Dirac Materials

similarities and differences between d-wave superconductors and Graphene

A.V. Balatsky

RMP, v 78, p 373, (2006)
http://theory.lanl.gov

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G. Volovik, V. Mineev - Landau

Ar. Abanov, J. X. Zhu, I. Martin, M. Salkola – Los Alamos

H. Dahal - BC

T. Wehling, A. Lichtenstein, K. Scharnberg,

R. Wiesendanger – U Hamburg

M. Katsnelson – U Niemegen

Dirac materials

Materials whose nontrivial electronic properties are a direct consequence of Dirac spectrum E = vk: specific heat ~T, penetration depth~T, optical conductivity~T^n,

Can be a collective state: 3He superfluid, heavy fermion, organic, high Tc superconductors, density wave states

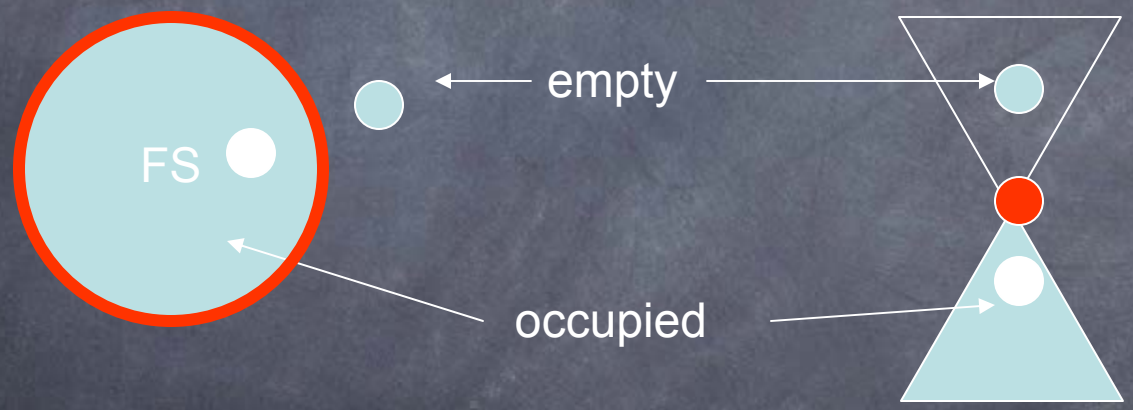
Band structure effect -- graphene

Not a Dirac equation (1928)

Dirac materials vs metals

Metals

Dirac materials
(3He included)



E = v(k-k_F)

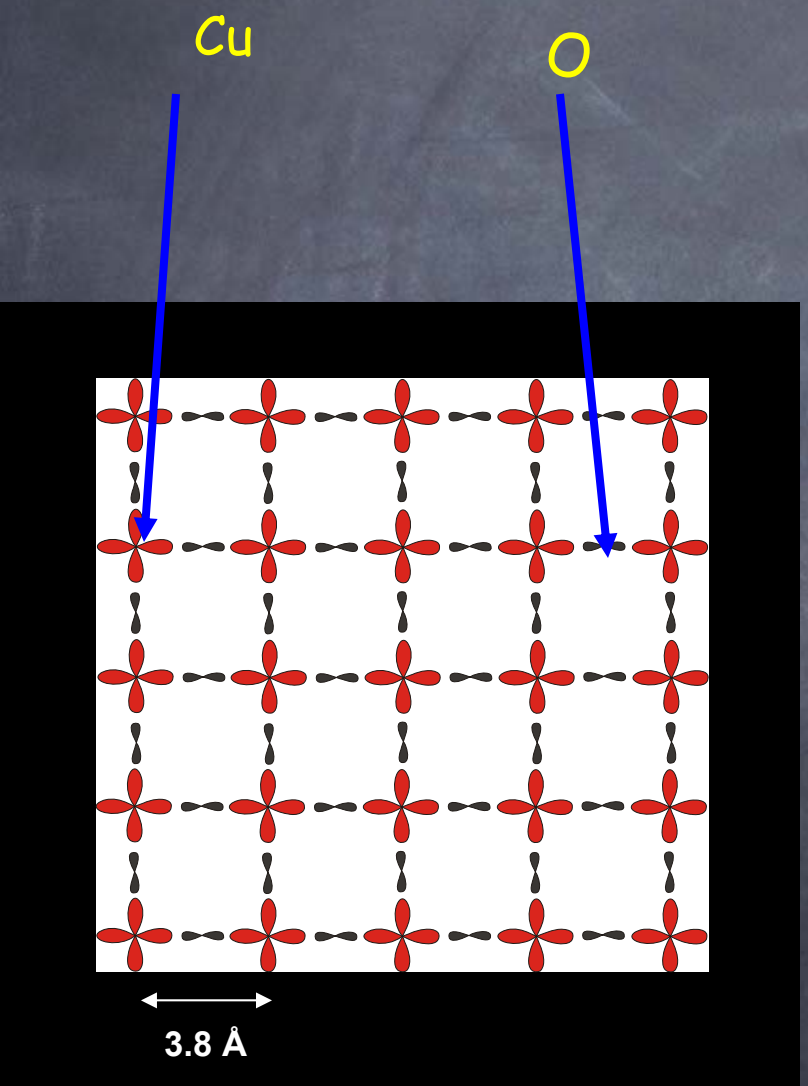
E = vk, k_F = 0

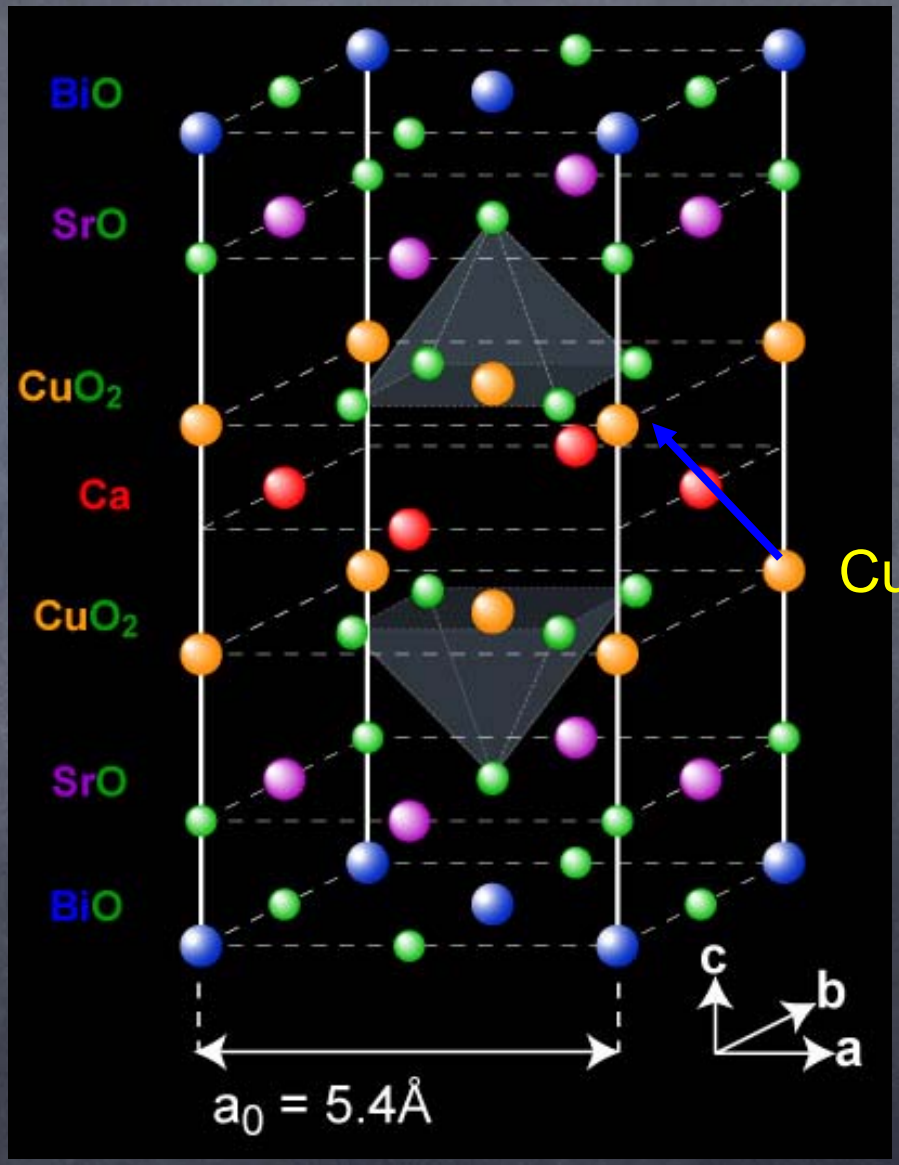
Dimensionality of zero energy states in one less(at least)
In the Dirac materials. Fewer excitations at low T.

- Narrow it down to d-wave SC and graphene
- Though please keep in mind He3, organic materials.
- Too diverse set to cover at once.

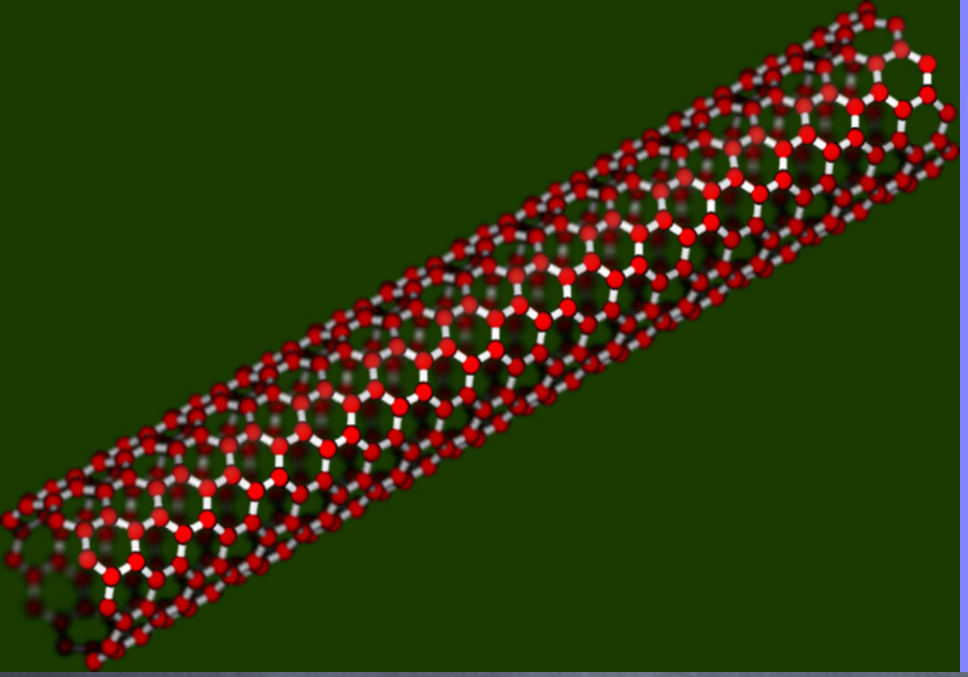
$Bi_2Sr_2CaCu_2O_{8+\delta}$

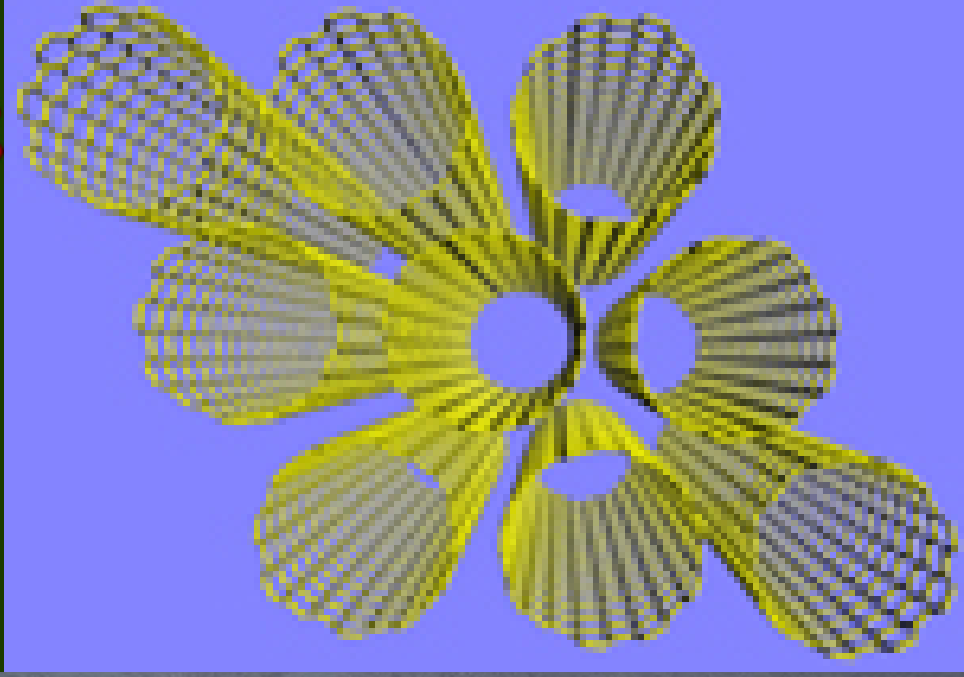
½ Unit Cell



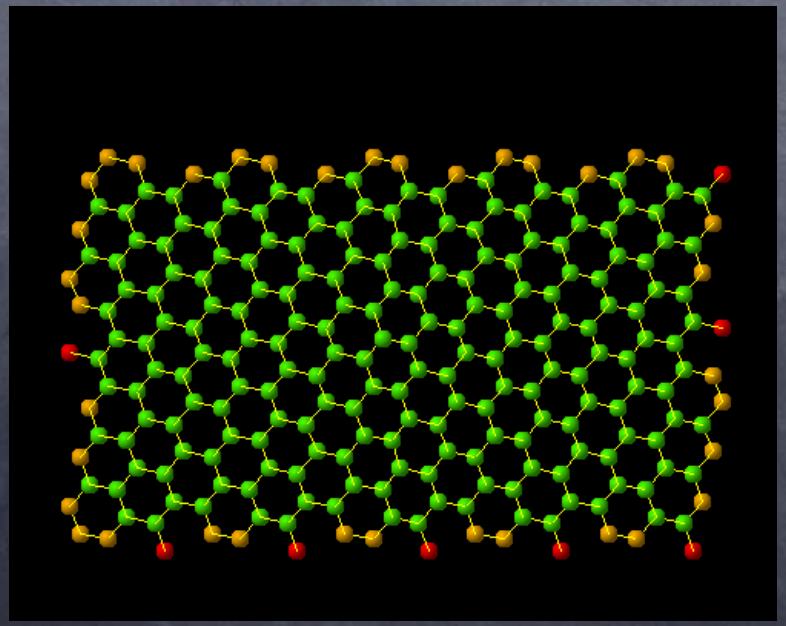


CuO_2 Laye



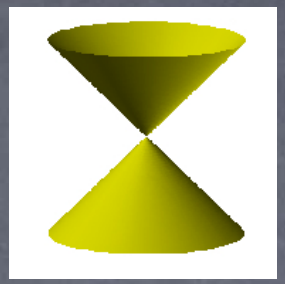


One dimensional: nanotubes



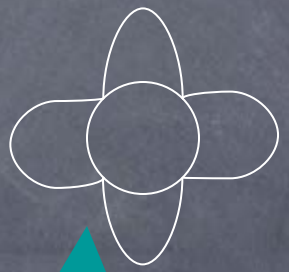
A. Geim, P Kim, deHeer

Dirac fermions in d-wave SC



Nodal excitations near gap nodes are exactly Dirac

Bogoliubov quasiparticles



$$H = \varepsilon(p)\tau_3 + \Delta(p)\tau_1$$

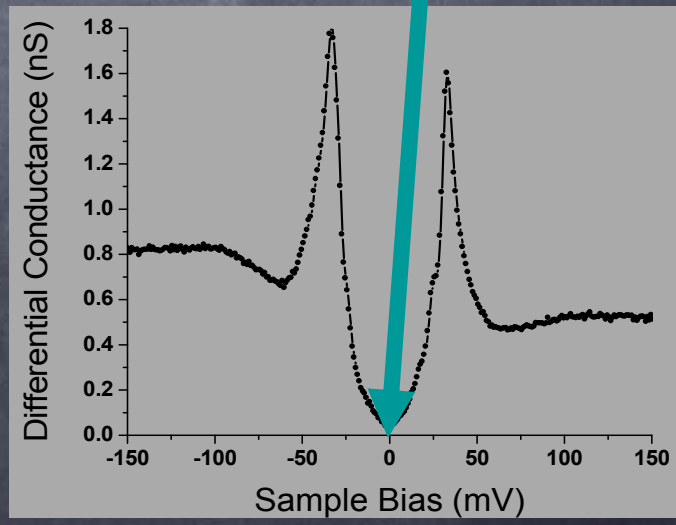
$$\Delta(p) = \Delta(p_x^2 - p_y^2)$$

Nodal points at p_x = p_y

$$E^2(p) = \left(\varepsilon^2(p) + \Delta^2(p)\right)$$

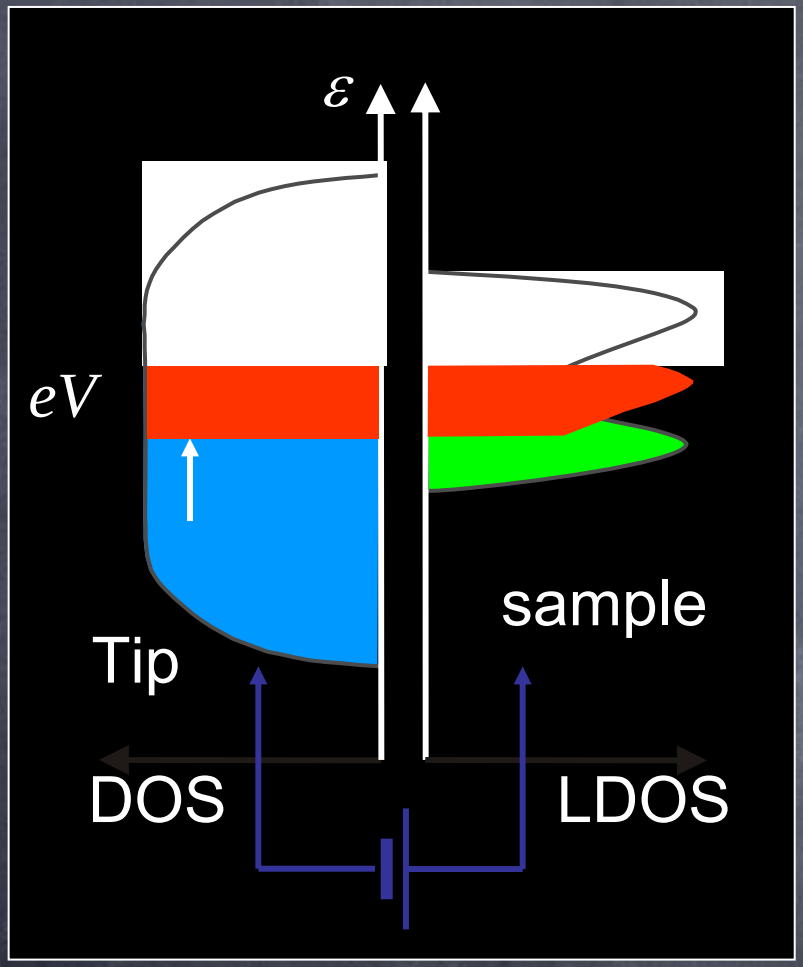
"non relativistic supersymmetry"

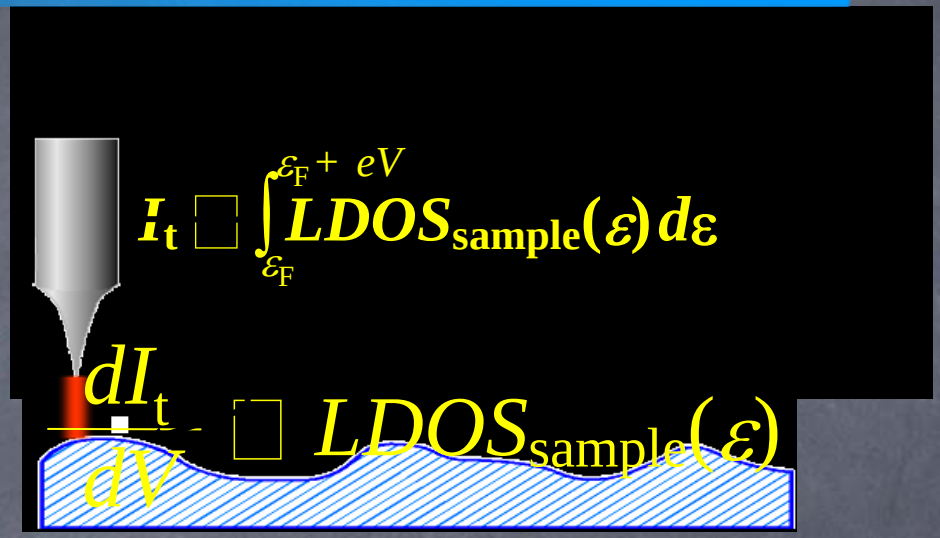
τ_2 as an operator that flips particles into holes.

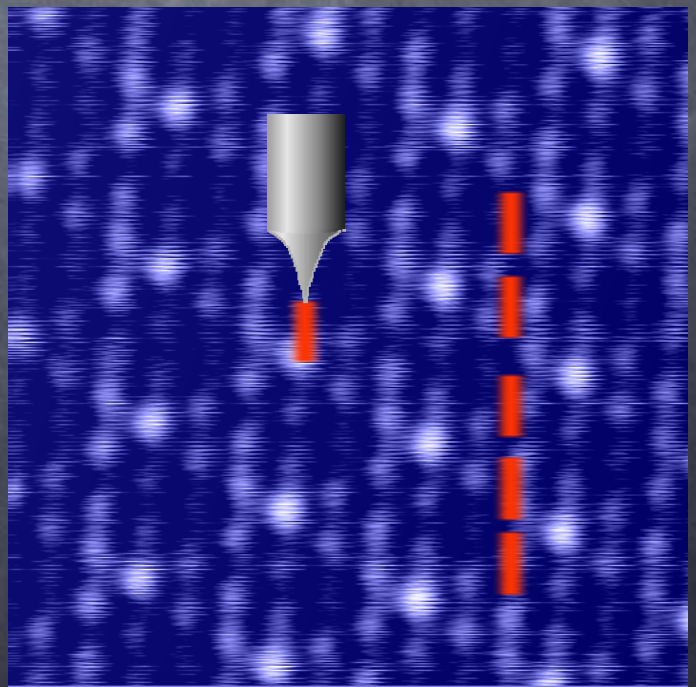


These nodal points are responsible for a lot of Interesting and puzzling physics in high-Tc materials

Local Probes:Scanning tunneling microscopy/spectroscopy







Spectroscopic map (LDOS map) can be obtained.

Similarities of physics of Dirac materials

- Impurity states in d-wave and in graphene
- Electronic nanoscale inhomogeneity in d-wave and in graphene
- Playbook of d-wave Dirac fermions is to be

repeated in graphene

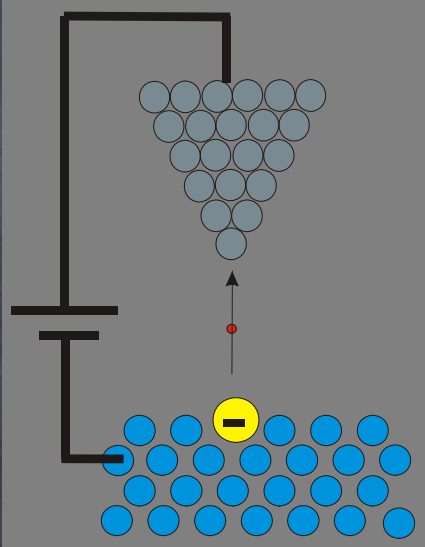
Except much faster, now that we know

what to look for

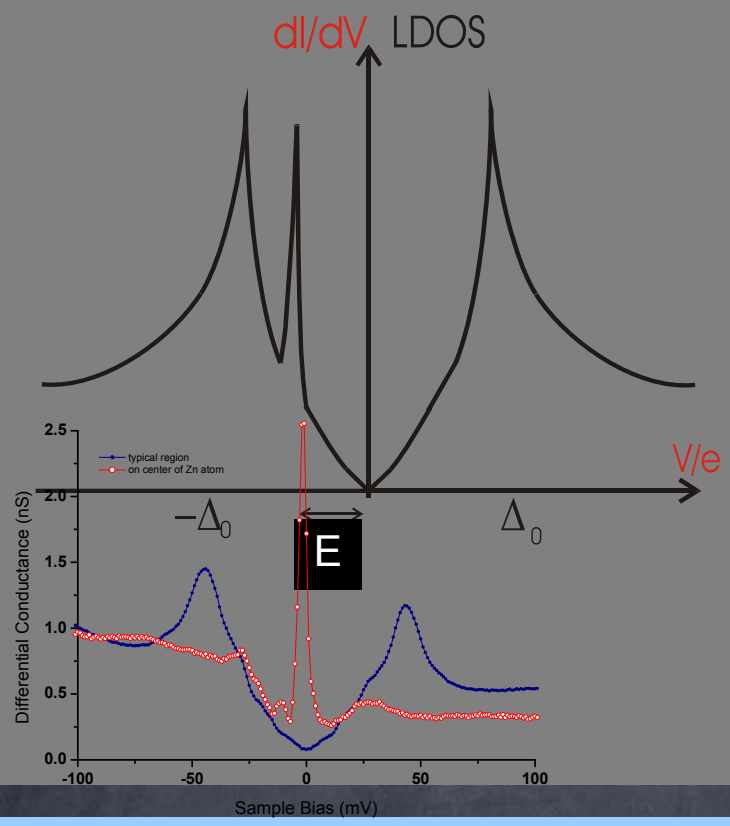
- More to be filled in: correlations, topological excitations, WC

Earlier work: d-SC Impurity Resonances

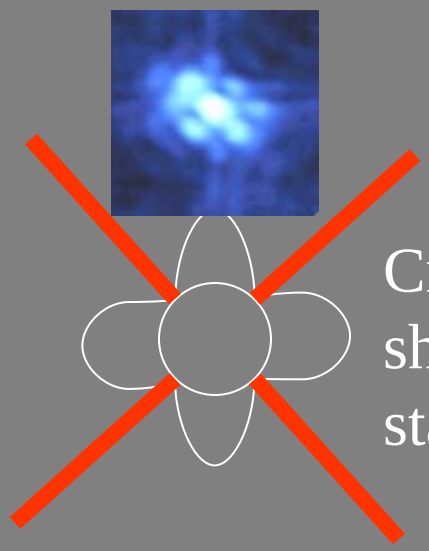
On-site potential
U>0



On-site LDOS



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



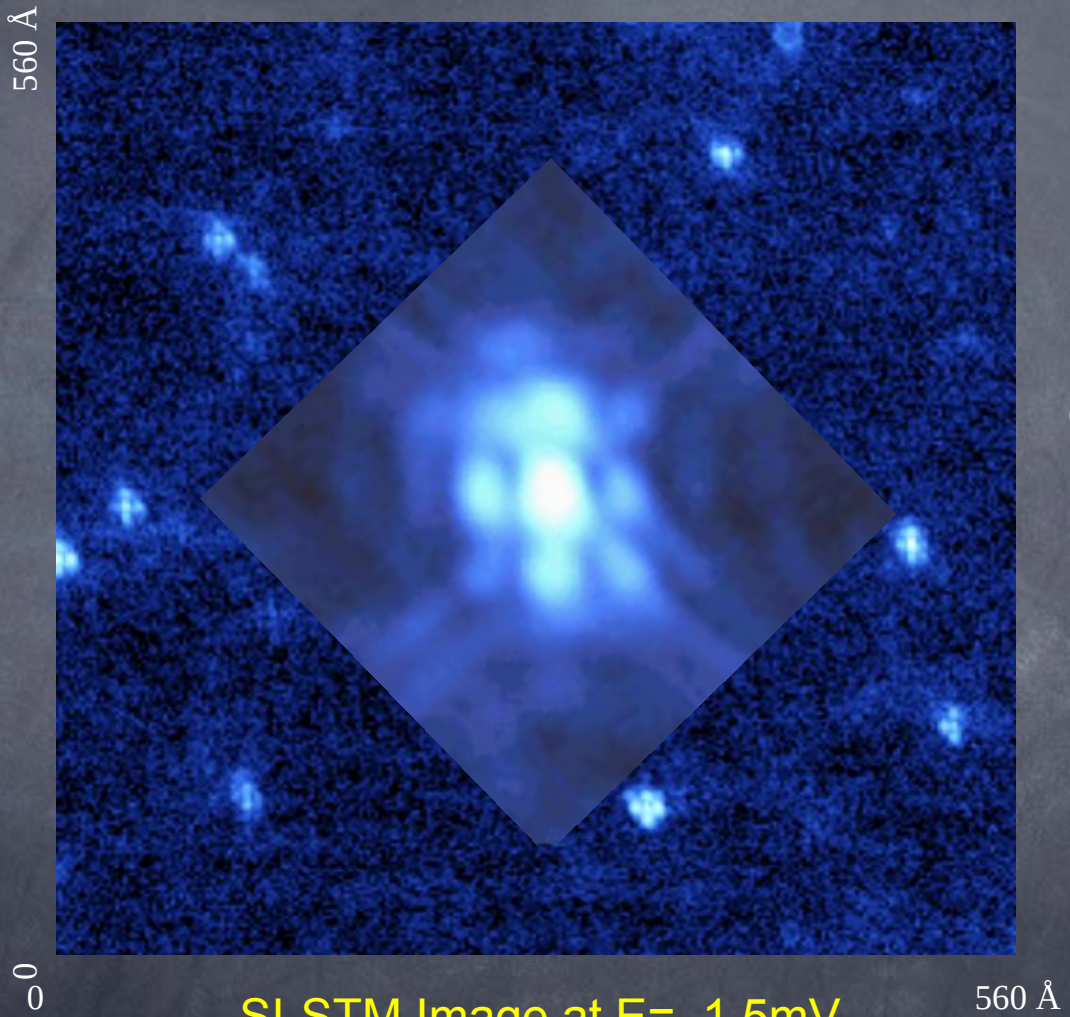
Cross shaped state

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

Balatsky, A.V., Salkola M.I., & Rosengren, A., *Phys. Rev.* ***B*** **51**, 15547 (1995).
A.V. Balatsky, I. Vekhter and J. X Zhu, Rev. Mod Phys, **78**, p 373, (2006)

Zn Impurity-State

~20
Zn atoms



Cross shaped
Impurity state
(due to 4 fold gap)

SI-STM Image at E=–1.5mV

$Bi_2Sr_2Ca(Cu_{1-x}Zn_x)_2O_{8+d}$: $x \cong 0.2\%$

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

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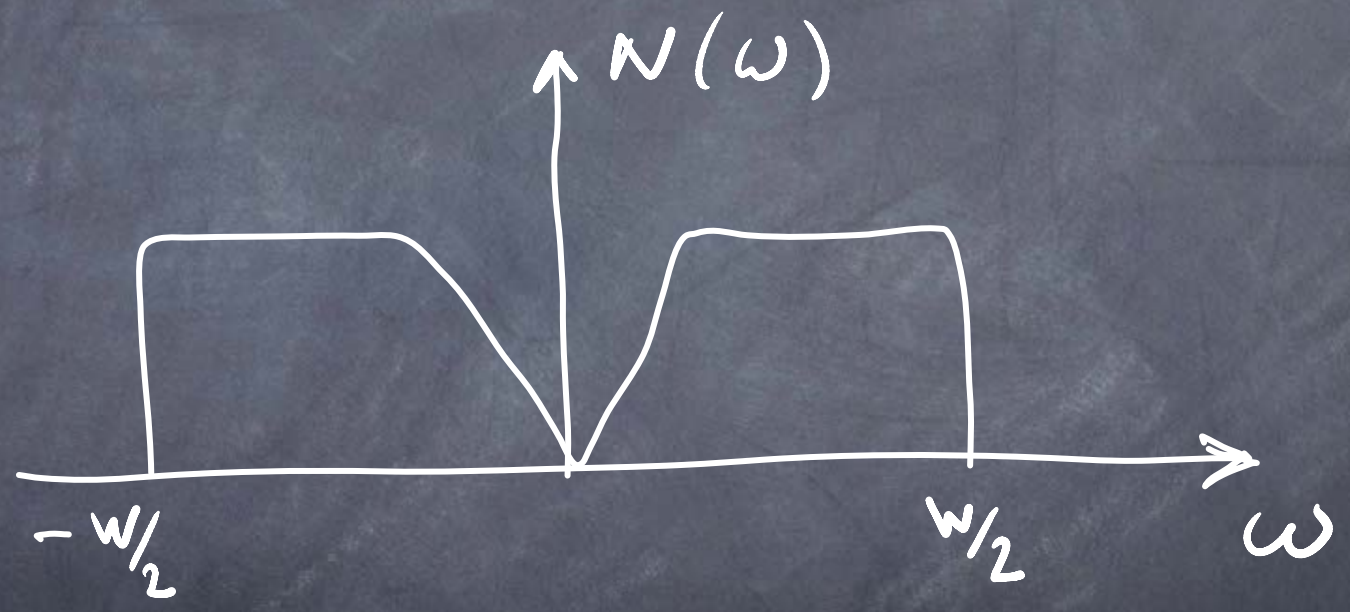
Impurity states in ANY Dirac point materials



$$T = \frac{U}{1 - U G(\omega)}$$

$$G(\omega) = \frac{1}{U} \leftarrow \text{small}$$

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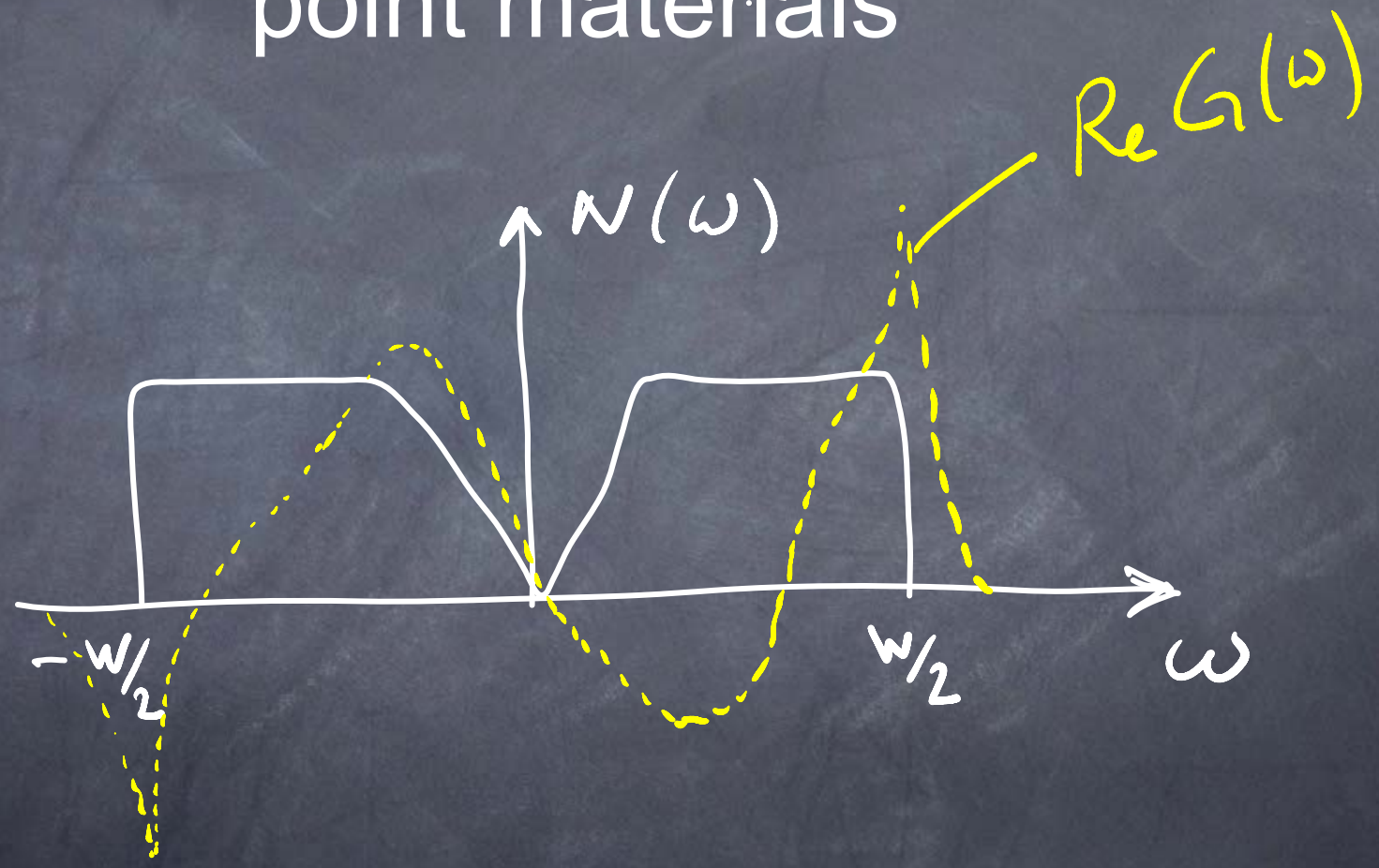
Impurity states in ANY Dirac point materials



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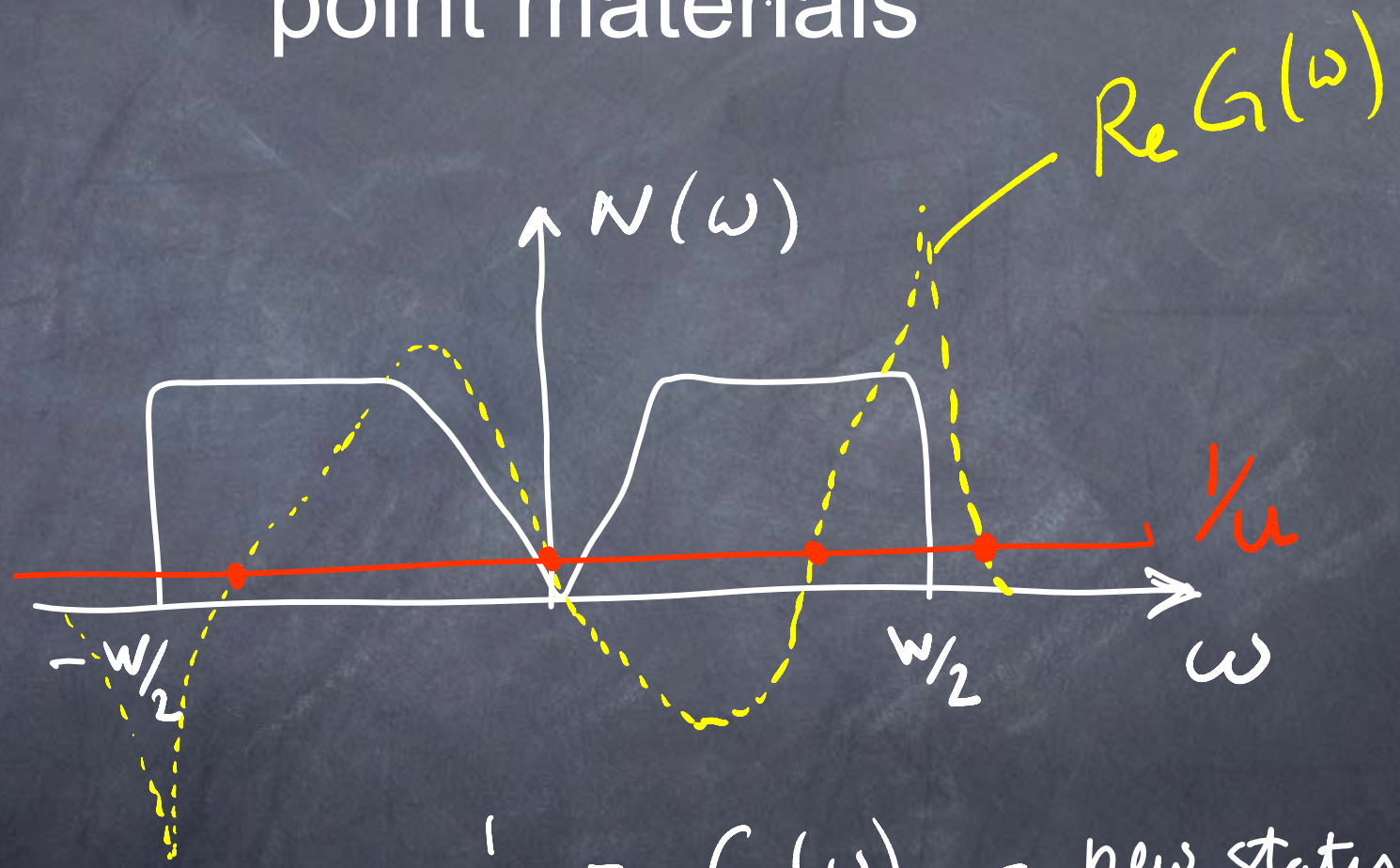

$$\frac{1}{u} = G(\omega)$$ - new states or resonances

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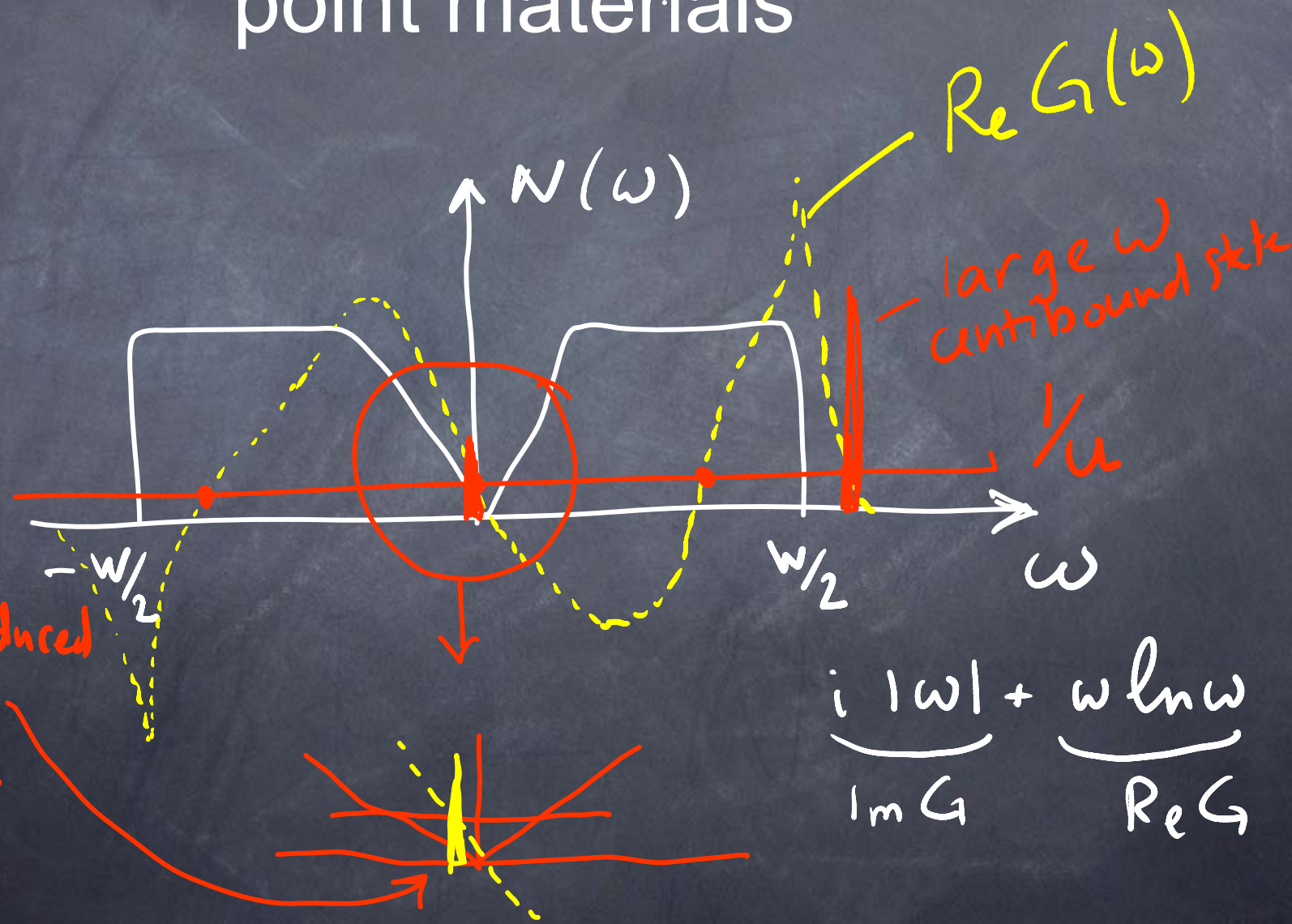
Impurity states in ANY Dirac point materials



$$\underbrace{i\,|\omega|}_{\mathrm{Im}\,G} + \underbrace{\omega \ln \omega}_{\mathrm{Re}\,G}$$

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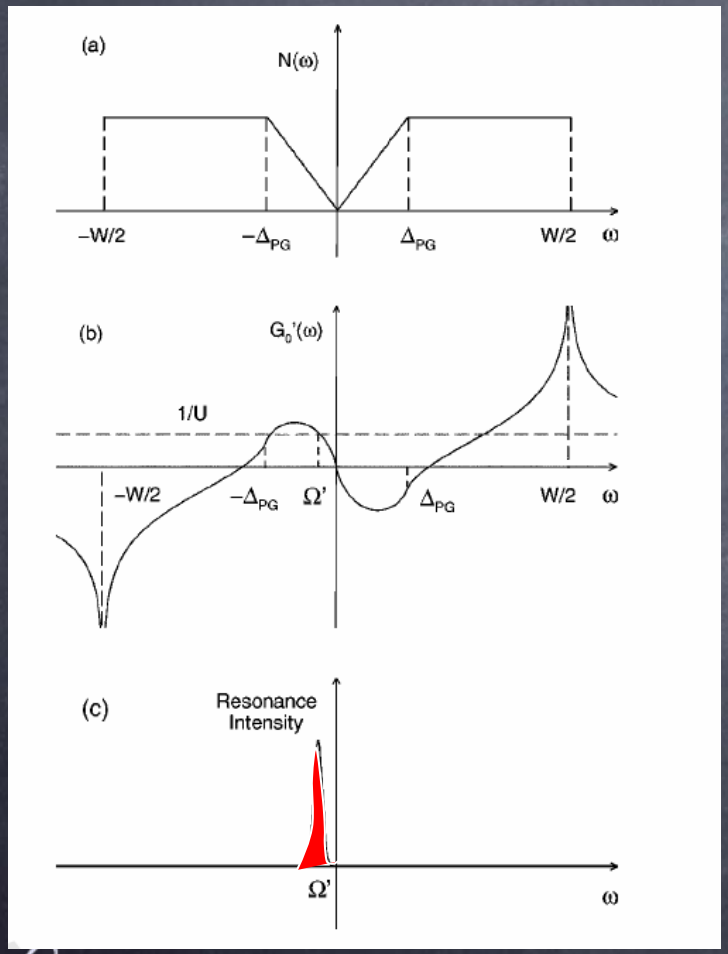
PHYSICAL REVIEW B, VOLUME 64, 0245XX

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-G0(Ω)U)

Hence the pole at G0(Ω) = 1/U

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

$$\Omega = \Omega' + i\Omega''$$

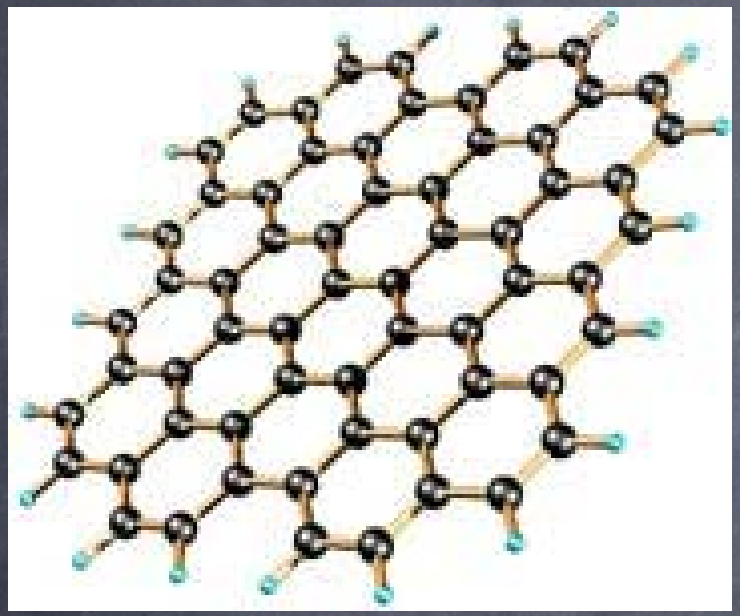
$$= -\frac{\Delta_{PG}}{2UN_0}\frac{1}{\ln|2UN_0|}\left[1 - \frac{1}{\ln|2UN_0|} + \frac{i\pi\ \mathrm{sgn}(U)}{2\ln|2UN_0|}\right],$$

H. Kruis et al, PRB 64, p 054501(2001); RMP 78, p373(06)

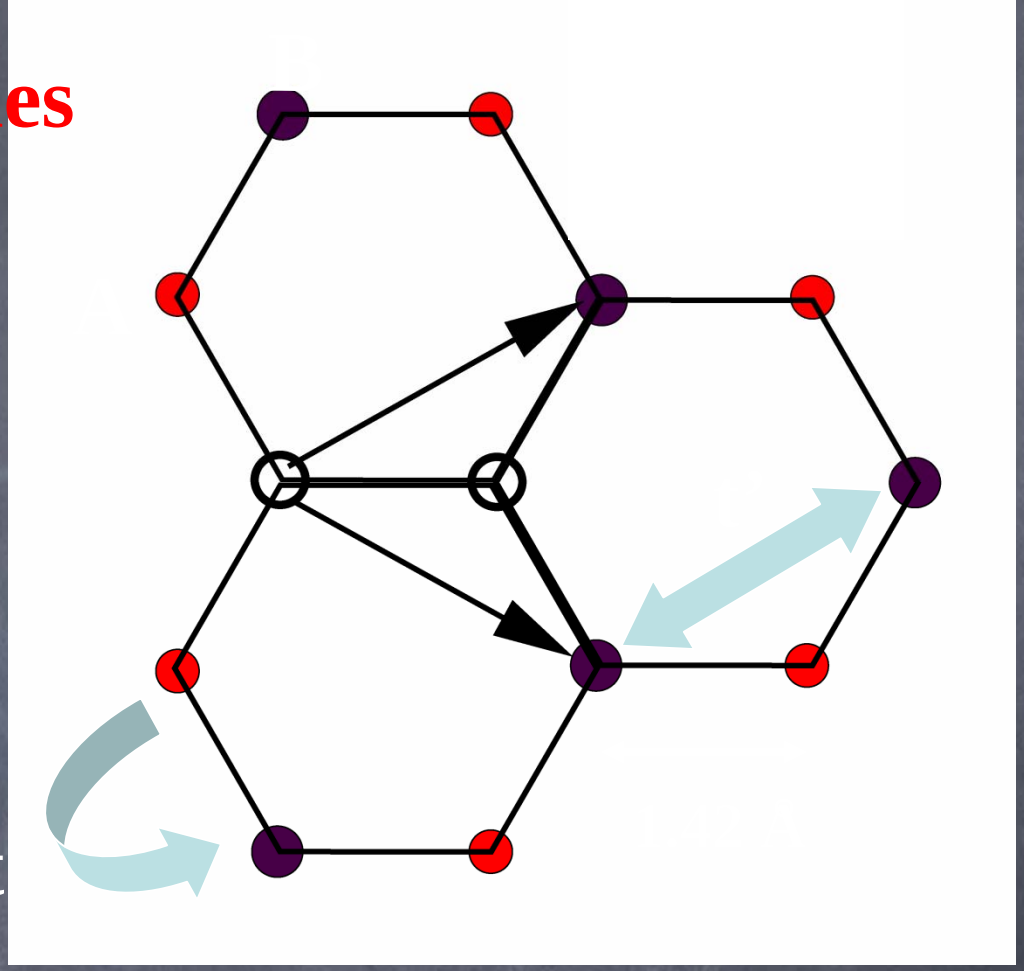
Electronic properties of graphene

- Repeating d-wave play book
- Proposal: to image local electronic properties, defects, dopants etc
- Role of impurities in superconducting graphene
- A. Geim “Graphene is a perfect system”

Electronic properties

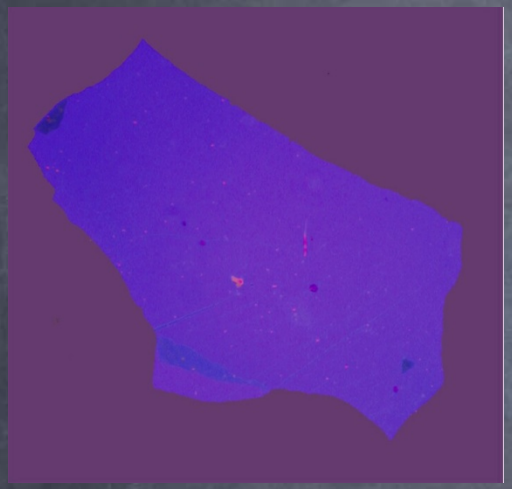


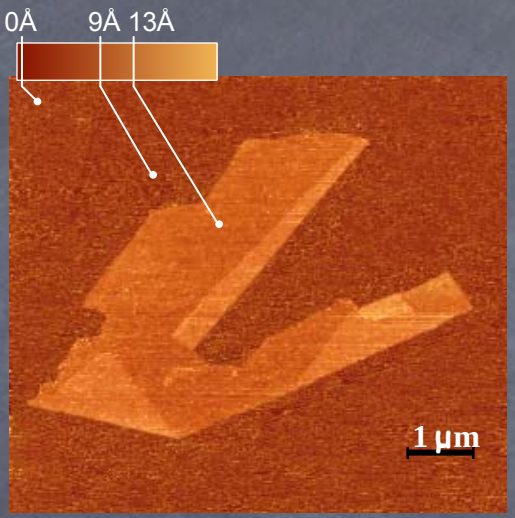
t

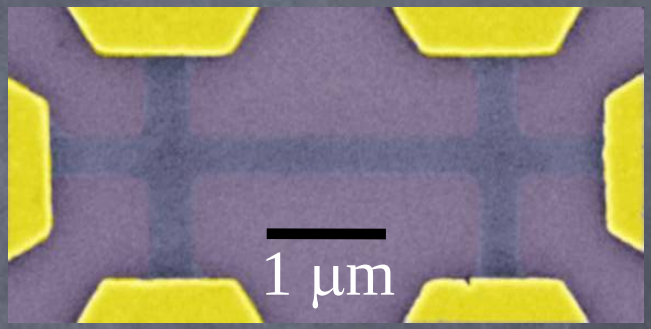


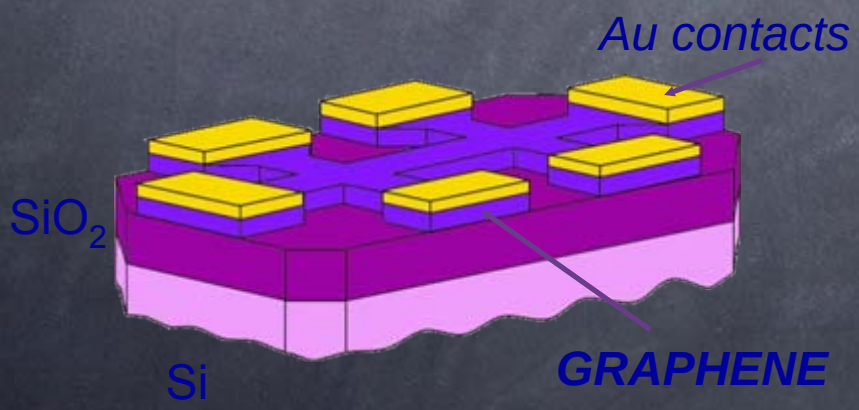
- 1 electron per π orbital: half-filled
- Kinetic energy: n.n. $t\ (\gamma_0) \sim 3$ eV
  n.n.n. $t' \sim 0.1$ eV

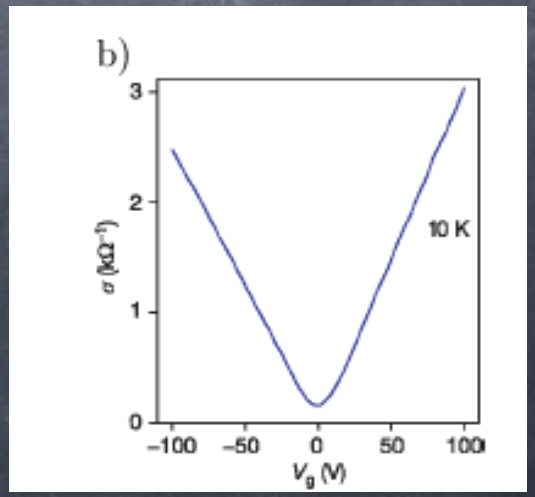
Robust samples:



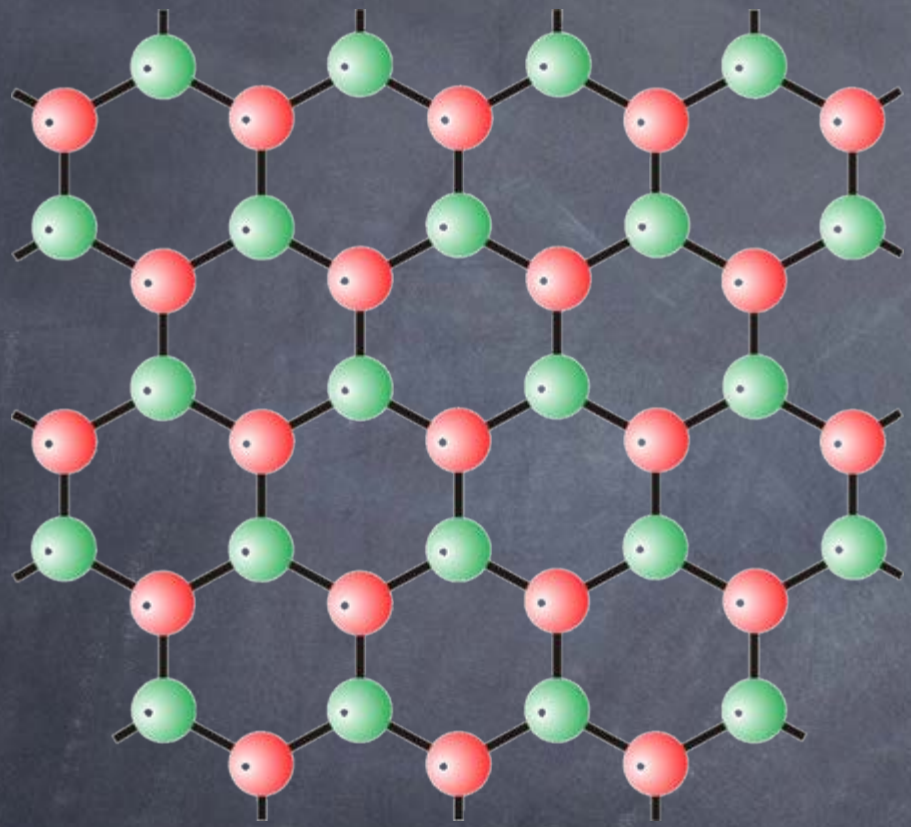


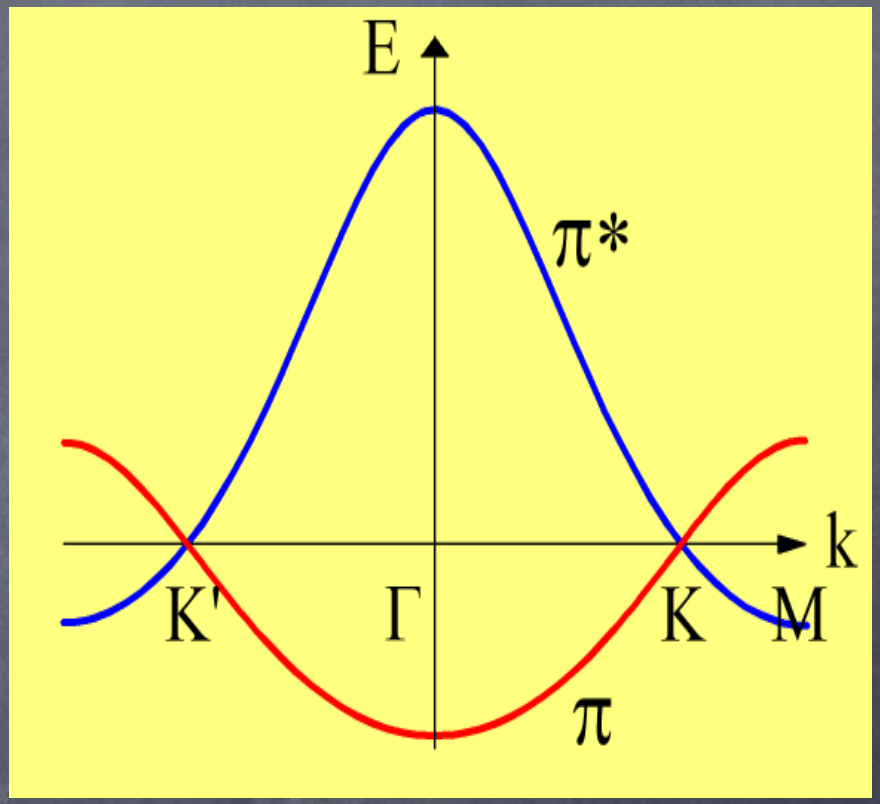






Chiral Fermions in Graphene





two sublattices → superposition of their wavefunctions → spinors (2 projections of pseudospin)

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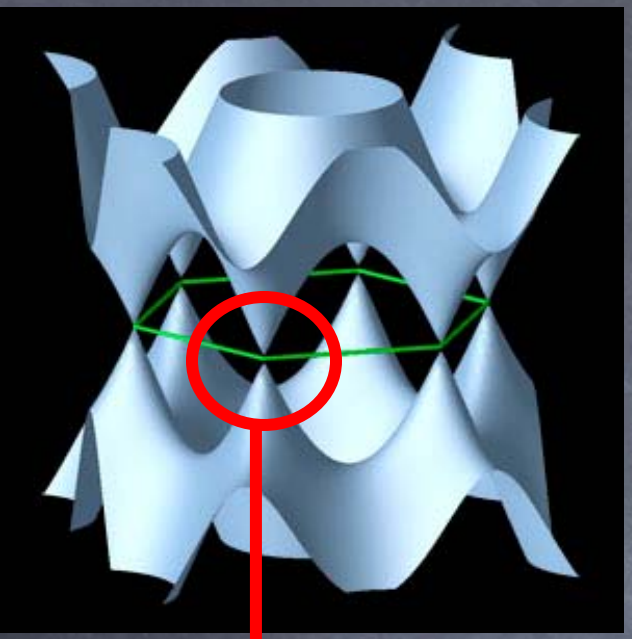
Dirac fermions in graphene

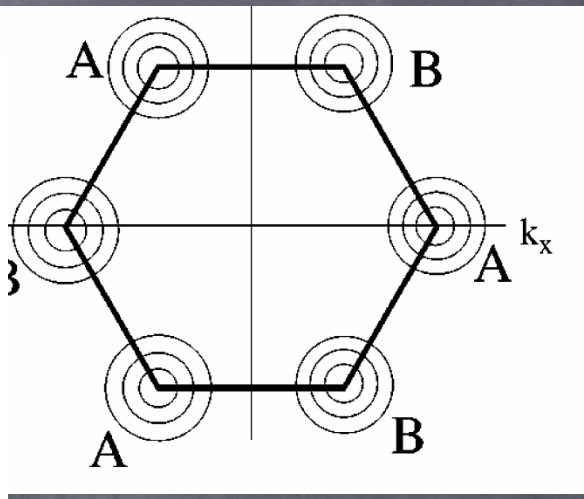


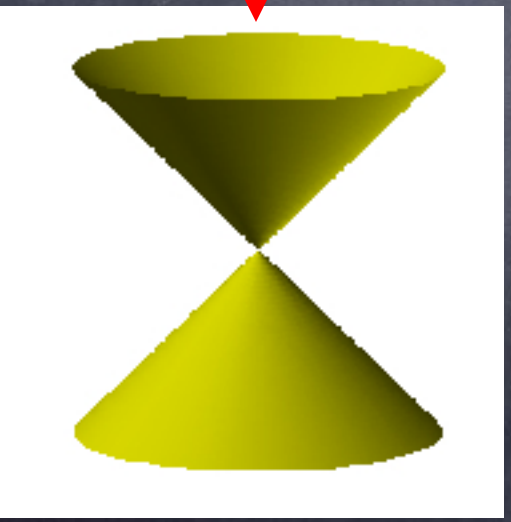
$$K.E. = \pm v\,|P|$$

$$K.E. = \pm\sqrt{m^2 v^4 + v^2 P^2}$$

$$m = 0$$

$$v \approx c/300$$



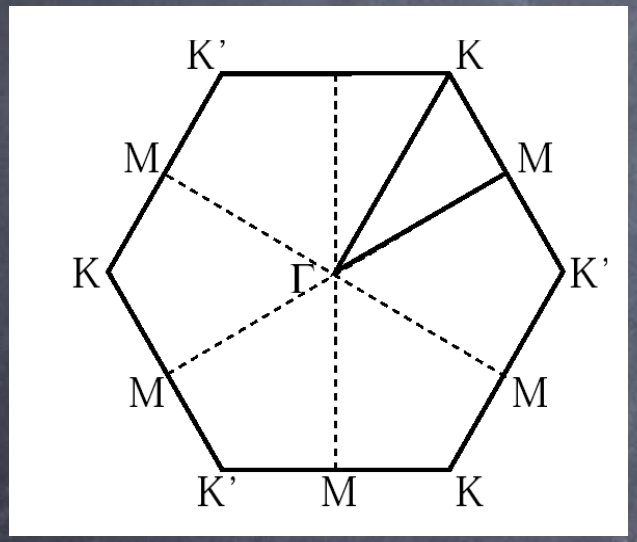


Low energy elementary excitations are two-dimensional Dirac-Fermions.

DOS is similar top d-wave SC because of nodal points

Dirac Fermions in Graphene

Brillouin zone

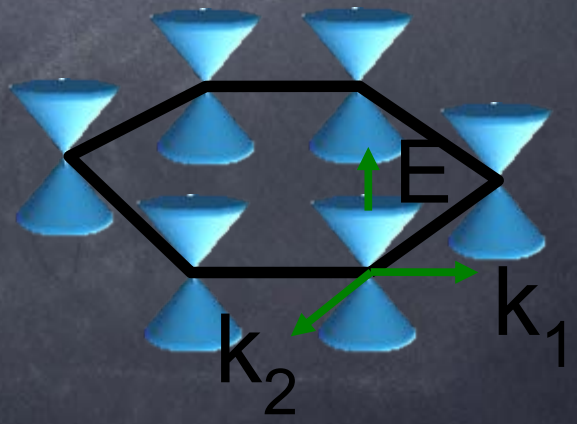


Tight binding model

$$H_k = \begin{pmatrix} 0 & \xi(k) \\ \xi^*(k) & 0 \end{pmatrix}$$

$$\xi(k) = t \sum_{j=1}^{3} e^{ik(b_j - b_1)}$$

$$H_{K\pm} = v_f \hbar (k_1 \sigma_1 \mp k_2 \sigma_2)$$



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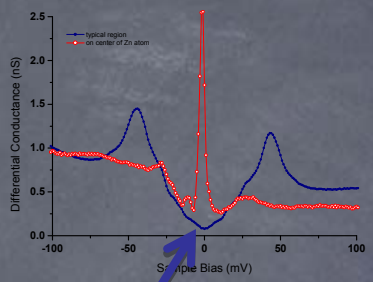
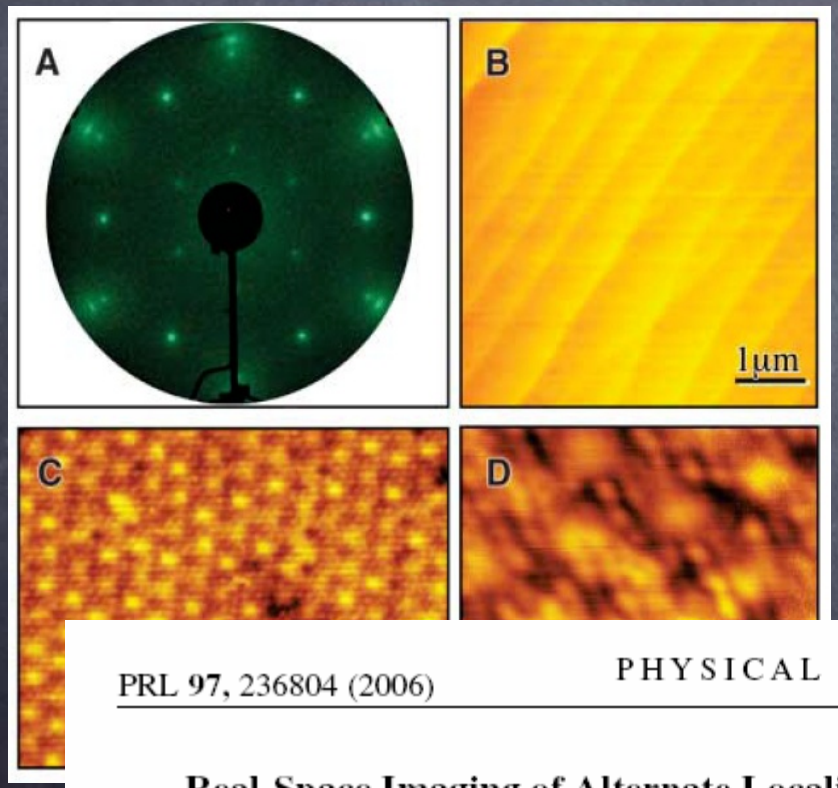
- Proposal: to image local electronic properties, defects, dopants etc
- Similarities with defects in d-wave
- Role of impurities in superconducting graphene
- A. Geim “Graphene is a perfect system”

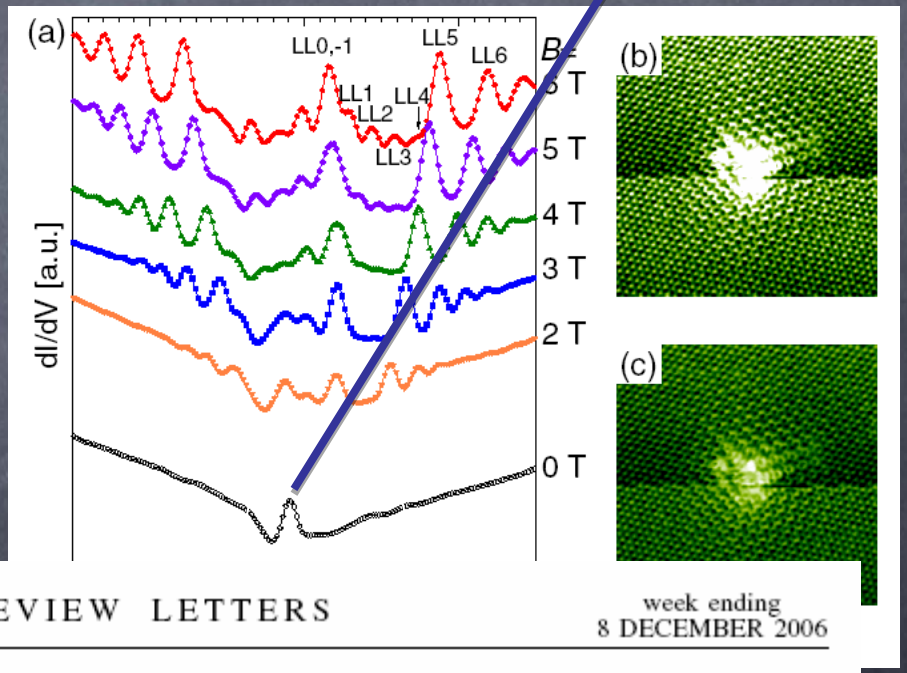
Graphene goes STM



Epitaxial Graphene

HOPG





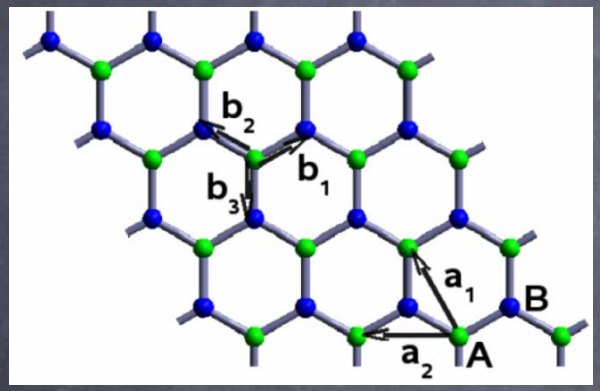
PRL 97, 236804 (2006) PHYSICAL REVIEW LETTERS week ending 8 DECEMBER 2006

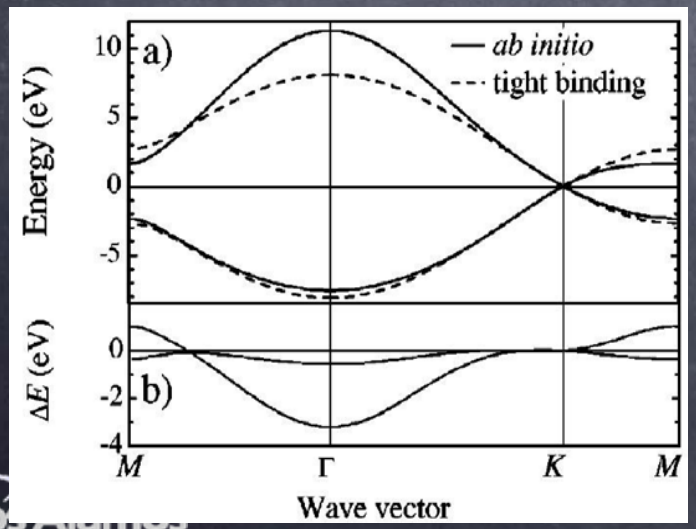
Real-Space Imaging of Alternate Localization and Extension of Quasi-Two-Dimensional Electronic States at Graphite Surfaces in Magnetic Fields

Y. Niimi,[1] H. Kambara,[1] T. Matsui,[1] D. Yoshioka,[2] and Hiroshi Fukuyama[1,*]

Modelling “dirty” graphene

Clean Graphene:





Tight binding model

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$$\xi(k) = t \sum_{j=1}^{3} e^{ik(b_j - b_1)}$$

Impurities:

$$V_{\text{imp}} = \sum_{ij} U_{ij} c_i^\dagger c_j$$

Fradkin, E. Critical-behavior of disordered degenerate semiconductors. II. Spectrum and transport properties in mean-field theory. *Phys. Rev. B* 33, 3263–3268 (1986).

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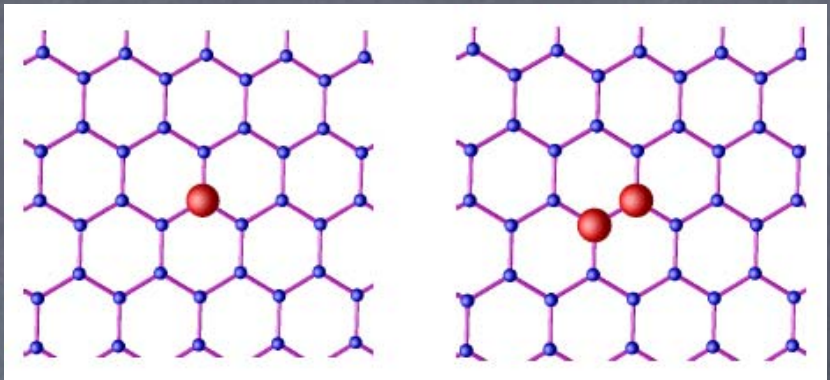
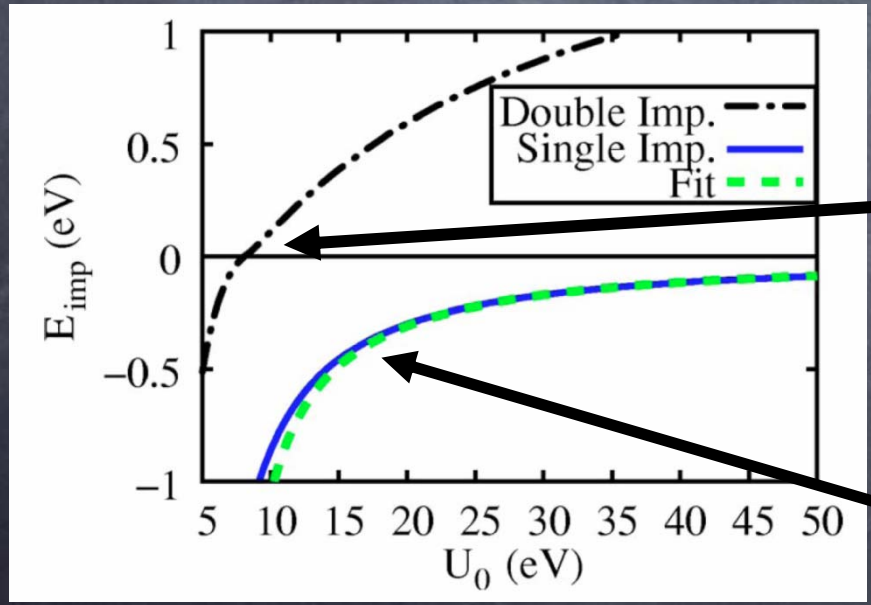
Single and double impurities

T. Wehling et. al., PRB 75, 125425 (2007)



Energy of impurity resonances:



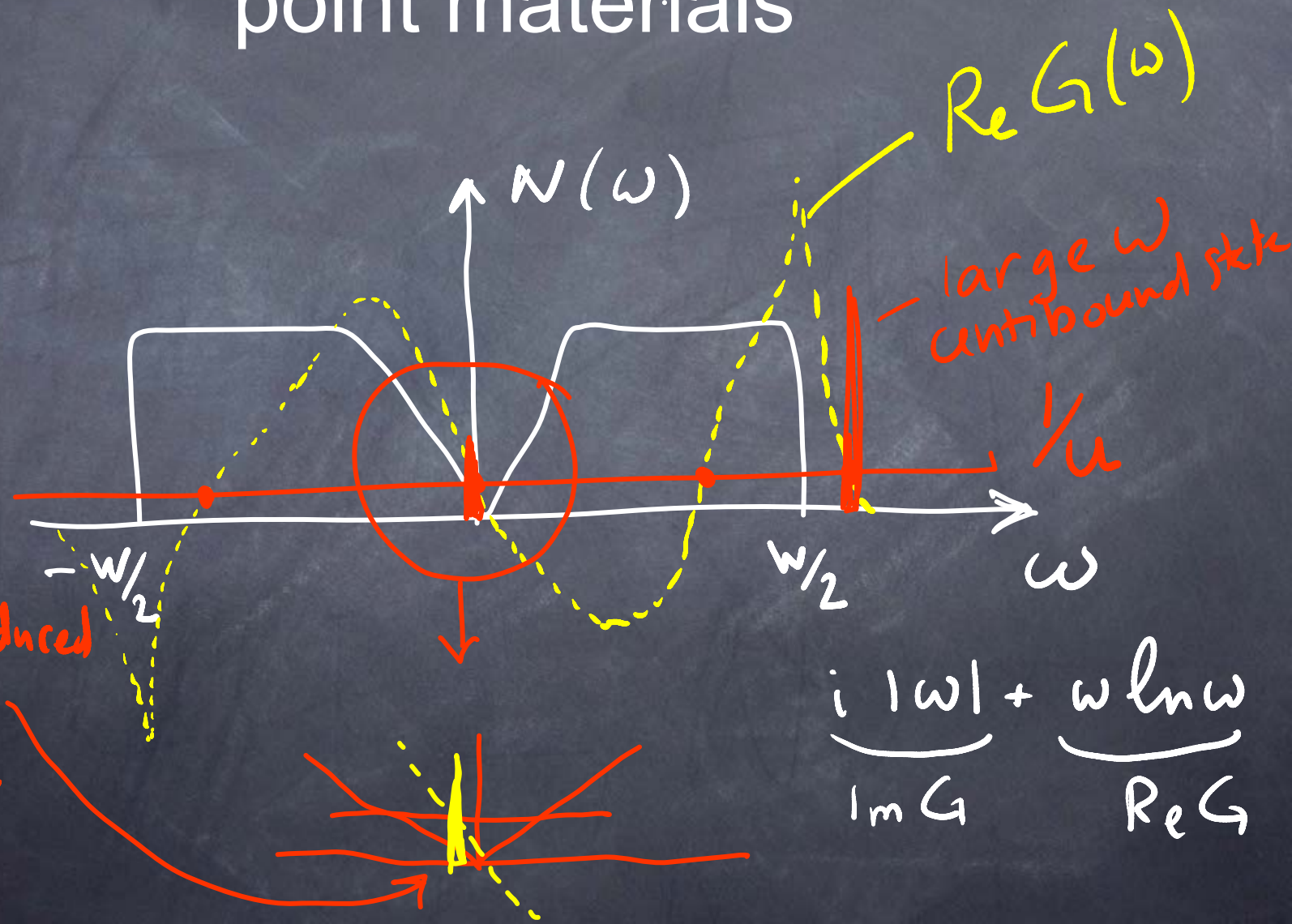
Double imp.:

$$U_0 - U_1 = 3t$$

Single imp.:

$$U_0 = \frac{W^2}{E_{imp} \ln \left| \frac{E_{imp}^2}{W^2 - E_{imp}^2} \right|}$$

Impurity states in ANY Dirac point materials



$$\underbrace{i\,|\omega|}_{\mathrm{Im}\,G} + \underbrace{\omega \ln \omega}_{\mathrm{Re}\,G}$$

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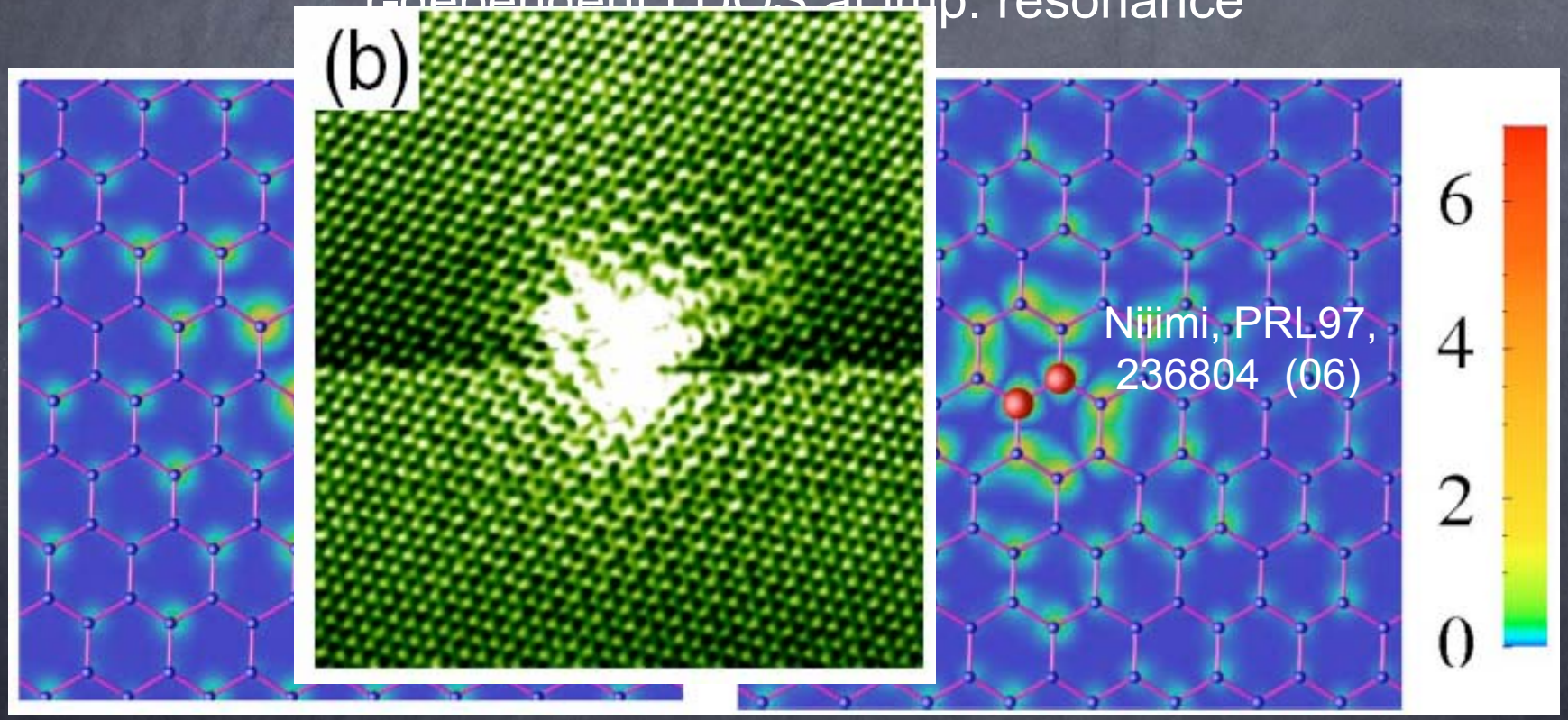
Real space signatures I

r-dependent LDOS at imp. resonance



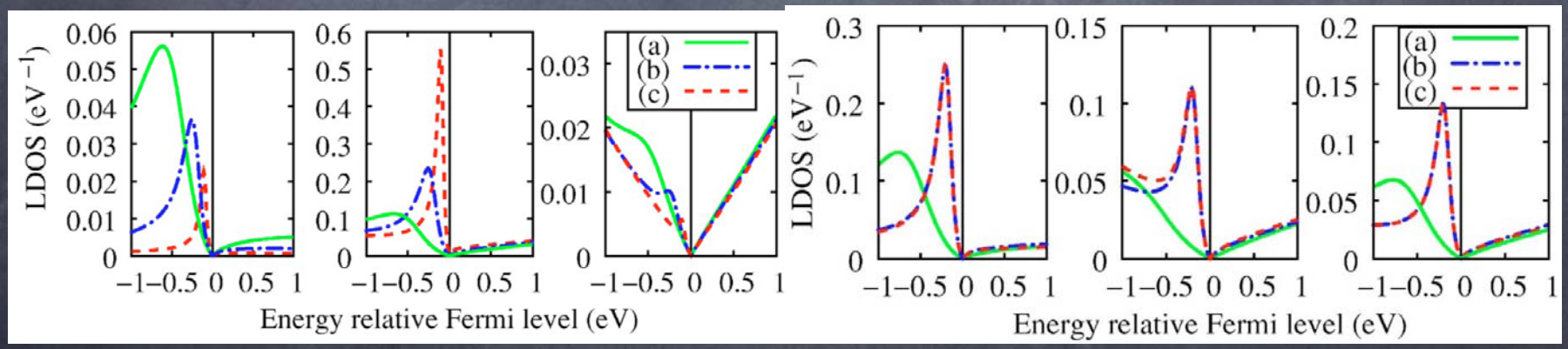
E_{imp}=0.1eV

Real space signatures II

Site projected LDOS

Single

Double



U_0=(a) 10 eV, (b) 20 eV, and (c) 40 eV

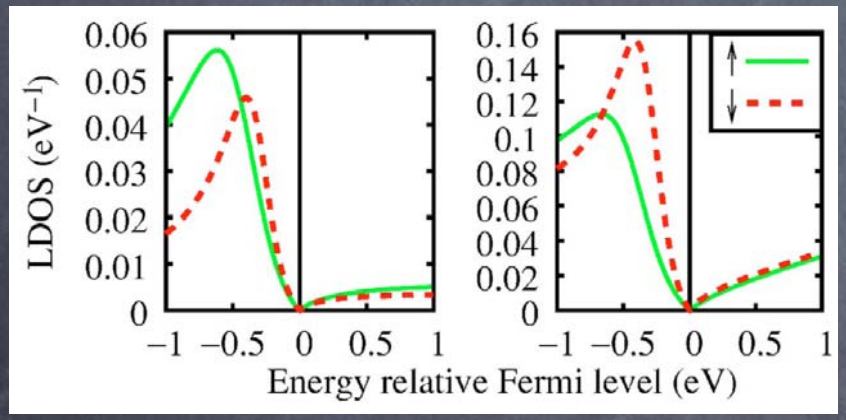
U_0=4 eV and U_1=(b) −2 eV

U_0=(a) 4 eV and (c) 6 eV

Magnetic Impurities

Possibility of fully spin-polarized imp. states

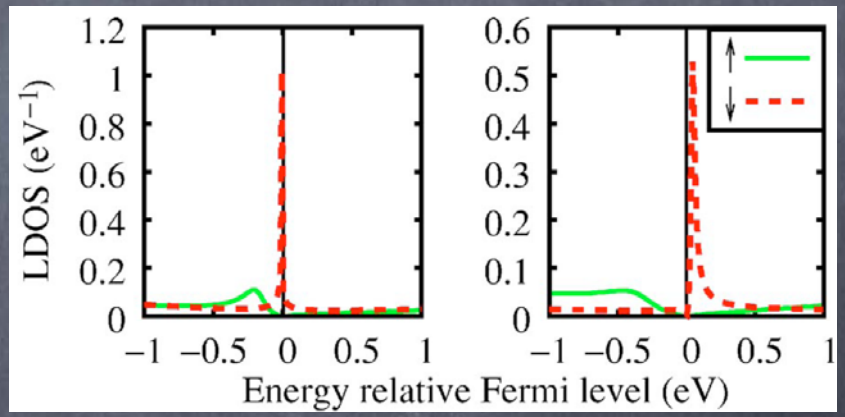
Single Impurity



$U_0 = 12$ eV and $J = 2$ eV

Imp. Site (left), NN (right)

Double Impurity



$U_0 = 5$ eV, $U_1 = -2$ eV, and $J = 1$ eV (left)

J=2eV (right)

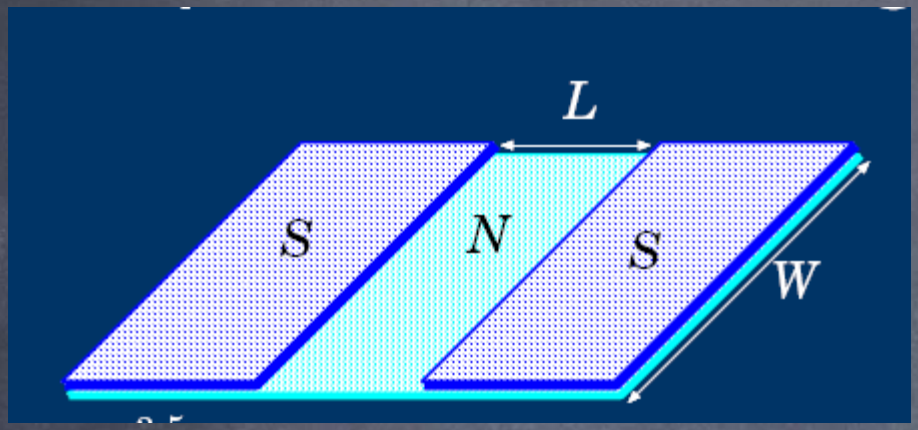
Power law decay of imp. states: δN~1/r ------> Long range exchange

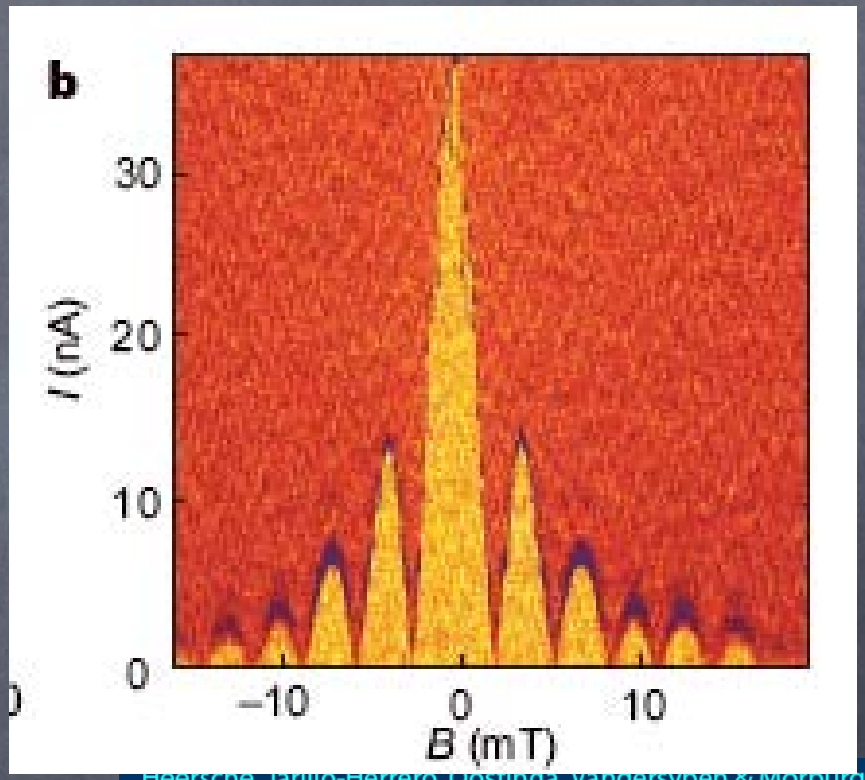
T. Wehling et. al., PRB 75, 125425 (2007)

Electronic properties of graphene

- Repeating d-wave play book
- Proposal: to image local electronic properties, defects, dopants etc
- Similarities with defects in d-wave
- Role of impurities in superconducting graphene
- A. Geim “Graphene is a perfect system”

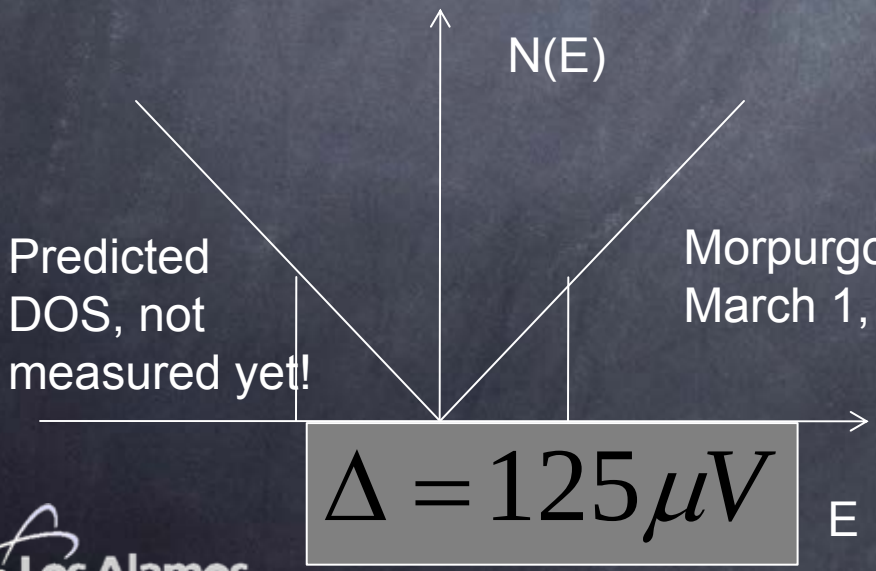
Superconducting graphene: proximity induced SC





Heersche, Jarillo-Herrero, Oostinga, Vandersypen & Morpurgo

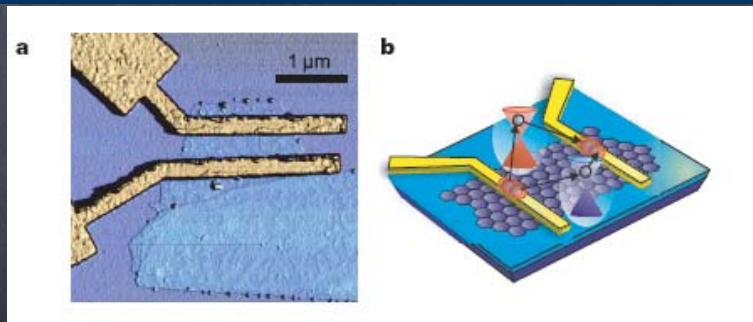
Titov & Beenakker



Predicted DOS, not measured yet!

Morpurgo, Nature, March 1, 2007

$$\Delta = 125 \mu V$$



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8*8 Bogoliubov de Gennes

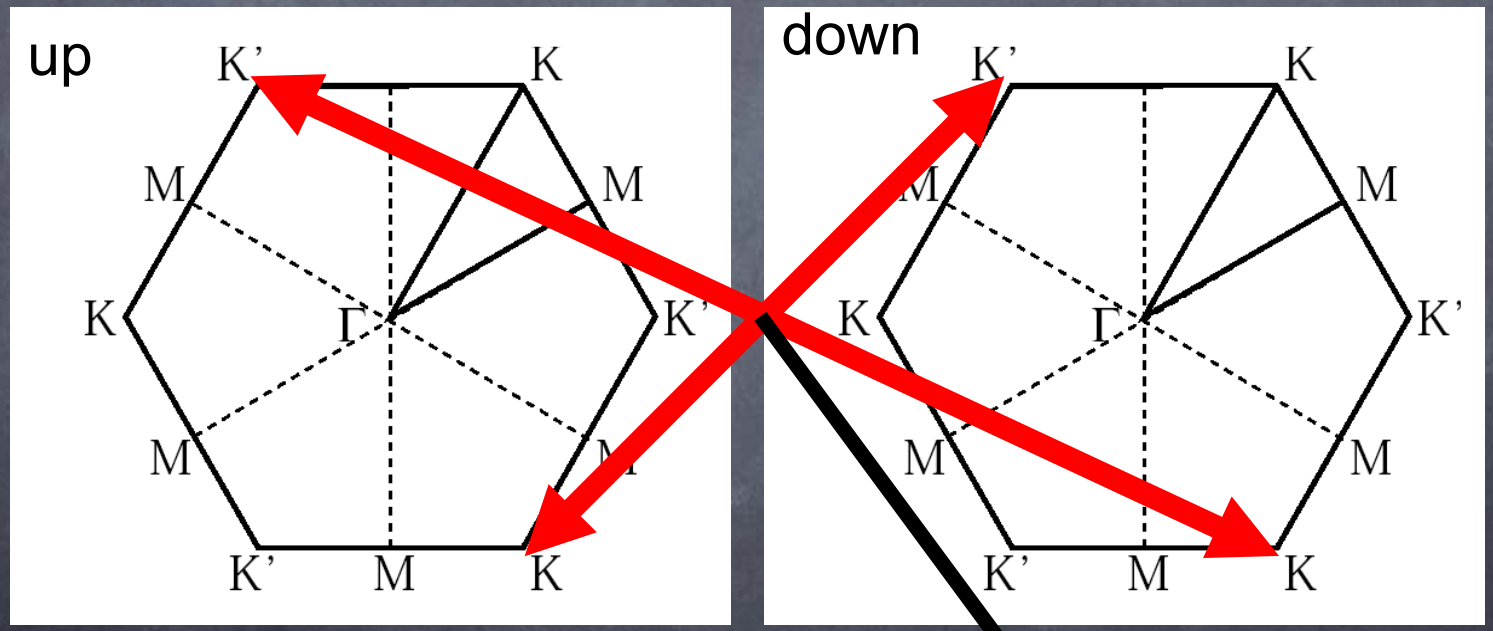
- One has to deal with 8 component spinors:

2 valley* 2sublattice*2(u, v) = 8 components

SC pairing in graphene really engages valleys in a nontrivial way

Superconducting graphene

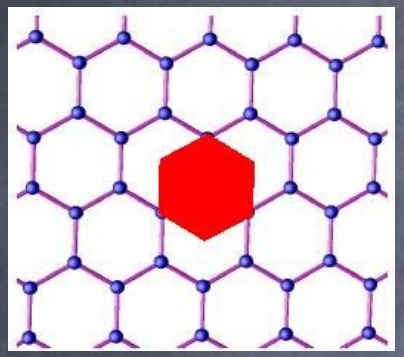
Proximity effect -> SC gap



$$H = -i\hbar v_f(\partial_1\sigma_1\otimes\tau_0 - \partial_2\sigma_2\otimes\tau_3)\otimes\Lambda_0 + \Delta\sigma_3\otimes\tau_0\otimes\Lambda_1$$

(C. Beenakker, PRL 97, 067007 (2006))

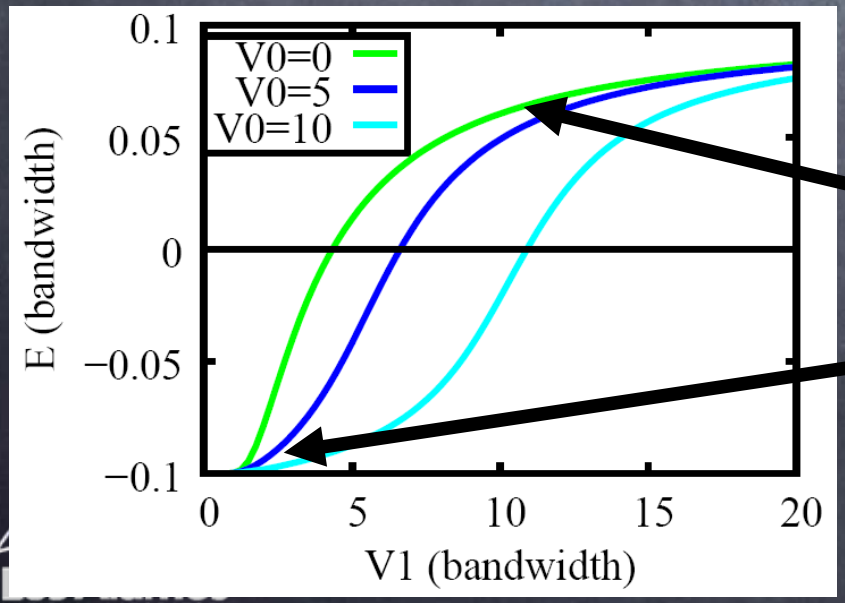
Impurities in SC graphene



Scalar (cell averaged) impurity

$$V_0\sigma_0 \otimes \tau_0 \otimes \Lambda_3 + V_1\sigma_0 \otimes \tau_0 \otimes \Lambda_0$$

Energy E of impurity state as function of potential V_1



Asymptotics

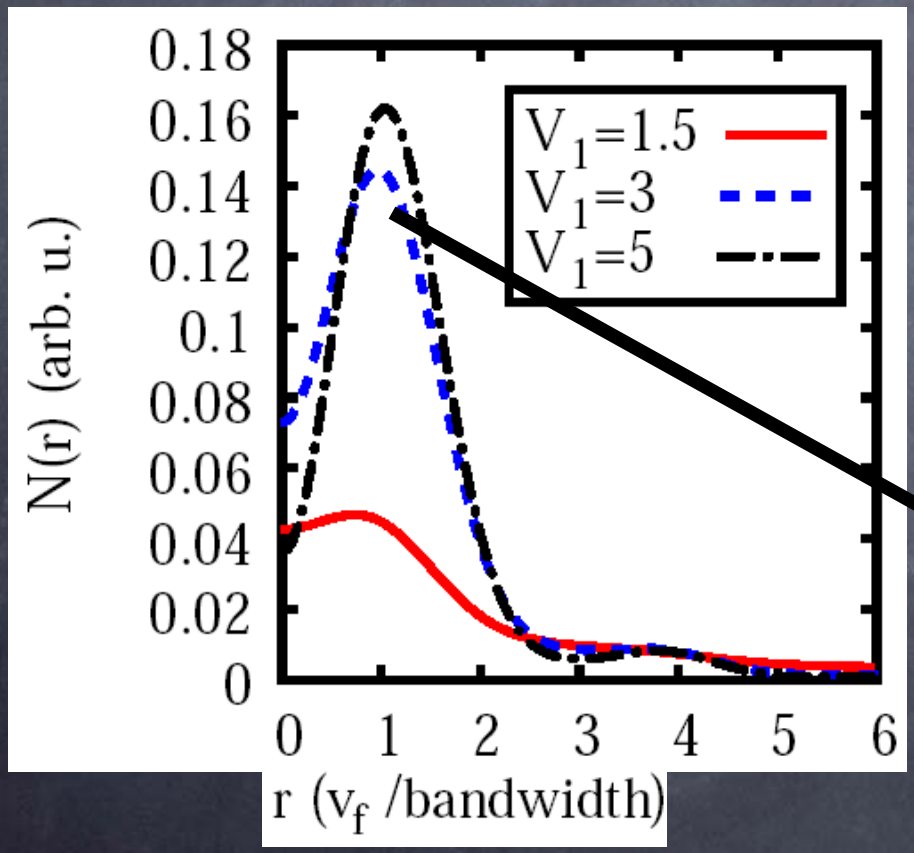
$$\delta\omega = -\frac{2\Lambda^2}{V_1 \ln\left(\frac{2\Delta}{V_1}\right)}$$

$$\delta\omega = \frac{\Lambda^2}{2\Delta} e^{-\Lambda^2/(\Delta V_1)}$$

(gap = bandwidth / 10)

Real space fingerprint of impurities

Density of intra gap imp. states



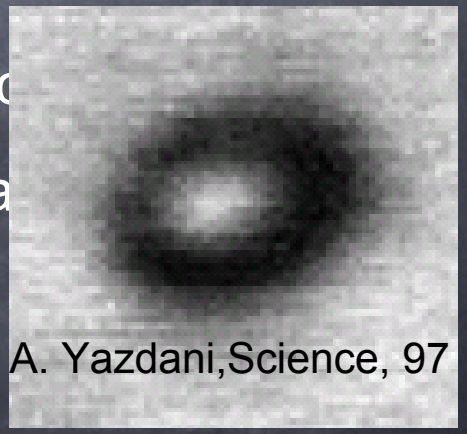
(gap = bandwidth/10)

Asymptotic decay

$$r^{-1} e^{-2r\sqrt{\Delta^2-\omega_0^2}/v_f}$$

Ringstruc

at consta



A. Yazdani,Science, 97

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Similarities of HighTc with Graphene II: nanoscale inhomogeneity

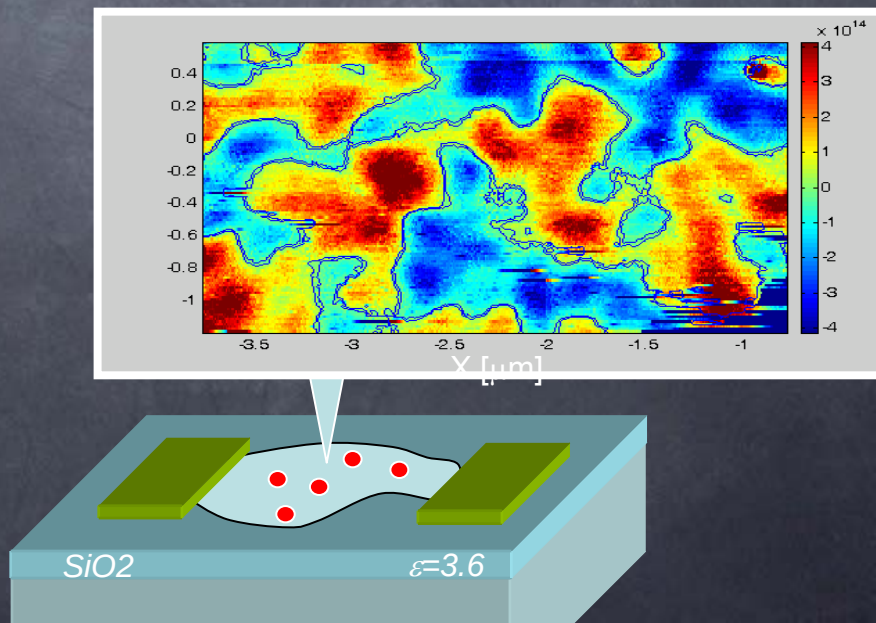
- Dirac spectrum of qp
- Micron mean free path, very clean
- Strong electronic (~ 50% charge)

inhomogeneity that coexists with

- the long mfp for low energy electrons

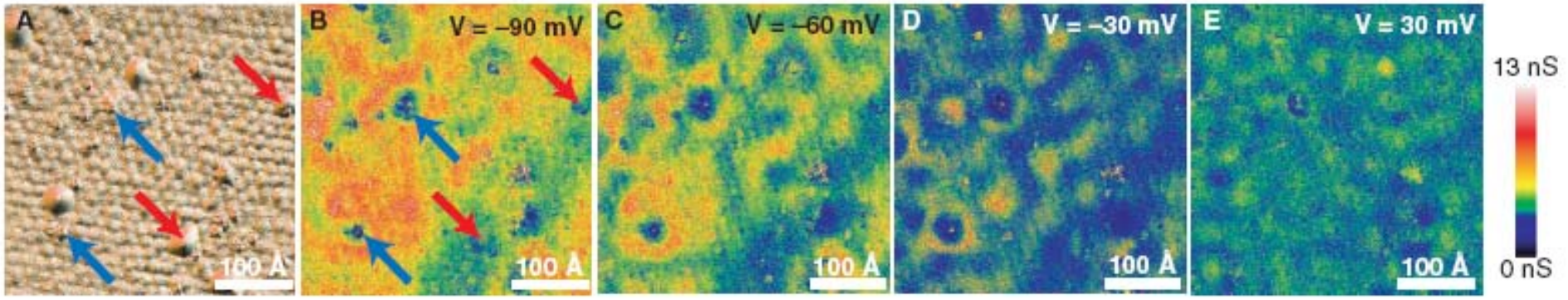
A.Yacobi

STM confirms similar inhomogeneity
Stroscio et al, E. Andrei et al



STM data by Stroscio

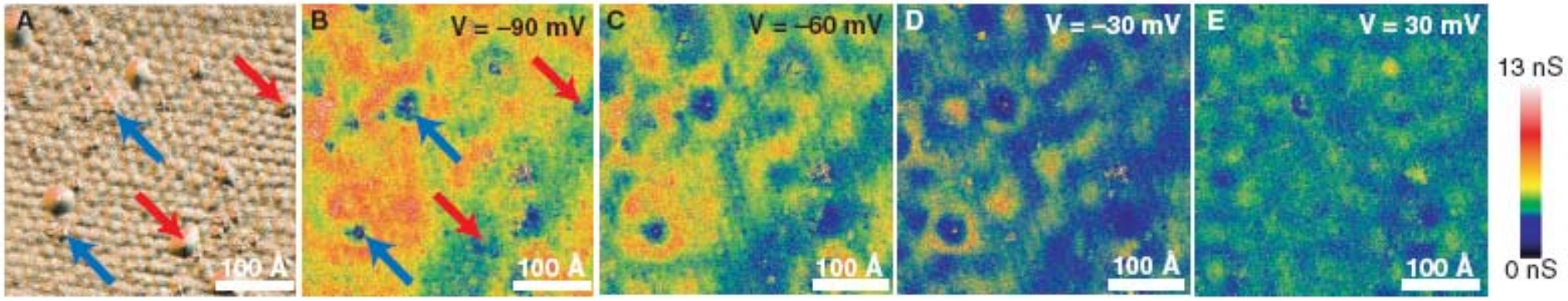
Science, v 317, p 219, 2007



Patterns are more homogeneous at lower doping

STM data by Stroscio

Science, v 317, p 219, 2007

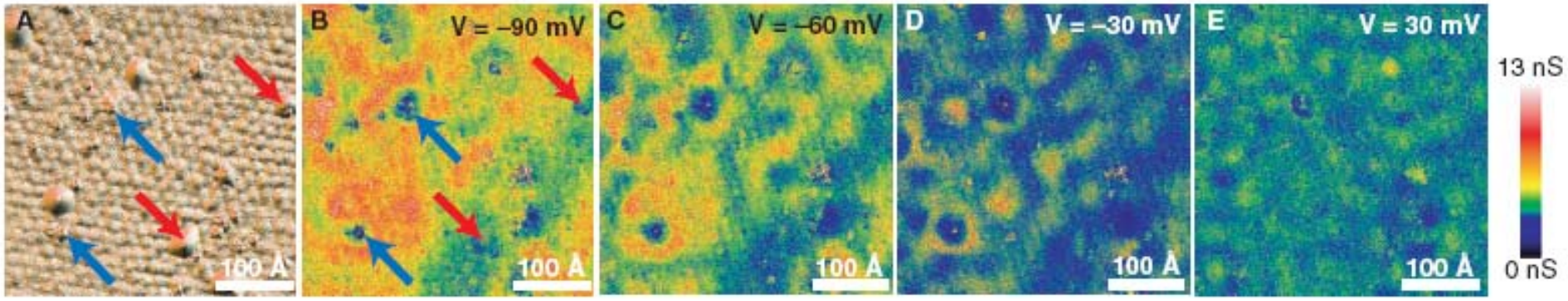


Patterns are more homogeneous at lower doping

low energy (DC states)

STM data by Stroscio

Science, v 317, p 219, 2007



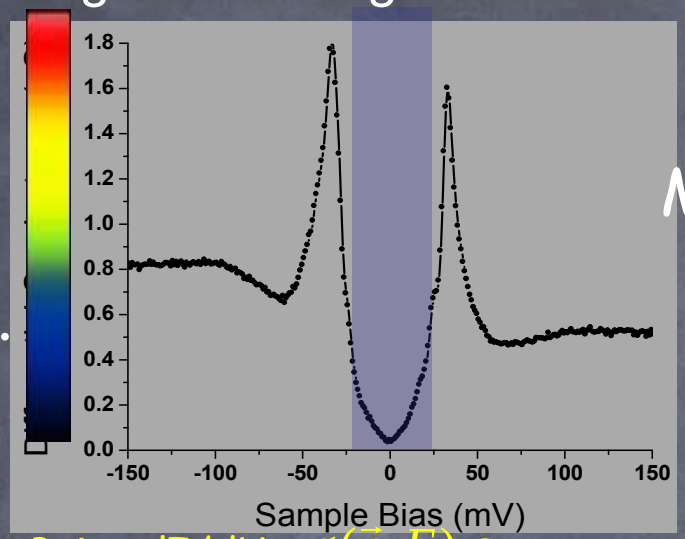
Patterns are more homogeneous at lower doping

low energy (DC states)

Inhomogeneity as an energy dependent property: low energies-homogeneous
Higher energies inhomogeneous

(1)

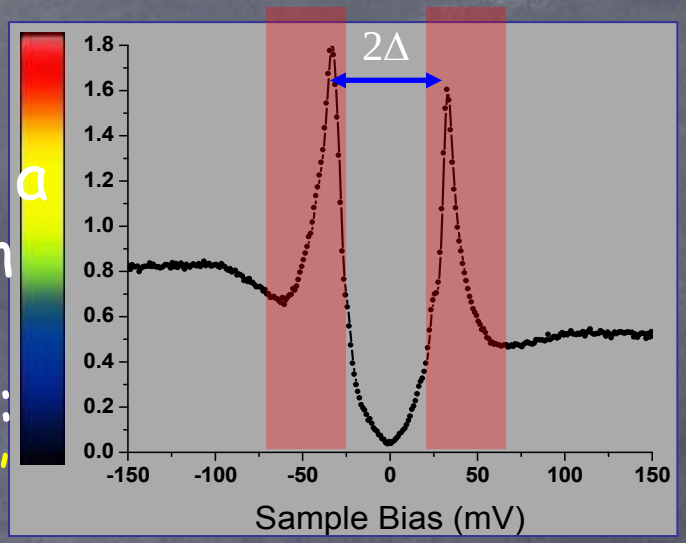
Map LDOS as E->0.



Point dI/dV $\equiv g(\vec{r},E)$ Spectrum

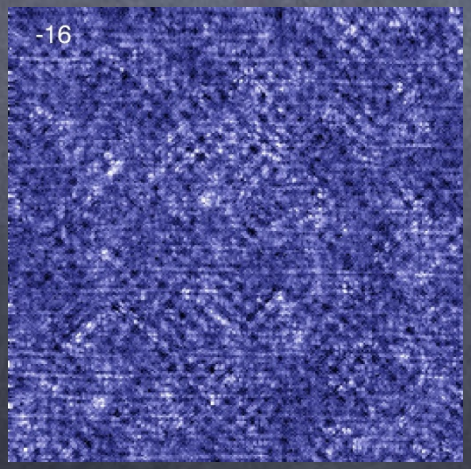
(2)

Map Δ as a function of location: 'gapmap'



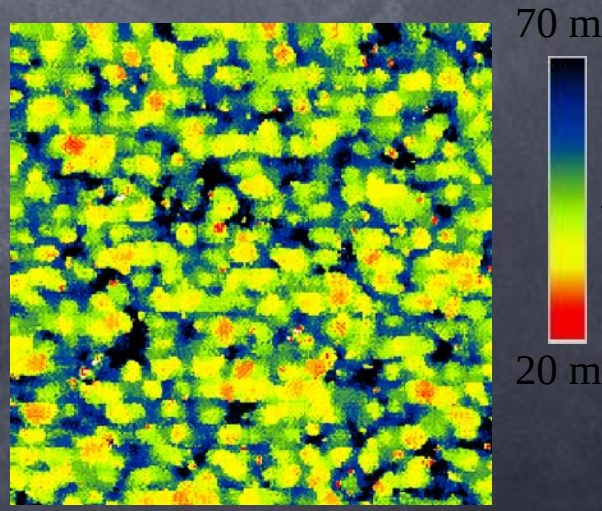
Point dI/dV $\equiv g(\vec{r},E)$ Spectrum

Weak, dispersive, LDOS modulations for all E<0.5Δ



$g(\vec{r},E=-16\,meV)$

Intense nanoscale disorder seen in 'gapmap'



Long mean free path can coexist with inhomogeneity $\Delta(\vec{r})$

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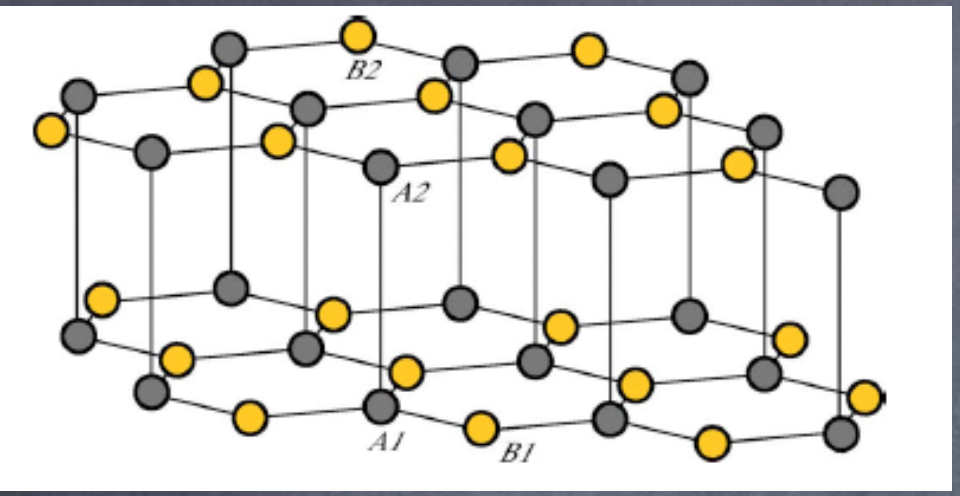
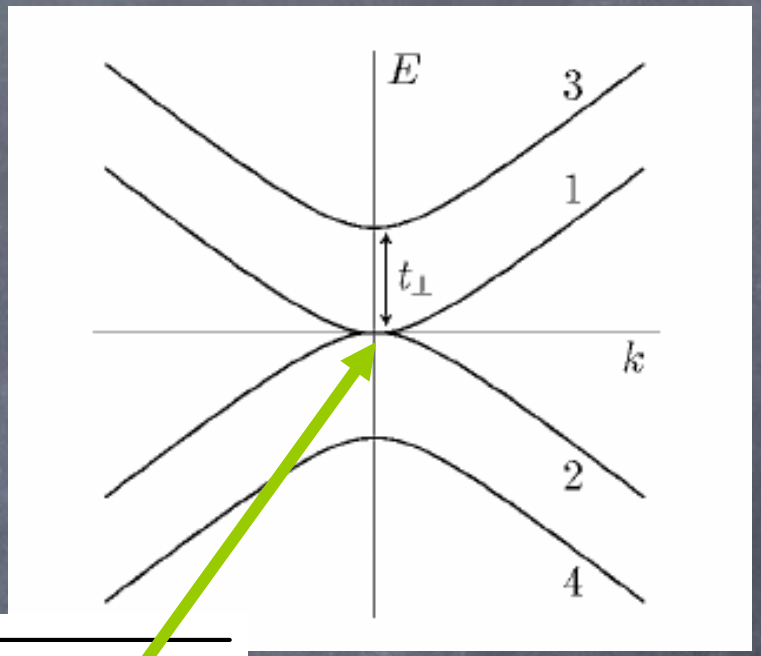
Nature 413, 282 (2001), *Nature 415*, 412 (2002)

Bilayer electronic structure





$$E_{1,2,3,4} = \pm t_\perp / 2 \pm \sqrt{(t_\perp / 2)^2 + p^2}$$

Kissing point that is highly susspectible to the gap opening: possible states:
Ferrimagnetisim (Stoner), AC Neto et al
Wigner Crystal/Commensurate CDW: AVB, H. Dahal et al.

Negative compressibility and Charge ordering in bilayer graphene

- CDW instability in Bilayer graphene due to parabolic “kissing point”
- Negative charge compressibility, A H C Neto etal, H. Dahal etal.

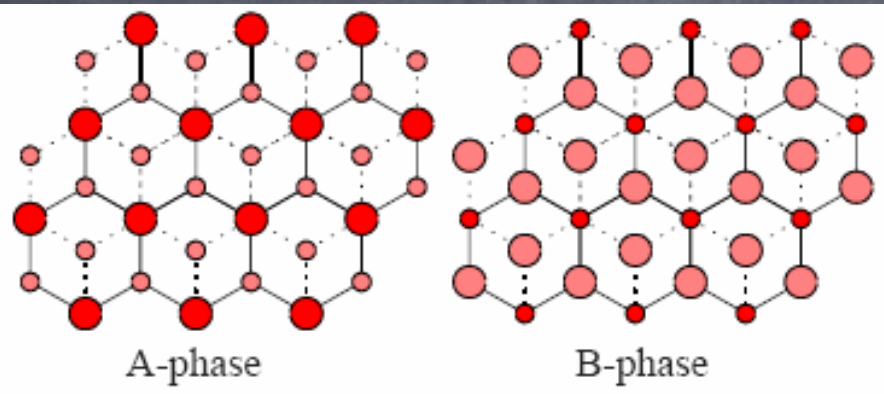
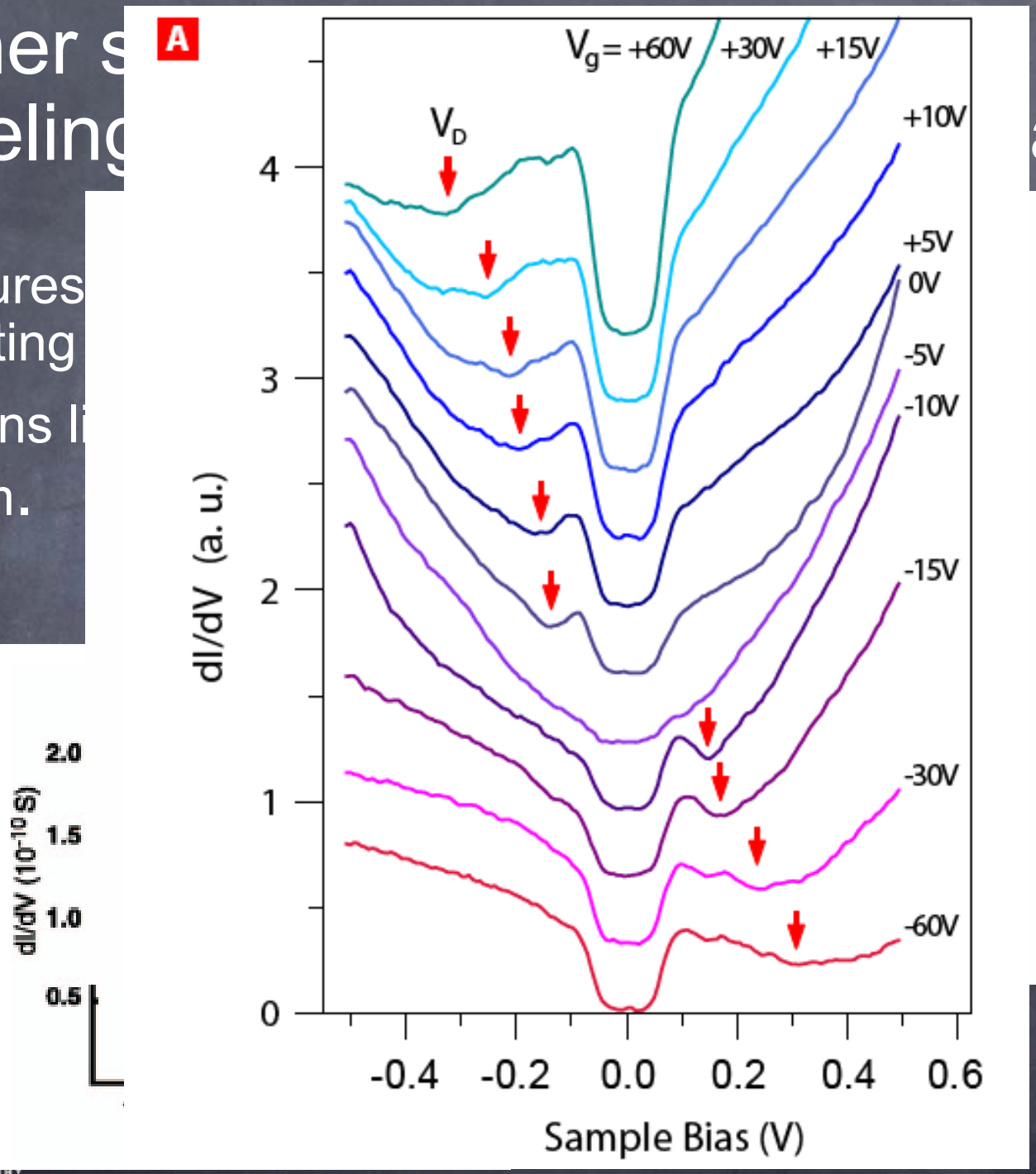


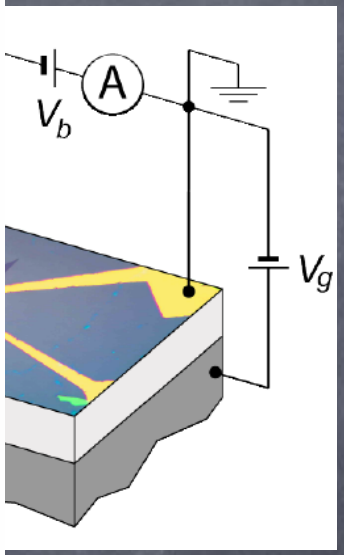
FIG. 2: (Color online) Charge distribution in ordered state of bilayer graphene is shown. Larger circles correspond to larger charge density on lattice sites. The sites connected by solid

H. Dahal, submitted 2007
arXiv:0706.1689

Another s
Tunneling aterials

- Signatures
interacting
- Fermions li
vaccum.





Crommie group
, UC Berkeley
submitted

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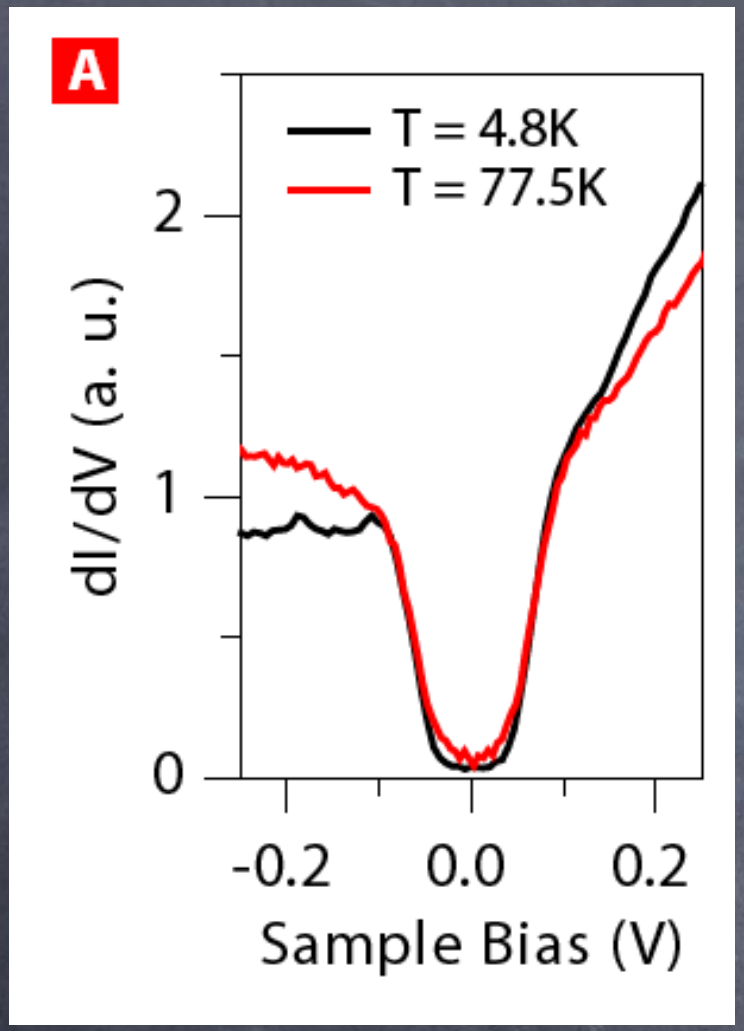
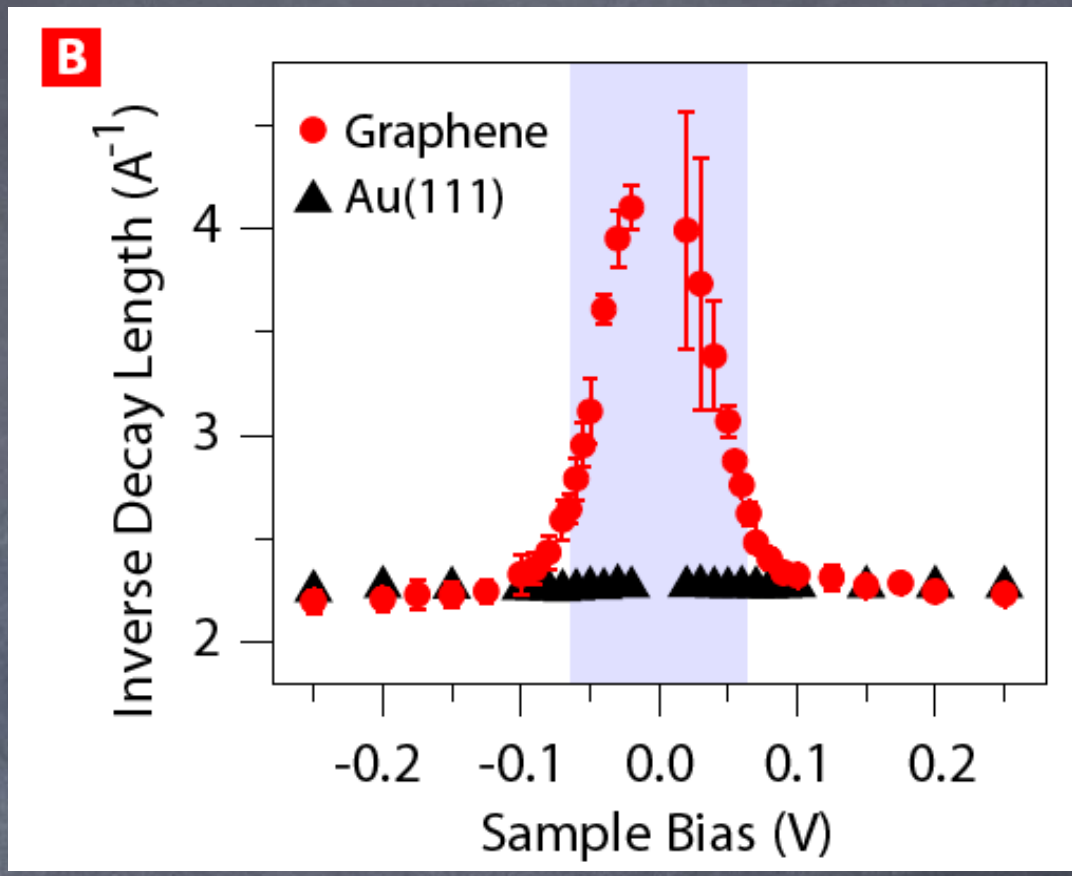


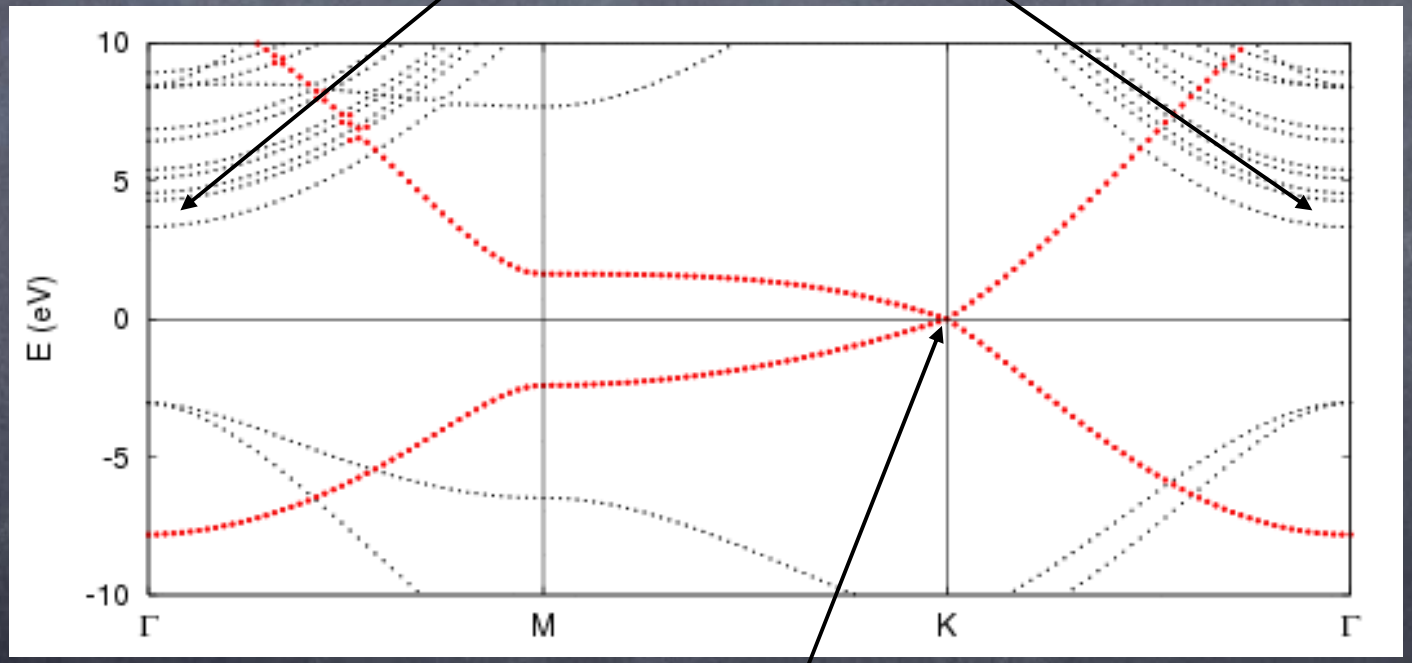


What is going on? Why we do not see a Dirac cone?
Conjecture:
Inelastic effect due to electron-phonon coupling. Phonon energy is 60 meV
And momentum that connects Gamma and K point.

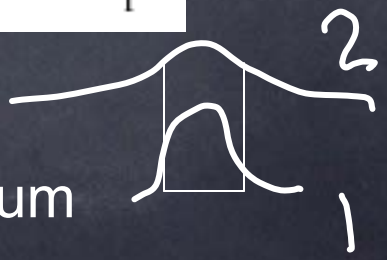
WEHLING et al, cond mat April 2008

Band structure and tunneling

Quasi free electron states (2)
$k_{||}=0$



Dirac electrons (1)



$k_{||}=1.7Å^{-1}$ ==> fast decay in the vacuum

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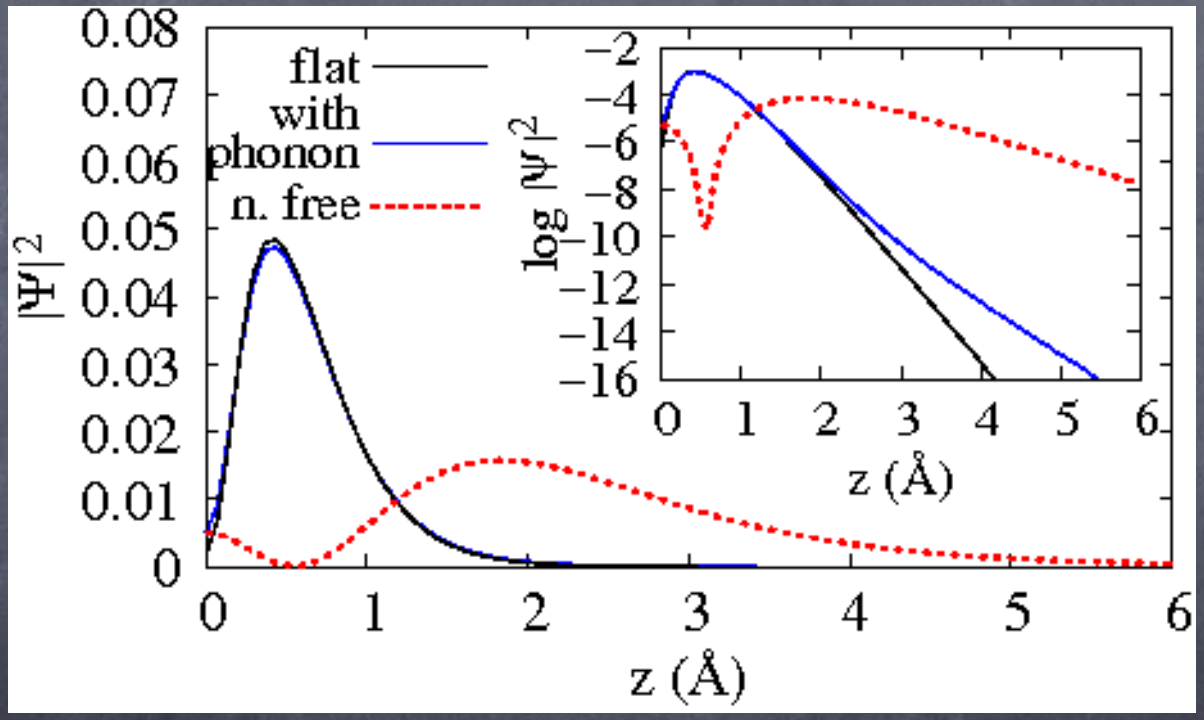
WEHLING et al, cond mat April 2008

Vacuum decay of graphene wave functions



Decay constants: π-band for flat graphene: $4 Å^{-1}$

π-band with frozen phonon: $2 Å^{-1}$

nearly free electron state: $1 Å^{-1}$

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WEHLING et al, cond mat April 2008

Electron phonon interaction

Scattering between the Dirac states and the quasi free states

$$V = \lambda \sum_{q,k} (d^\dagger_{k+q} c_q + c^\dagger_{k+q} d_q)(a_k + a^\dagger_{-k})$$

→ Non zero DOS $N_\sigma(E)$ in quasi free channel for $|E|>\omega_a$

Tunnelling through quasi free states greatly enhanced:

$$\mathrm{d}I/\mathrm{d}U \sim |\Psi_\sigma|^2 N_\sigma(E) + |\Psi_\pi|^2 N_\pi(E)$$

with

$$|\Psi_\sigma/\Psi_\pi|^2 \propto e^{1.9\text{Å}^{-1} z}$$ → 10^4 for z = 5 Å

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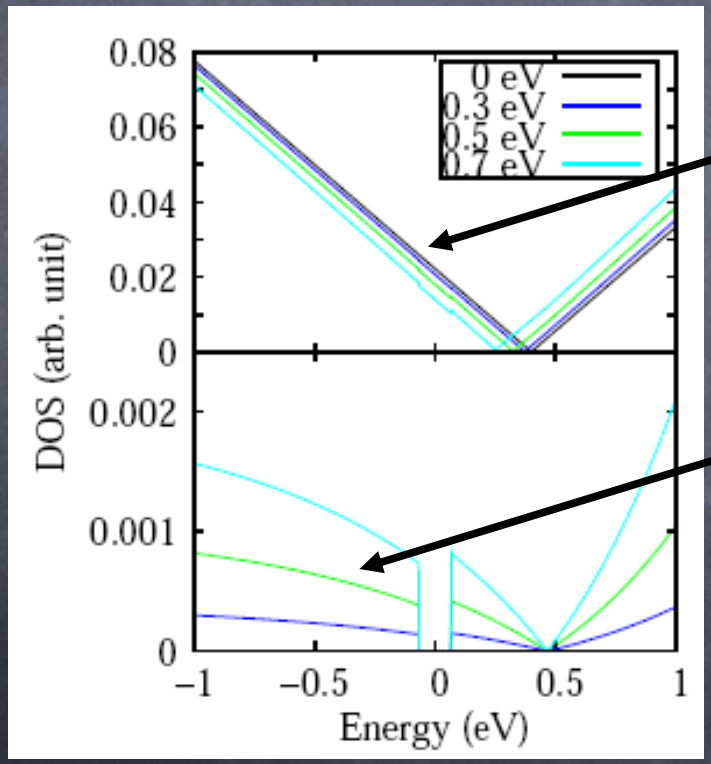
WEHLING et al, cond mat April 2008

Tunnelling vs. total DOS

Density of states for different coupling constants (λ=0-0.7eV)



total DOS virtually unaffected

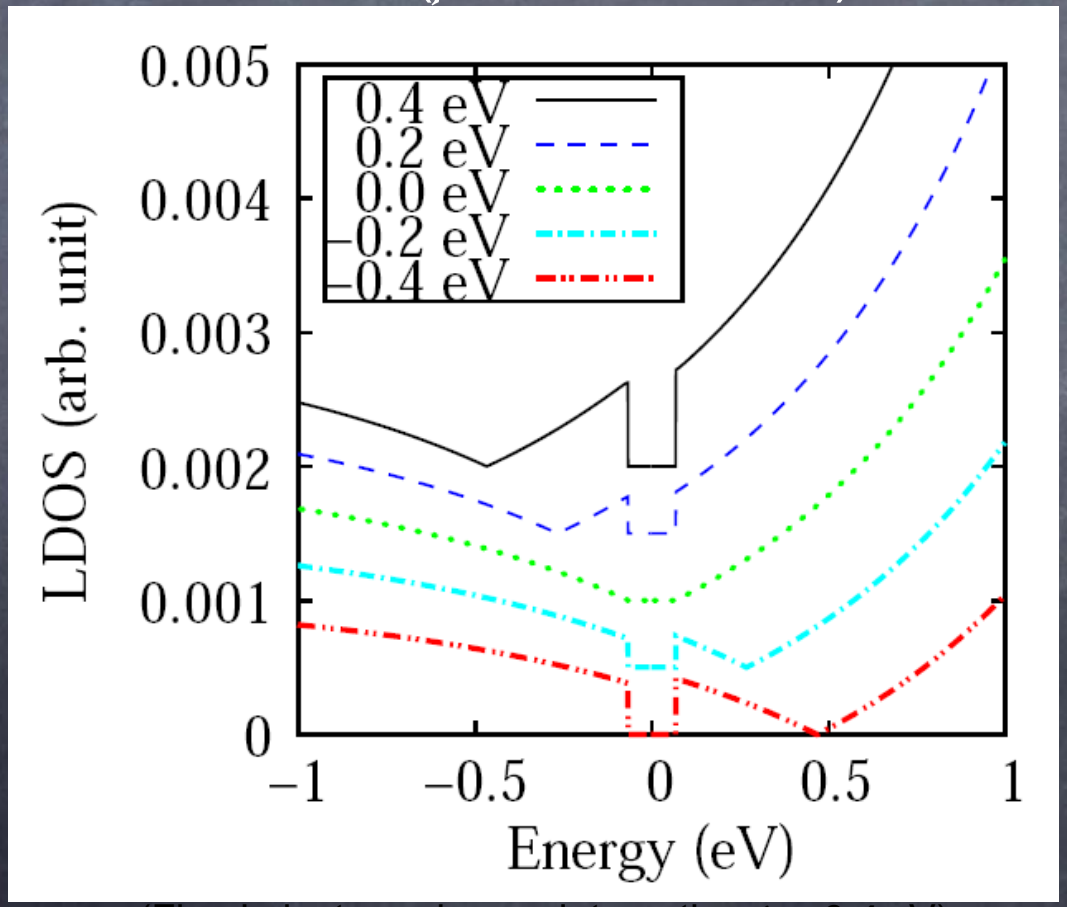
nearly free states' DOS

(Fixed doping. Chemical potential μ = *0.4* eV)

WEHLING et al, cond mat April 2008

STS for different amounts of doping

DOS of quasi free electron channel for different chemical potentials (μ=-0.4...+0.4eV)



(Fixed electron phonon interaction λ = *0.4* eV)

Conclusion and future directions

- Strong cimilarities across classes: Dirac fermions as one realization of correlated and low dimensional electronics.
- Growing list of materials with similar properties:
- Similar physics of Impurity states in high-Tc and in Graphene, normal and superconducting.
- Expect new physics at nanoscale that has no precedent in “nicely behaving” bulk materials.
- Electronic inhomogeneity and impurity states is a reality in graphene inspite of micron mfp. Similar story to highTc
- One needs adequate tools both theoretical and experimental to address inhomogeneity, frustration and local correlations.