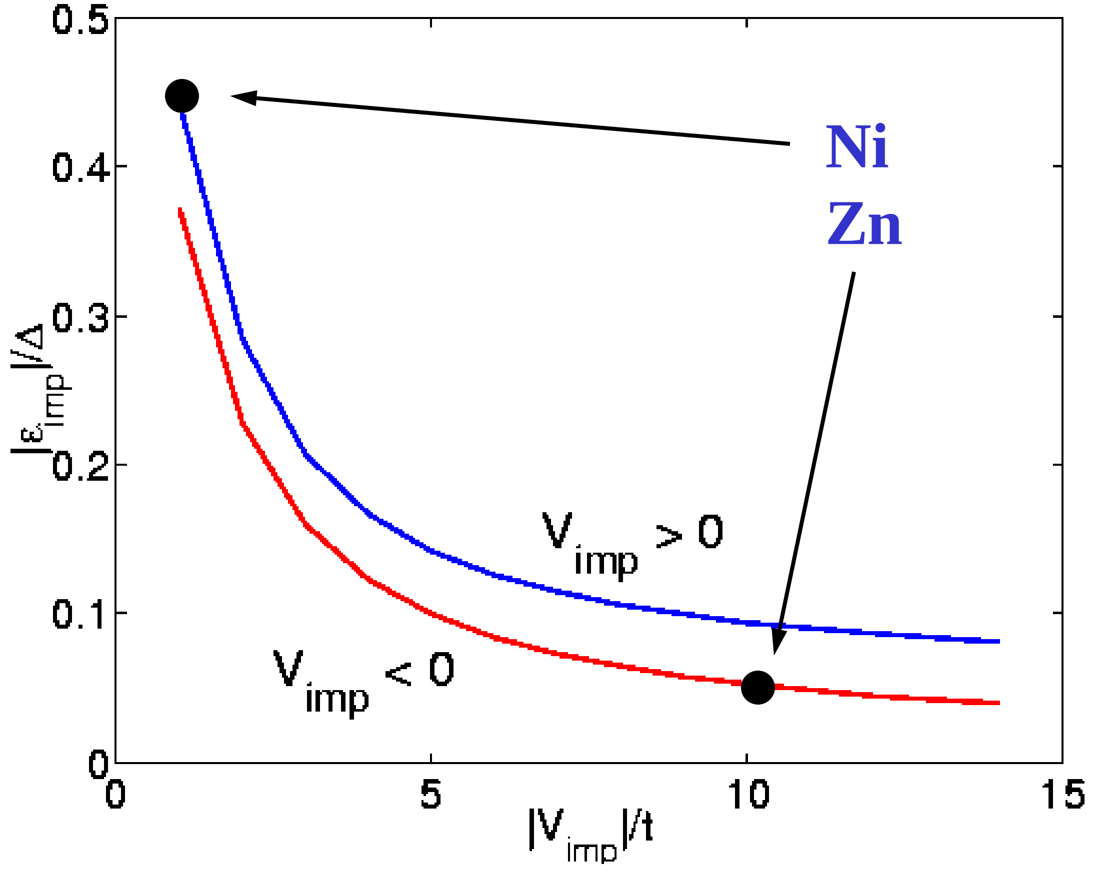
Experiment:

Impurity level splitting caused by Ni spin

ε = 9 & 18 meV



Potential impurity in BSCCO (0.16 doping)



Ni – weak repulsive
8 electrons in 3*d*

Zn – strong attractive
10 electrons in 3*d*
(filled shell)

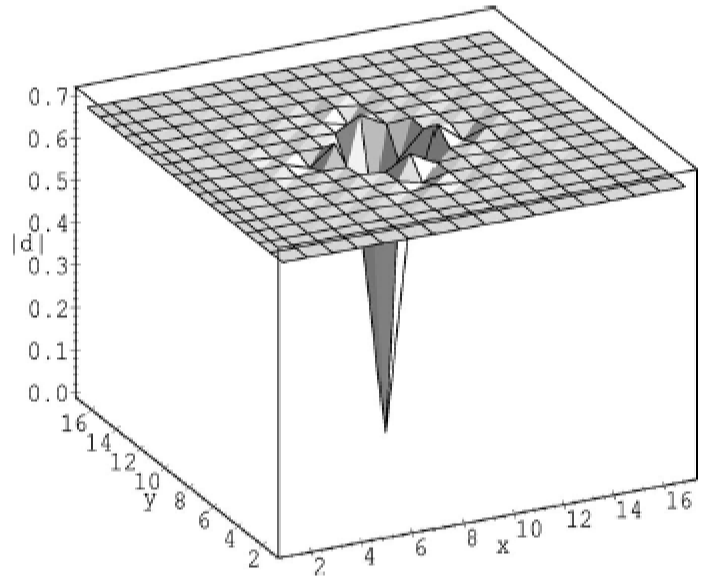


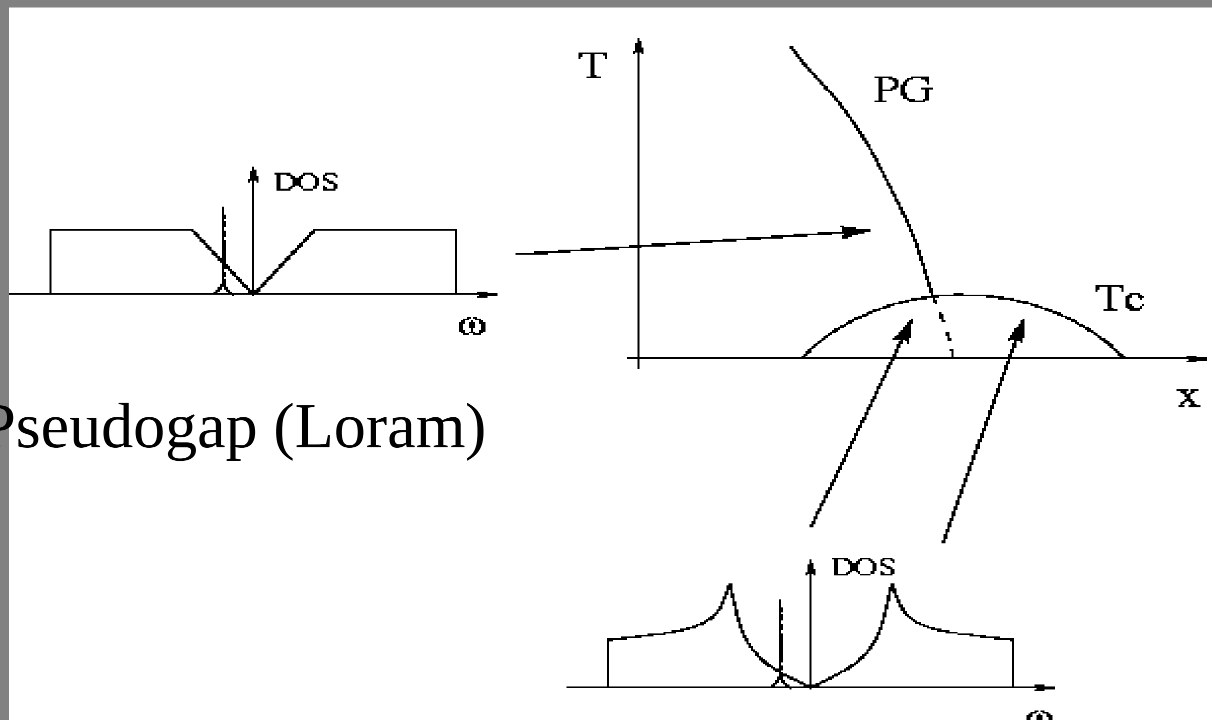
FIG. 5. Self-consistently determined gap function near the scalar impurity in a 2D *d*-wave superconductor. The gap suppression is strongly localized near the impurity site aside from weak oscillating tails. From Franz *et al.*, 1996.

Gap is suppressed on the atomic scale

Not only on scale of coherence length as GL would

Lead us to believe.

Impurity as a probe of Pseudogap (PG) Regime



Pseudogap (Loram)

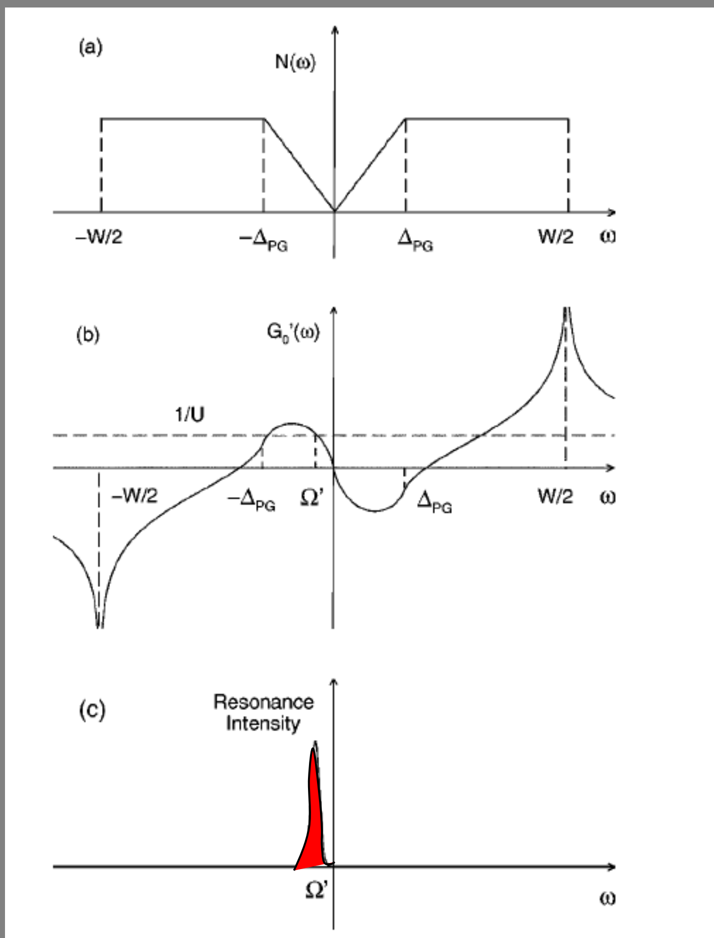
Vanishing of density of states at the fermi level is sufficient for formation of impurity state.

H. Kruis, I. Martin and AVB
PRB, 2002

PHYSICAL REVIEW B, VOLUME 64, 0245XX

Impurity-induced resonant state in a pseudogap state of a high-T_c superconductor

H. V. Kruis,[1,2] I. Martin,[2] and A. V. Balatsky[2]



$T = U/(1-G_0(\Omega)U)$

Hence the pole at $G_0(\Omega) = 1/U$

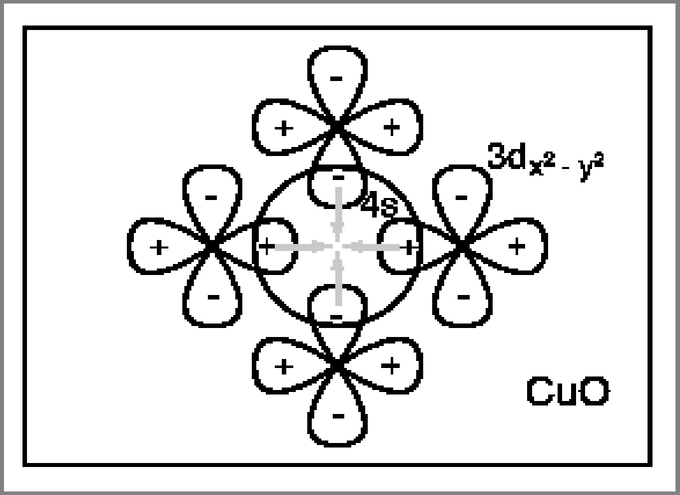
$$G_0(\Omega) = -\frac{2\Omega N_0}{\Delta_{PG}}\left[\ln\left|\frac{\Delta_{PG}}{\Omega}\right| + 1 - \frac{i\pi \ \mathrm{sign}(U)}{2}\right] = \frac{1}{U}.$$

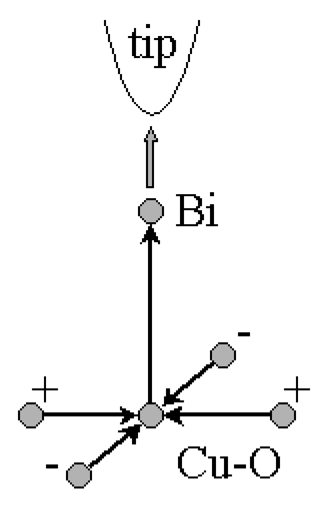
$$\Omega = \Omega' + i\Omega''$$
$$= -\frac{\Delta_{\mathrm{PG}}}{2UN_0}\frac{1}{\ln|2UN_0|}\left[1 - \frac{1}{\ln|2UN_0|} + \frac{i\pi \ \mathrm{sgn}(U)}{2\ln|2UN_0|}\right],$$

H. Kruis et al, PRB 64, p.054501(2001); RMP 78, p37

Role of the Interlayer Tunneling

Ψ_{ij} – value impurity state wavefunction on site (i,j)





Martin, Balatsky, Zaanen (2000)

Intensity in CuO layer:

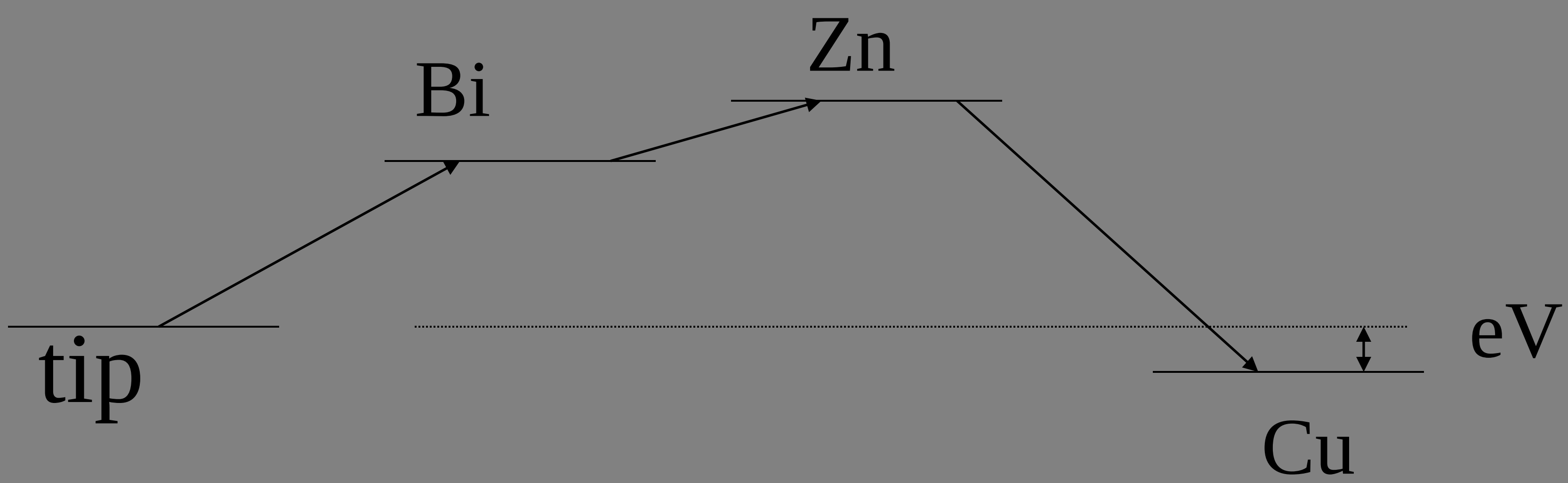
$$A_{ij} = |\,\Psi_{ij}\,|^2$$

Intensity in BiO layer:

$$A_{ij} = |\,\Psi_{ij-1} + \Psi_{ij+1} - \Psi_{i-1j} - \Psi_{i+1j}|^2 \sim |\, \cos kx - \cos ky \,|$$

Direct tunneling (tip to CuO) is exponentially suppressed:

t ~ exp(-r/d), d~0.5A



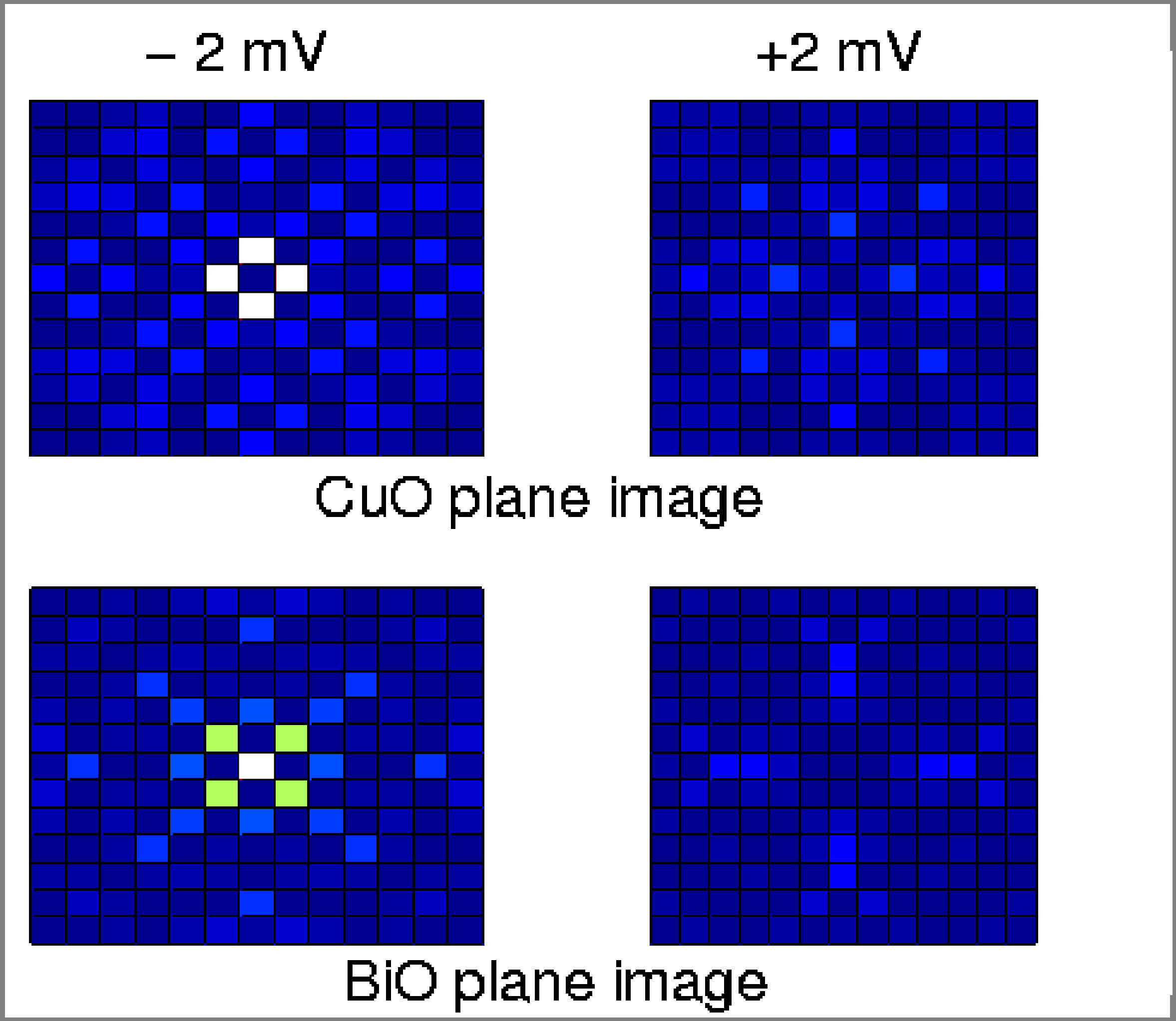
Hopping via virtual states on Bi and Zn(Ni)

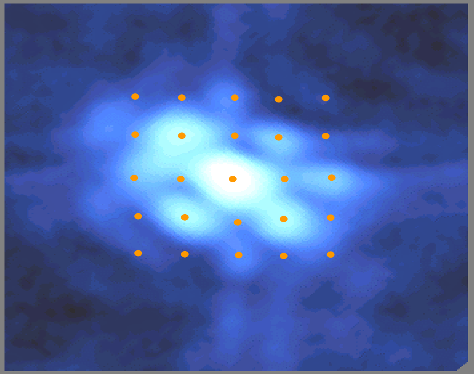
One uses the easiest available path. In this case direct tunneling into Cu-O plane is exponentially suppressed.

$$N_{eff}(r,\omega) = \int d\phi \, \mathrm{t}(\phi) N(r,\phi,\omega) \text{-}$$

surface seen Density of States

BiO vs. CuO plane image





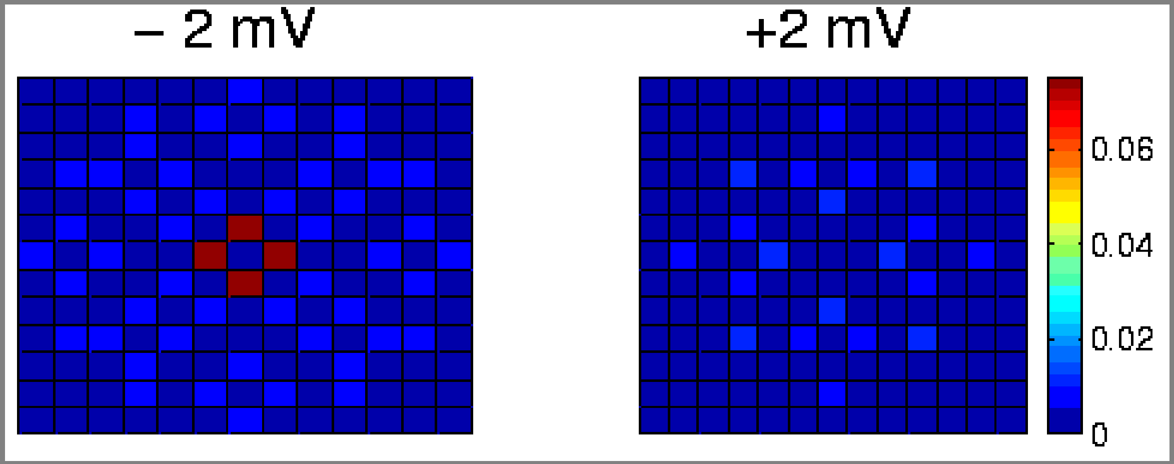
Experiment!

Zn: Strong potential imp

Theory

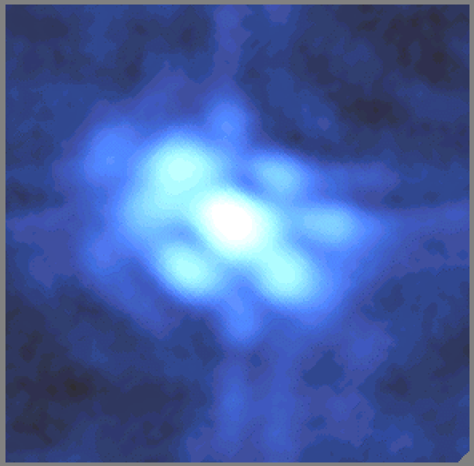
V_{imp}= -10 t = -4 eV

doping 16%



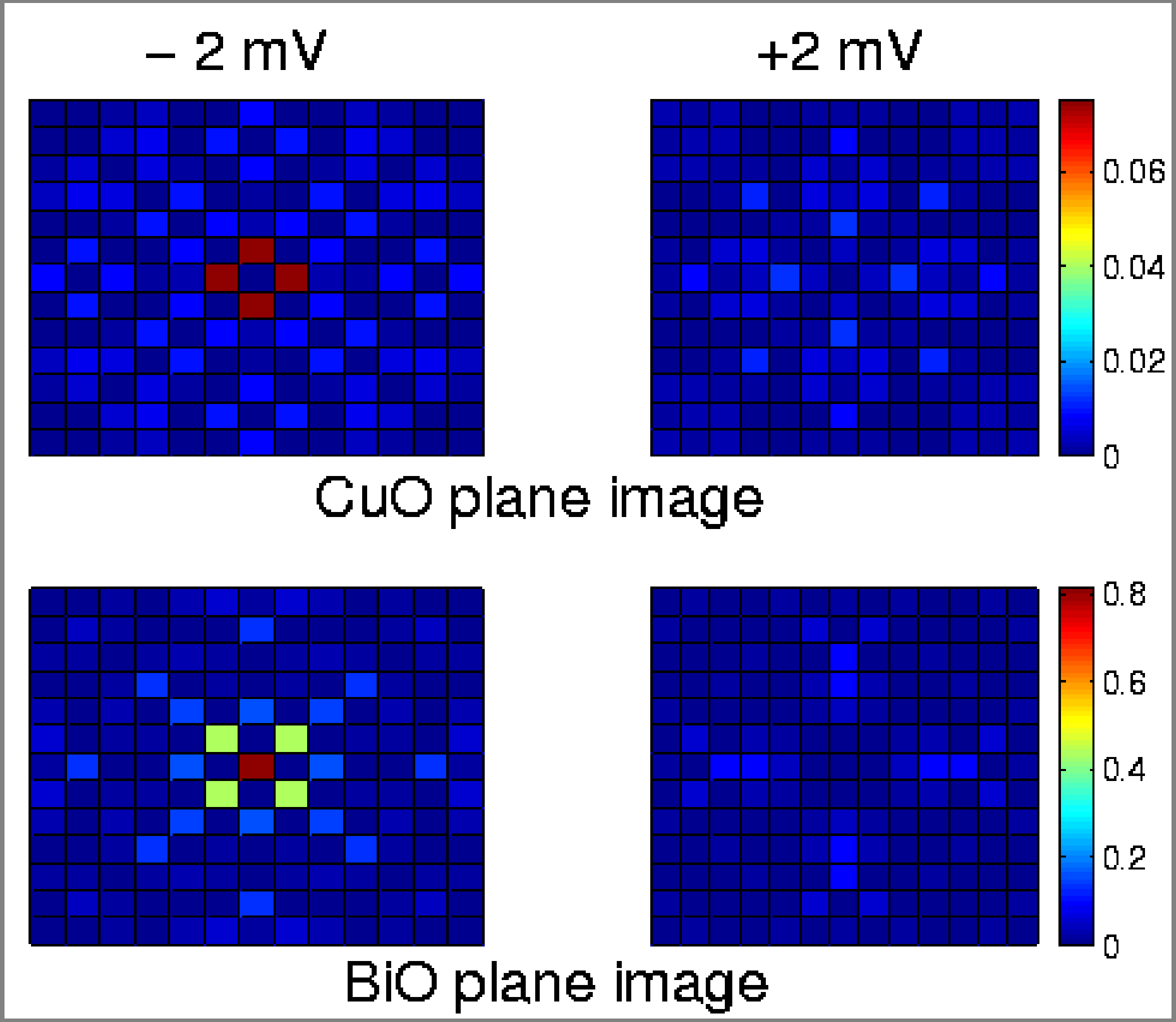
Experiment

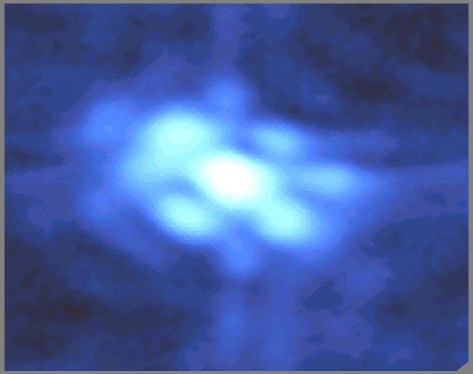
S.H. Pan et al



Impurity site has to be bright!!!

BiO vs. CuO plane image

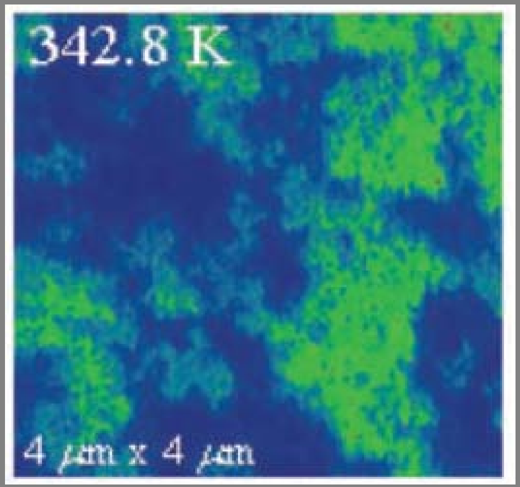




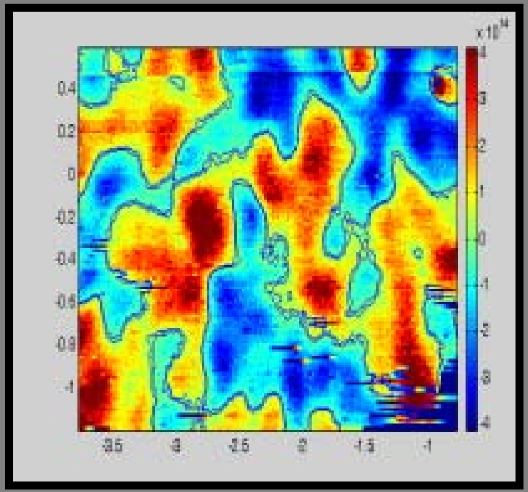
Experiment!

Why local nanoscale probes are useful

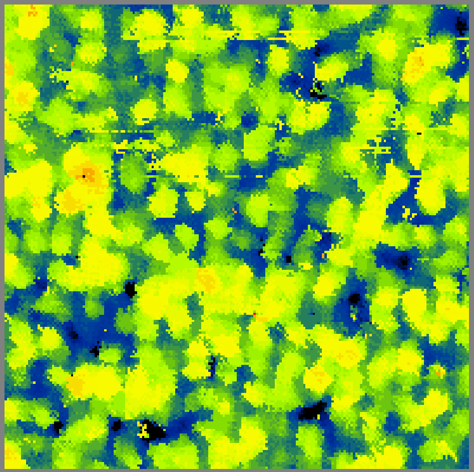
Examples (incomplete list)



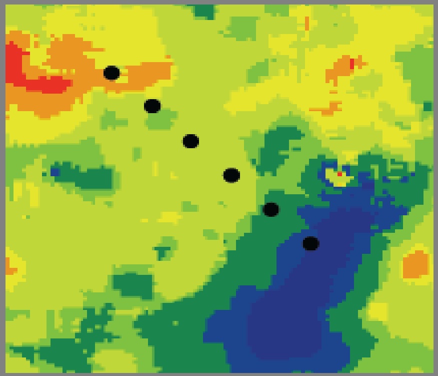
MIT in VO2 Basov
Science, v 318,
1759 (2007)



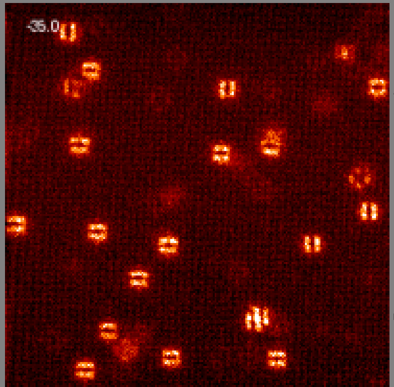
A. Yacobi
J. Stroscio



Gap inhomogeneity
In high Tc oxides
J.C. Davie, S.H. Pan, A. Yazdani

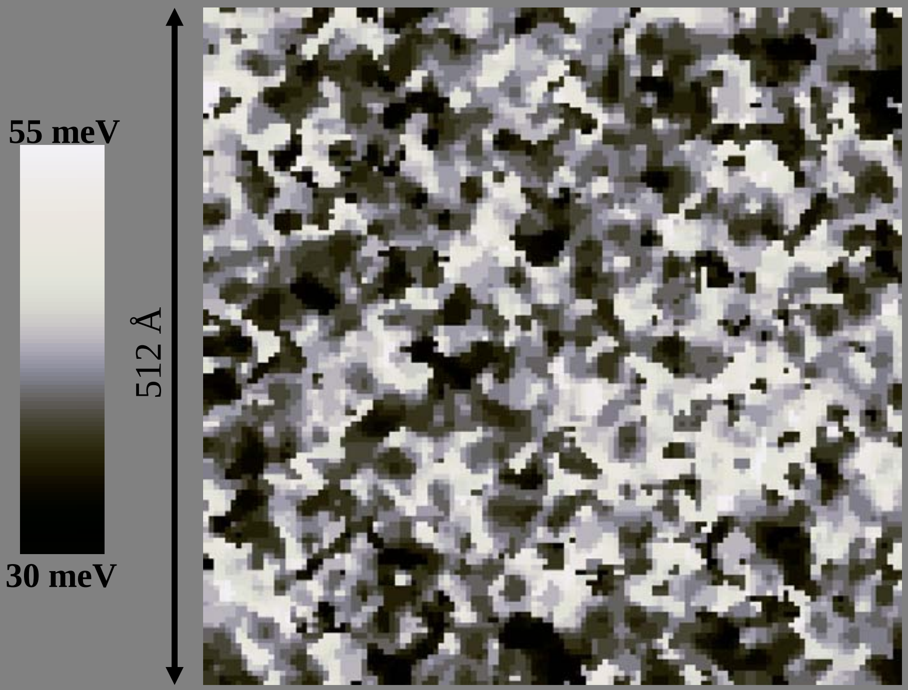


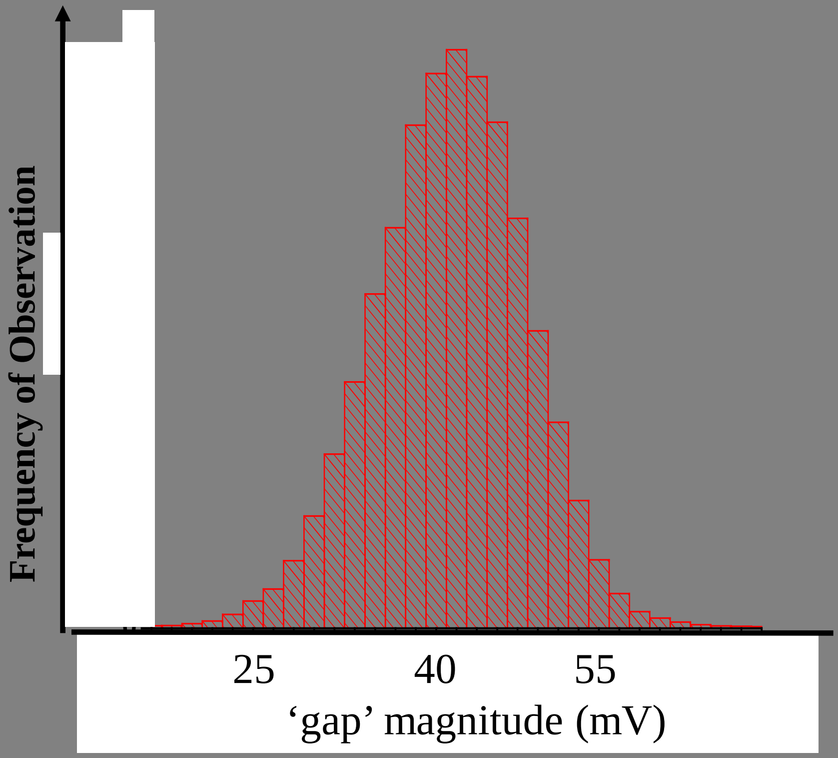
Gap inhomogeneity in
novel FeAs
superconductors,
J. Hoffman et al



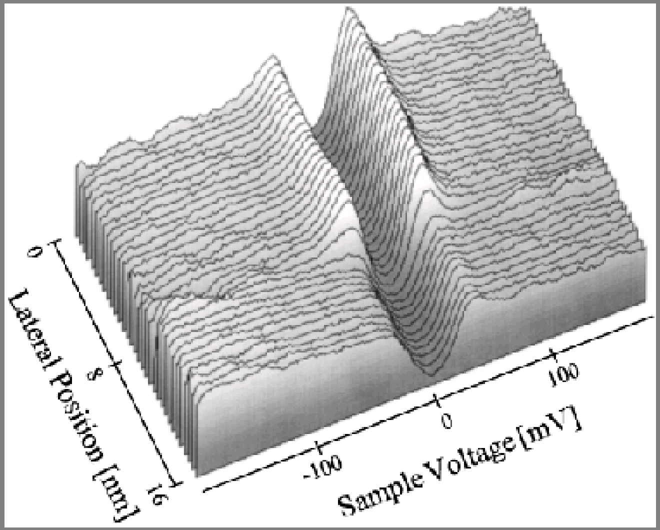
URu2Si2inhomo
geneity in dI/dV
at 35 mev
JC Davis et al

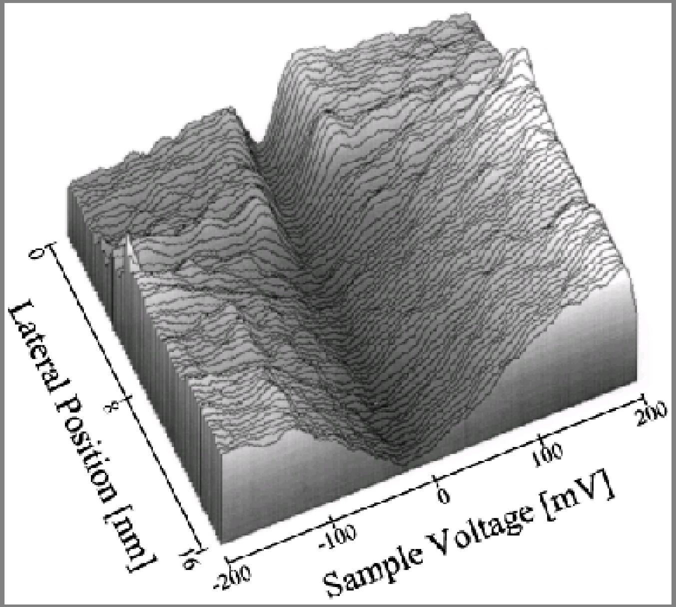
Gap Map, BSCCO (0.5%Ni)

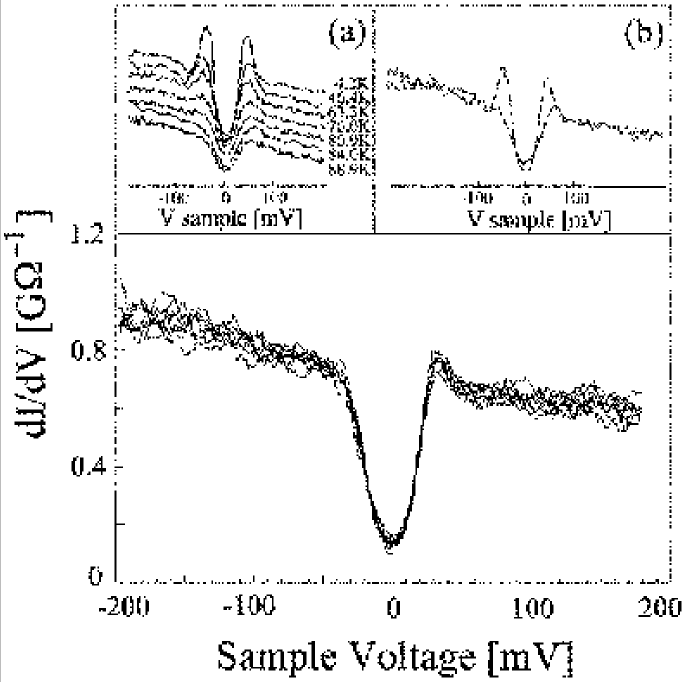




Cren, et al, PRL (2000)
Bi2212 film



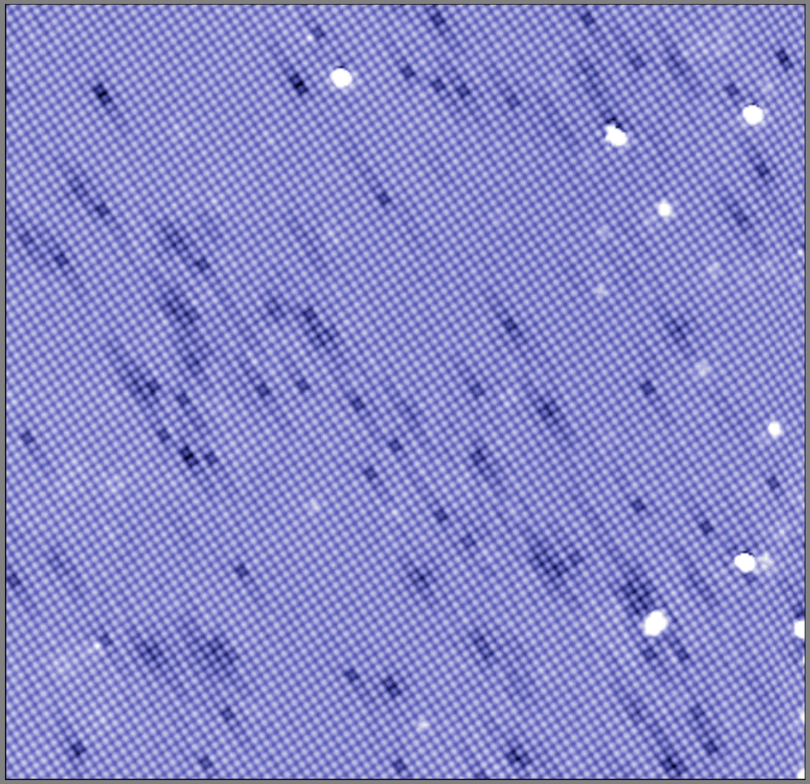




BaO vs BiO

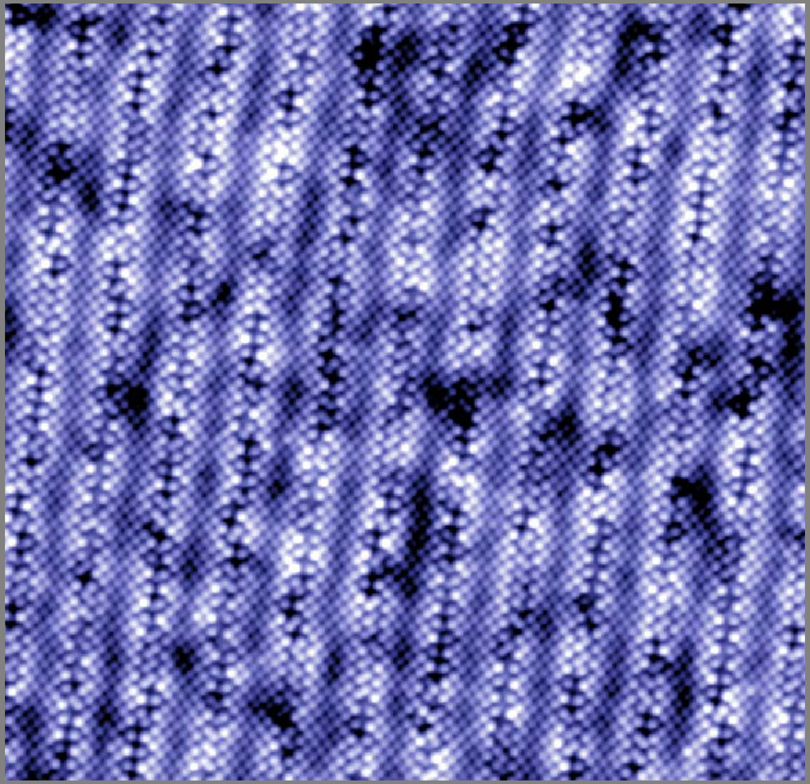
YBCO

YBCO - BaO plane



300 Å

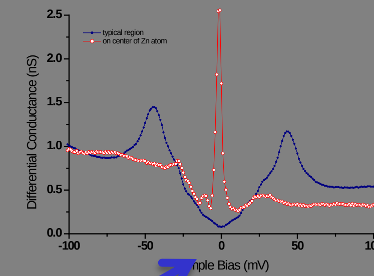
BSCCO - BiO plane



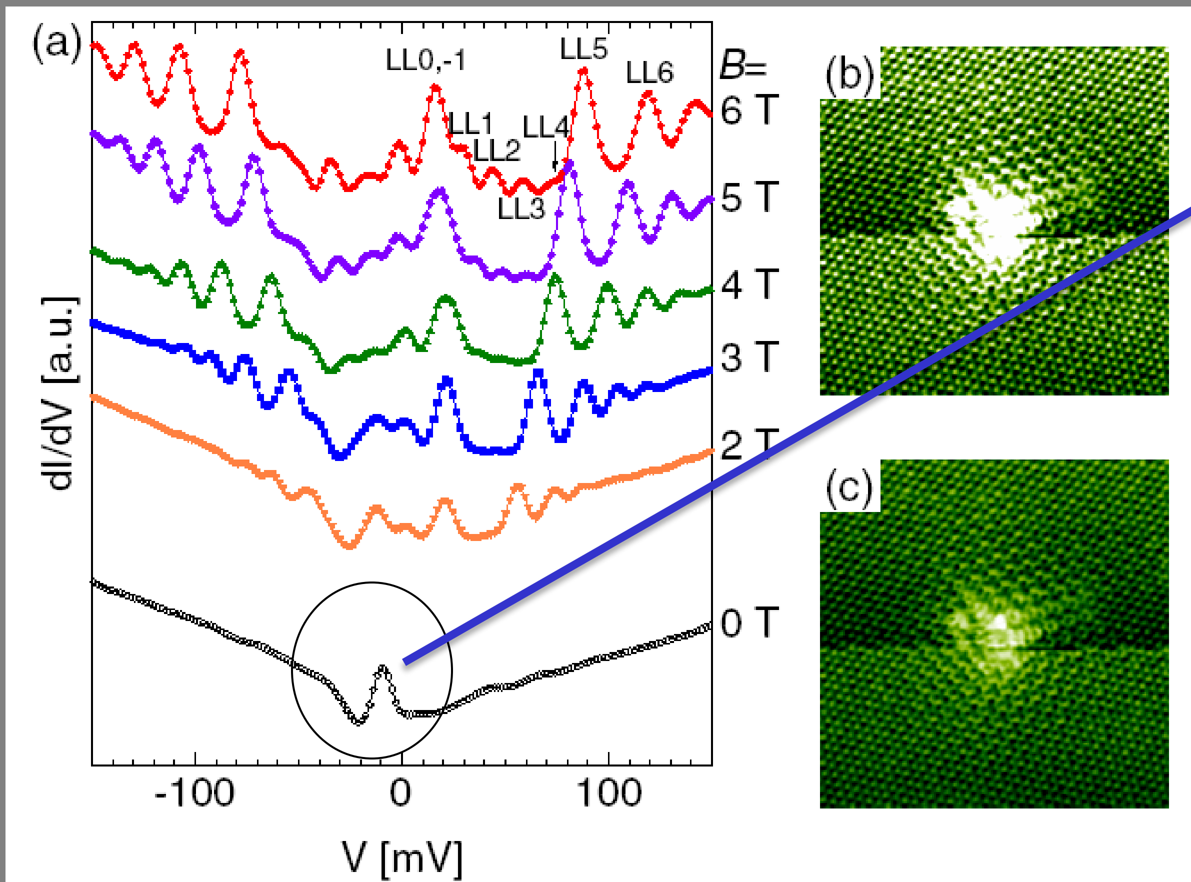
280 Å

Do equivalent nanoscale electronic structure variations exist in YBCO? **Probably not. If they do they are probably weaker and more ordered.**

Impusity states
and STM on Graphene



HOPG



Y. Niimi et. al., PRL 97, 236804

Conclusion

Impurity and defects in correlated states
Are important in that enable new properties

Or make identification of an unknown state easier

One would need right set of tools: experiment…

Theory: investigate local features, no average lifetime
Average scattering potential etc.

A lot of correlated materials do show variety of
inhomogeneous competing states.

Thanks

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