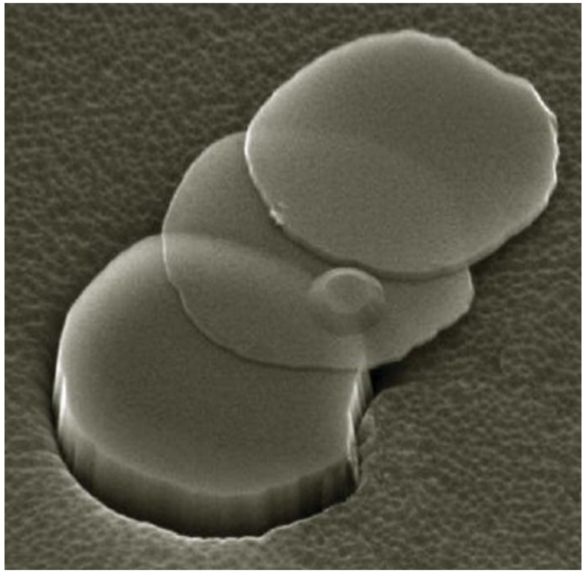
EPFL

Emergent relativistic physics in materials

Oleg Yazyev


graphite (3D crystal) = stack of graphene layers (2D crystals)

graphene = CERN on a table

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Exercise on graphene from Solid State Physics

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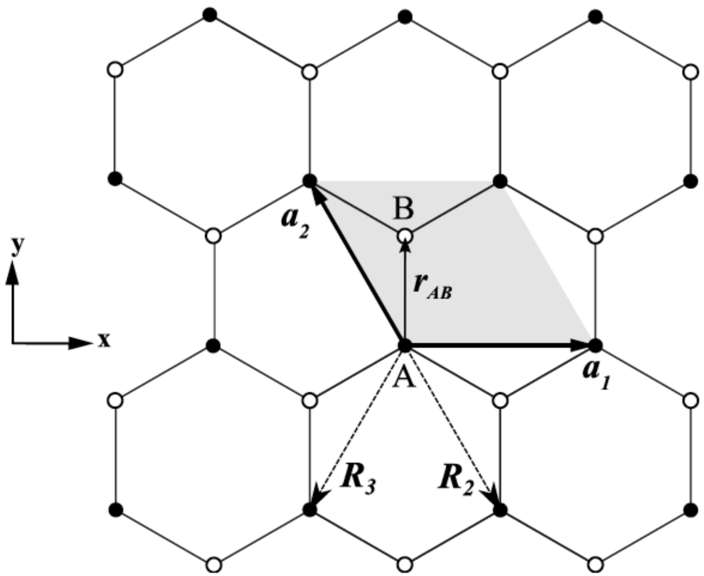
Atomic lattice
(honeycomb lattice of C atoms)



Hamiltonian (tight-binding)

$$H^{\mathbf{k}} = \begin{bmatrix} \langle\phi_A^{\mathbf{k}}|H|\phi_A^{\mathbf{k}}\rangle & \langle\phi_A^{\mathbf{k}}|H|\phi_B^{\mathbf{k}}\rangle \\ \langle\phi_B^{\mathbf{k}}|H|\phi_A^{\mathbf{k}}\rangle & \langle\phi_B^{\mathbf{k}}|H|\phi_B^{\mathbf{k}}\rangle \end{bmatrix} = \begin{bmatrix} \varepsilon_A^{\mathbf{k}} & \Delta^{\mathbf{k}} \\ \Delta^{\mathbf{k}*} & \varepsilon_B^{\mathbf{k}} \end{bmatrix}$$

$$\mathbf{d}_1 = \mathbf{r}_{AB} = a\left(0, \frac{1}{\sqrt{3}}\right)$$

$$\mathbf{d}_2 = \mathbf{r}_{AB} - \mathbf{a}_2 = a\left(\frac{1}{2}, -\frac{1}{2\sqrt{3}}\right)$$

$$\mathbf{d}_3 = \mathbf{r}_{AB} - \mathbf{a}_1 - \mathbf{a}_2 = a\left(-\frac{1}{2}, -\frac{1}{2\sqrt{3}}\right)$$

$$\Delta^{\mathbf{k}} = -\gamma \sum_{\mathbf{d}_i} e^{i\mathbf{k}\mathbf{d}_i}$$

$$= -\gamma\left(e^{ik_y a/\sqrt{3}} + e^{i(k_x a/2 - k_y a/2\sqrt{3})} + e^{i(-k_x a/2 - k_y a/2\sqrt{3})}\right)$$

$$= -\gamma\left(e^{ik_y a/\sqrt{3}} + e^{-ik_y a/2\sqrt{3}}(e^{ik_x a/2} + e^{-ik_x a/2})\right)$$

$$= -\gamma\left(e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}}\cos(k_x a/2)\right)$$

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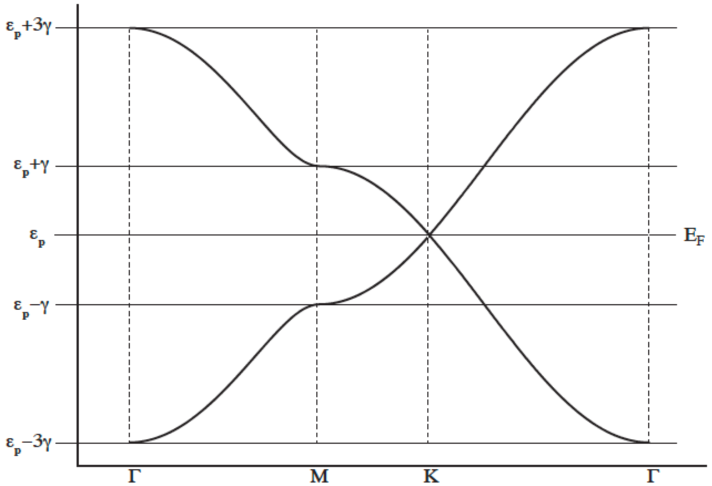
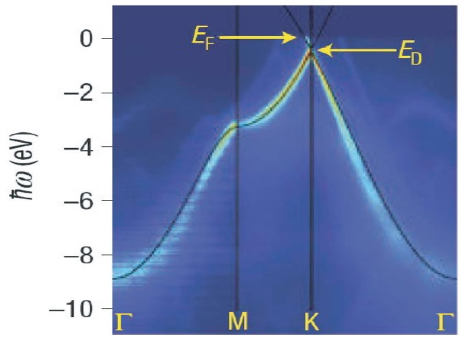
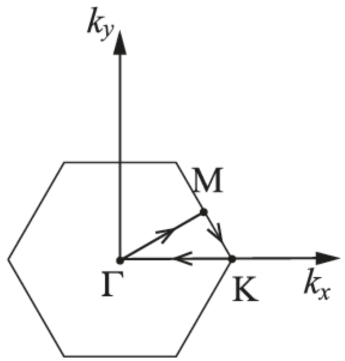
Band structure

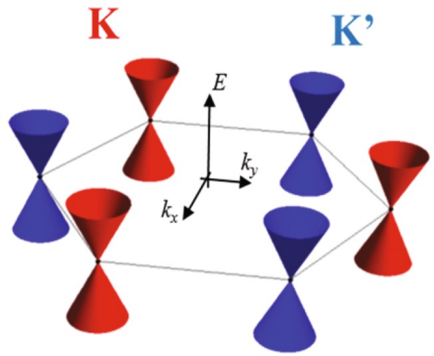
$$E(\mathbf{k}) = \varepsilon_p \pm \gamma \sqrt{1 + 4\cos^2\frac{k_x a}{2} + 4\cos\frac{k_x a}{2}\cos\frac{k_y a\sqrt{3}}{2}}$$





Brillouin zone





“Relativity” in graphene

Oleg Yazyev

Expanding the Hamiltonian around point *K* (*K*’), $\kappa = k - K$ lead to two-dimensional Dirac equation

$$\hat{H} = \pm\hbar v_F \boldsymbol{\sigma} \cdot \boldsymbol{\kappa} \qquad E_s(\kappa) = s\hbar v_F |\boldsymbol{\kappa}|$$

but with zero mass (“massless” Dirac fermions). Remember $E = \sqrt{(mc^2)^2 + (cp)^2}$

$s = +1$ and -1 corresponds to electrons and holes (antiparticles)

$\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ and $\boldsymbol{\kappa} = (\kappa_x, \kappa_y)$

Bloch states are 2-spinors containing wavefunction amplitude on sites *A* and *B* (“pseudospin”). Pseudospin is directed along momentum $\boldsymbol{\kappa}$ for $s = +1$ (and opposite for $s = -1$) – “chirality”.

Note 1: $v_F = \dfrac{2d\gamma}{2\hbar} \approx c/300$ = 1000 km/s

Note 2: At point *K*’ everything is opposite. “Intervalley” scattering must be excluded – only smooth potential variations are allowed

Note 3: Lorentz invariance is approximate – low energies

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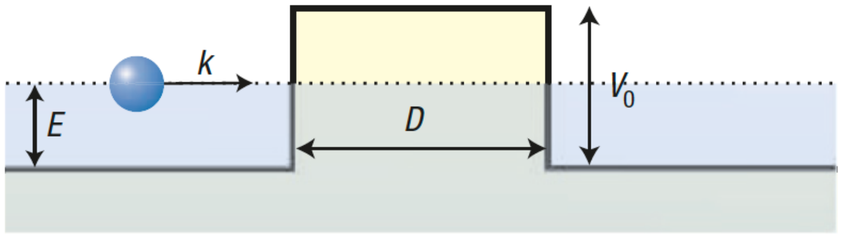
#1: Klein paradox

Tunneling through potential barrier



- Non-relativistic physics

  Transmission probability *T* decays exponentially with V_0 and *D*

- Relativistic physics

  For $V_0 > mc^2$, *T* becomes weakly dependent on V_0 and approaches perfect transparency ($T \sim 1$) for very high values of V_0

  Why? For $V_0 > mc^2$, this potential is attractive to anti-particles. Matching particle and antiparticle wavefunctions across the barrier result in perfect transmission.

  Why difficult to measure? Requires potential drop of $\sim mc^2$ over $\sim \hbar/mc$, which corresponds to electric fields $>10^{16}$ V/m.

Klein, O. Die reflexion von elektronen an einem potentialsprung nach der relativistischen dynamic von Dirac. Z. Phys. 53, 157–165 (1929).

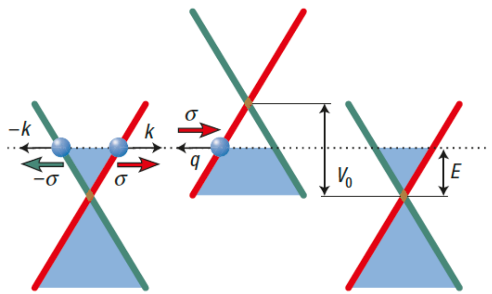
Klein tunneling in graphene

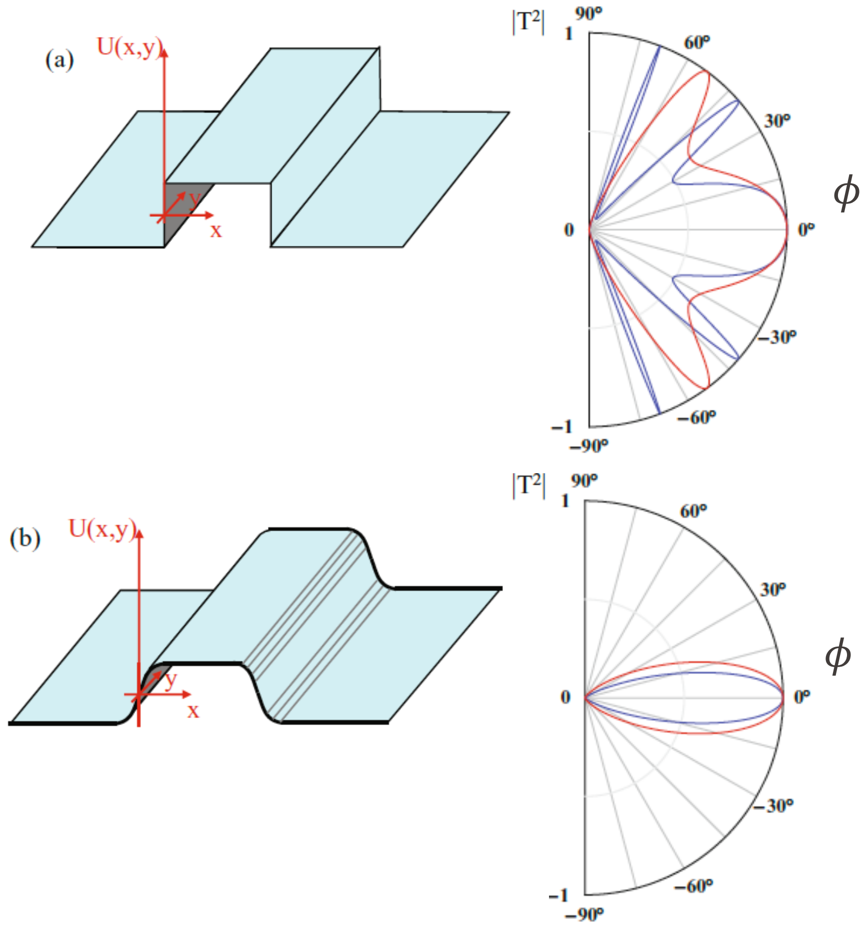
- Two components of the spinor wavefunction incident at angle ϕ

$$\psi_1(x,y) = \begin{cases} (e^{ik_x x} + re^{-ik_x x})e^{ik_y y}, & x < 0, \\ (ae^{iq_x x} + be^{-iq_x x})e^{ik_y y}, & 0 < x < D, \\ te^{ik_x x + ik_y y}, & x > D, \end{cases}$$

$$\psi_2(x,y) = \begin{cases} s(e^{ik_x x + i\phi} - re^{-ik_x x - i\phi})e^{ik_y y}, & x < 0, \\ s'(ae^{iq_x x + i\theta} - be^{-iq_x x - i\theta})e^{ik_y y}, & 0 < x < D, \\ ste^{ik_x x + ik_y y + i\phi}, & x > D, \end{cases}$$

- Electrons and holes are the conjugated particles and antiparticles



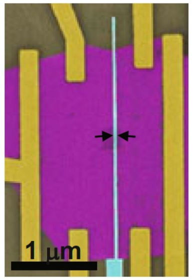


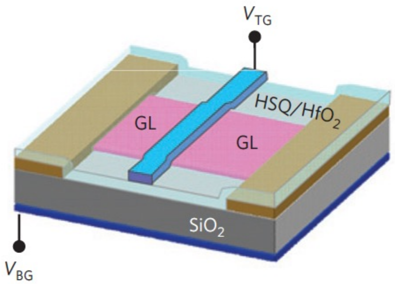
Katsnelson, M. I., Novoselov, K. S. & Geim, A. K. Chiral tunnelling and the Klein paradox in graphene. Nature Phys. 2, 620–625 (2006).

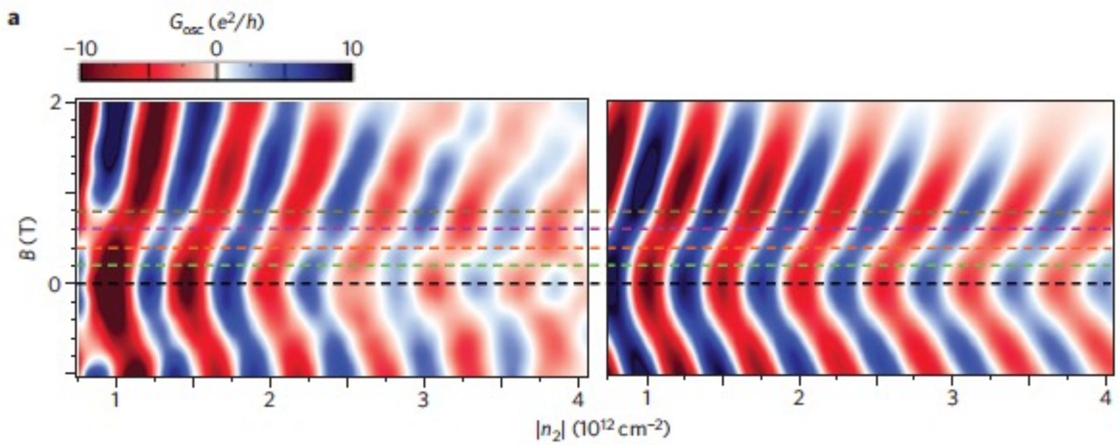
Experimental confirmation

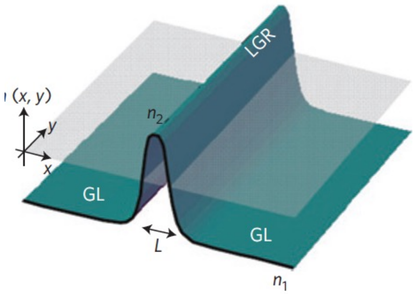
- Problem: one cannot inject electrons with a predefined momentum

- Observed indirectly through the phase shift in conductance oscillations





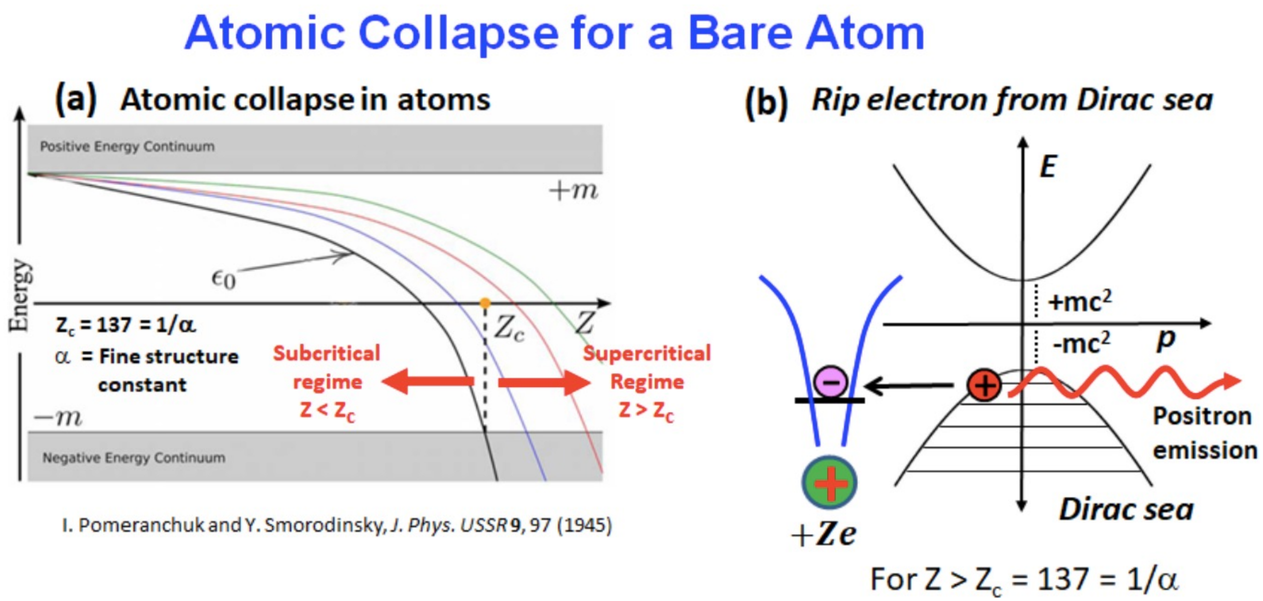




Young, A. F. & Kim, P. Quantum interference and Klein tunnelling in graphene heterojunctions. Nature Phys. 5, 222–226 (2009).

#2: Atomic collapse in atoms

- In ultraheavy atoms, the energy of the lowest atomic 1*s* orbital may reach the Dirac sea (negative energy continuum of antiparticles)
- Classically, this corresponds to an electron falling onto nucleus and knocking out positron (“atomic collapse”)
- Problem: requires $Z > 137$ elements (“supercritical” nuclei)

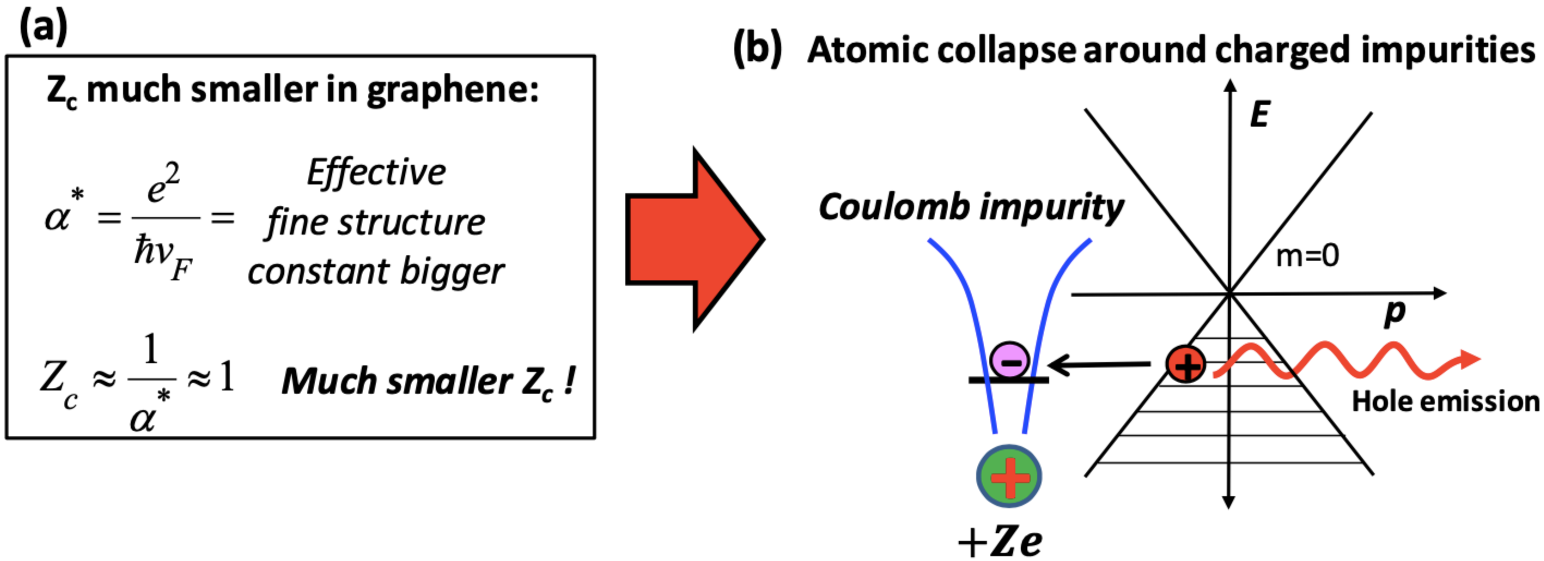


Pomeranchuk, I. & Smorodinsky, Y. On the energy levels of systems with Z >137. J. Phys. USSR 9, 97–100 (1945).

Atomic collapse in graphene

- In graphene, only Z ~ 1 is required
- Would result in a resonant state at *E* = 0 that corresponds to periodic spiraling in and out the charged impurity

Atomic Collapse for an Impurity in Graphene



A. V. Shytov, M. I. Katsnelson & L. S. Levitov, "Atomic Collapse and Quasi--Rydberg States in Graphene", Physical Review Letters 99, 246802 (2007); V. M. Pereira, J. Nilsson & A. H. Castro Neto, "Coulomb Impurity Problem in Graphene", Physical Review Letters 99, 166802 (2007).

Scanning tunneling microscopy

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Imaging Electrons via STM

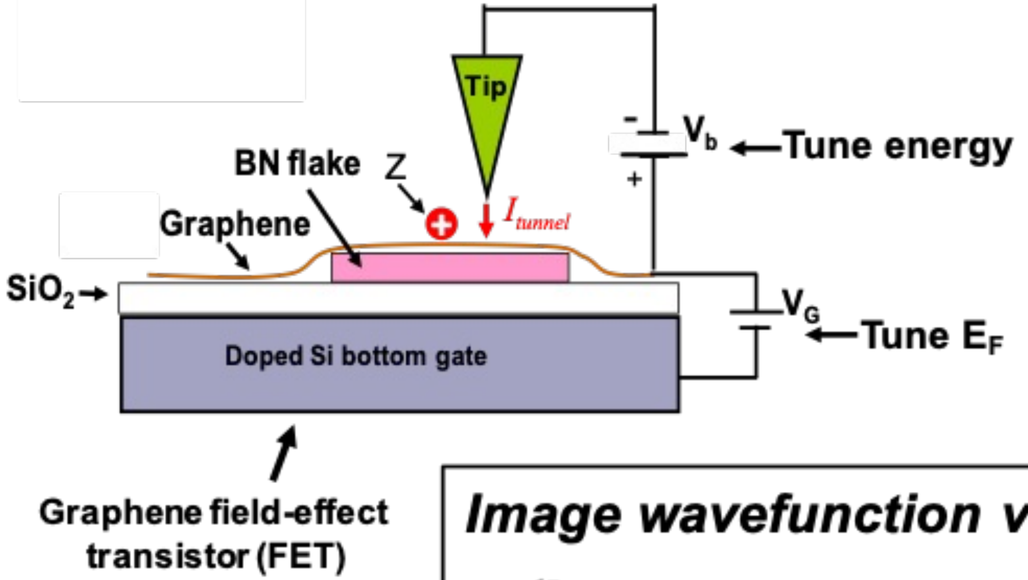


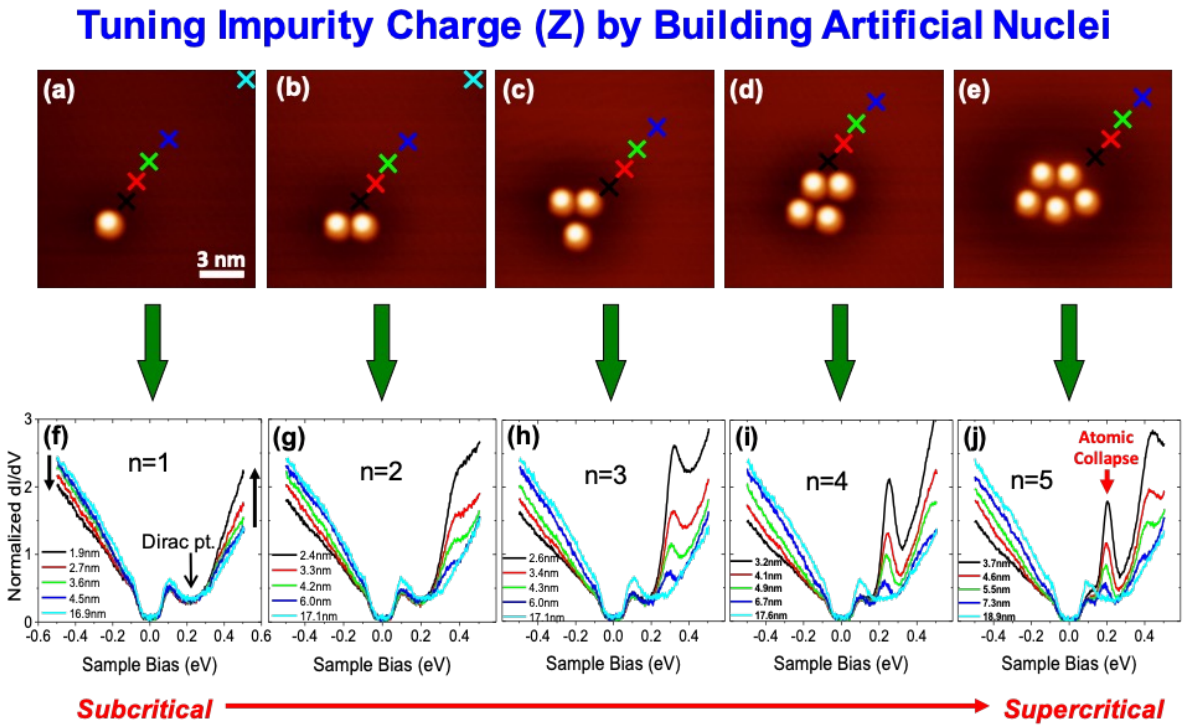
Image wavefunction via dI/dV:

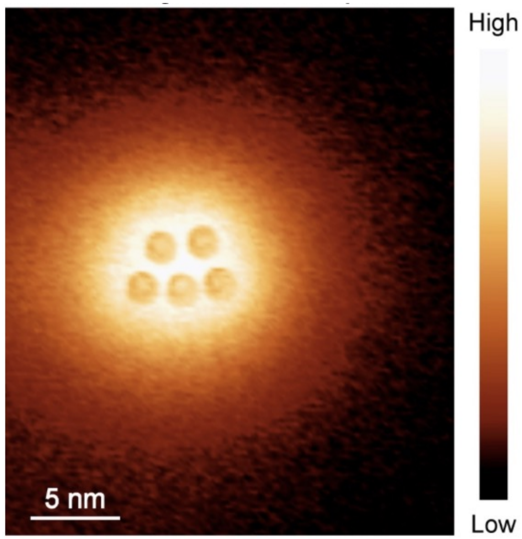
$$\frac{dI}{dV}(V) \propto LDOS(\vec{r}, E_F + eV)$$

$$= \sum_k |\psi_k(\vec{r})|^2 \, \partial\left(E_k - \left(E_F + eV\right)\right)$$

Scanning tunneling microscopy

- Atomic collapse state at the charged Ca ions on the surface of graphene





Y. Wang, D. Wong, A. V. Shytov, V. W. Brar, S. Choi, Q. Wu, H.-Z. Tsai, W. Regan, A. Zettl, R. K. Kawakami, S. G. Louie, L. S. Levitov & M. F. Crommie, "Observing Atomic Collapse Resonances in Artificial Nuclei on Graphene", Science 340, 734 (2013).

Oleg Yazyev

#3: Zitterbewegung (trembling motion)

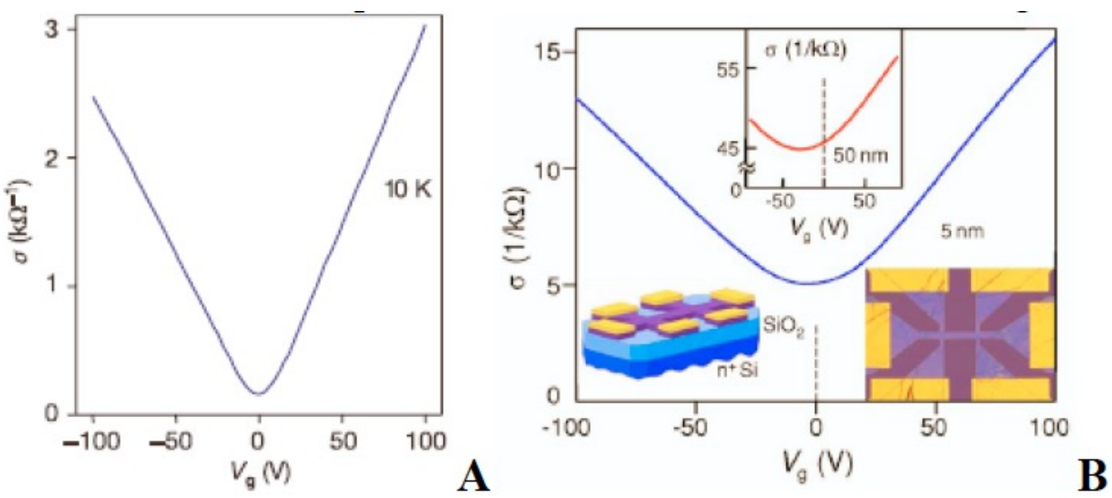
- Rapid apparent fluctuation of the position of relativistic particles as a result of interference between positive and negative energy states.
- No solid experimental observations, frequencies of the order of $2mc^2/\hbar$ (~10^{21} Hz)

Breit, Gregory (1928). "An Interpretation of Dirac's Theory of the Electron". *Proceedings of the National Academy of Sciences.* ***14*** *(7): 553–559;* Schrödinger, E. (1930). *Über die kräftefreie Bewegung in der relativistischen Quantenmechanik* [*On the free movement in relativistic quantum mechanics*] (in German). pp. 418–428.

Minimal conductivity in graphene

- Manifestation of Zitterbewegung – minimum conductivity

$$\sigma_{min} = \frac{4e^2}{h}$$



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K.S. Novoselov et al., Science 306, 666 (2004); M.I. Katsnelson, Zitterbewegung, chirality, and minimal conductivity in graphene, Eur. Phys. J. B 51, 157–160 (2006).