Relativistic Phenomena in Graphene: Optics, Atomic Collapse, Invisible States.

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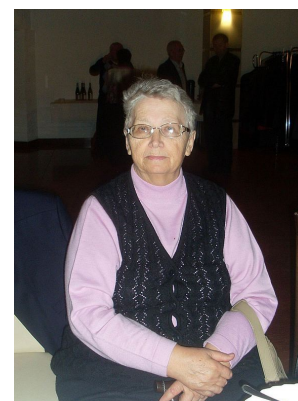
Київ, Жовтень 2015

...або: На добраніч, діти!

Дід Панас (Укр. Телебачення)

УФМЛ (старий будинок)

Виктор Товиевич Топоров, физика
(now in NY)

Нина Григорьевна Серикова,
математика

University of Exeter:

– Consistently in the top 10 UK league tables

– Quantum Systems and Nanomaterials group,
  Prof. A.K.Savchenko Center for NanoScience

– Graphexeter (S. Russo): flexible, transparent, well-conducting form
   of doped graphene; potential ITO replacement for touchscreens

– Other activities: Astro(exoplanets), Electromagnetic metamaterials,
                          Biophysics, Centre for Doctoral Training in MetaMat.

How a condensed matter (or solid-state) physicist looks at the world

Nominally (HEP): the world is made of electrons and protons (or quarks), held together by EM and strong forces.

However, solids often look as if they were made of something else: their transport, optical, etc properties suggest that their constituents are different particles known as <u>quasiparticles.</u>

If it walks like a duck, quacks
like a duck,
swims like a duck
– then it is a duck
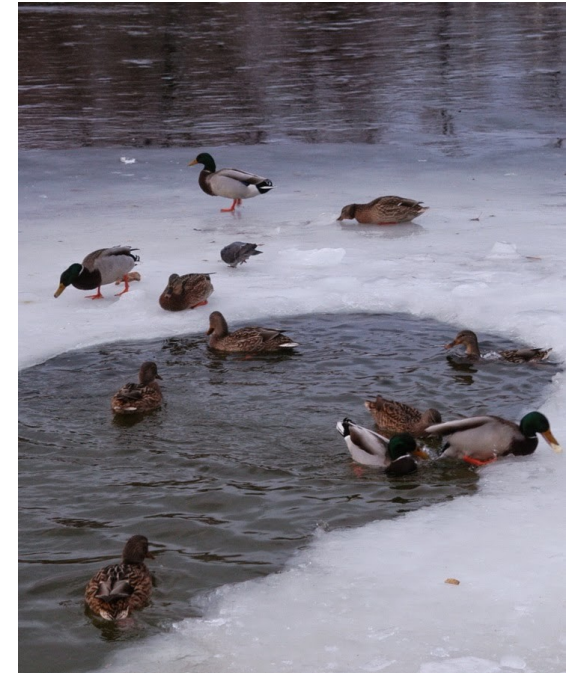
(and not a random mix of quarks and leptons)

The properties of quasiparticles can be very different from those of electrons:

– Mass (energy dispersion, dispersion law for deBroglie waves)

– Charge/spin

– Statistics (Bosons / Fermions / neither)

– Internal quantum numbers

$$\epsilon(\boldsymbol{p}) = \hbar\omega(\boldsymbol{k}) \qquad \boldsymbol{p} = \hbar\boldsymbol{k}$$

Exc. energy   (Quasi)momentum, defined modulo reciprocal
(above the g.s.)   lattice vector

E.g.: for a nonrelativistic electron $\qquad \epsilon = \dfrac{m\boldsymbol{v}^2}{2} = \dfrac{\boldsymbol{p}^2}{2m}, \qquad \boldsymbol{p} = m\boldsymbol{v}$
      in a vacuum

рил, что за Ландау он пошел бы на каторгу.

Дипломная работа Чука касалась свойств металлов при очень низких температурах. Первым делом для этой цели нужно было изучить теорию металлов, но без излишней мишуры и ненужных деталей. Для этого очень подходящей оказалась обзорная статья Р. Пайерлса в «Ergebnisse der exakten Naturwissenschaften», написанная по-немецки. Статью эту вместе с Чуком изучал и я. Ландау и нам вслед за ним нравилось в этой статье то, что в ней с самого начала электрон рассматривается не как свободная частица, а как некоторая квазичастица, обладающая определенными энергией и квазиимпульсом, причем зависимость энергии от квазиимпульса может быть произвольной. Впоследствии эту зависимость, которую стали называть произвольным законом дисперсии, вроде бы «переоткрыли» заново, хотя она была известна с 1928 г. после классической работы Ф. Блоха. Не дай бог, если бы при изучении свойств электронов проводимости в металле в материалах, представляемых Ландау, или, как мы их называли, формулярах, он увидел бы квадратичный, а не произвольный закон дисперсии — был бы колоссальный «разгон»! Используя общий закон дисперсии электронов в кристалле, Чук

*А.И.Ахиезер, о работе в теоротделе УФТИ в Харькове (~1935), из кн. «Воспоминания о Л.Д. Ландау»*

Well-known examples of charge-carrying quasiparticles in metals and semiconductors:

– (Quasi)Electrons and (Quasi)holes in semiconductors (effective mass)

– Cooper pairs formed by electrons in superconductors, due to attractive forces mediated by phonons

– Excitons (bound states of electrons and holes)

# Artificial solids: a portal into a strange man-made universe of unusual quasiparticles
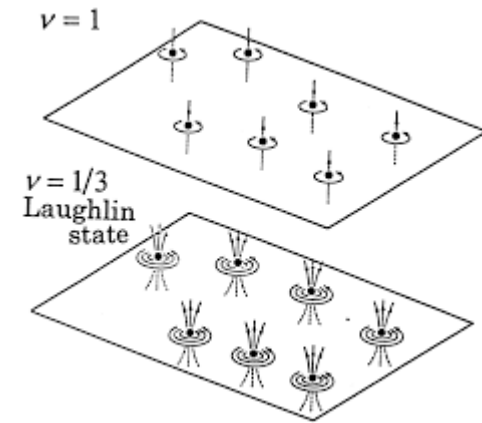
- Semiconducting 2D quantum wells (~1980):
  fractionalized charges in FQHE, unusual statistics
  (NP 1998: Laughlin, Stormer, Tsui); quantum computing??

- One-dimensional quantum wires (~1990), nanotubes,:
  polymers: fractional charges, spin-charge separation

- Cold atoms in optical traps

- Graphene (2004), topological insulators, dihalcogenides:
  Dirac fermions (dispersion, internal quantum numbers, chirality)
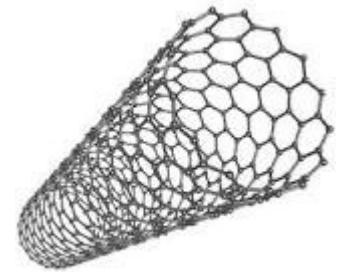
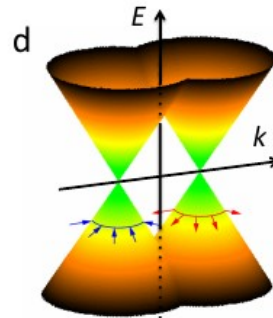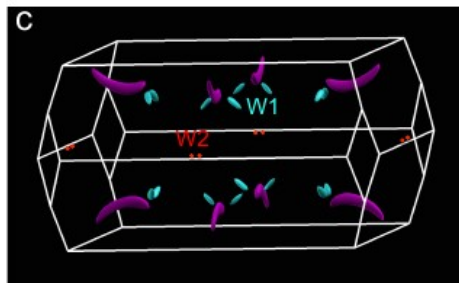# Artificial solids: a portal into a strange man-made universe of unusual quasiparticles

Figure 1
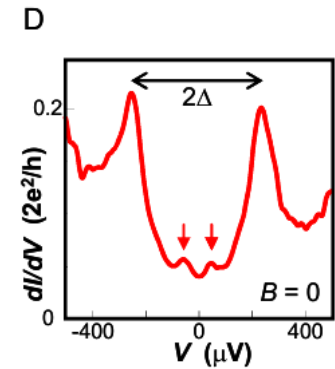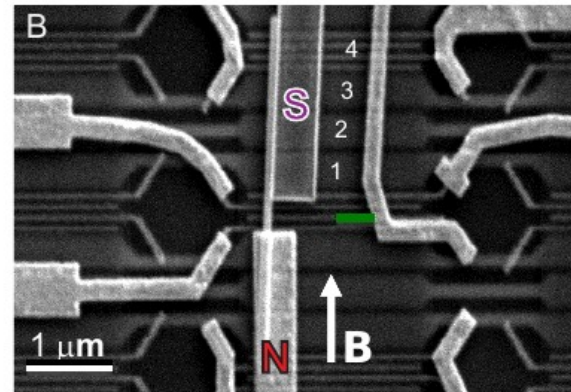
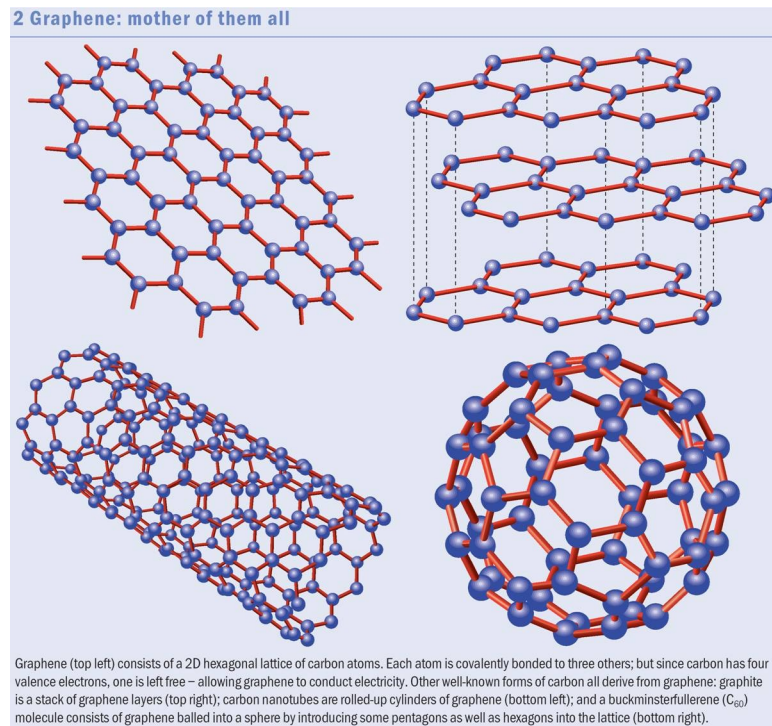*V.Mourik et al, Science 336, 1003 (2012)*

Recent developments:

- Majorana fermions in superconducting junctions (~2012): unusual statistics
- 2015: Weyl fermions in TaAs: chiral relativistic particles, the 3d version of graphene / topological insulators

$$H = v\boldsymbol{\sigma} \cdot \boldsymbol{p}$$

B.Lv et al, Nature Physics 11, 724 (2015)

Graphene: one(or two or three) -atom-thick 2D solid

2 Graphene: mother of them all

Graphene (top left) consists of a 2D hexagonal lattice of carbon atoms. Each atom is covalently bonded to three others; but since carbon has four valence electrons, one is left free – allowing graphene to conduct electricity. Other well-known forms of carbon all derive from graphene: graphite is a stack of graphene layers (top right); carbon nanotubes are rolled-up cylinders of graphene (bottom left); and a buckminsterfullerene (C_{60}) molecule consists of graphene balled into a sphere by introducing some pentagons as well as hexagons into the lattice (bottom right).
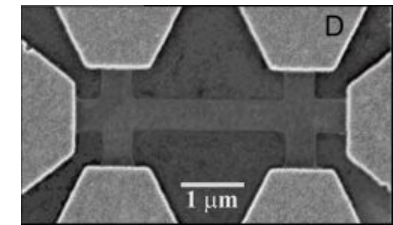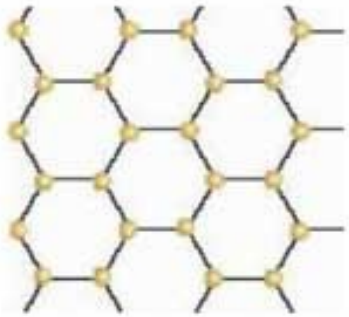
Andre Geim

Kostya Novoselov

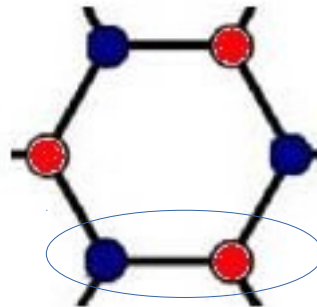In graphite, carbon forms two-dimensional planes which can be extracted, processed and experimented upon (NP 2010)

Novoselov et al, Science <u>306</u>, 666 (2004)
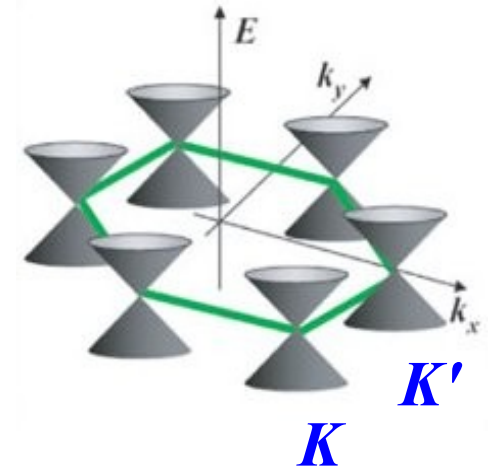
Dirac Fermions in Monolayer Graphene

Two sublattices

$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$

unit cell

K′

K

– The wave function of electrons in graphene has a non-trivial internal structure, owing to symmetries of the lattice.
– As a result, electron states are described by a two-dimensional version of Dirac equation, with no mass term

$$\hat{H} = v_F \left(\hat{\sigma}_x \, \hat{p}_x + \hat{\sigma}_y \, \hat{p}_y \right) \qquad \epsilon = \pm v_F |\boldsymbol{p}| \qquad R.P.Wallace\ (1947)$$

Pauli matrices

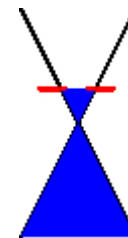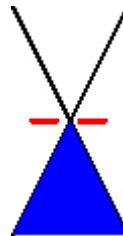– However, this pseudo-relativistic motion is rather slow: $v_F \approx \dfrac{c}{300}$

– True 2D crystal

– Conductive (can be probed by transport measurements, scanning tunneling microscopy)

– The surface can be open: «hands-on experience» with a scanning tunneling probe, or an atomic force microscope

– Super-strong, super-thin, super-everything…

– **Unusual electron dispersion, chirality, control over dispersion, internal degrees of freedom (pseudospin)**

– Control over electron density (and theFermi level position, and the carrier electric charge) via gating; quantum effects at room temperature
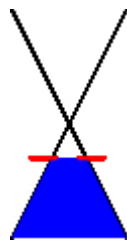
Hole doping   Neutrality point   Electron doping

Pseudospin and Chirality (monolayer)

$$\hat{H} = v_F(\hat{\sigma}_x \hat{p}_x + \hat{\sigma}_y \hat{p}_y) = v_F \begin{pmatrix} 0 & p_x - i\,p_y \\ p_x + i\,p_y & 0 \end{pmatrix}$$
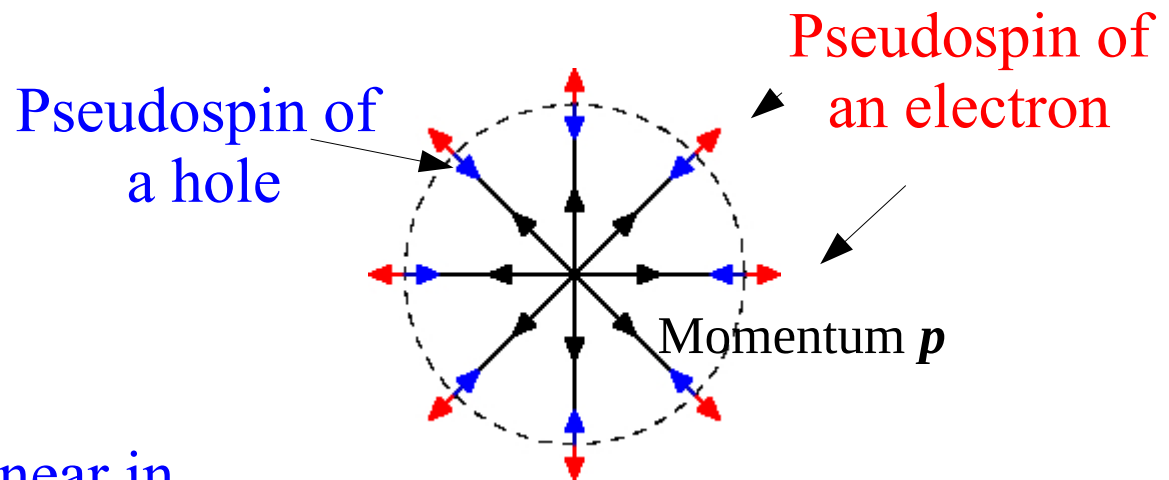
(Energy dispersion
Is now a matrix
In the pseudospin space)

Linear dispersion: $\epsilon_k = \pm v_F |\boldsymbol{p}|$

Hence, there are two bands, electron and holes, and they differ
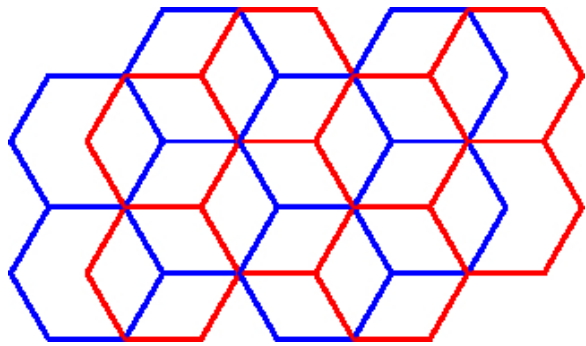by the alignment between the pseudospin and the momentum.

Pseudospin of
an electron

Pseudospin of
a hole

$\nu(\epsilon)$

ϵ
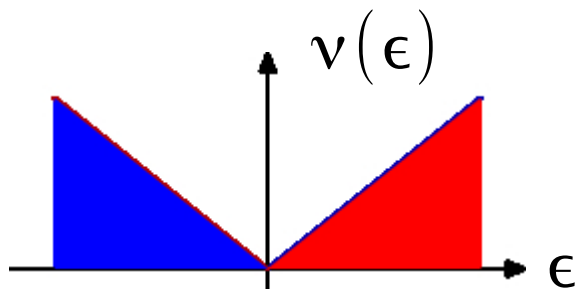
Momentum $\boldsymbol{p}$

The density of states (DOS) is linear in
energy and hence is suppressed at ε=0,
almost like a gap.

"Massive" Chiral Particles in Bilayers

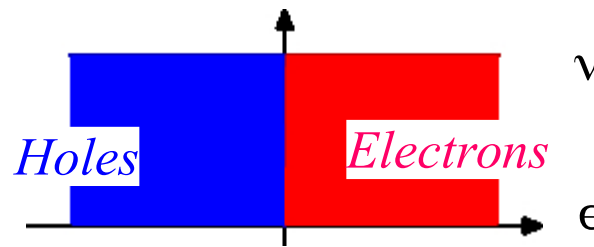In bilayer graphene with *A-B* stacking, interlayer tunneling makes the kinetic energy quadratic in momentum:

$$H_{bi} = \frac{1}{2m^*} \begin{vmatrix} 0 & (p_x - i\,p_y)^2 \\ (p_x + i\,p_y)^2 & 0 \end{vmatrix} + U(x,y)$$
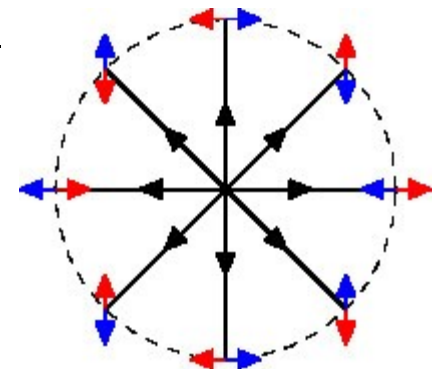
McCann, Falko (2006)

The effective mass («semiconducting» order of magnitude): $m^* \approx 0.036\, m_e$

The states of free carriers are given by chiral w.f.'s, and fill two continua:

$$\epsilon_k = \pm \frac{\hbar^2 k^2}{2m}$$

$$\nu(\epsilon) = \frac{m^*}{2\pi\hbar^2}$$

Holes   *Electrons*

Pseudospin rotates at the double speed,
Berry phase of 2π, degenerate QH level at $\varepsilon = 0$

Common features:

– The pseudospin is aligned with momentum, although the alignment is different between monolayers and bilayers. This is known as chirality

– No energy gap between electrons and holes: coexistence of electron-like and hole-like states is possible.
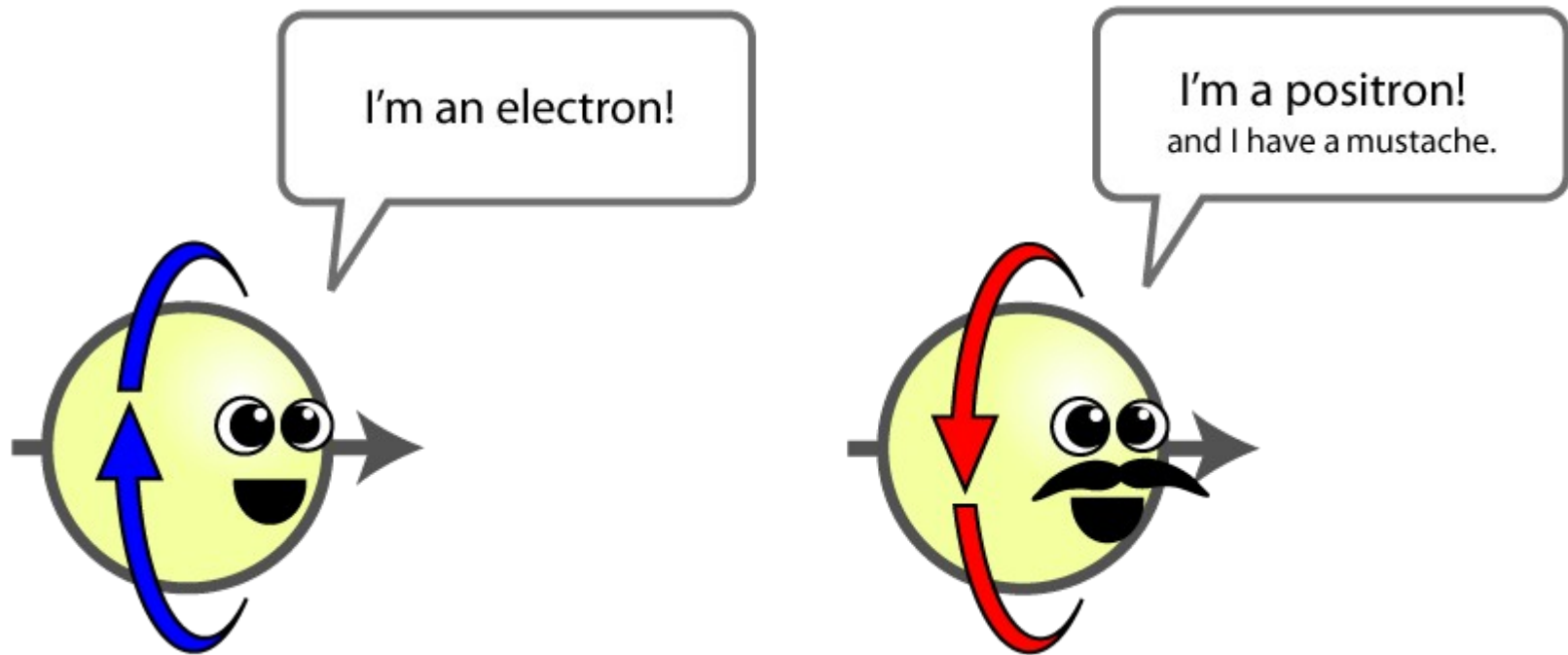
From quantumdiaries.org (Helicity, chirality, mass, and the Higgs)

The dispersion laws and chirality can be probed in quantum transport experiments, e.g., in Quantum Hall measurements (Hall conductivity in strong magnetic fields)
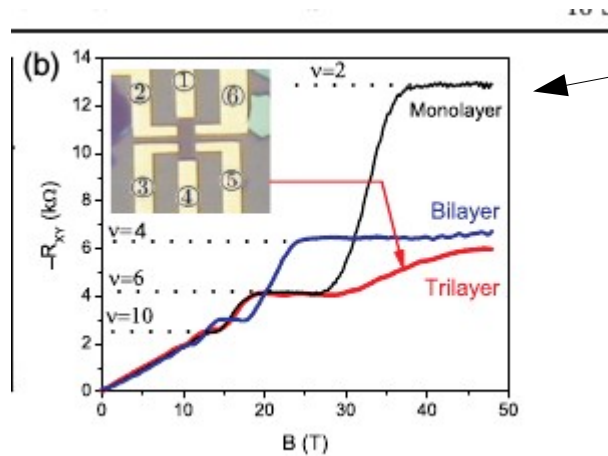

Half-integer QHE (hallmark of Dirac fermion behaviour)

Due to different properties of dispersion and chirality, transport properties can be altered by adding only one extra layer.
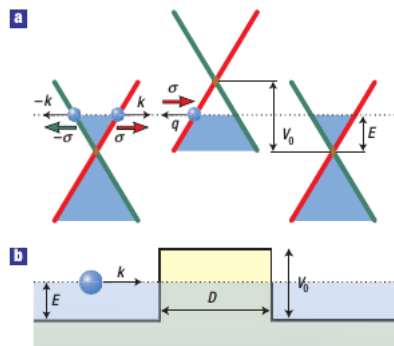
A.Kumar et al, PRL **107,** 126806 (2011)

"Optics" in Graphene heterojunctions

Polarisation matters: when the incoming light is incident at Brewster's angle, it is reflected in fully polarised state (numerous applications in optics: sunglasses, photography, golography)
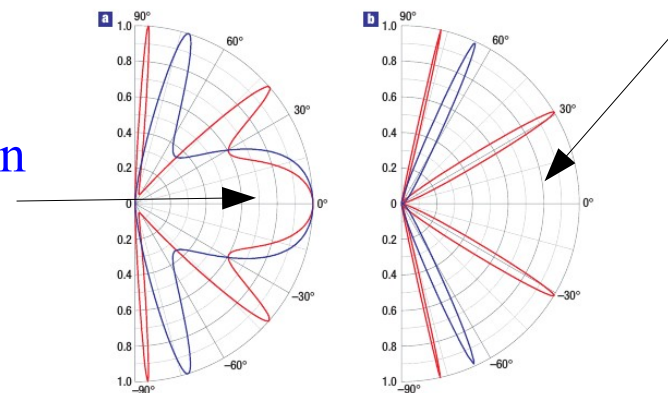
Incident ray (unpolarised)

Reflected ray (polarised)

θ_B

From wikipedia

Refracted ray (slightly polarised)
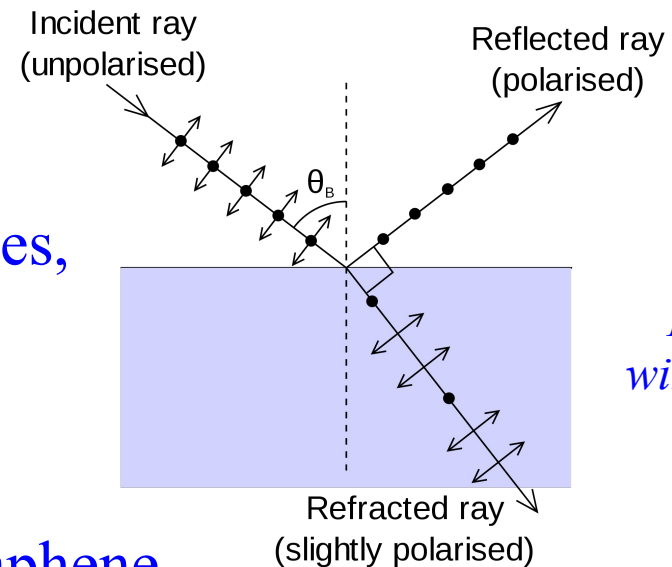
Klein paradox: electrons in monolayer graphene are perfectly transmitted through a *pn*-junction

Perfect reflection (bilayer)

Perfect transmission at θ=0 (mono)

Katsnelson, Novoselov, Geim, Nat Phys 2, 620 (2006)

Figure 2 **Klein-like quantum tunnelling in graphene systems. a,b,** Transmission probability *T* through a 100-nm-wide barrier as a function of the incident angle for single- (**a**) and bi-layer (**b**) graphene. The electron concentration *n* outside the barrier is chosen as 0.5×10^{12} cm^{-2} for all cases. Inside the barrier, hole concentrations *p* are

"Optics" in Graphene heterojunctions
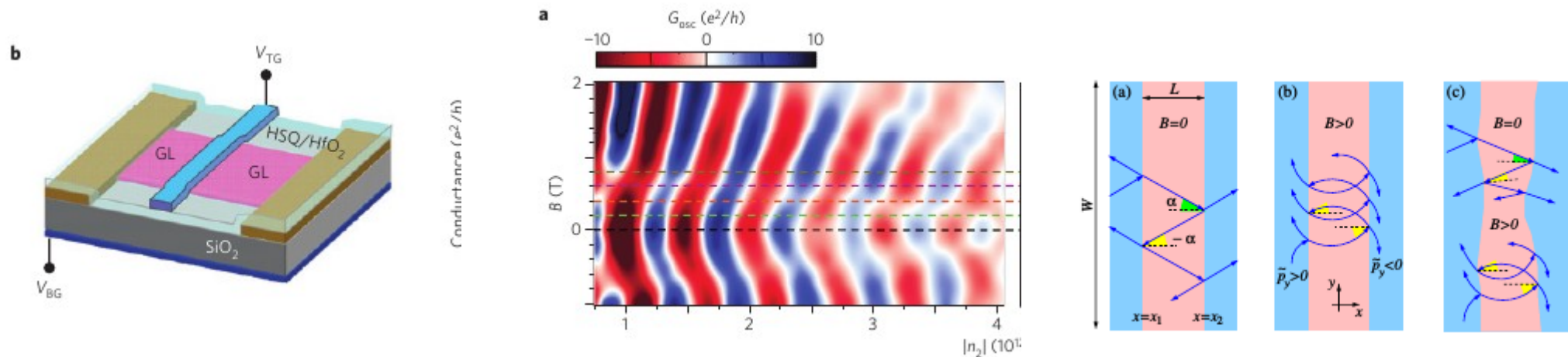
Away from normal incidence: negative refraction index ($n = -1$);
due to opposite velocities of electrons and holes

$$p_{y,e} = p_{y,h} \qquad \boldsymbol{v}_{e,h} = \frac{d\,\epsilon_{e,h}}{d\,\boldsymbol{p}} = \pm v\,\hat{\boldsymbol{p}}$$

This enables construction of the Veselago lens (perfect geometrical optics, aberration free)
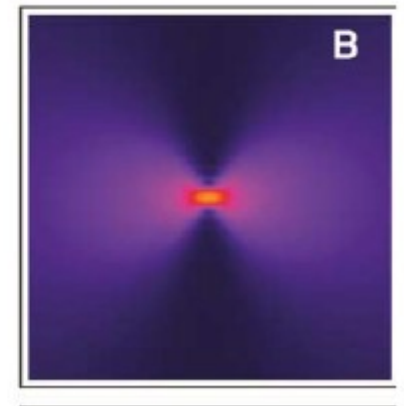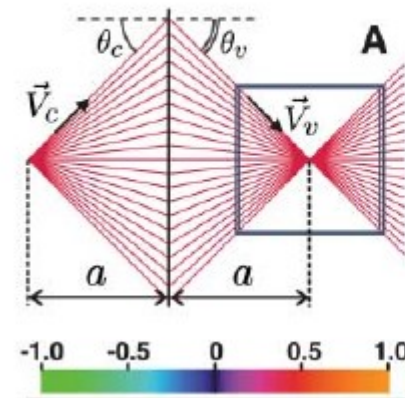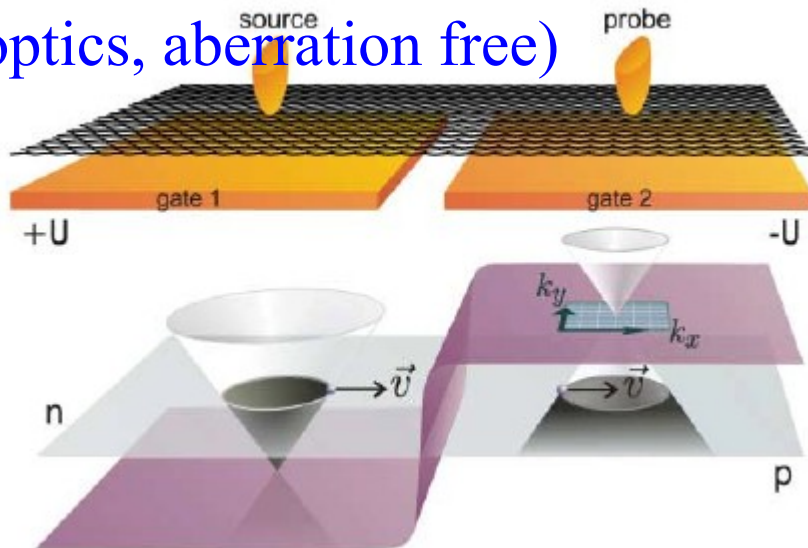
Electron interferometer: detecting reflectionless Klein tunneling from the phase shift
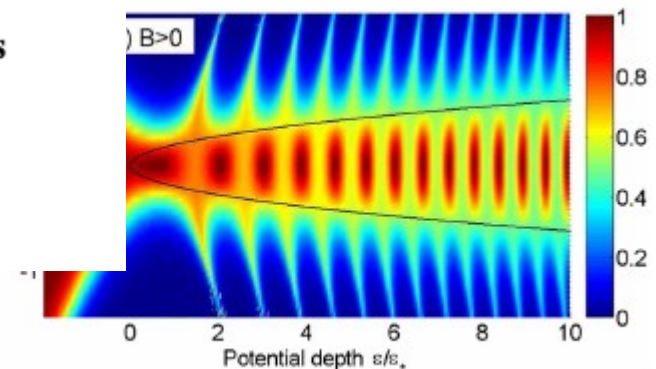

*Young and Kim, Nat.Phys. **5**, 222 (2008)*

Klein Backscattering and Fabry-Pérot Interference in Graphene Heterojunctions

Andrei V. Shytov,[1] Mark S. Rudner,[2] and Leonid S. Levitov[2]

[1]*Department of Physics, University of Utah, Salt Lake City, Utah 84112, USA*
[2]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

Monolayer graphene: relativistic dispersion
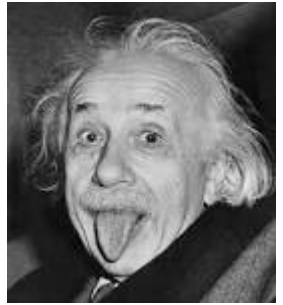
– At large enough energies, all particles become relativistic

$$E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$E = \sqrt{p^2 c^2 + m^2 c^4} = \begin{cases} mc^2 + \dfrac{p^2}{2m} & p \to 0 \quad \text{Non-relativistic} \\[3mm] cp & E \gg mc^2 \quad \text{Ultrarelativistic} \end{cases}$$

– Particle's velocity can never exceed the speed of light

– What are the consequences for quantum theory?

Relativistic theory of an electron: Dirac equation

$$\left[\gamma_\mu\left(-i\hbar\partial_\mu - eA_\mu\right) - m\right]\Psi = 0$$

4x4 matrices

Wave function is a 4-component vector

Free solutions: $\epsilon(p) = \pm\sqrt{p^2 c^2 + m^2 c^4}$

$E(p)$

Electron states, empty (conduction band)

$2mc^2$ Mass gap, no free states

Positron (or hole) states forming Dirac sea (valence band)
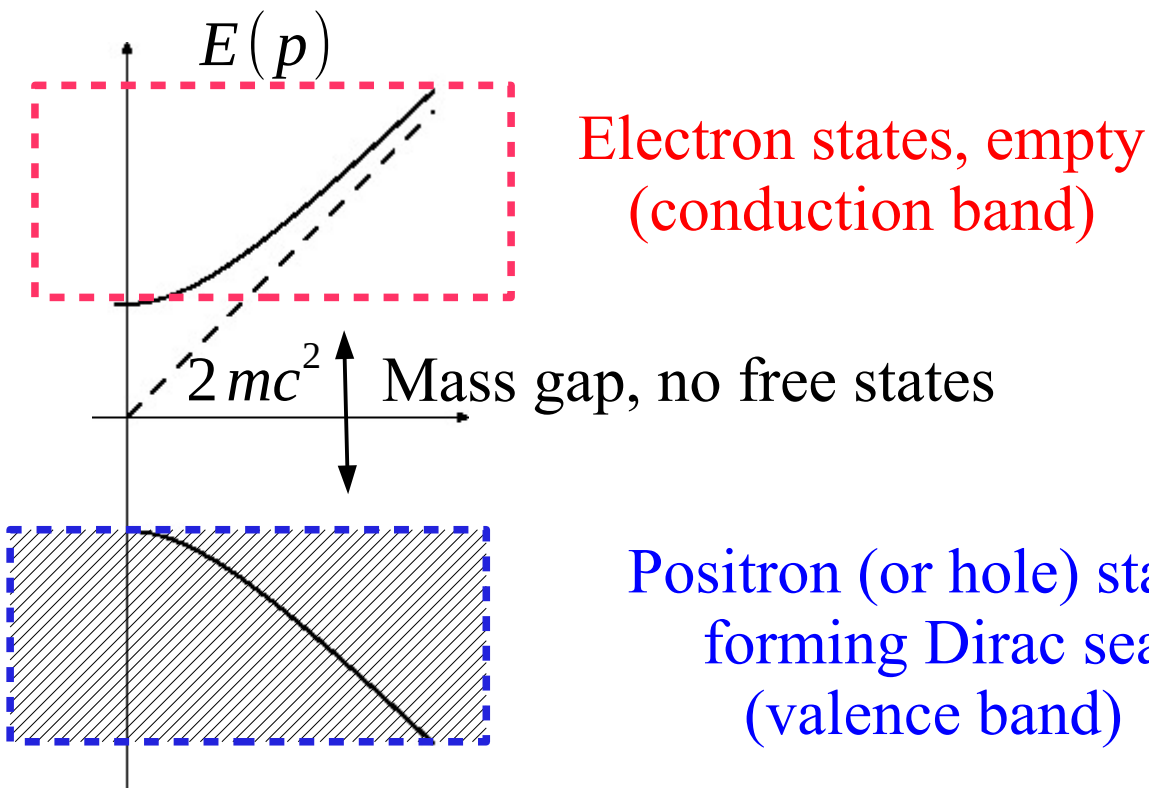
This quantum relativistic particle has 4 internal states; two of these can be identified with particle's spin-up and spin-down states..

The other two states are the two spin states for an antiparticle (HEP) or a hole (CM).

Supercritical atom

Collapse, vacuum reconstruction
(Z > Zc = 170)
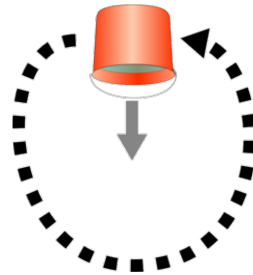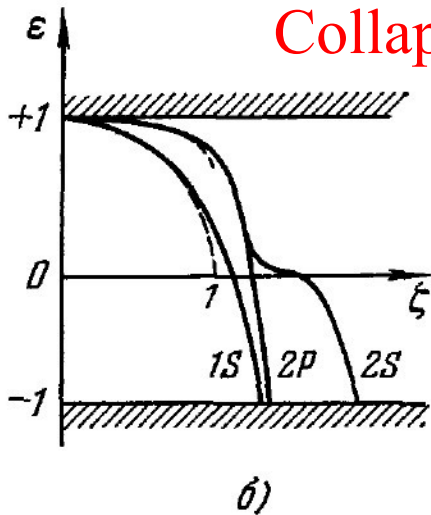
Gershteyn, Zeldovich (1969)
Popov (1970)

– Electron state embedded into Dirac sea is hybridised with positron states, this gives rise to a resonant level of finite width, which can be treated as a complex energy level

electrons

$$E = E_0 - i\,\Gamma$$

Position   Width (tunneling rate)

positrons
(holes)

– The energy can be lowered by filling up the localised level => spontaneous positron emission; discharging the supercritical nucleus

Atomic collapse can be modeled by charged impurities in graphene:

Atomic Collapse and Quasi–Rydberg States in Graphene

A. V. Shytov,[1] M. I. Katsnelson,[2] and L. S. Levitov[3]
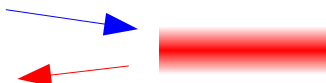
[1]Brookhaven National Laboratory, Upton, New York 11973-5000, USA
[2]Radboud University of Nijmegen, Toernooiveld 1 6525 ED Nijmegen, The Netherlands
[3]Department of Physics, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, Massachusetts 02139, USA
(Received 6 August 2007; published 14 December 2007)

Charge impurities in graphene can host an infinite family of Rydberg-like resonance states of massless Dirac particles. These states, appearing for supercritical charge, are described by Bohr-Sommerfeld quantization of *collapsing* classical trajectories that descend on point charge, in analogy to the hydrogenic Rydberg states relation with planetary orbits. Strong tunnel coupling of these states to the Dirac continuum leads to resonance features in scattering on the impurities that manifest themselves in transport properties and in the local density of states.

– The collapse occurs at a much lower critical charge ($Z\sim1$ vs 170)

– Manifestations: quasistationary states, resonances in tunneling

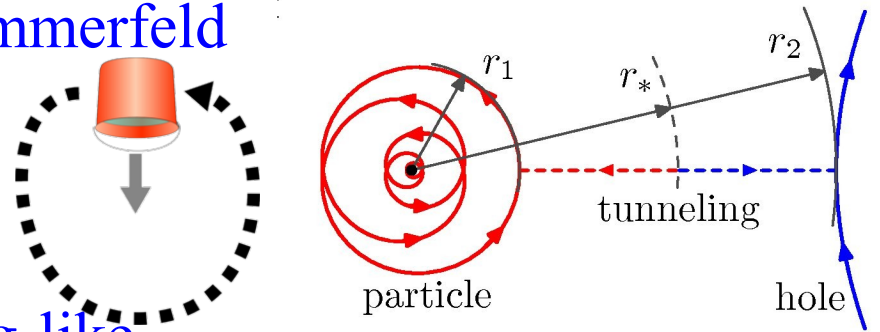– Strong effects in vacuum polarization (impurity charge is screened)

Semiclassical picture of collapse

The classical motion can be analysed employing energy and momentum consesrvation:

$$v_F^2\left(p_r^2+\frac{M^2}{r^2}\right)=\left(\epsilon+\frac{Ze^2}{r}\right)^2$$

The radial momentum obeys the Bohr-Sommerfeld quantisation rule:

$$\int_{r_0}^{r_1} p_r\, dr=\pi\hbar n$$

particle   tunneling   hole

This gives a spectrum of shallow Rydberg-like states

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

Their decay due to Klein tunneling can be found from the WKB approximation:

$$\gamma\equiv\sqrt{\beta^2-\left(m+\frac{1}{2}\right)^2}$$

$$\beta\equiv\frac{Ze^2}{\hbar v_F \kappa}$$

$$\Gamma_n\sim|\epsilon|e^{-2S_{tun}/\hbar}\sim|\epsilon_n|e^{-2\pi\beta}\quad S_{tun}\equiv\int_{r_1}^{r_2} p_r\, dr$$

Note the angular momenta are half-integer (due to the Berry phase)
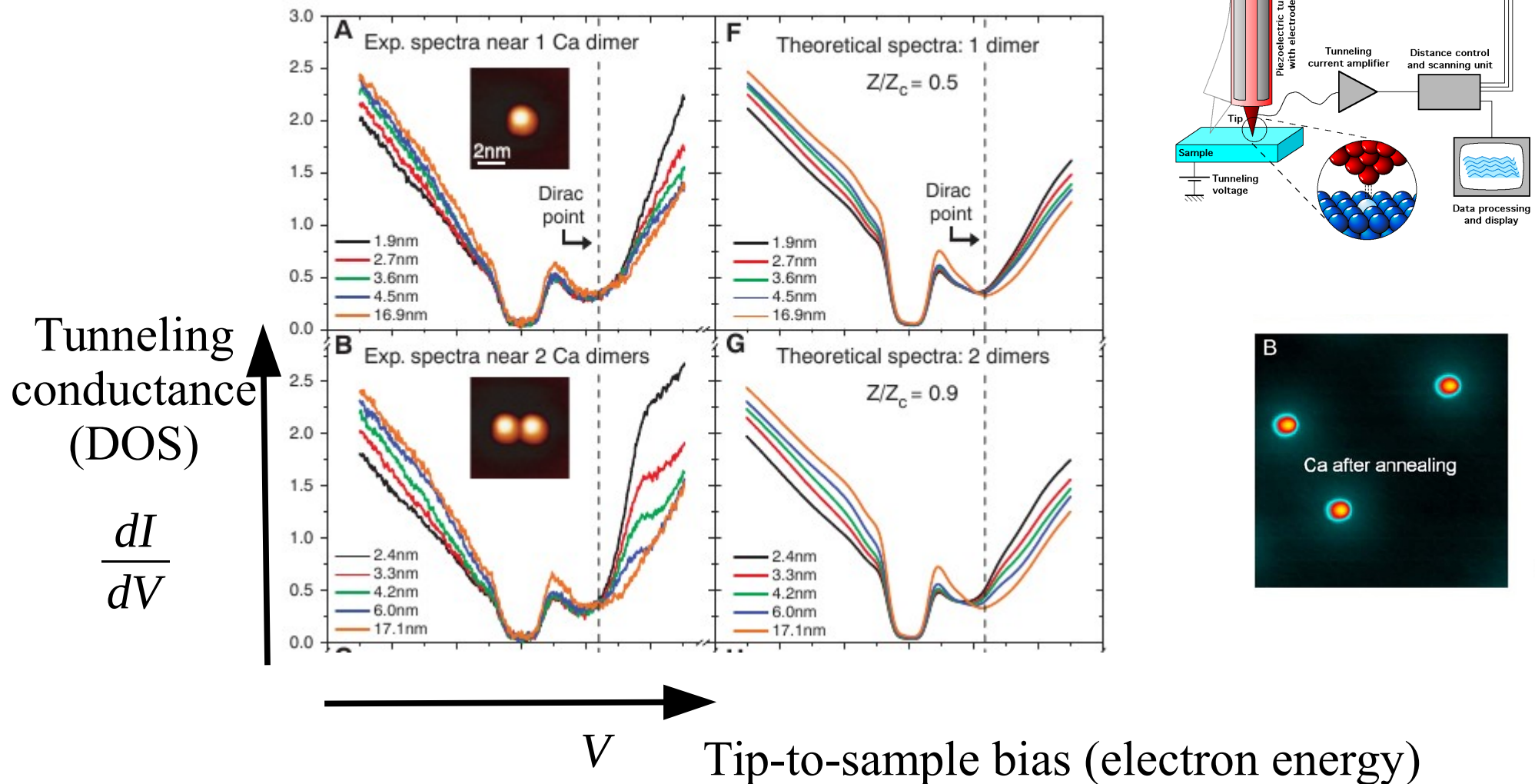
$$M=\hbar\left(m+\frac{1}{2}\right)$$

Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene

Yang Wang,[1,2]* Dillon Wong,[1,2]* Andrey V. Shytov,[3] Victor W. Brar,[1,2] Sangkook Choi,[1]
Qiong Wu,[1,2] Hsin-Zon Tsai,[1] William Regan,[1,2] Alex Zettl,[1,2] Roland K. Kawakami,[5]
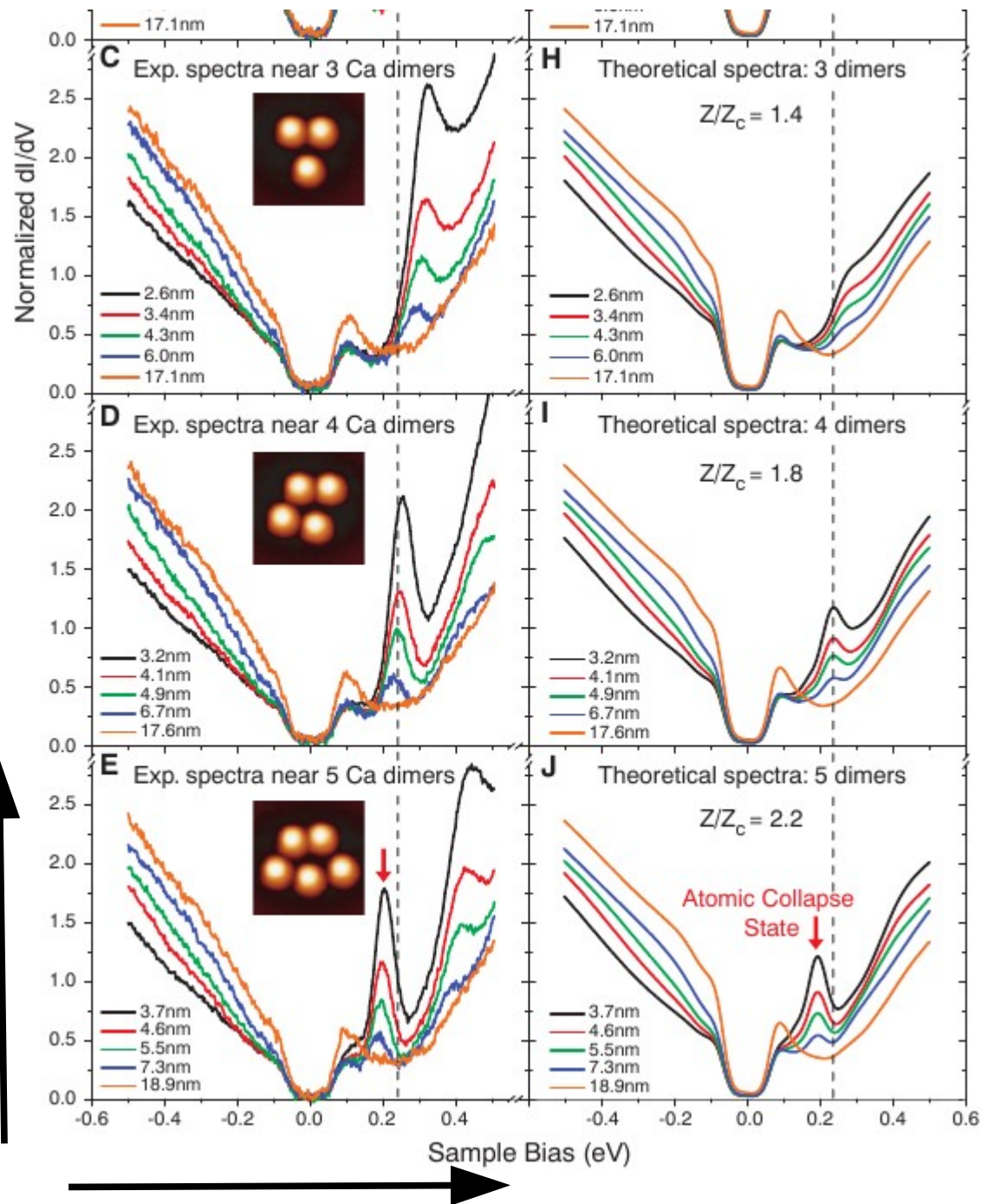Steven G. Louie,[1,2] Leonid S. Levitov,[4] Michael F. Crommie[1,2]†

Relativistic quantum mechanics predicts that when the charge of a superheavy atomic nucleus surpasses a certain threshold, the resulting strong Coulomb field causes an unusual atomic collapse state; this state exhibits an electron wave function component that falls toward the nucleus, as well as a positron component that escapes to infinity. In graphene, where charge carriers behave as massless relativistic particles, it has been predicted that highly charged impurities should exhibit resonances corresponding to these atomic collapse states. We have observed the formation of such resonances around artificial nuclei (clusters of charged calcium dimers) fabricated on gated graphene devices via atomic manipulation with a scanning tunneling microscope. The energy and spatial dependence of the atomic collapse state measured with scanning tunneling microscopy revealed unexpected behavior when occupied by electrons.
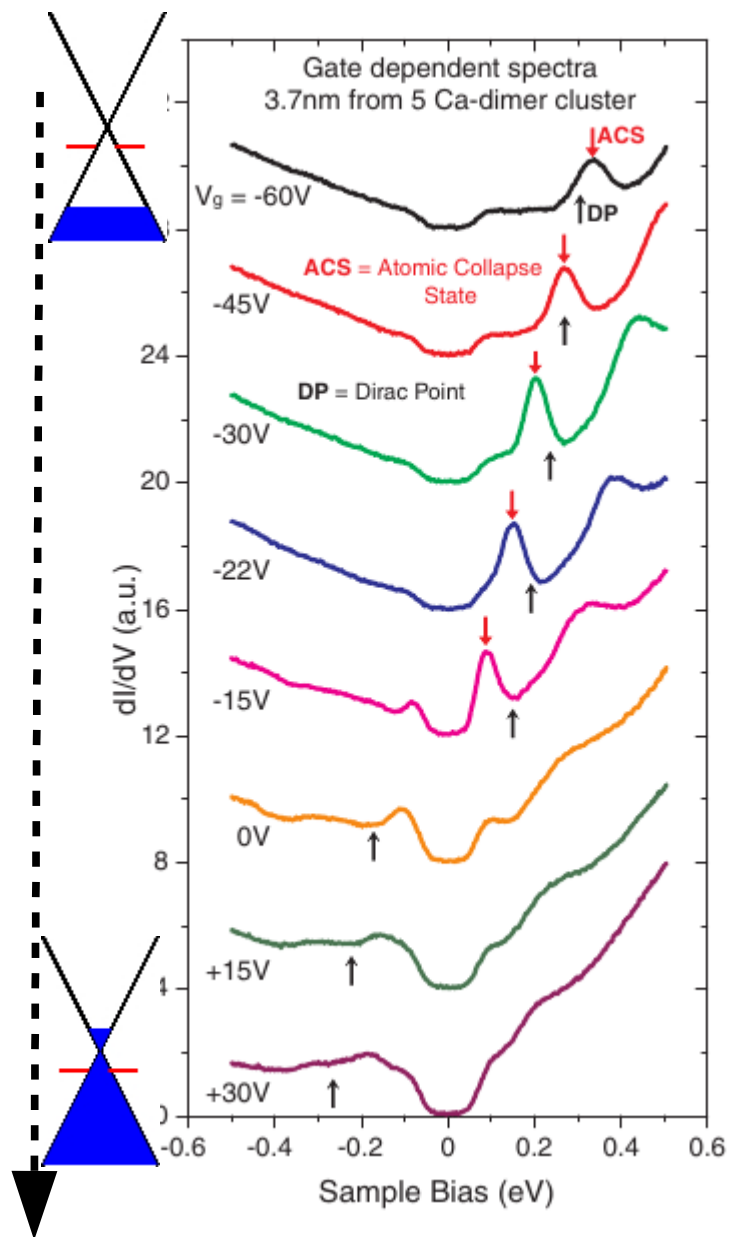
- Ca dimers on graphene have two states, charged and uncharged
- They can be moved around by an STM tip, and the charge states can be manipulated
- Thus, one can make «artificial atoms» and study them via tunneling spectroscopy.

Tunneling conductance (DOS)

$$\frac{dI}{dV}$$

V Tip-to-sample bias (electron energy)

C   Exp. spectra near 3 Ca dimers

Normalized dI/dV

2.6nm	
3.4nm	
4.3nm	
6.0nm	
17.1nm	

H   Theoretical spectra: 3 dimers

$Z/Z_c = 1.4$

2.6nm	
3.4nm	
4.3nm	
6.0nm	
17.1nm	

D   Exp. spectra near 4 Ca dimers

3.2nm	
4.1nm	
4.9nm	
6.7nm	
17.6nm	

I   Theoretical spectra: 4 dimers

$Z/Z_c = 1.8$

3.2nm	
4.1nm	
4.9nm	
6.7nm	
17.6nm	

E   Exp. spectra near 5 Ca dimers

3.7nm	
4.6nm	
5.5nm	
7.3nm	
18.9nm	

J   Theoretical spectra: 5 dimers

$Z/Z_c = 2.2$

Atomic Collapse State

3.7nm	
4.6nm	
5.5nm	
7.3nm	
18.9nm	

Sample Bias (eV)

Tunneling conductance (DOS)

Tip-to-sample bias (electron energy)

«In theory, theory and experiment are always the same. Experimentally, they are always different»

Features not explained by simple theory based on the single-particle Dirac equation:

– The resonance is sensitive to doping

– Sometimes, it occurs on the wrong side w.r.t. the Dirac point.

– Distance dependence of peak intensity.

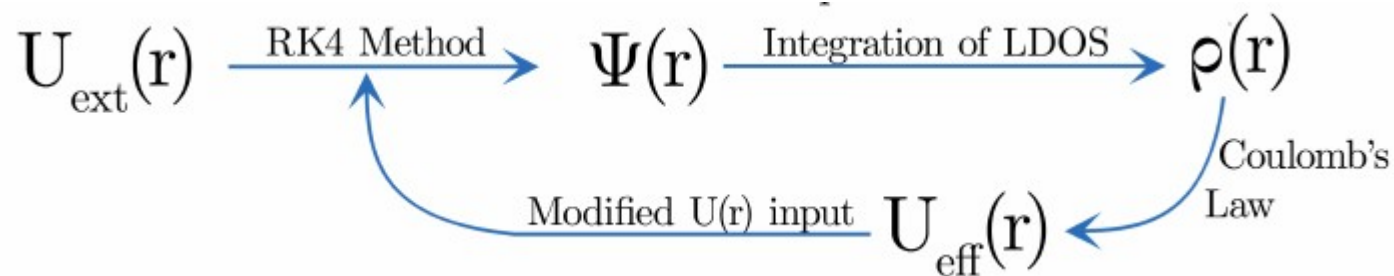Must be due to some many-body effects.

Electron density (Gate voltage)

The recent MPhys project:

A Self-Consistent Analysis of Coulomb Impurity States in Graphene: The Role of Screening

G. Pope, S. R. Taylor, Supervisor: Dr. A. V. Shytov

$$U_{ext}(r) \xrightarrow{\text{RK4 Method}} \Psi(r) \xrightarrow{\text{Integration of LDOS}} \rho(r)$$

$$\text{Modified } U(r) \text{ input} \quad U_{eff}(r) \xleftarrow{\text{Coulomb's Law}}$$

Aim: obtain a self-consistent solution numerically, by determining the potential from collapsing wave functions.
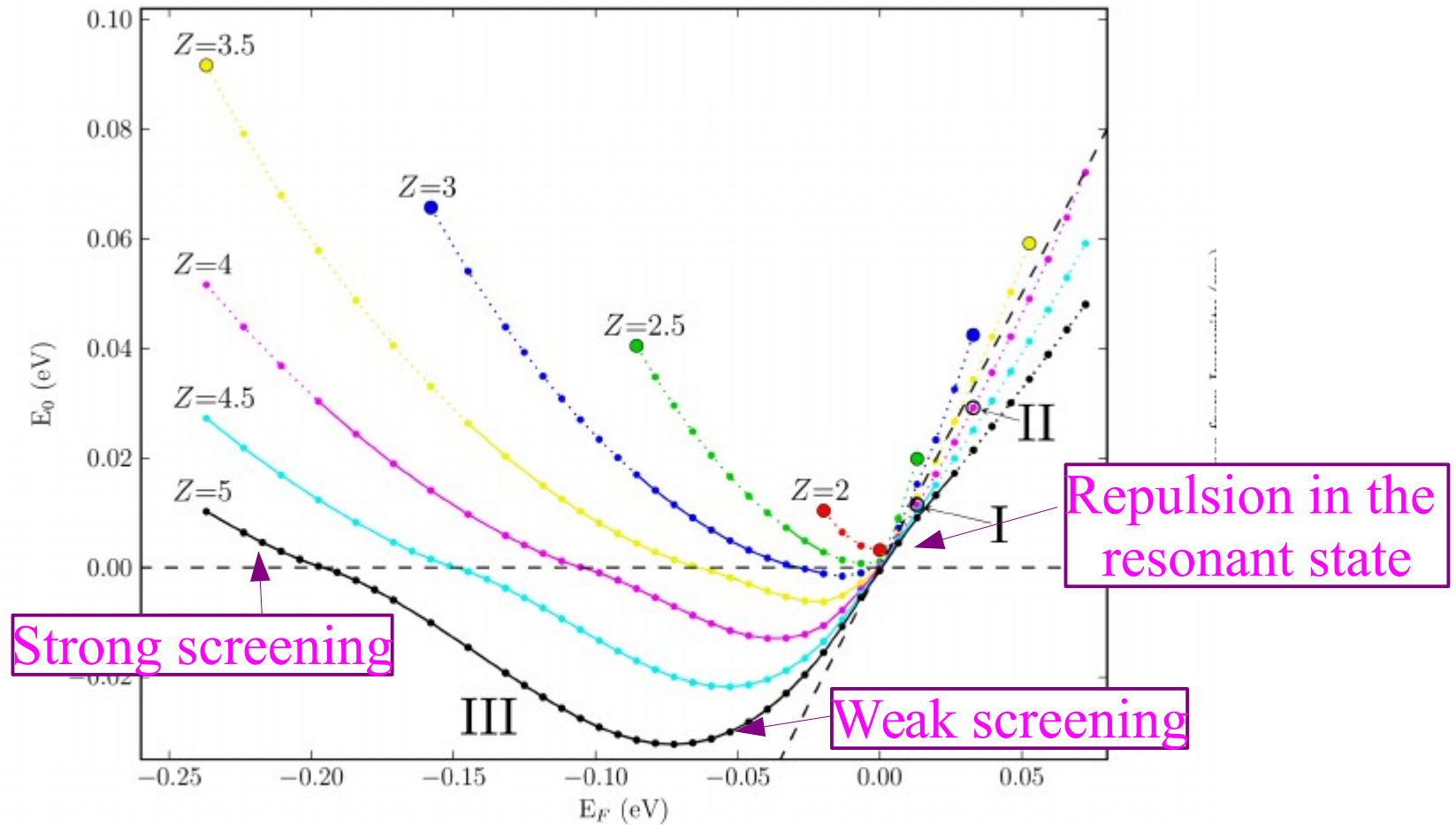(Basically, it is a Hartree approach.)

S.R.T., G.P., A.S., In preparation

Figure 4: energy of the LDOS collapsing peak with changing E_F for varying impurity charge Z. The dashed diagonal line shows $E_F = E_0$, the dashed horizontal line shows $E_0 = 0$.
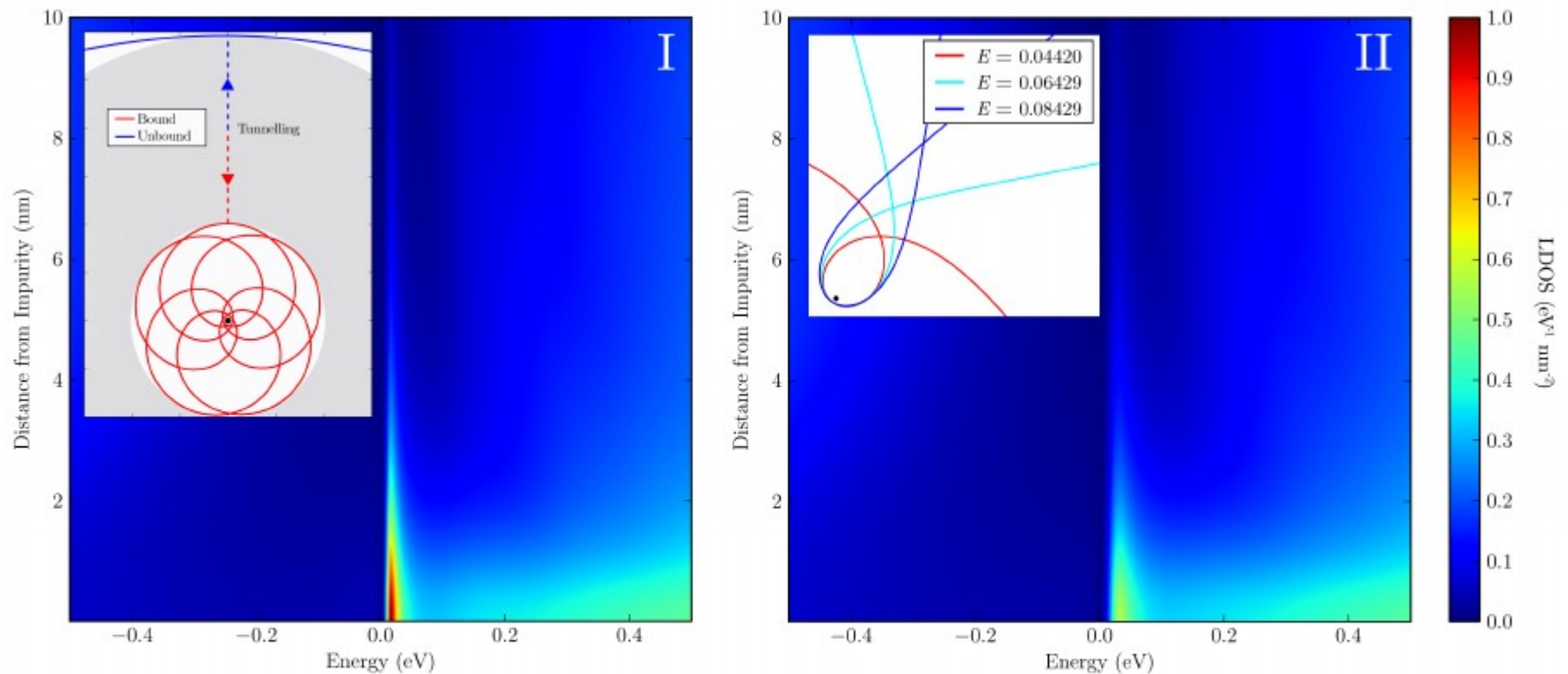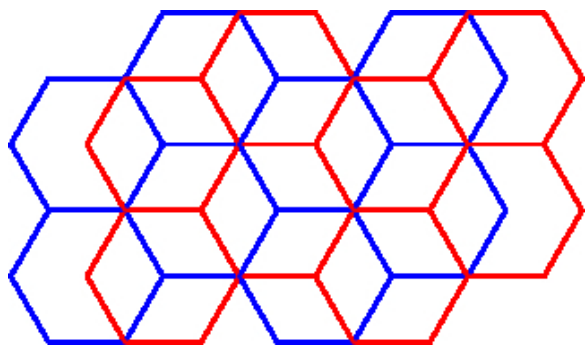
Resonant peak position

Gate voltage (electron density)

Figure 5: **LDOS for $Z = 4$.** We see for E_F=0.02 (I) the signature resonance of a quasi-bound state. The inset shows electron trajectories for a system with a classically forbidden region (grey), however electrons are not truly bound due to quantum tunnelling through the barrier. For E_F=0.05 (II) where there is no classically forbidden region, we see pseudo-resonance in the LDOS. The inset shows that there is no bound trajectory for the peak energy (red).

Weak resonances at positive energies describe slinging trajectories, and thus are precursors to the fully developed collapse

"Massive" Chiral Particles in Bilayers

In bilayer graphene with *A-B* stacking, interlayer tunneling makes the kinetic energy quadratic in momentum:

$$H_{bi} = \frac{1}{2m^*}\begin{vmatrix} 0 & (p_x - i\, p_y)^2 \\ (p_x + i\, p_y)^2 & 0 \end{vmatrix} + U(x,y)$$
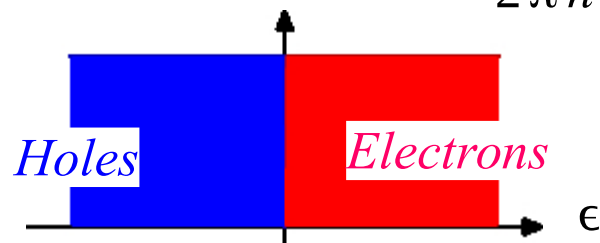
McCann, Falko (2006)

The effective mass: Note the phase!

$$m^* \approx 0.036\, m_e$$

The states of free carriers are given by chiral w.f.'s, and fill two continua:

$$\nu(\epsilon) = \frac{m^*}{2\pi\hbar^2}$$

$$\Psi_{\boldsymbol{k}}^{\pm} = \begin{pmatrix} e^{-i\varphi_k} \\ \pm e^{i\varphi_k} \end{pmatrix} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \qquad \epsilon_{\boldsymbol{k}} = \pm\frac{\hbar^2 \boldsymbol{k}^2}{2m}$$

Holes   *Electrons*

ϵ

Pseudospin rotates at the double speed,
Berry phase of 2π, degenerate QH level at $\varepsilon = 0$

Can bilayer graphene host a bound state? (and, what would it look like?)

– The quadratic dispersion (ignoring the sign) suggests a conventional bound state of a massive particle ...

$$\epsilon_k = \pm \frac{\hbar^2 k^2}{2m}$$

– … but such a state would immediately decay into the continuum, via hybridisation/tunneling/....

$$\nu(\epsilon) = \frac{m^*}{2\pi\hbar^2}$$
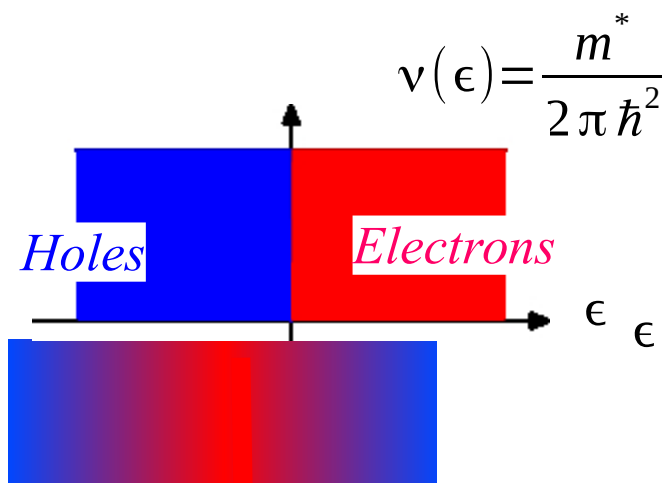
The flat DOS indicates a large number of available final states.

Holes   *Electrons* ϵ

Localised states are destroyed unless this coupling is suppressed.
Is it?
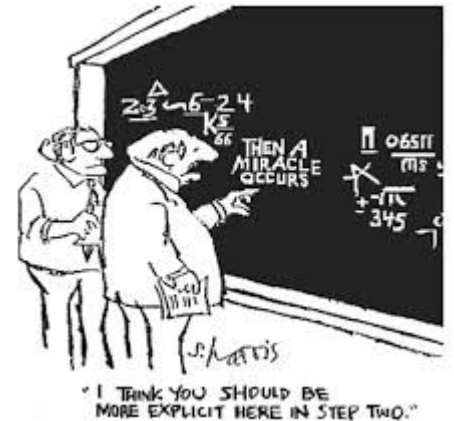
The equation for the wave function in bilayer graphene

$$\Psi(r,\varphi)=e^{iM\varphi}\begin{pmatrix} e^{-i\varphi}\left[u(r)+v(r)\right] \\ e^{i\varphi}\left[u(r)-v(r)\right] \end{pmatrix}$$

decouple in the s-wave channel($M = 0$):

$$\left[\epsilon-U(r)\right]u = -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{1}{r^2}\right)u$$

$$-\left[\epsilon-U(r)\right]v = -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{1}{r^2}\right)v$$

"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

These equations describe two completely decoupled particles:

– *u(r)*: the electron with positive parabolic dispersion, affected by the potential *U(r)*

– *v(r)*: the hole with negative parabolic dispersion, affected by *-U(r)*
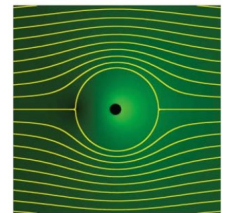
Both electrons and holes are described by the Schrödinger eqn for a massive non-chiral particle in the *p*-wave channel.

Hence:

– Bilayer graphene can host a localised electron-like state immersed into a continuum of hole-like states.

– Hence the level is *cloaked*: it cannot be probed by looking at decoupled hole states.
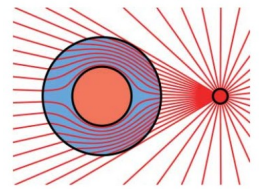
*U.Leonhardt, Science **312**, 1777 (2006)*
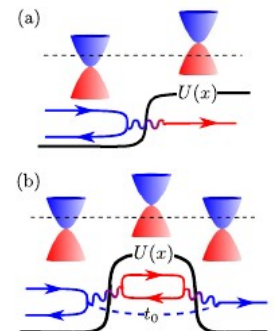

Pendry et al, ibid, p.1780

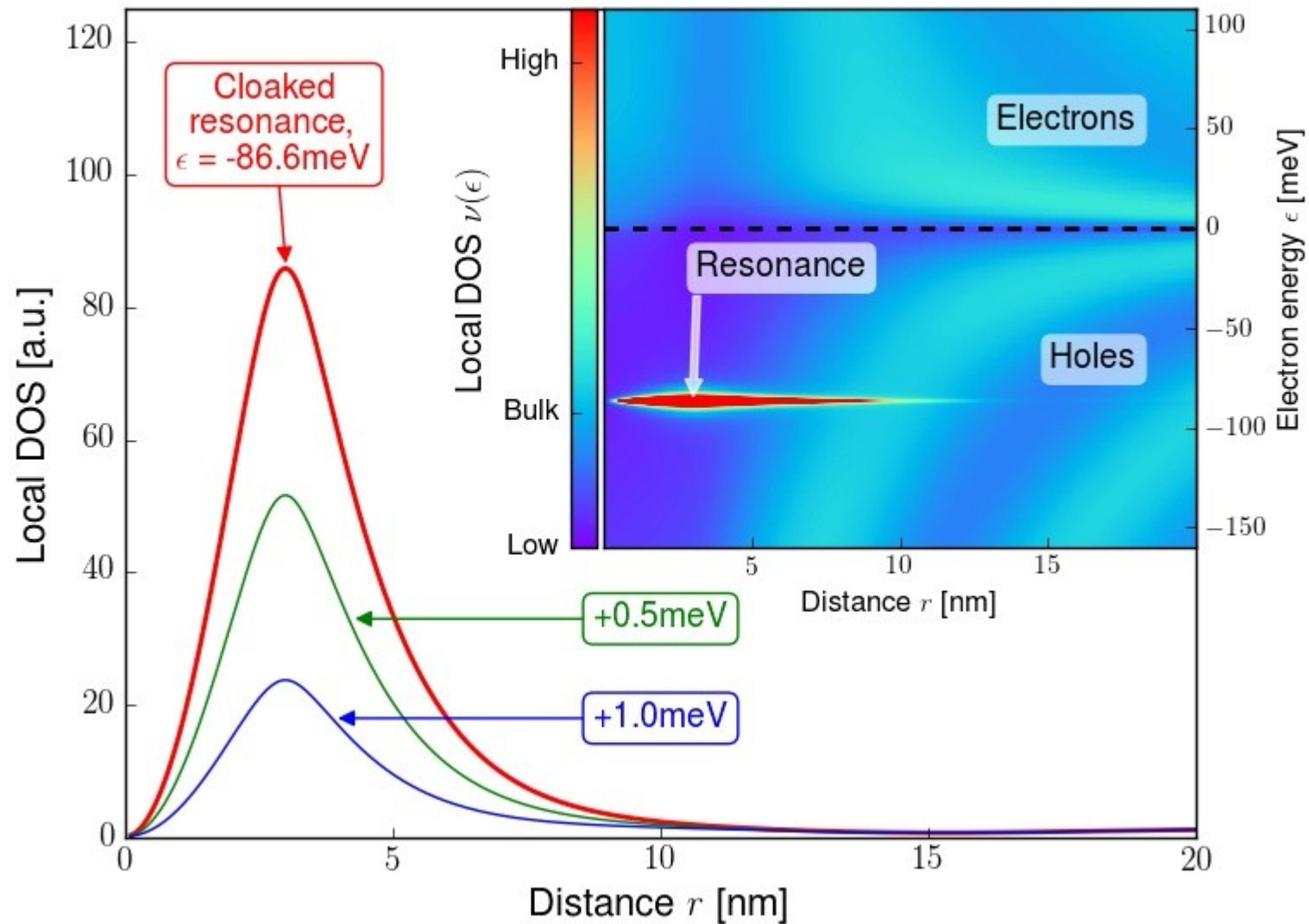**Chirality-Assisted Electronic Cloaking of Confined States in Bilayer Graphene**

Nan Gu,[1] Mark Rudner,[2] and Leonid Levitov[1]

[1]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
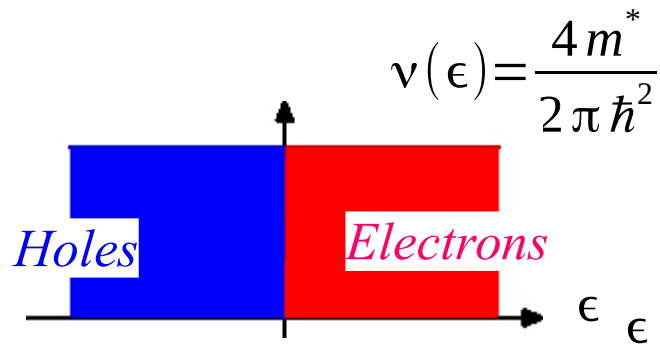[2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

The LDOS near a charged ring, *R*=3nm, *Z* = 12
The cloaked peak can be seen as a narrow (0.6meV) resonance

Ring geometry is better

$$\nu(\epsilon) = \frac{4\,m^*}{2\,\pi\,\hbar^2}$$

Holes   *Electrons*

ϵ ϵ

– Large DOS => strong RPA screening

– No impurity states (Coulomb potential is suppressed)

$$U > \frac{\hbar^2}{m^*\,a^2}$$

– The criterion is easier to satisfy in large-scale geometries

– Quantum corrals

– STM tip gating

Weakly Confined
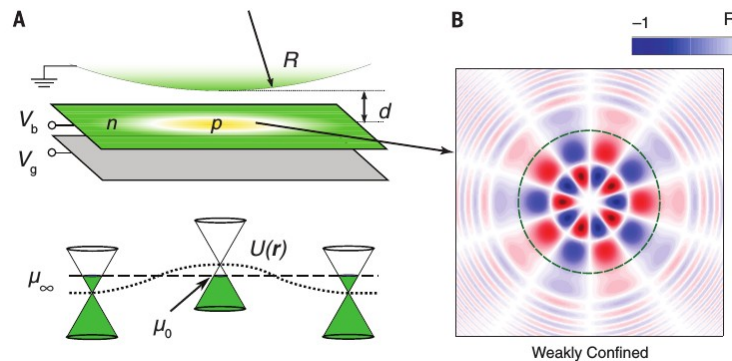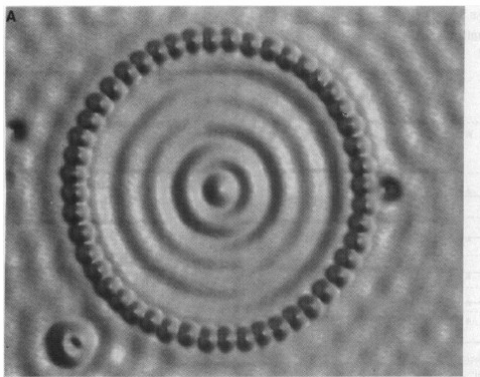
48 Fe-atoms, from M.F.Crommie et al, Science 262, 218 (1993)

From Zhao et al, Science 348, 672 (2015)

Conclusions:

– In bilayer graphene, there is a new kind of localized
   states: cloaked levels

– They could be engineered in quantum corral geometris
   and detected via STM measurements

Two-particle states in monolayer graphene

– For two particles in graphene, with energies $\epsilon_i = \pm v |\boldsymbol{p}_i|$ and opposite momenta, there are 4 quantum states with energies $2pv$, $-2pv$, 0, 0.

– The zero-energy degeneracy is lifted if one includes the quadratic term in the dispersion:

$$\hat{H}_i = v\, \boldsymbol{p}_i \cdot \boldsymbol{\sigma}_i - \frac{\boldsymbol{p}_i^2}{4m^*} \qquad m^* \approx 3 - 5\, m_e$$

– Interestingly, the sign of this term turns out to be negative, so that the pair behaves as a particle with negative mass.

– For a repulsive interaction between the particles, a metastable state Exists. (Cooper-pair-like)

– ??? How to excite and detect ???

Graphene and other nanoscale systems host quasiparticles with unusual properties. Quantum mechanics of such particles is yet to be fully explored.

Дякую за увагу
Questions?