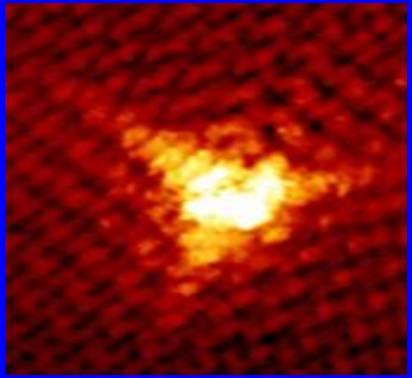
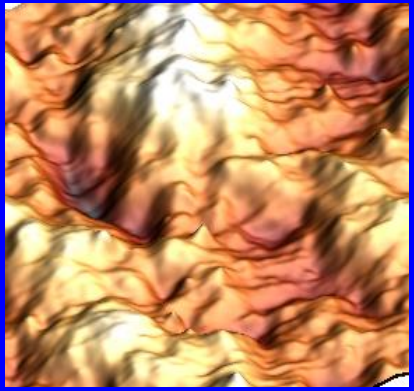
Interaction of Dirac electrons with spins and point charges

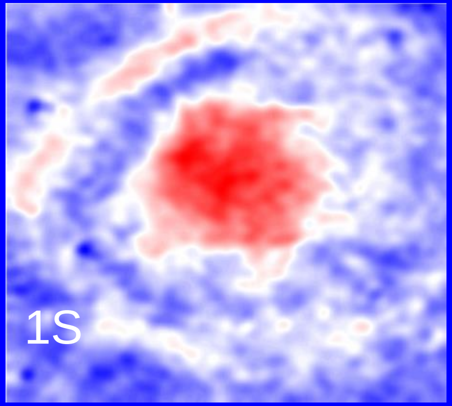
Vacancies in graphene



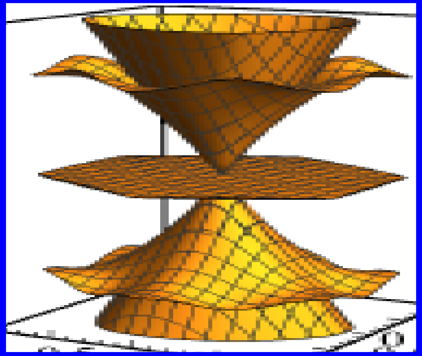
Vacancy Magnetic moment and Kondo screening



Vacancy Charge and Tunable artificial atom



Twisted bilayer graphene



Eva Y. Andrei

LECTURE NOTES POSTED AT:

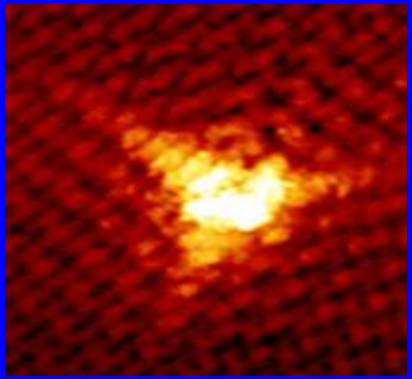
http://www.physics.rutgers.edu/~eandrei/links.html#trieste18

Summer School on Collective Behaviour in Quantum Matter

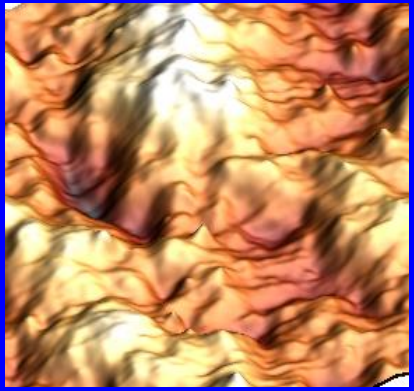
ICTP

Interaction of Dirac electrons with spins and point charges

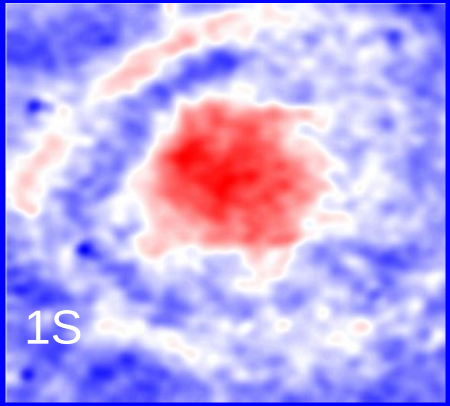
Vacancies in graphene



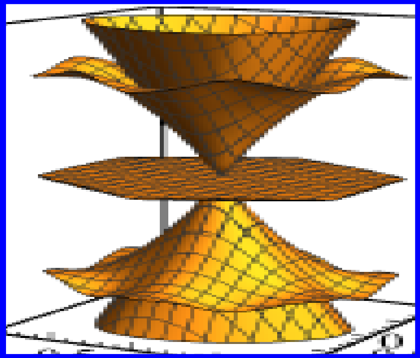
Vacancy Magnetic moment and Kondo screening



Vacancy Charge and Tunable artificial atom



Twisted bilayer graphene

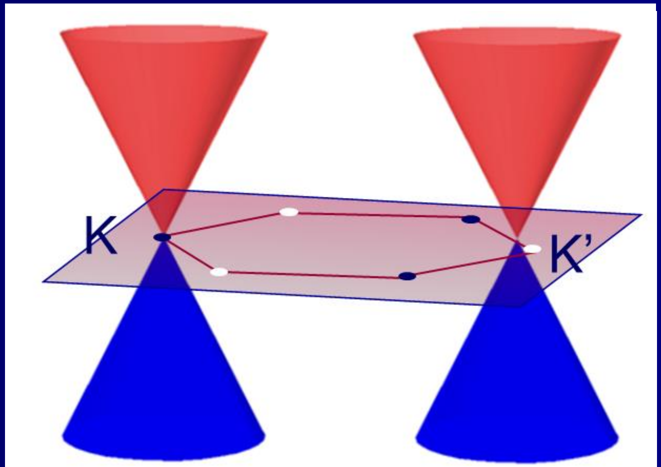


- Engineering electronic properties
  - Density of states and Landau levels in graphene
  - Scanning tunneling microscopy (STM) and spectroscopy (STS)
  - Defects:
    - Atomic collapse and artificial atom
    - Kondo effect
  - Substrate:
    - Twisted graphene

Andrei

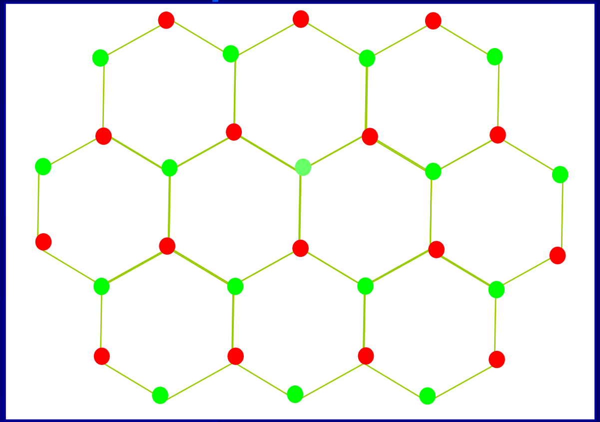
Density of states

Band structure



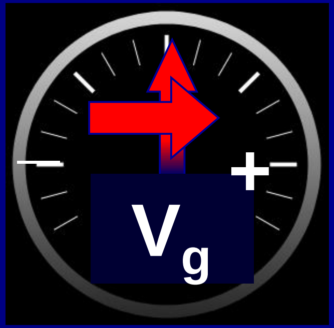
$$E = v_F p$$

Ultra-relativistic
Chiral quasiparticles



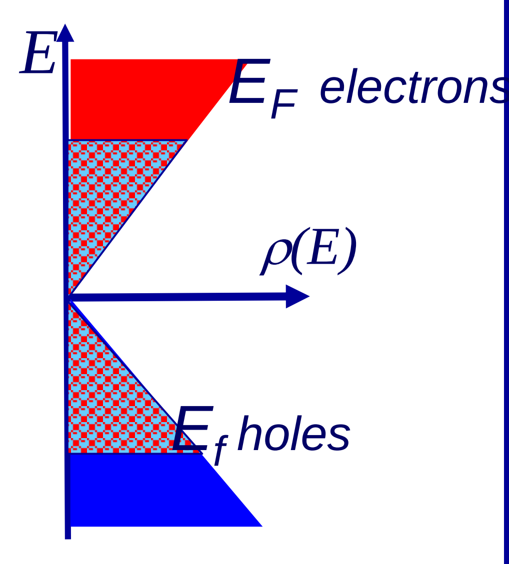
sp^2 Carbon

$$\rho(E) = 3^{3/2} a^2 \frac{|E|}{\pi(\hbar v_F)^2}$$



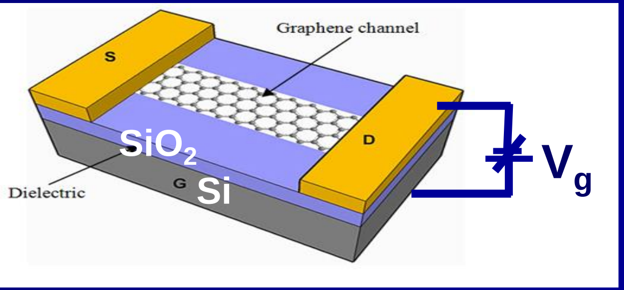
1V $\mapsto$ 7x10^{10} cm^{-2}

Density of states



Ingredients:

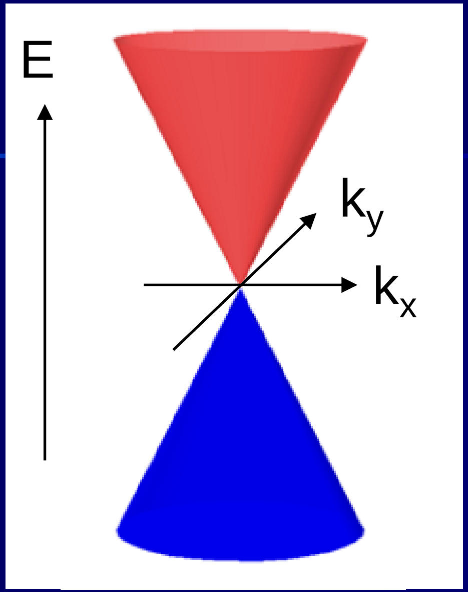
1. 2D
2. Honeycomb structure
3. Identical atoms



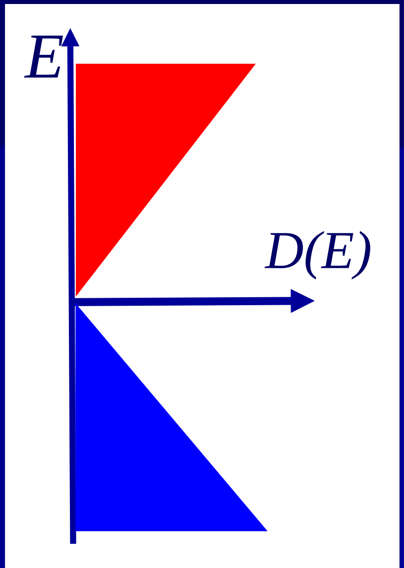
E.Y. Andrei

Landau levels in graphene from Dirac-Weyl equation

Band structure

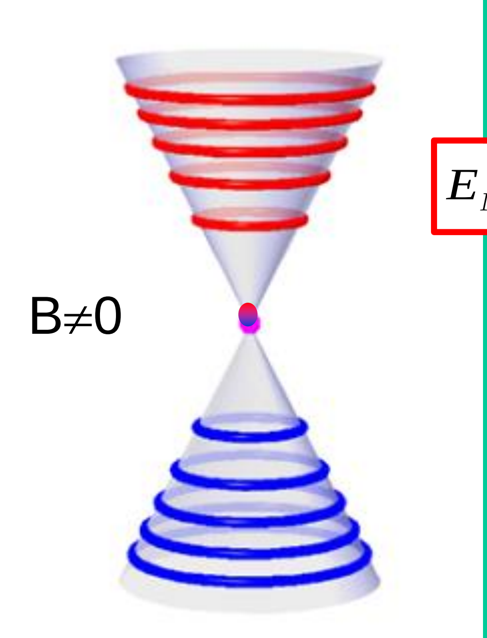


Density of states



$$H = v_F \begin{pmatrix} 0 & \vec{\sigma}.\vec{p} \\ -\vec{\sigma}^*.\vec{p} & 0 \end{pmatrix}$$

$$H = v_F \begin{pmatrix} 0 & \vec{\sigma}.(\vec{p}-e\vec{A}) \\ -\vec{\sigma}^*.(\vec{p}-e\vec{A}) & 0 \end{pmatrix}$$



Finite B → Landau Levels

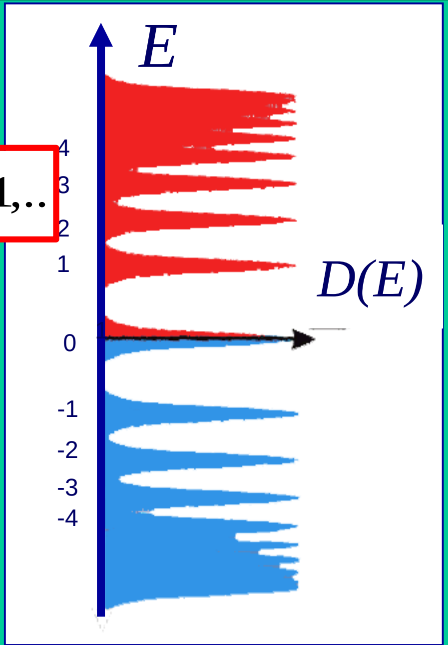
$$E_N = \pm v_F \sqrt{2e\hbar B|N|} = \pm\hbar\omega_c\sqrt{2|N|}; \quad N = 0, \pm1, ..$$

$$\hbar\omega_c = \hbar v_F / l_B \approx 35\sqrt{\mathrm{B}}\ \mathrm{meV}$$

$$l_B = \sqrt{\hbar / eB} = 25/\sqrt{\mathrm{B}}\ \mathrm{nm}$$

$$Degeneracy: g = 4g_0; \qquad \phi_0 = h/e$$

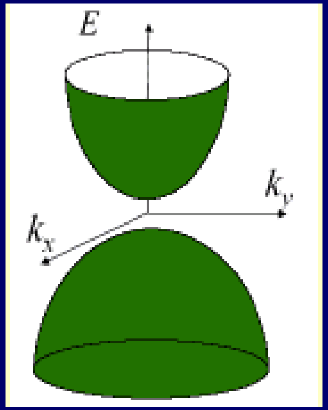
$$Orbital\ \ Degeneracy\ \ \boldsymbol{g_0} = B/\phi_0 = 2.5\times10^{14}\ m^{-2}B[T]$$

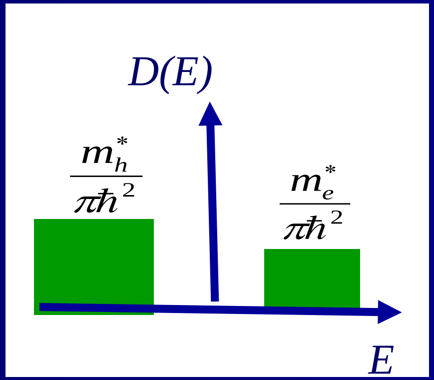


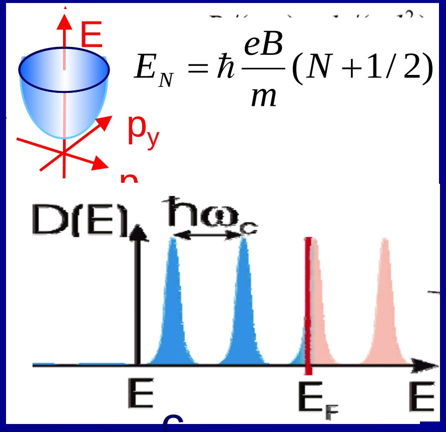
Graphene and conventional 2d electron systems

Low energy excitations | Density of states | Landau levels

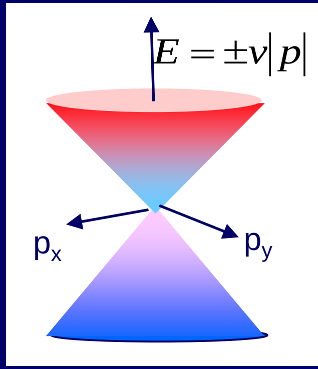
Conventional semiconductor

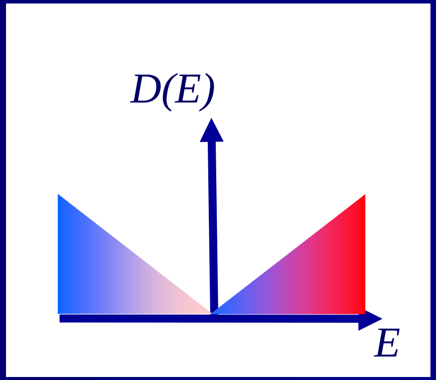


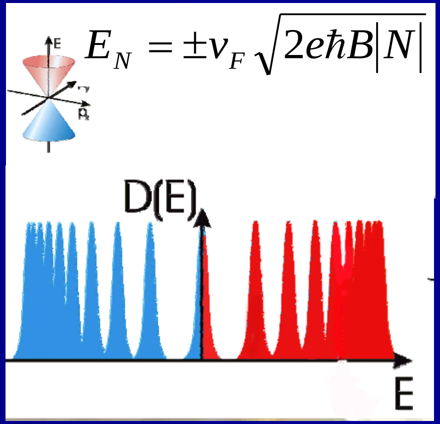




Graphene



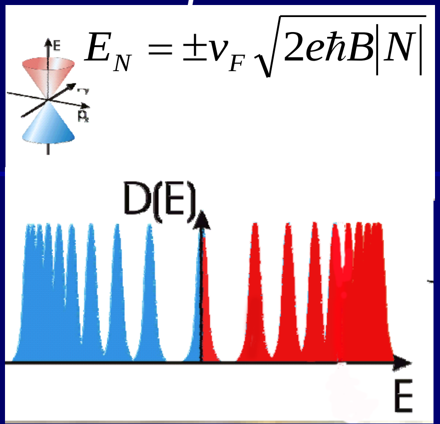




E.Y. Andrei

Landau levels: graphene and conventional 2D ES

Graphene

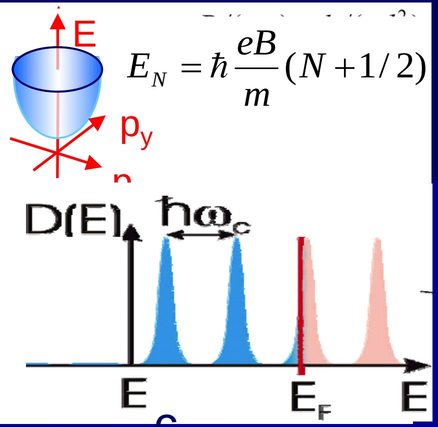


$$E_N = \pm v_F \sqrt{2e\hbar B|N|} = \hbar\omega_c \sqrt{2|N|}; \quad N = 0, \pm 1, \ldots$$
$$\omega_c = v_F / l_B = v_F \sqrt{eB/\hbar}$$

- $E_{N=0}$ =0 Berry phase π
- Electron hole symmetric
- E ~ $N^{1/2}$ Level
- E ~ $B^{1/2}$
- g_i=4

$$\hbar\omega_c \approx 33\sqrt{\mathrm{B}}\,[\mathrm{meV}/\mathrm{T}^{1/2}]$$

Conventional 2DES



$$E_N = \hbar\omega_c (N + 1/2) \quad N = 0, 1, 2, \ldots$$
$$\omega_c = eB/m$$

- Gap at E=0 Berry phase =0
- Either electrons OR holes.
- Equally spaced levels
- E~B
- g_i=2

$$\hbar\omega_c \approx 1.4B[\mathrm{meV}/\mathrm{T}] \quad \mathrm{GaAs}$$

$$l_B = \sqrt{\hbar/eB} = 25/\sqrt{\mathrm{B}}\ \mathrm{nm}$$

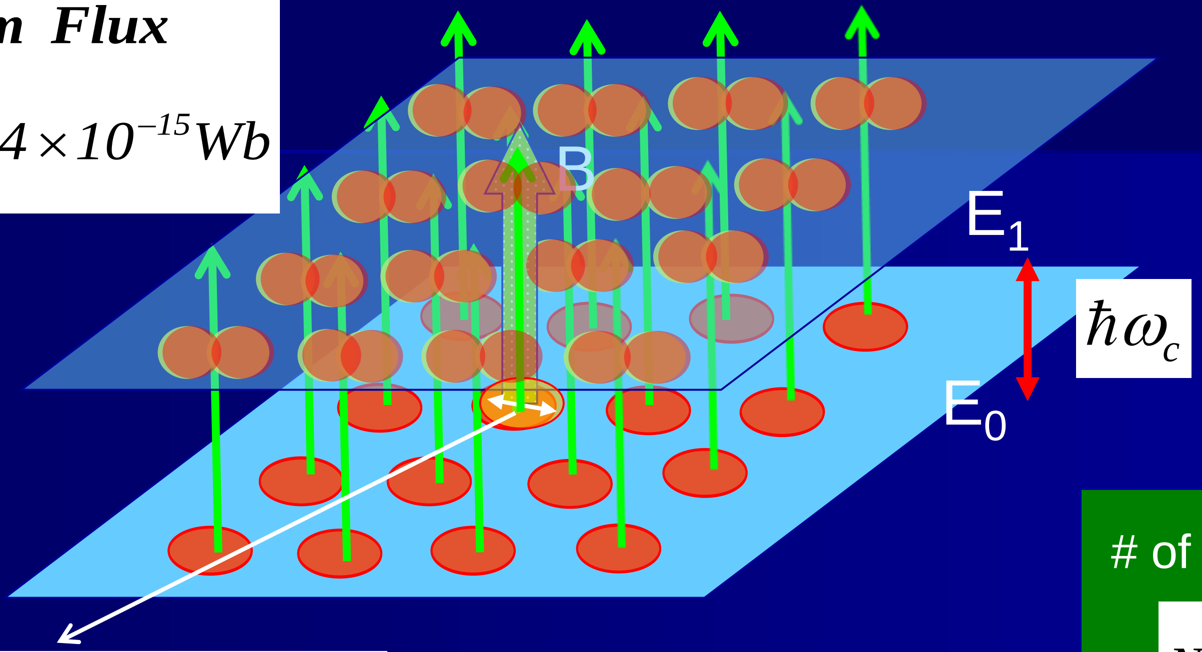
$$g_0 = B/\phi_0 = 8.5 \times 10^{14} \times B[Tm^{-2}]$$

E.Y. Andrei

Populating Landau levels

Quantum Flux

$$\phi_0 = \frac{h}{e} = 4\times10^{-15}Wb$$



$$l_B = \sqrt{\hbar / eB} = 25/\sqrt{\mathrm{B}}\ \mathrm{nm}$$

Flux line ⟷ Electronic state

Flux Density B/ϕ_0

$$Orbital\ \ Degeneracy\ \ \mathrm{g_o} = B/\phi_0 = 2.5\times10^{14}\ \mathrm{Tm^{-2}}$$

$$Total\ \ Degeneracy\ \ g_i\mathrm{g_o} = 4\mathrm{g_o}$$

\# of filled Landau levels

$$N = \frac{n_s}{g_i g_0} = \frac{1}{g_i}\frac{n_s\phi_0}{B}$$

\# of electrons per flux line

$$g_i N = \frac{n_s}{g_0}$$

Summary

Quantum unit of flux

$$\phi_0 = \frac{h}{e} = 4.14\cdot 10^{-7}\,\text{gauss}\cdot\text{cm}^2\ \ [\text{Tesla}\cdot\text{m}^2]$$

$$\Rightarrow \frac{\Phi}{\phi_0} = N \quad \text{flux enclosed by cyclotron orbit}$$

Onsager relation :k-space area of cyclotron orbit

$$S(k_N)l_B^2 = 2\pi(N + 1/2 - \gamma/2\pi)$$

$$\gamma = \text{Berry Phase}$$

Landau level energy

Non-relativistic

$$E_N = \hbar\frac{eB}{m}(N+1/2)$$

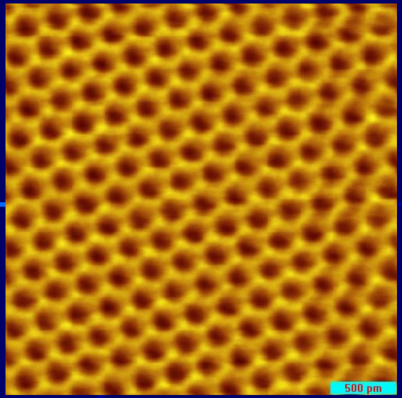
Ultra-relativistic (graphene)

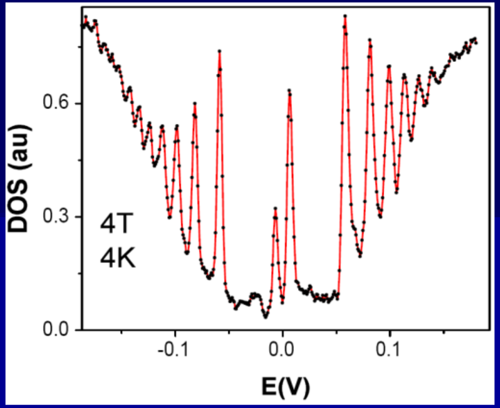
$$E_N = \pm v_F\sqrt{2e\hbar B|N|}$$

degeneracy: $g_i g_o$

$$4\frac{B}{\phi_0} \qquad 2\frac{B}{\phi_0}$$

Scanning tunneling microscopy and spectroscopy





- Engineering electronic properties
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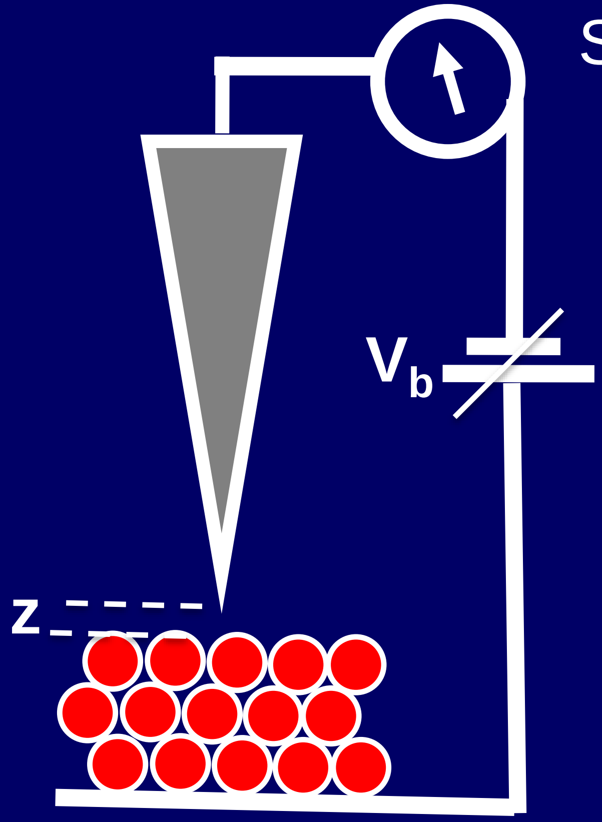
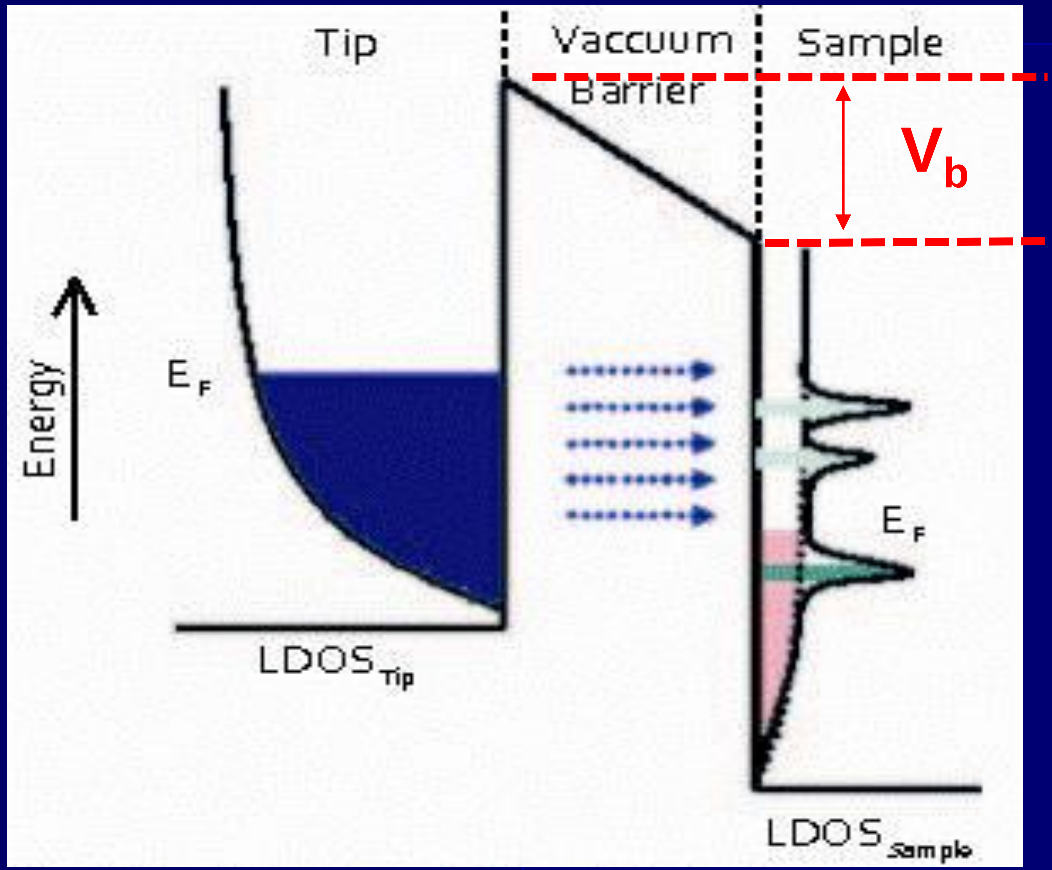
Scanning Tunneling Microscopy (STM



STM measures tunnel current across a vacuum barrier

$$I(r,z,V) \propto \left[\int_0^{eV_b} \rho(r,\varepsilon) d\varepsilon \right] \exp^{-z(r)\kappa}$$



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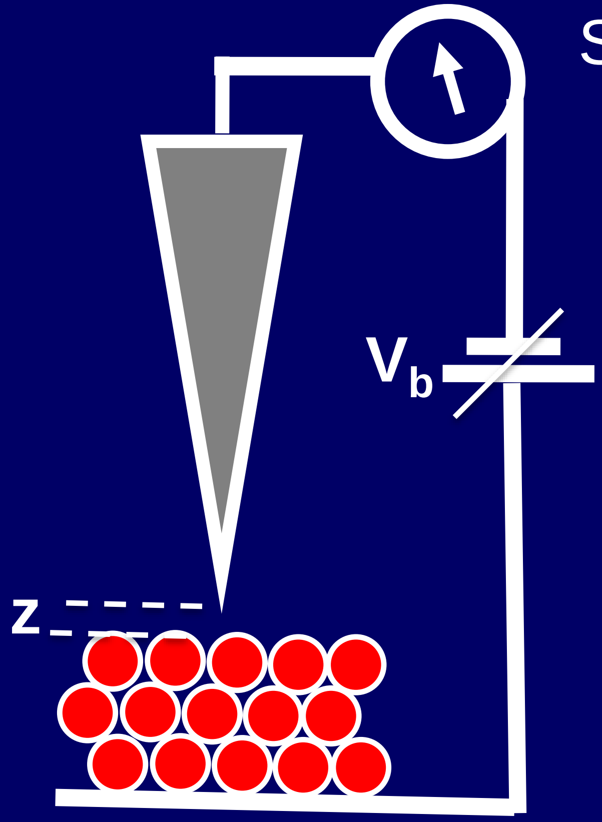
Scanning Tunneling Microscopy (STM



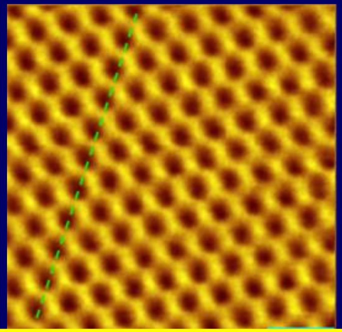
STM measures tunnel current across a vacuum barrier

$$I(r,z,V) \propto \left[\int_0^{eV_b} \rho(r,\varepsilon)\, d\varepsilon \right] \exp^{-z(r)\kappa}$$

I ,V_b constant

Topography:
Imaging Atoms

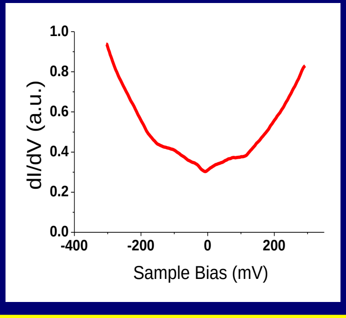
$$I(r,z) \propto \exp^{-z\kappa(r)}$$



z constant

Spectroscopy:
Density of states

$$dI/dV_b \propto \rho(r,V_b)$$



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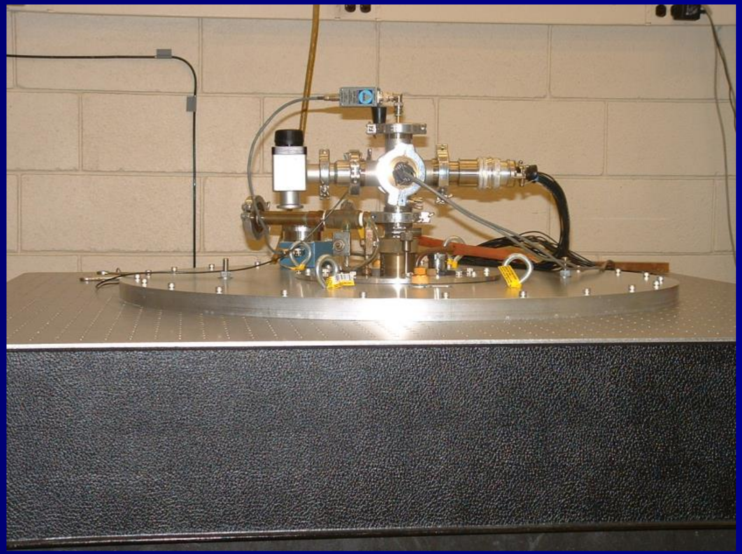
Rutgers Low Temperature High field STM

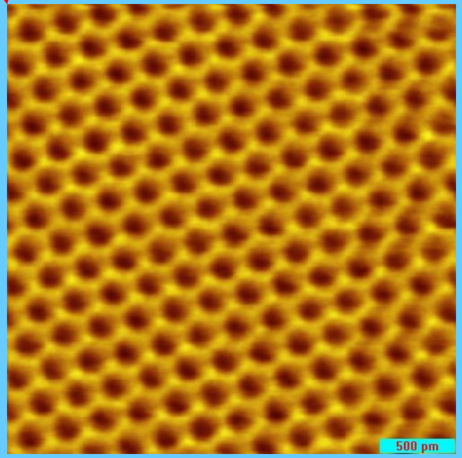
- Rutgers STM
  - Temperature T=4 (2K)
  - Magnetic field B=13 (15T)
  - Scan range 10^{-10} -10^{-3} m



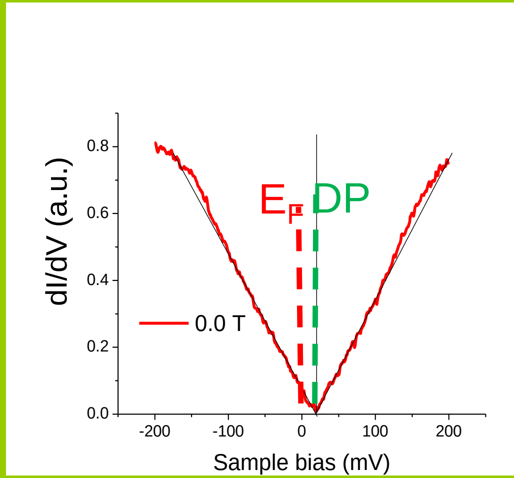
- Topography $\mapsto$ structure
- Spectroscopy $\mapsto$ Density of states B=0
- Spectroscopy $\mapsto$ Density of states B>0

Graphene on Graphite : the Perfect substrate

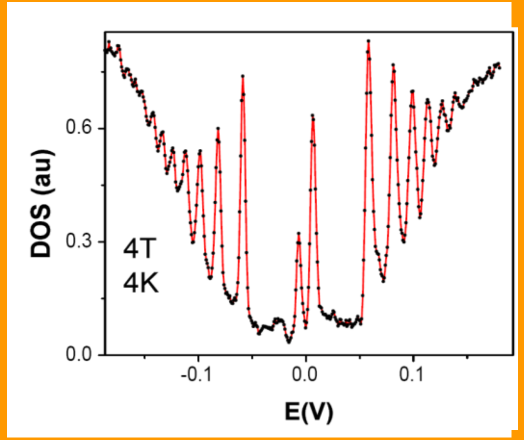
topography



B=0 spectroscopy



B>0 spectroscopy



- Local doping
- Electron-phonon coupling

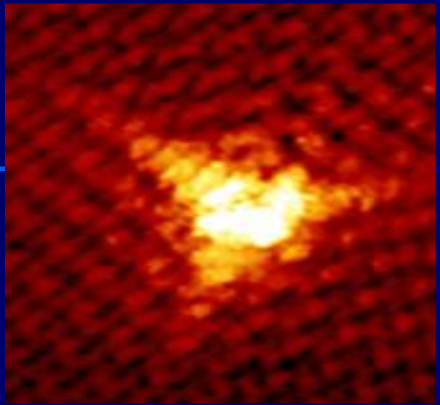
$$E_N = \pm v_F \sqrt{2e\hbar B|N|}$$

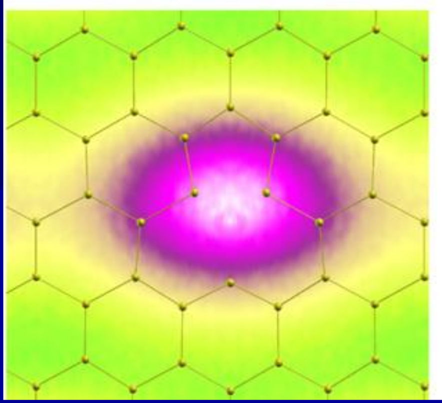
- Local Fermi velocity
- Quasiparticle lifetime
- Coupling to substrate

G. Li , E.Y. A - Nature Physics, (2007)
G. Li, A. Luican, E. Y. A., Phys. Rev. Lett (2009)

E.Y. Andrei

Vacancies: Inducing local magnetic moments and charge





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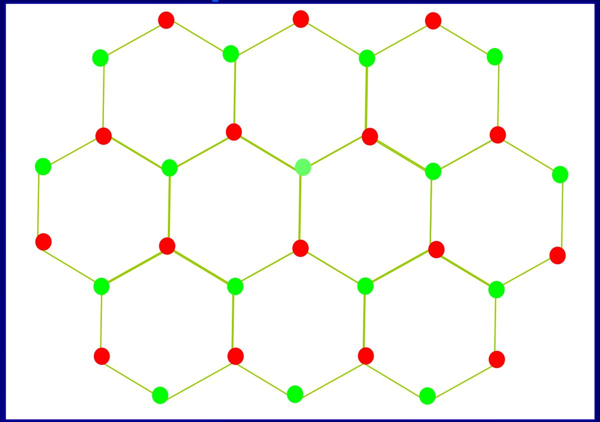
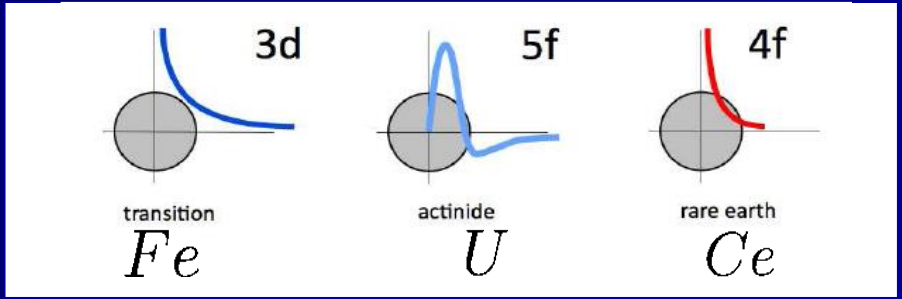
    Twisted graphene

Perfect Graphene

Magnetism: Spin of localized electrons in partially filled inner d or f shell .



sp^2 Carbon

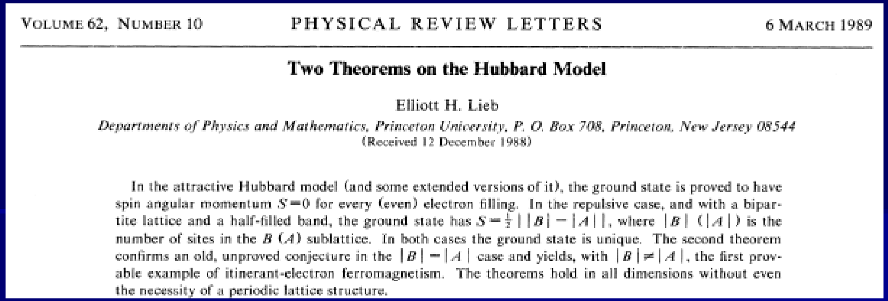


Carbon

- *No d, f electrons*
- *But partially filled p shell*

Graphite, graphene, …, Carbon allotropes
? Non-Magnetic ?

Magnetism and Perfect Graphene



VOLUME 62, NUMBER 10 PHYSICAL REVIEW LETTERS 6 MARCH 1989

Two Theorems on the Hubbard Model

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(Received 12 December 1988)

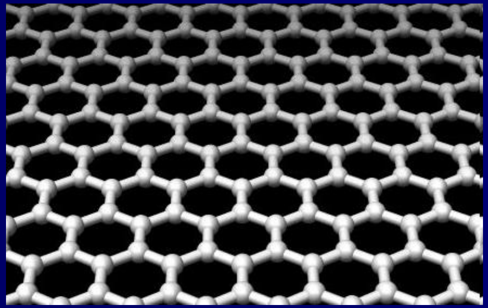
In the attractive Hubbard model (and some extended versions of it), the ground state is proved to have spin angular momentum $S=0$ for every (even) electron filling. In the repulsive case, and with a bipartite lattice and a half-filled band, the ground state has $S=\frac{1}{2}||B|-|A||$, where $|B|$ ($|A|$) is the number of sites in the B (A) sublattice. In both cases the ground state is unique. The second theorem confirms an old, unproved conjecture in the $|B|=|A|$ case and yields, with $|B|\neq|A|$, the first provable example of itinerant-electron ferromagnetism. The theorems hold in all dimensions without even the necessity of a periodic lattice structure.

...repulsive Hubbard model + **bipartite lattice** + **half-filled** band:

spin of ground state with N_A, N_B populated sites:

$$S= 1/2(N_A- N_B)$$

Pristine graphene (graphite) $N_A=N_B \rightarrow S=0$



Perfect graphene Non-Magnetic!

Vacancies $\rightarrow N_A>N_B \mapsto$ magnetic moment

Material	χ_v ($\times 10^{-5}$)
Superconductor	-10^5
Pyrolytic carbon	−40.9
Bismuth	−16.6
Mercury	−2.9
Silver	−2.6
Carbon (diamond)	−2.1
Lead	−1.8
Carbon (graphite)	−1.6
Copper	−1.0
Water	−0.91

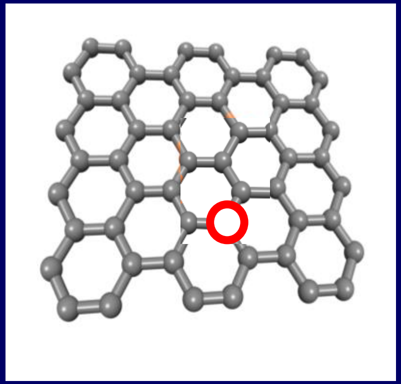
A.H. Castro Neto et al. Solid State Commun. (2009).
T. Wehling,. Phys. Lett. (2009)
O. Yazyev, et al Rep. Prog. (2010).
M. Vojta *et.al*, EPL, 90 (2010) 27006
T. O. Wehling, Phys. Rev. B 81, 115427(2010)
J. O. Sofo, et al Phys. Rev. B 85, 115405 (2012)

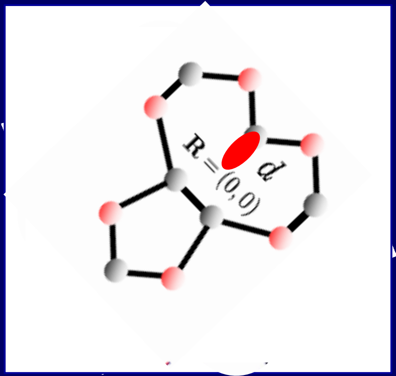
E.Y. Andrei

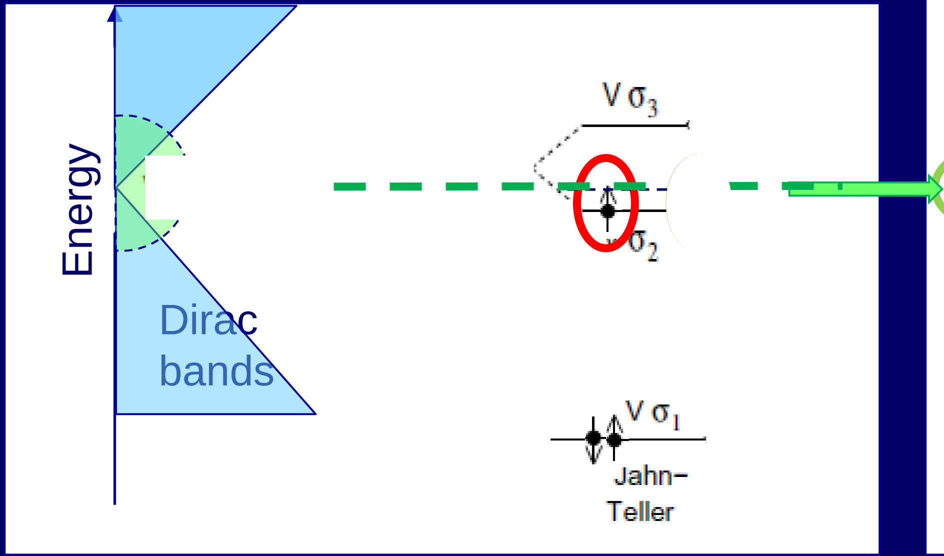
Imperfect Graphene – Vacancy Magnetic Moment

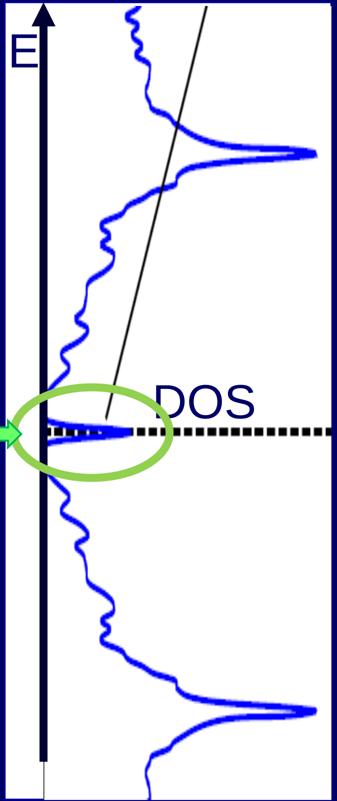
Yazyev & Helm (2007),
Popovi’c, Nanda, Satpathy (2012)

remove
Carbon atom









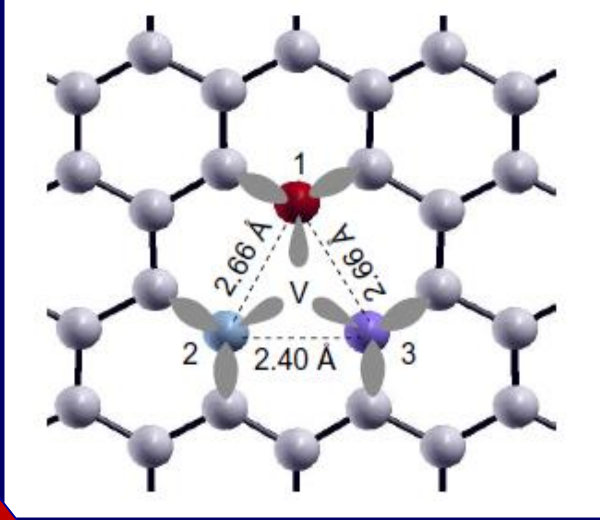
Broken
AB
symmetry

σ Dangling bond ↦ localized state ↦ $1\mu_B$

p_z ↦ quasi-localized state on other sublattice ↦ ~$0.5\text{-}0.7\mu_B$

Zero mode peak at ~Dirac Point

Vacancy Properties



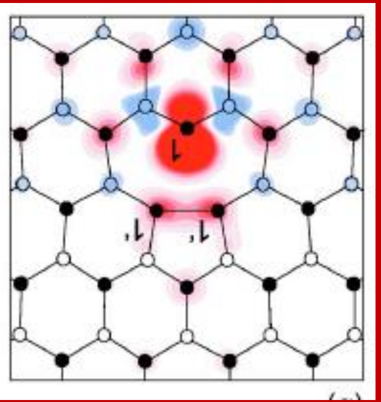
Interaction of ultra-relativistic electron with magnetic moment?

Interaction of ultra-relativistic electron with Point charge ?

Magnetic

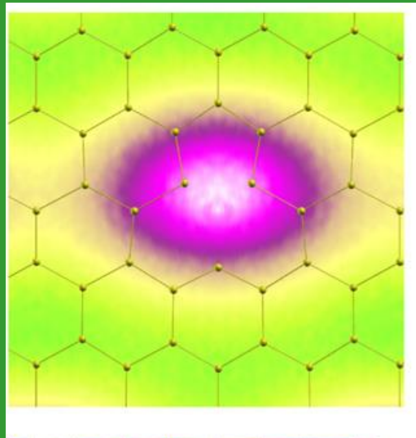
Charge

~ $1.7\mu_B$



Yazyev & Helm (2007)

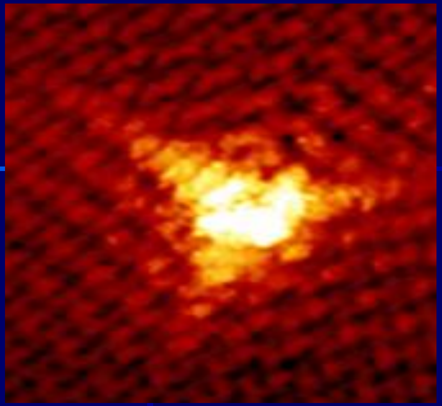
Charge ~ +1|e|

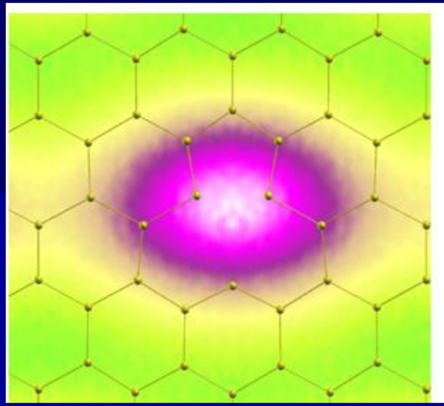


Y Liu et al (2015)
Padmanabhan & Nanda (2016)

Andrei

➤ Vacancy Charge and Tunable artificial atom

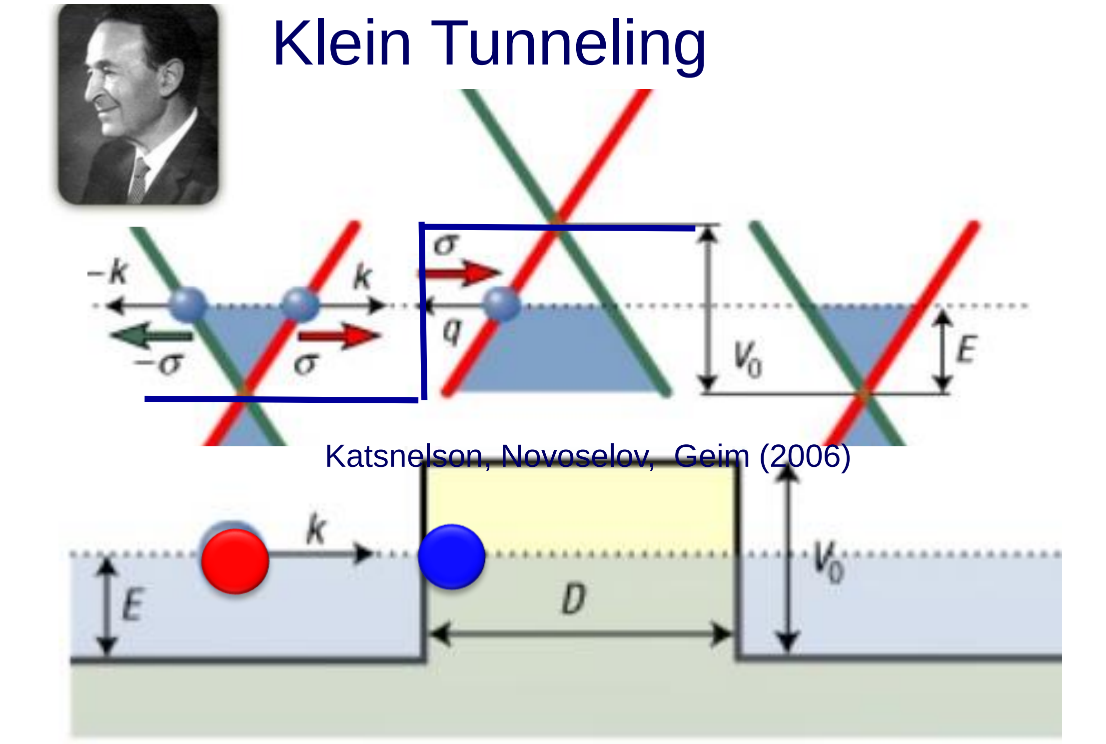




❖ Engineering electronic properties
- Density of states and Landau levels in graphene
- Scanning tunneling microscopy (STM) and spectroscopy (STS)
- Defects:
  Atomic collapse and artificial atom
  Kondo effect
- Substrate:
  Twisted graphene

Pristine graphene

Pseudospin + chirality $\mapsto$ Klein tunneling



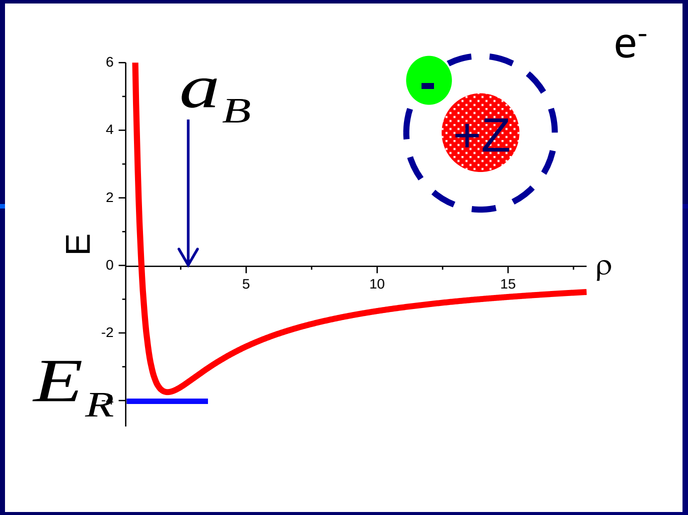
Katsnelson, Novoselov, Geim (2006)

No electrostatic confinement

- No quantum dots
- No switching
- No guiding

Can one use a point charge to control the carriers?

Electron in 1/r potential : Bohr atom



Non relativistic classical

$$KE = \frac{p^2}{2m};\ PE = -\frac{Ze^2}{r}$$

Semiclassical approximation

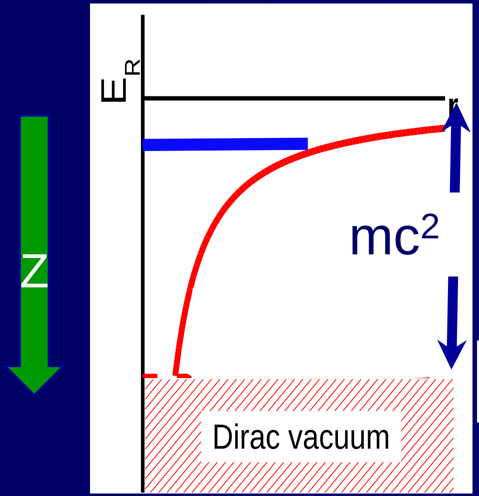
$$p \rightarrow \frac{\hbar}{r}$$

$$E(\rho) \approx mc^2\left(\frac{1}{2\rho^2} - \frac{\beta}{\rho}\right)$$

Compton wavelength $\quad \lambda\!\!\!^-_c = \frac{\hbar}{mc}, \quad \rho = \frac{r}{\lambda\!\!\!^-_c}$

Coulomb coupling constant $\quad \beta \equiv Z\alpha$

Fine structure constant $\quad \alpha \equiv \frac{e^2}{\hbar c} \sim \frac{1}{137}$



$\beta << 1$

$\beta \approx 1 \Rightarrow E_R \approx mc^2$

Z>>1 Must Include relativistic effects

$$\frac{p^2}{2m} \rightarrow \sqrt{(pc)^2 + (mc^2)^2}$$

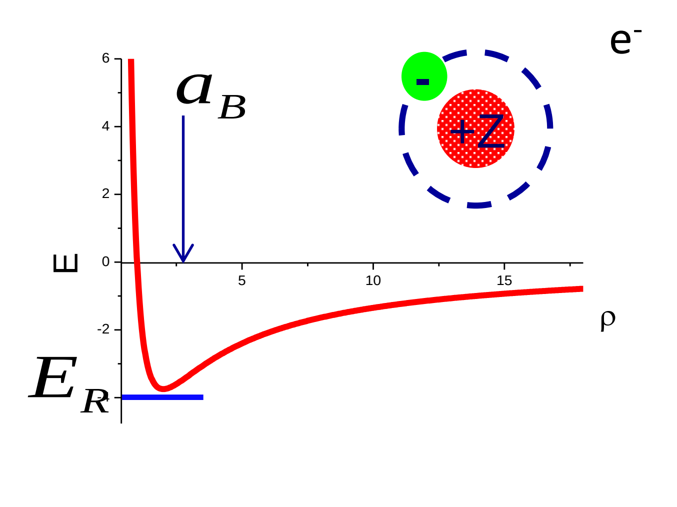
Length scale: Bohr radius $\quad a_B = \frac{\lambda\!\!\!^-_c}{\beta}$

Energy scale (Rydberg) $\quad E_R = -\frac{1}{2} mc^2 \beta^2$

QM ensures stability of the atom

E.Y. Andrei

Electron in 1/r potential : Bohr atom



relativistic massive particle

$$E = mc^2(1/2\rho^2 - \beta/\rho)$$

$$E = mc^2(\sqrt{1/\rho^2 + 1} - \beta/\rho)$$

$$E_R = \frac{1}{2}mc^2\beta^2 \xrightarrow[Z=1]{} 13.6eV$$

$$\xrightarrow[Z>>1,\beta\sim 1]{} \sim mc^2$$

Z>>1 Must Include relativistic effects

$$\frac{p^2}{2m} \rightarrow \sqrt{(pc)^2 + (mc^2)^2}$$

Bohr radius $a_B = \frac{\lambdabar_c}{\beta} \Rightarrow \frac{\lambdabar_c}{\beta}\sqrt{1-\beta^2}$

Rydberg $E_R = -\frac{1}{2}mc^2\beta^2 \Rightarrow mc^2\sqrt{1-\beta^2}$

Bohr atom: QM+ Relativity ↦ Atomic Collapse

Dirac 1928: Total energy of Electron near nucleus of charge Z :

$$E_R = mc^2\sqrt{1-\beta^2}$$

$$\beta_c \equiv Z_c\alpha \approx 1$$

$Z_c \sim 1/\alpha = 137$

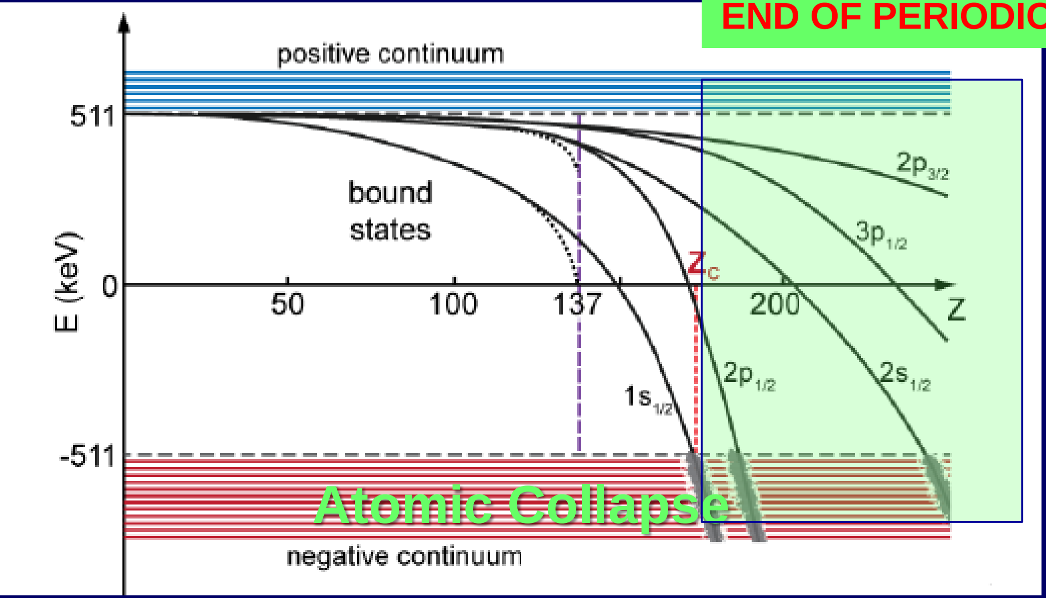
$$\beta \geq 1 \Rightarrow \text{No solution}$$

Regularize problem
finite size nucleus: $r_0 \sim 10^{-15}$ m

$\beta_c \sim 1.24 \mapsto Z_c \sim 170$

Pomeranchuk and Smorodinskii (1945)

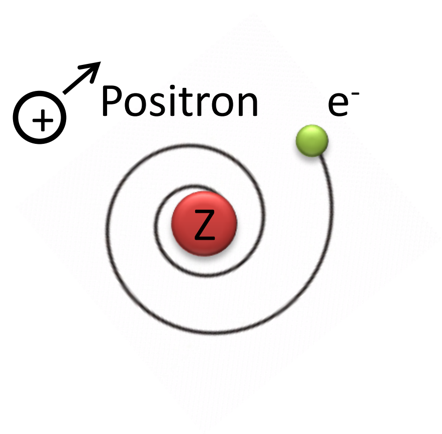
$Z_c \sim 170$
END OF PERIODIC TABLE



118	2
Uuo	8
	18
	32
	32
Ununoctium	18
(294)	8

In fact Periodic table ends earlier

Atomic Collapse



Spontaneous positron emission

QM+RELATIVITY :
atom collapses

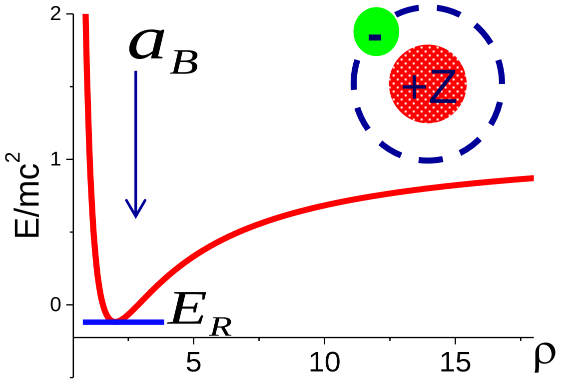
E.Y. Andrei

Relativistic Electron in 1/r potential

relativistic massive Bohr atom

$$E \approx mc^2(\sqrt{1/\rho^2+1}-\beta/\rho)$$

2D, m=0, c=v_F



Length scale

$$a_B = \frac{\lambda_c}{\beta}\sqrt{1-\beta^2}$$

Energy scale

$$E_R = mc^2\sqrt{1-\beta^2}$$

$\beta_c=1 \mapsto Z_c \sim 137$

relativistic massless Bohr atom

$$E \approx \frac{\hbar v_F}{r}(\frac{1}{2}-\beta)$$

Compton wavelength

$$\lambda_c = \frac{\hbar}{mc}, \quad \rho = \frac{r}{\lambda_c}$$

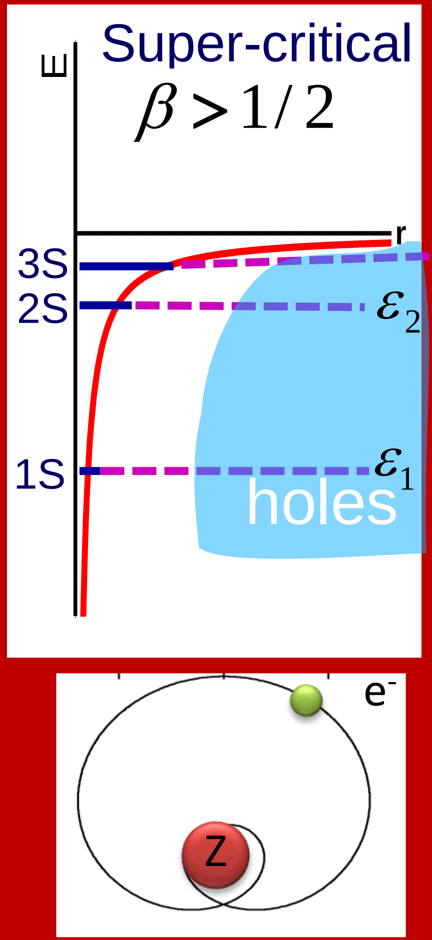
Coulomb coupling constant

$$\beta \equiv Z\alpha$$

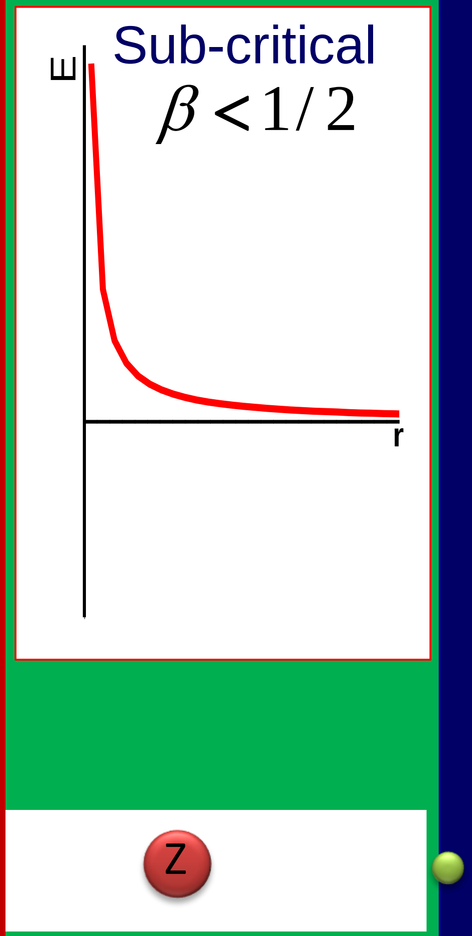
Fine structure constant

$$\alpha \equiv \frac{e^2}{\hbar c} \sim \frac{1}{137}$$

Ultra-relativistic Electron in 1/r potential



$$|\epsilon_n| = \frac{Ze^2}{r_0} e^{-\pi n\hbar/\gamma}$$

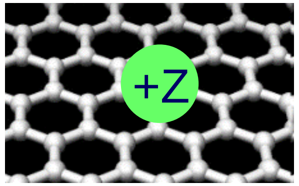


No bound states
Klein tunneling

Shytov, Katsnelson, Levitov 07
Pereira, Nilsson, Castro Neto 07

Ultra-relativistic Bohr atom

Graphene



$$E \approx \frac{\hbar v_F}{r}\left(\frac{1}{2} - \beta\right)$$

$$\beta = Z\alpha_g \qquad \alpha_g = \alpha \frac{c}{\kappa v_F} \approx 2$$

Dielectric constant

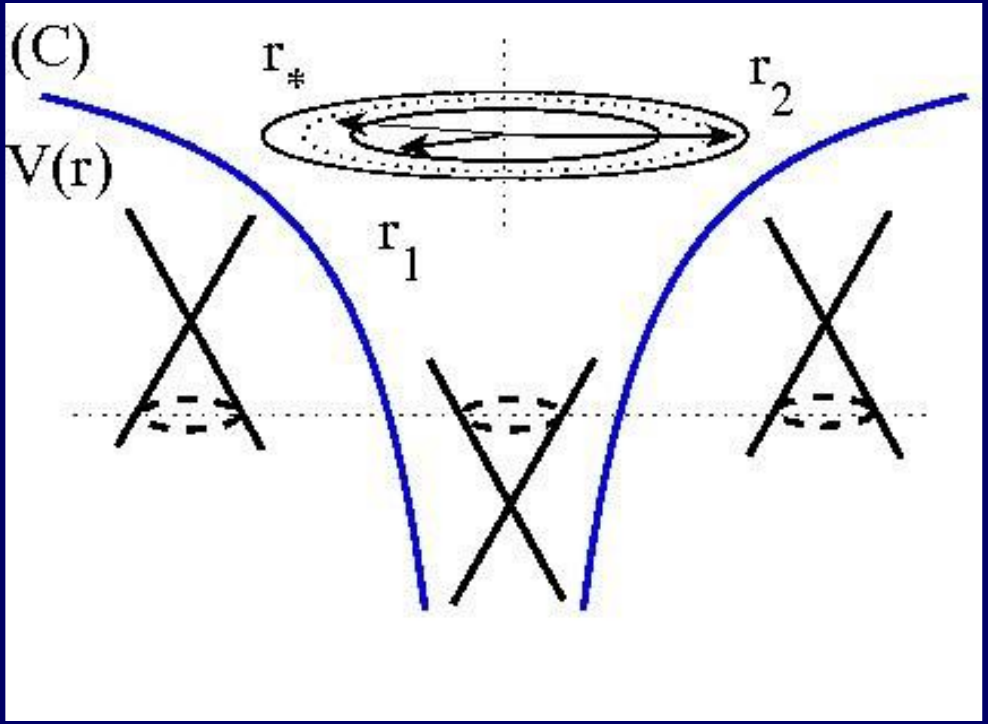
Scale free

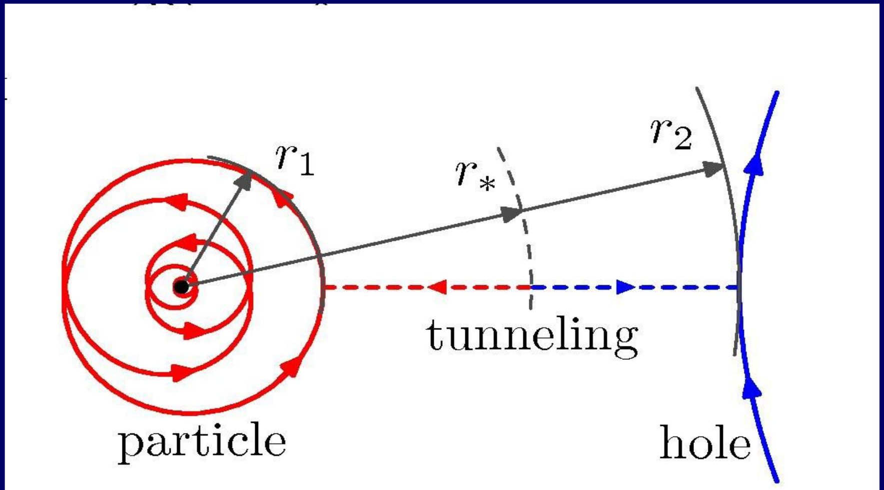
Critical charge $\mapsto$ Quantum Phase transition

$\beta_c = 1/2$ $Z_c \sim 1$

O. Ovdat et al Nat. Comm. **8**, 507 (2017)

Ultra-relativistic Case





$$r_{1,2} = \frac{Ze^2 \pm M}{\epsilon}$$

$$r^* = \frac{e^2 Z}{\kappa E} = \beta \lambda_C$$

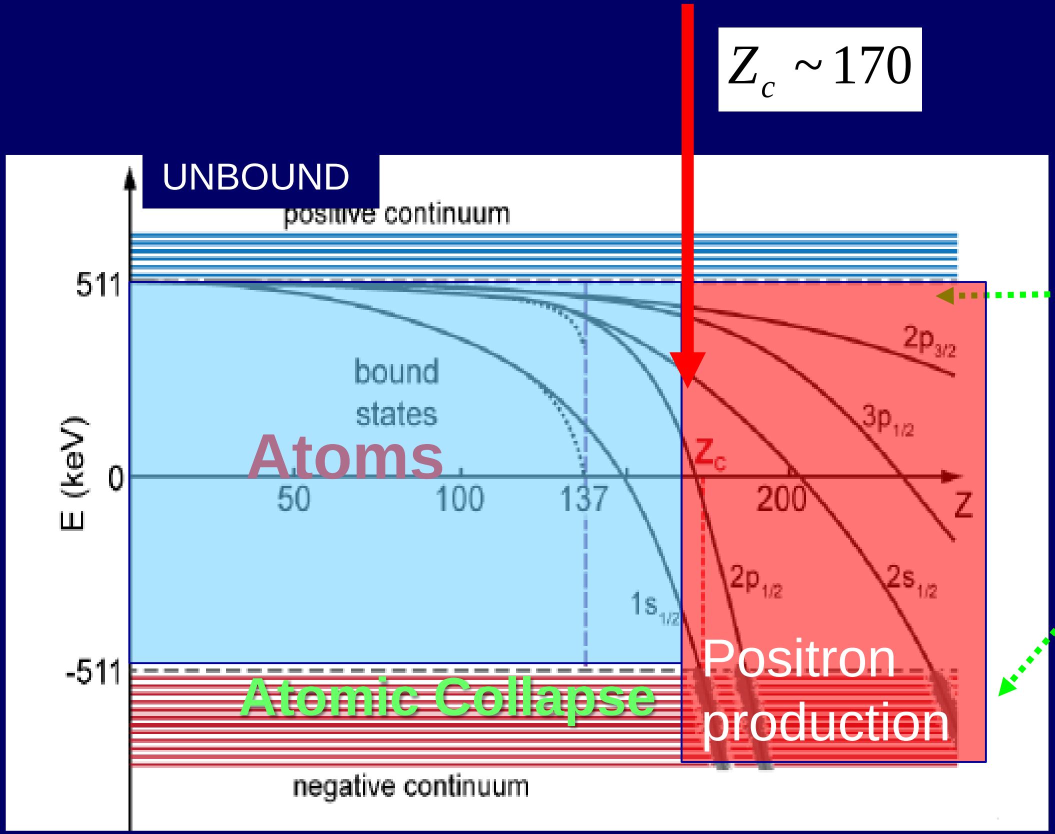
$$M = (m + 1/2)\hbar \quad angular \quad momentum$$

- Type of carriers is reversed as E_F crosses DP
- Klein tunneling couples electron-like states at small r to hole-like states at large r

Shytov, Katsnelson, Levitov 07
Pereira, Nilsson, Castro Neto 07

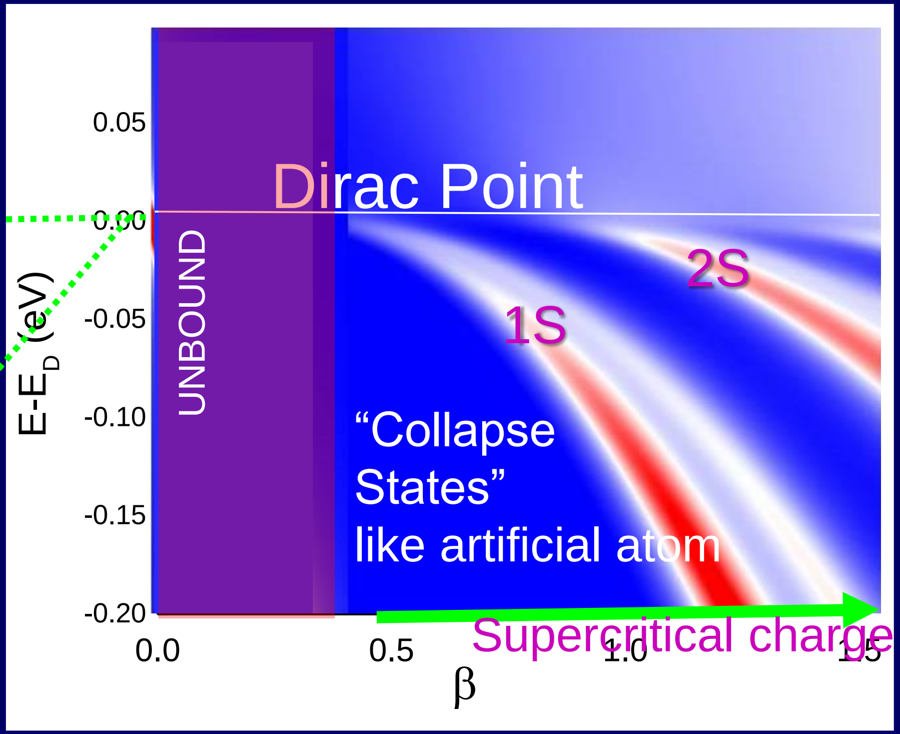
What is the experimental signature of Atomic collapse

ATOM



Schwinger (1950)
Zeldovich (1970)

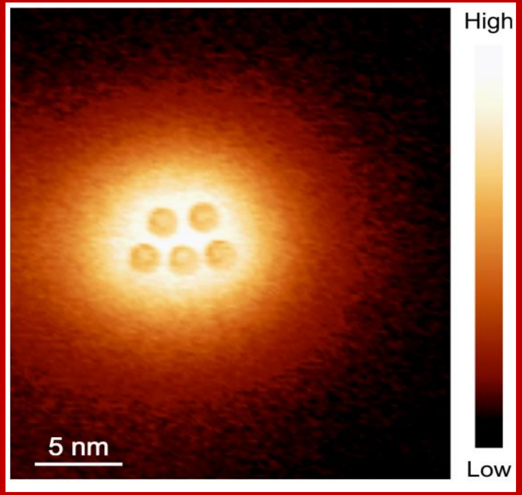
GRAPHENE + CHARGE

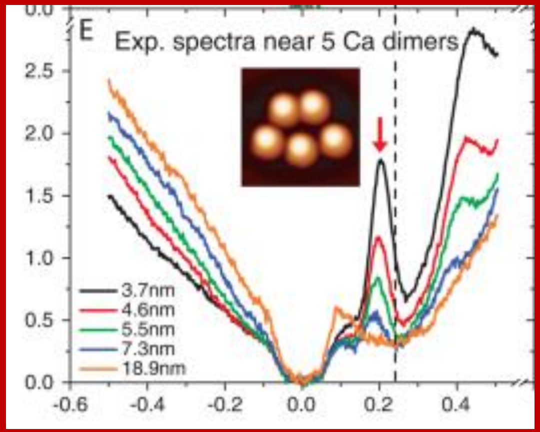


D. Moldovan, M.R. Masir, F. Peeters,

E.Y. Andrei

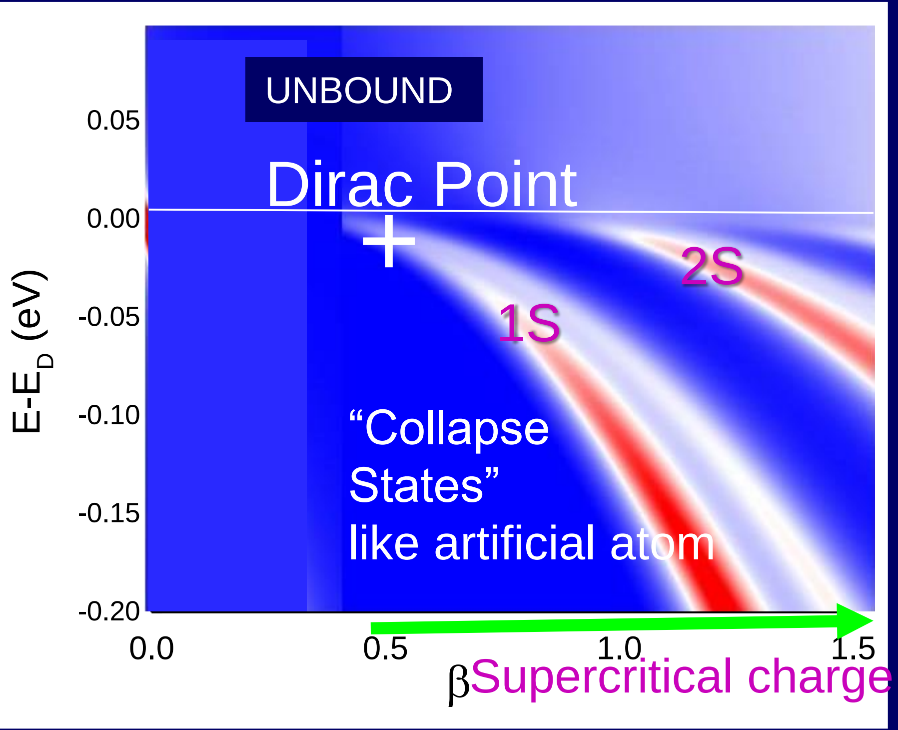
What is the experimental signature of Atomic collapse





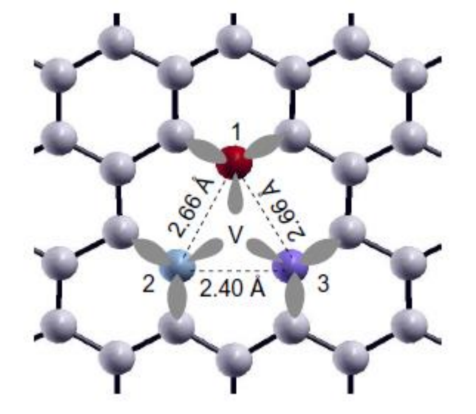
Wang et al Science 2013

GRAPHENE + CHARGE



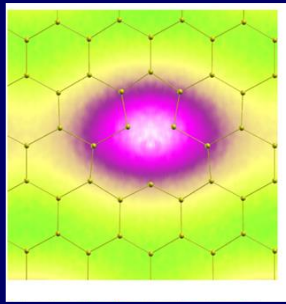
D. Moldovan, M.R. Masir, F. Peeters,

Can one host a stable charge in graphene?

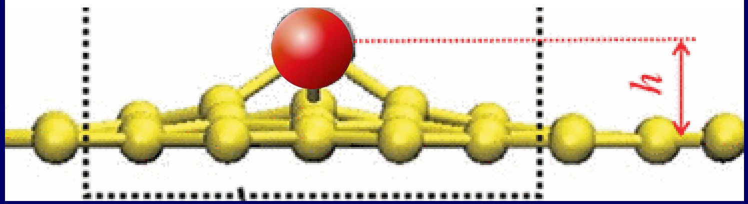


Ground state

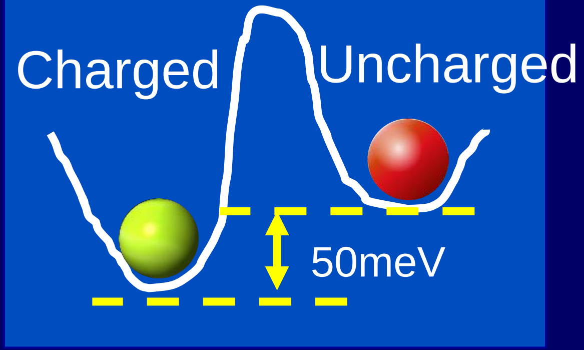
Charge ~ +1|e|



Metastable (+50meV)



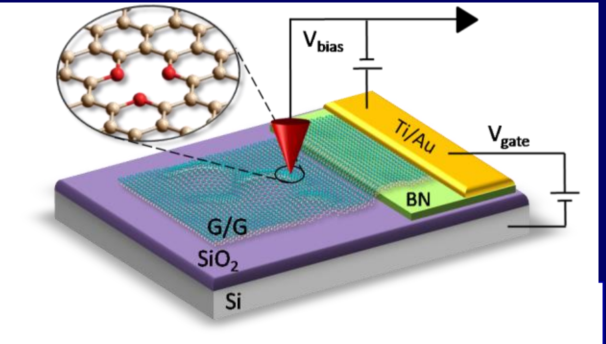
Uncharged metastable state
Stabilized by strain or substrate

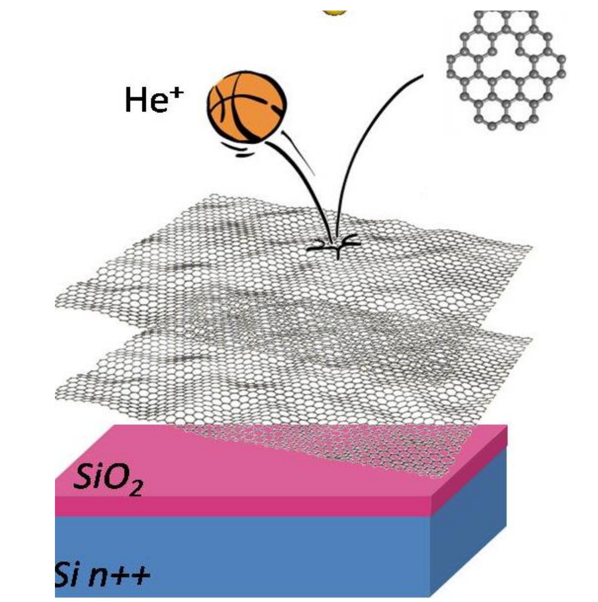


Y Liu et al (2015)
Padmanabhan & Nanda (2016)

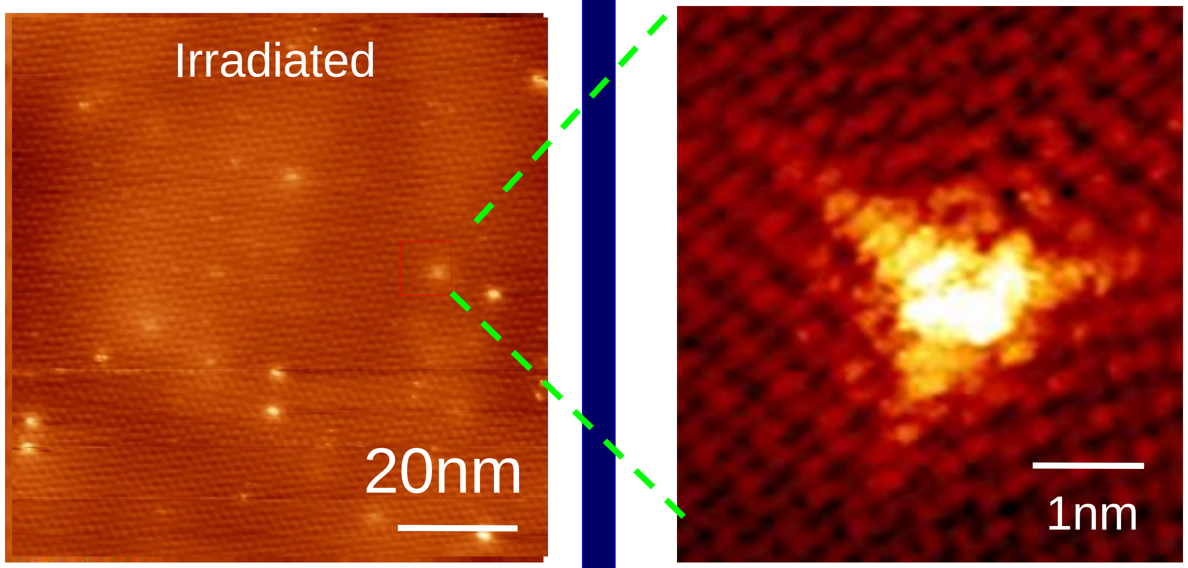
E.Y. Andrei

Making Vacnacies in graphene





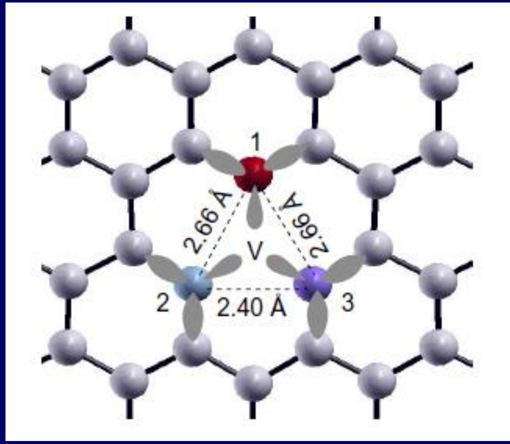
STM Topography



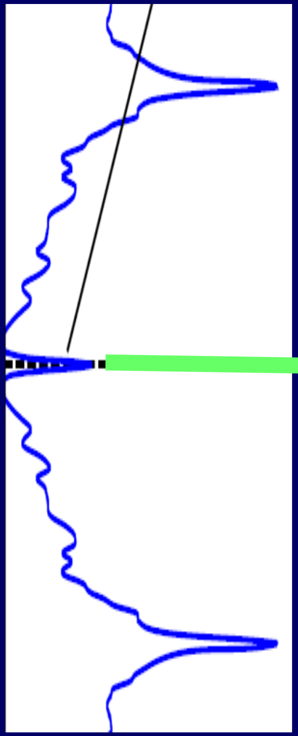
Single atom vacancy ➔ triangular structure.

M. M. Ugeda, *et al* PRL 104, 096804 (2010).

Charged Vacancy Spectrum - Artificial Atom

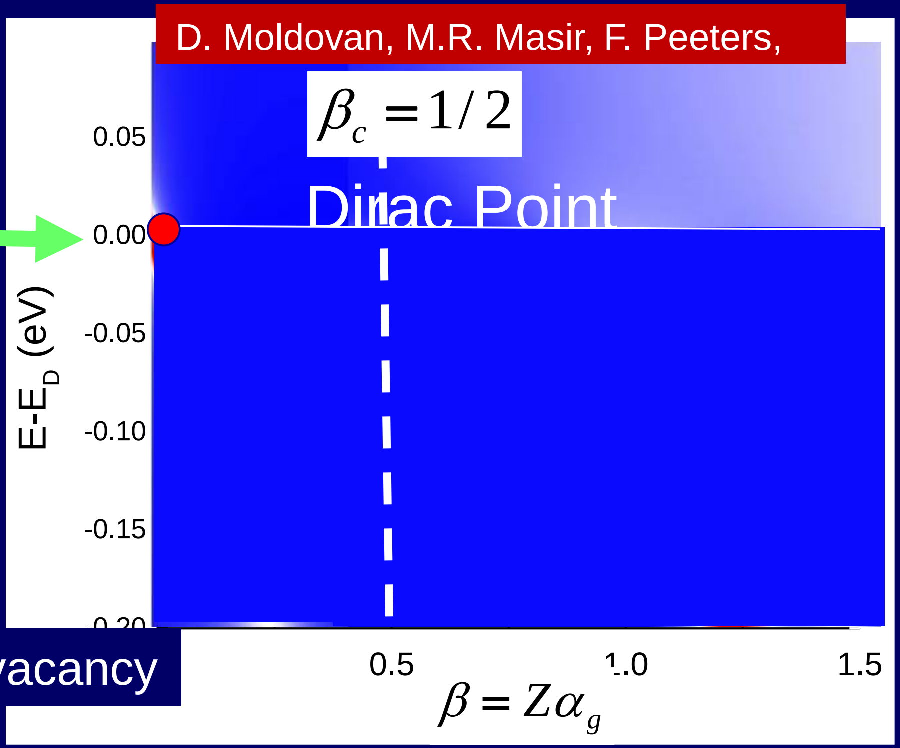


Neutral vacancy



Zero mode

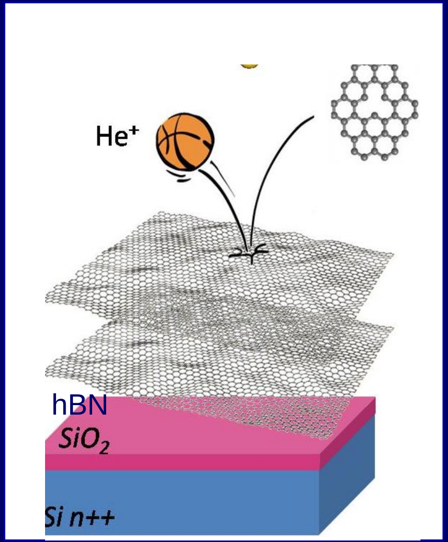
Charged vacancy

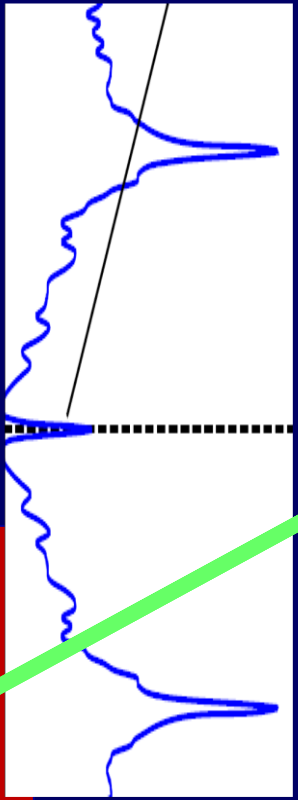


- ❖ Zero mode measures vacancy charge
- ❖ No zero mode in perfect graphene

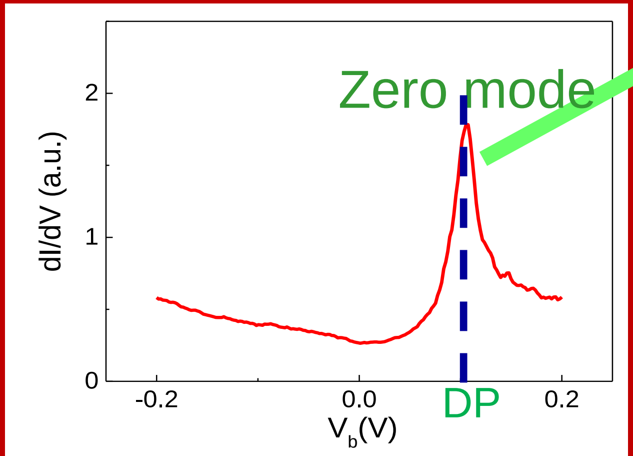
J. Mao et al, Nature Physics 2016

Vacancy in Graphene/hBN



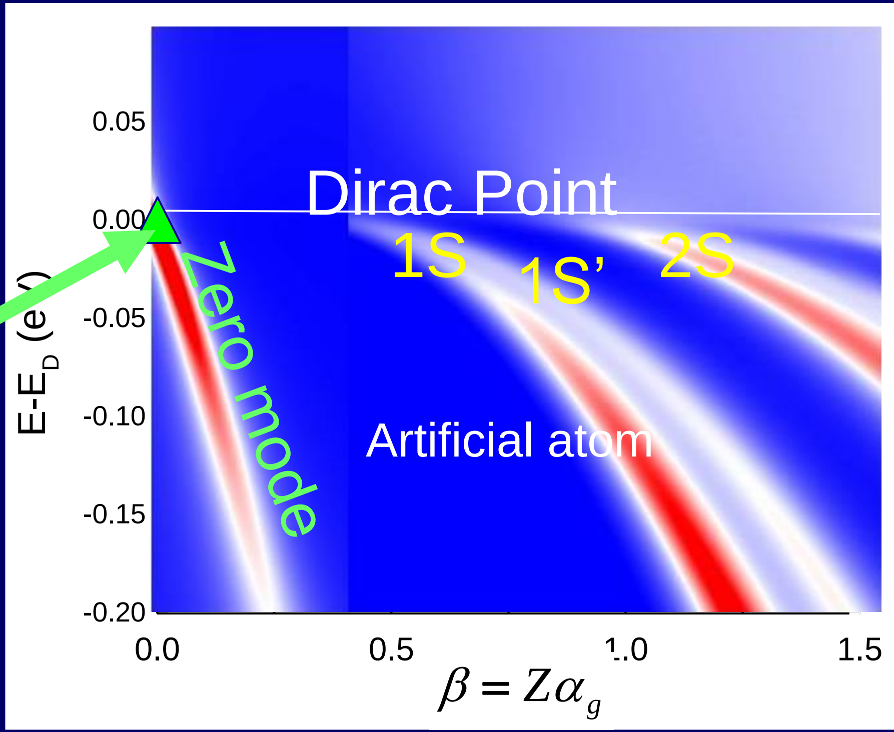


As prepared vacancy



Negligibly small charge!

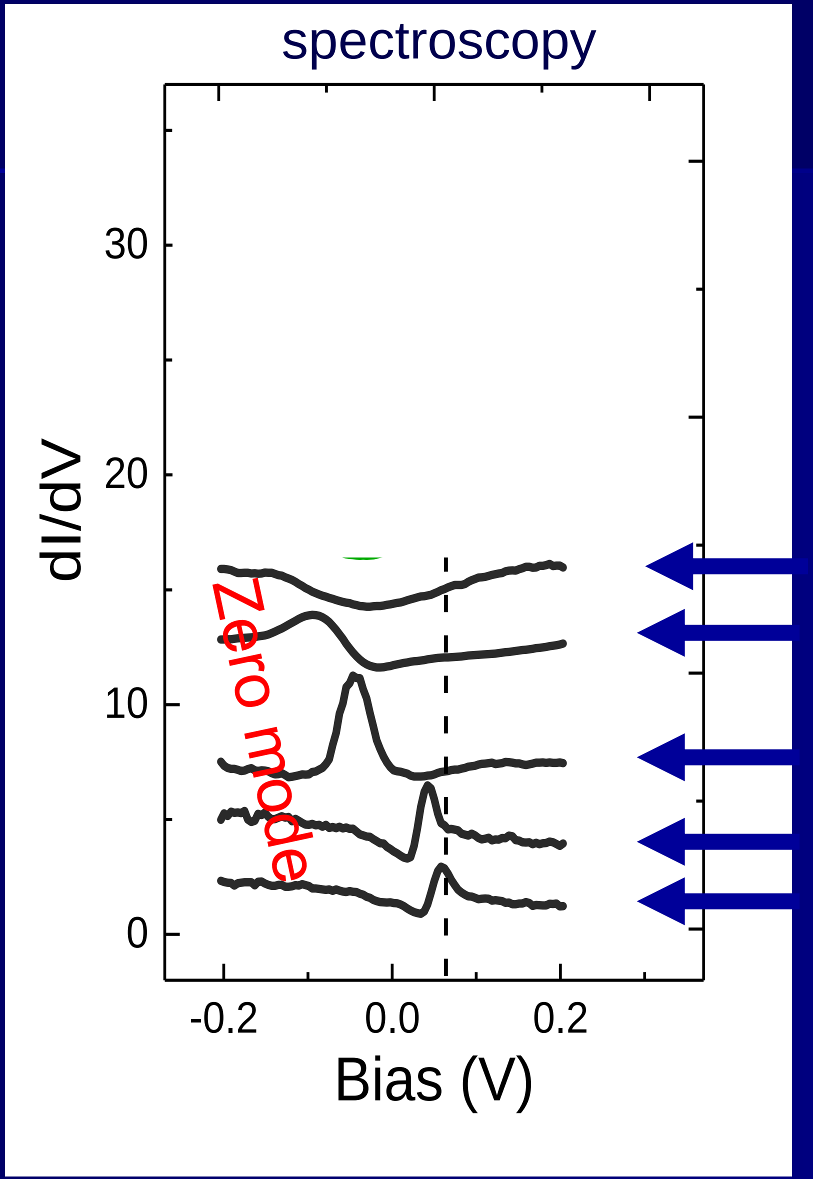
J. Mao et al Nature Physics 2016

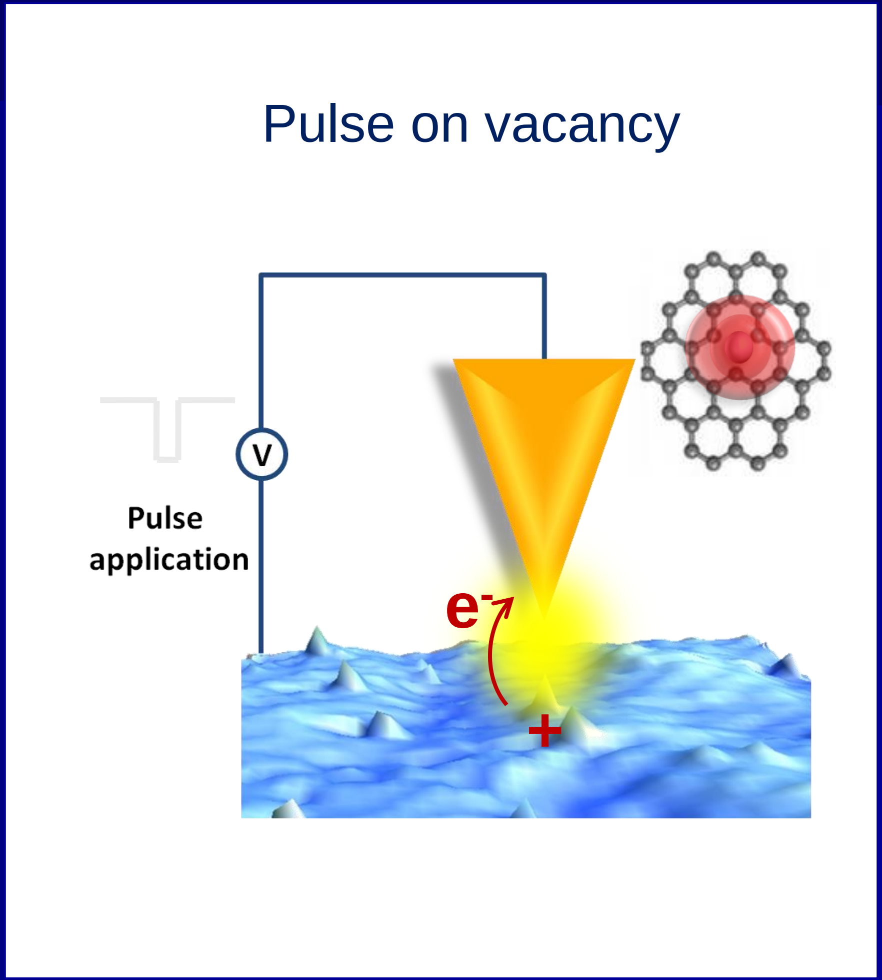


Zero mode measures vacancy charge

E.Y. Andrei

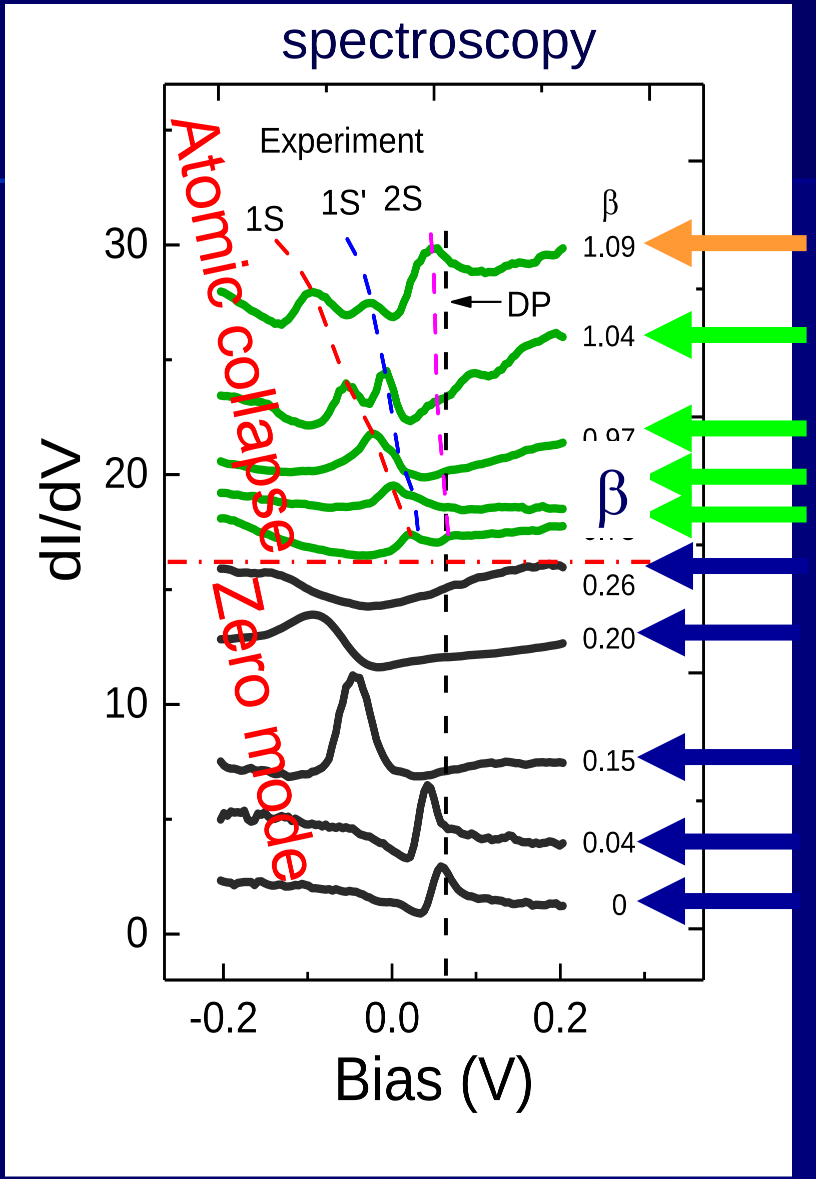
Charging a Vacancy

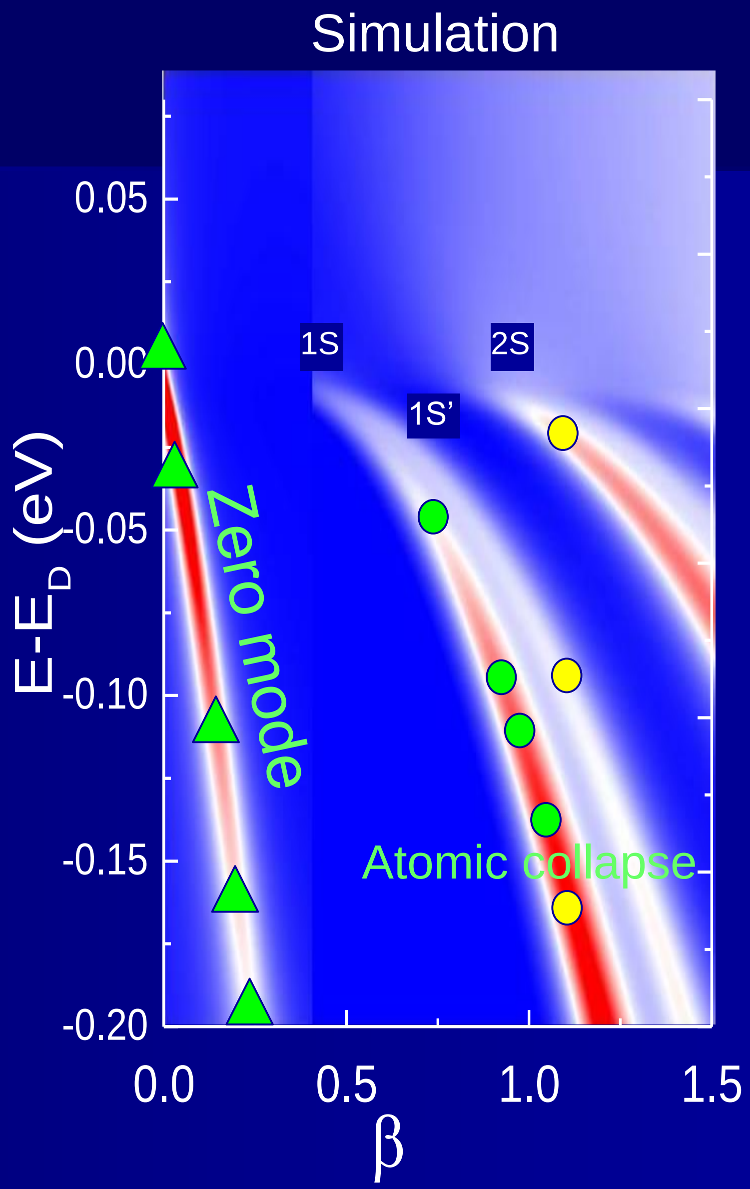




J. Mao et al, Nature Physics 2016

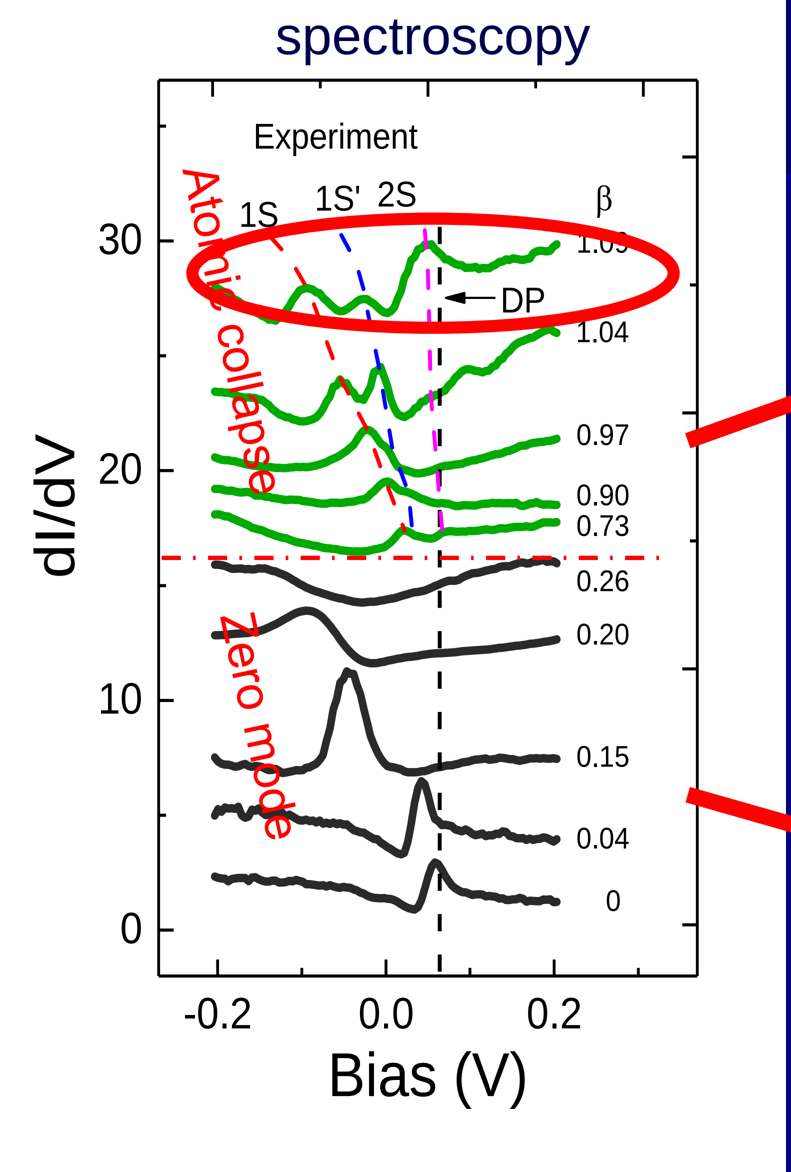
Charge Buildup



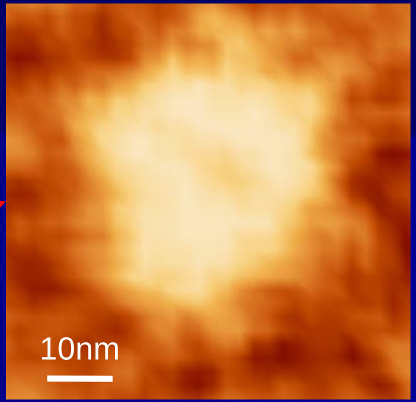


E.Y. Andrei

Charge Buildup



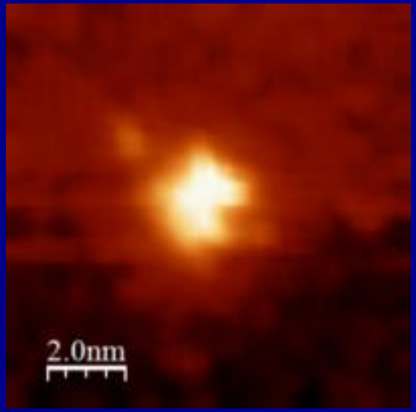
1S



Collapse peaks extended ~ 20nm

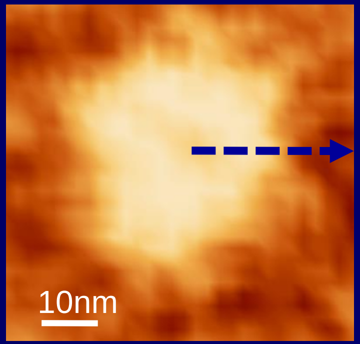
ZM peak tightly localized ~ 2nm

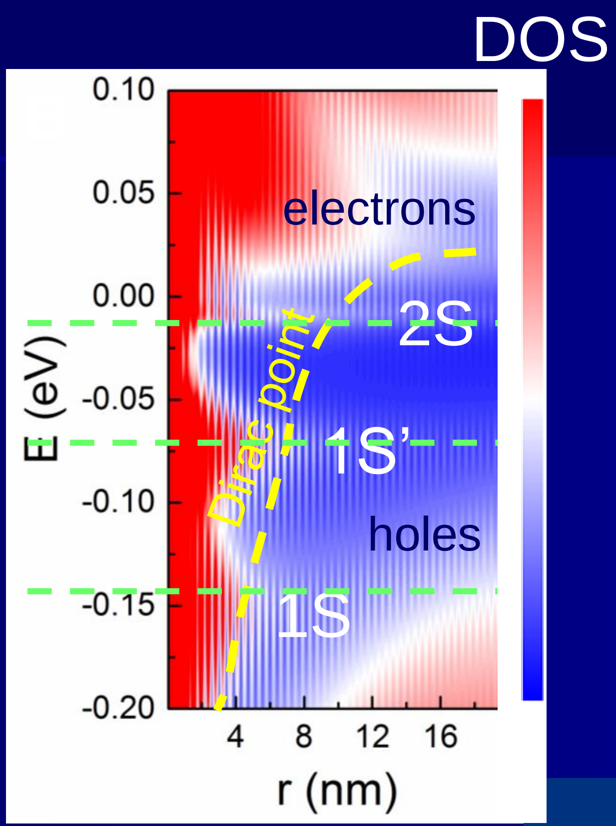
Zero mode peak

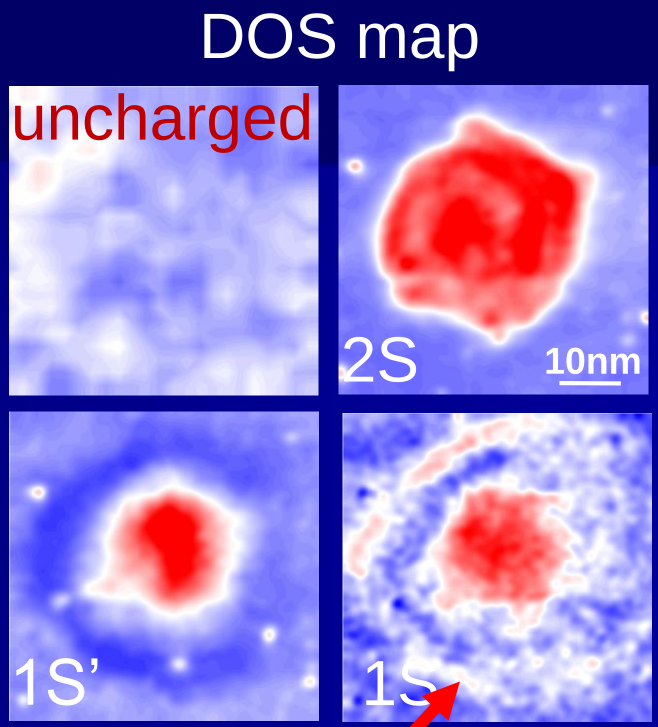


J. Mao et al, Nature Physics 2016

Spatial Dependence -Artificial Atom







Captured electron state surrounded by halo of hole states

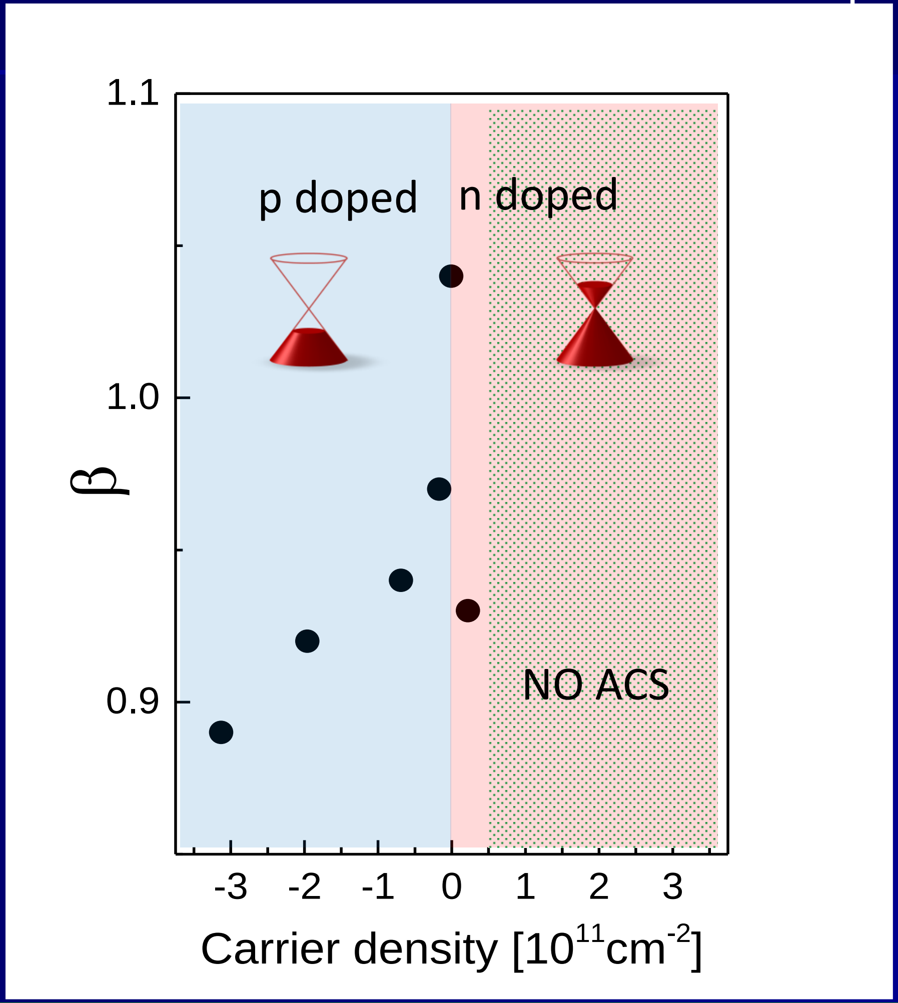
mechanism to confine electrons in graphene

J. Mao et al, Nature Physics 2016

Asymmetric Screening

J. Mao et al Nature Physics 2016

Gate dependence



Gate controlled switch for trapping and releasing carriers

Summary of part III

- QED Fine structure constant measures strength of electromagnetic interaction
- IN QED interactions is weak $\mapsto$ periodic table could survive to Z~137

$$\alpha_{QED} = \frac{e^2}{\hbar c} \approx \frac{1}{137}$$

$$Rydberg = \frac{Z^2 m e^4}{2\hbar^2} = \frac{1}{2} mc^2 (Z\alpha)^2$$

- In graphene fine structure constant is large $\mapsto$ strong interactions

$$\alpha_{graphene} = e^2 / \kappa \hbar v_F \approx 1$$

- "Atomic collapse" observable already for Z ~1

Question we can ask:
Physics at large α?