Supercritical phenomena in graphene with charged impurities: Table top realization of relativistic quantum mechanics

Davron Matrasulov

Turin Polytechnic University in Tashkent, Uzbekistan

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OUTLINE

- Condensed matter (table-top) Lab. For QED in 2 dimensions
- Supercritical phenomena in relativistic quantum mechanics
- Relativistic atoms and molecules
- Relativistic electron-dipole system
- Charged impurities in graphene
- Planar atoms in graphene
- Planar molecules in graphene
- Dipole type impurities

Graphene as unusual material and facility for fundamental studies

- Why graphene is so attractive?
- *Broad spectrum of practical applications*
- *Powerful testing ground for (2+1)-dimensional QED*
- *New way for other two-dimensional materials*

Physical properties

- Zero effective mass of quasiparticles
- Velocity of quasiparticles is more than 300 times less than that of light speed
- Gapless band structures
- Linear dispersion relation
- Nevertheless, their dynamics is described by ultrarelativistic Dirac equation
- Coupling constant is 300 times larger than that of fine structure constant

Condensed matter laboratory for testing of relativistic quantum mechanics and QED in two dimensions

- Graphene is unique testing ground for many QED effects such as:
- Vacuum polarization
- Schwinger pair creation
- Klein Tunneling
- Darmstadt effect
- Casimir effect
- Etc.

Supercritical phenomena in relativistic QM

Energy space in the relativistic quantum mechanics consist of upper continuum (analog of the conduction band in condensed matter), lower continuum called “Dirac sea” (analog of valence band) and the gap between them

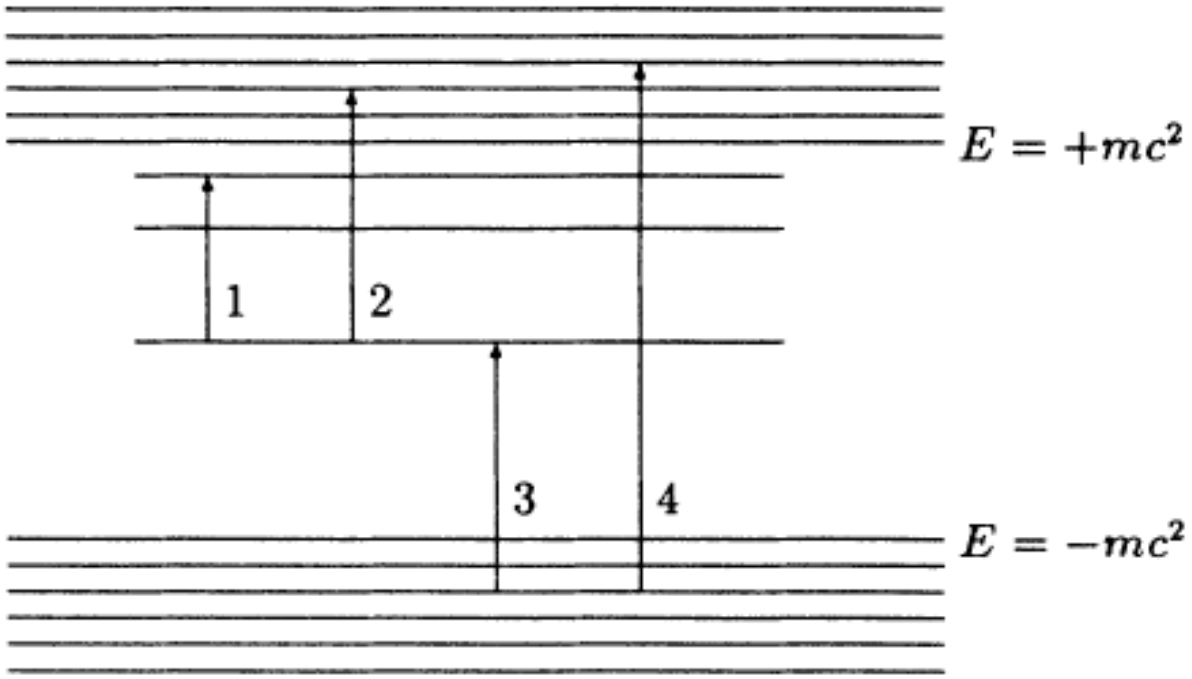
The phenomena occurring near the Dirac sea, i.e. for the energies close to lower continuum are called supercritical phenomena.

Such phenomena as electron-positron pair production by Schwinger mechanism, Klein tunneling, vacuum polarization etc. are the supercritical phenomena.

Supercritical phenomena in relativistic QM

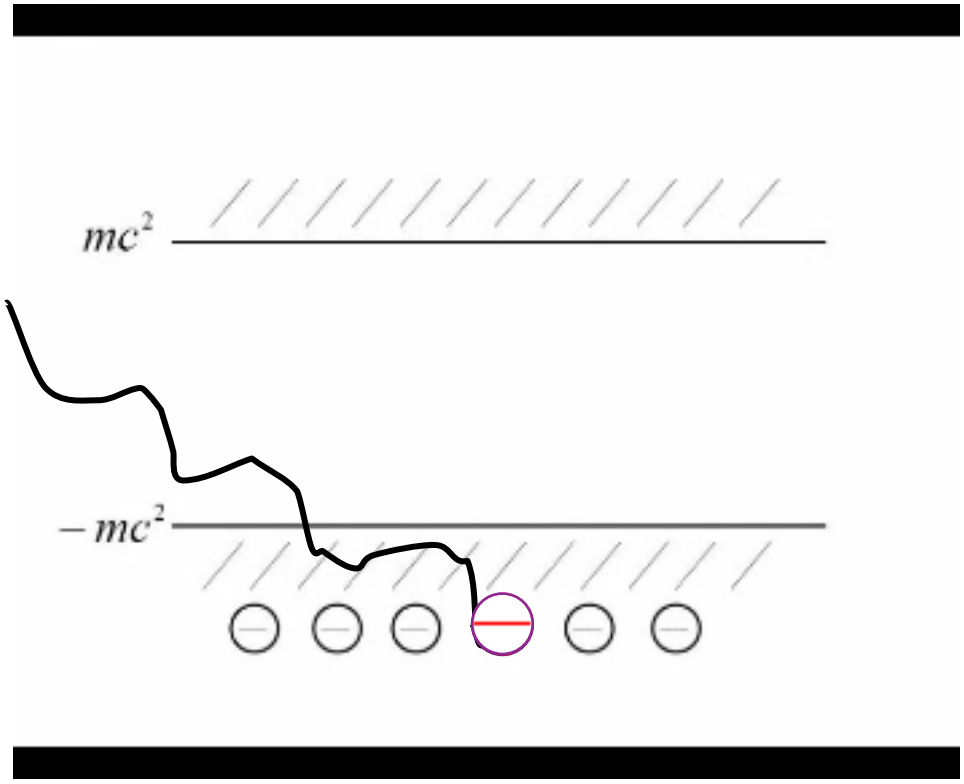
- Vacuum polarization
- Electron-positron pair creation
- Klein tunneling
- Casimir effect

Transitions in Dirac spectrum



Spectrum of the Dirac equation. Indicated are possible atomic Excitations: (1) excitation, (2) ionization, (3) pair creation with capture, and (4) direct pair creation.

Schwinger Mechanism for Pair Production



Relativistic Coulomb problem

Electron motion in strong Coulomb field is relativistic

Relativistic Coulomb problem $(m = c = \hbar = 1)$

$$\left[\vec{\alpha}\vec{p} + \beta - \frac{Z\alpha}{r}\right]\psi = E\psi$$

$$E = \left[\sqrt{1 + \left(\frac{Zj}{j + n_r}\right)^2}\right]^{-1}$$

$$n_r = 0,1,2,3, \dots , \qquad j = \sqrt{\varkappa^2 - Z^2\alpha^2} \qquad \alpha = \frac{1}{137}$$

Supercritical states in strong Coulomb field

$$H = \vec{\alpha}\,\vec{p} + \beta\, mc^2 - \frac{z\alpha}{r} \qquad \alpha = \frac{1}{137}$$

Ground state energy

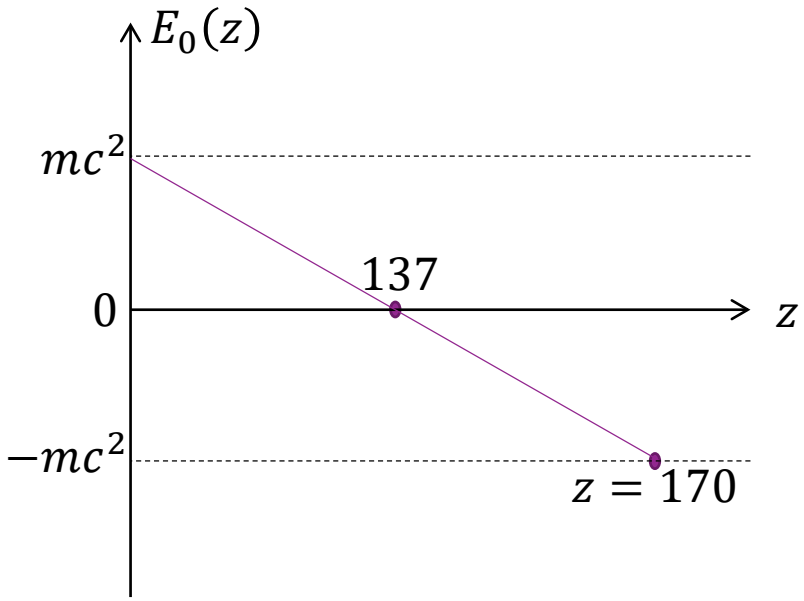
$$E_0(z) = mc^2\sqrt{1 - z^2\alpha^2}$$

For $z > 137$ E_0 becomes imaginary

(**Pomeranchuk & Smorodinsky,** 1945)

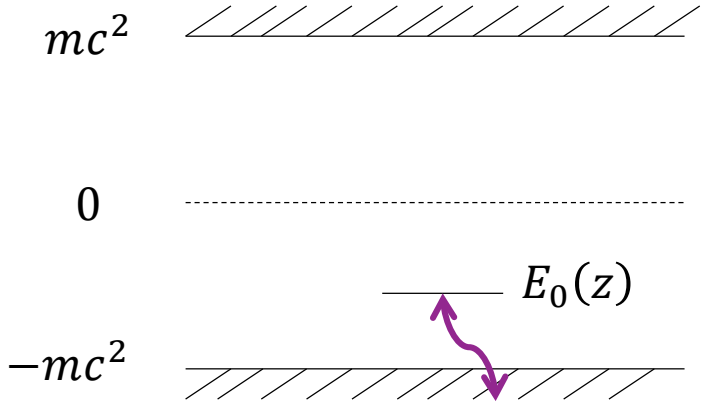
Regularized problem

$$V(r) = \begin{cases} f(r) & r \le r_0 \\ -\dfrac{z\alpha}{r} & r > r_0 \end{cases}$$



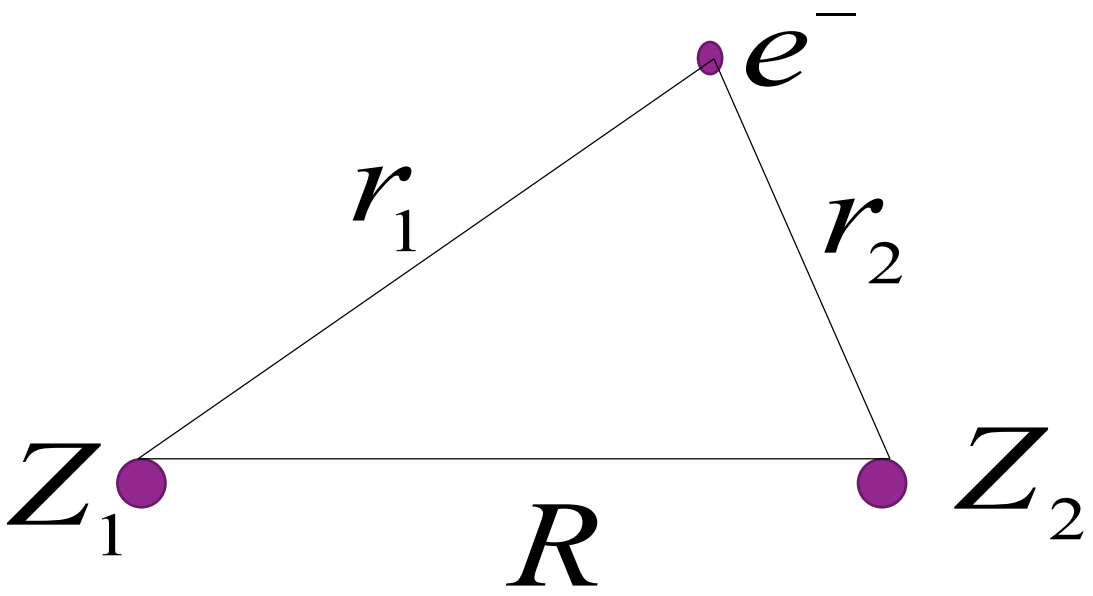
Pair production strong Coulomb field

Pair production in strong field occurs in diving of (empty) levels into the Dirac sea



Pair production in collision of two heavy ions

$$\left[\alpha p + \beta m - \frac{Z_1\alpha}{r_1} - \frac{Z_2\alpha}{r_2}\right]\psi = E\psi$$



$$Z_1 + Z_2 \geq 170$$

Ya.B. Zeldovich, V.S. Popov. Sov. Phys. Usp. **14,** 673 (1972)

QED in graphene

Usual QED

Coupling constant

$$\alpha = \frac{1}{137}$$

QED in graphene

Coupling constant

$$\alpha_g = \frac{300}{137}$$

Relativistic planar and 3D Coulomb problems

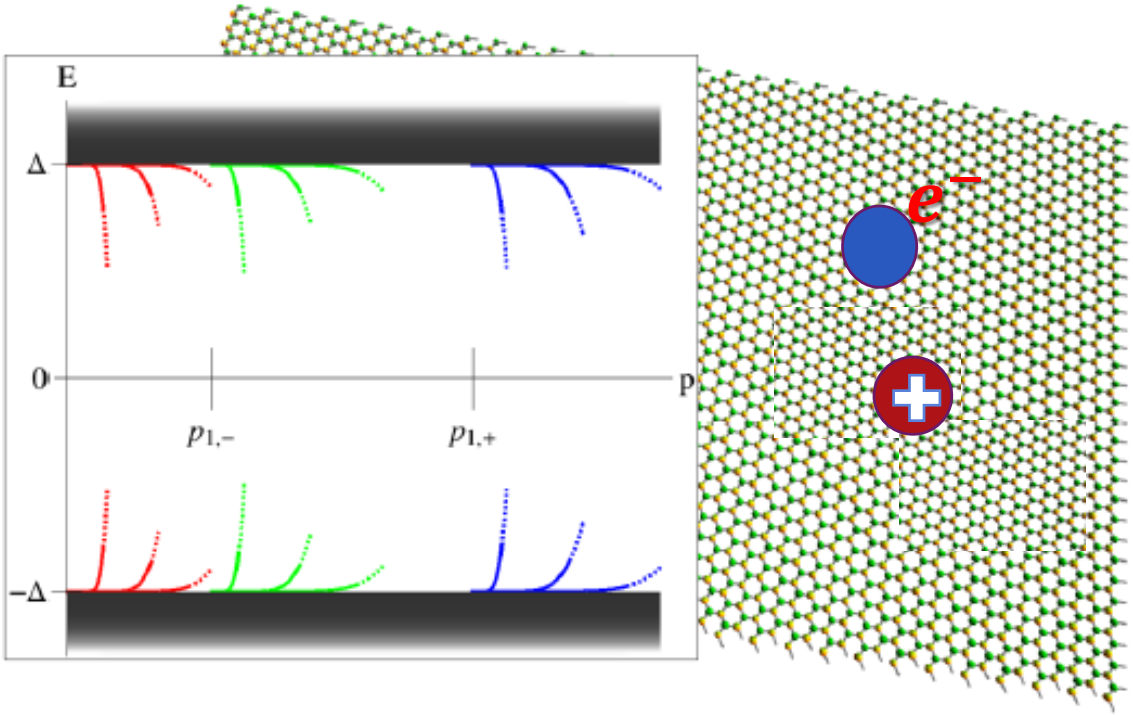
3D-system: $$E_0 = \sqrt{1 - Z^2\alpha^2}$$

2D-system: $$E_0 = \sqrt{1 - 4Z^2\alpha^2}$$

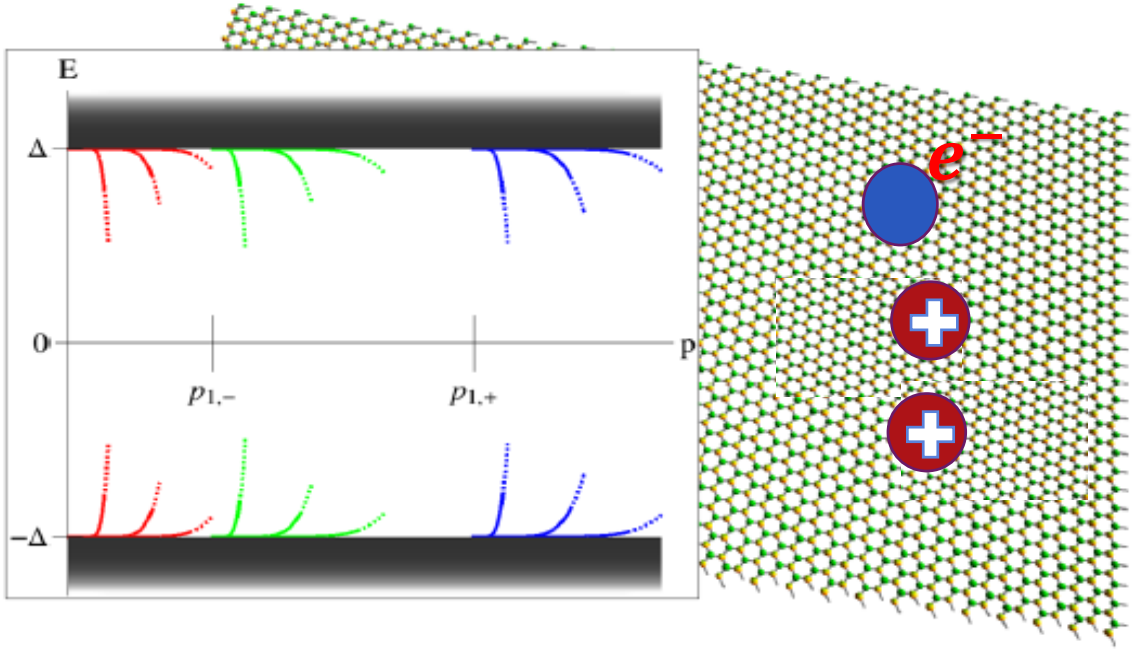
Planar relativistic atoms in graphene

Charged impurities in graphene allow to create two-dimensional relativistic atoms and molecules as the electron motion in the Coulomb field of such charges are described by Dirac equation.

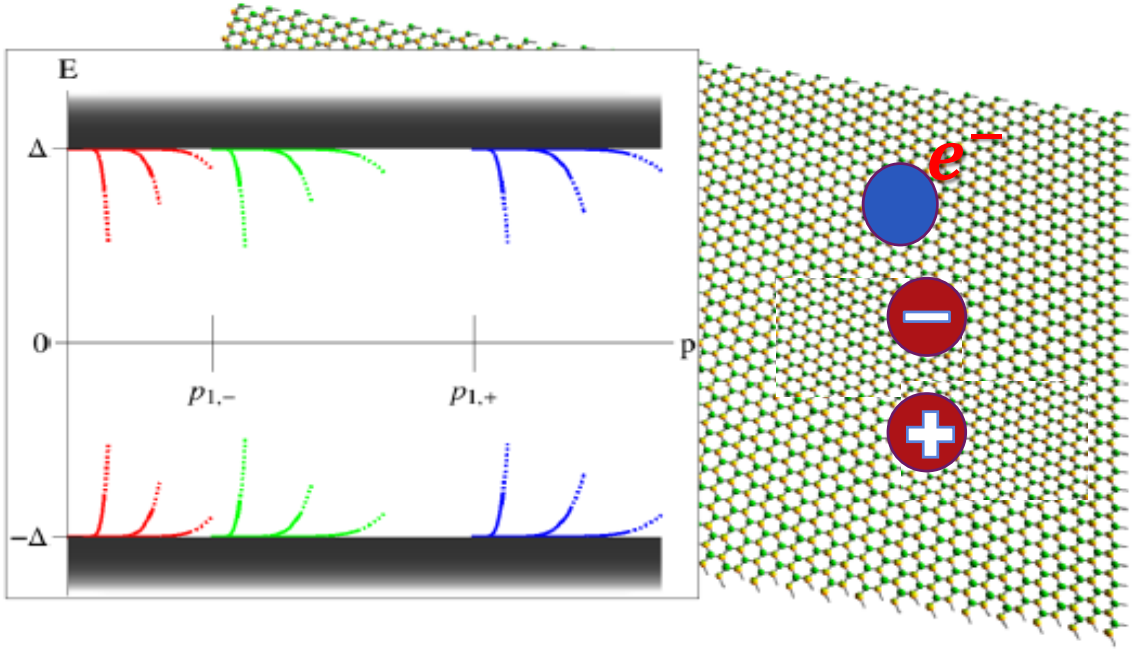
Charged impurities in graphene: Planar atoms



Charged impurities in graphene: Planar molecules



Charged impurities in graphene: Relativistic electron-dipole system



Supercritical phenomena in graphene induced by charged impurities

- Charged impurities in graphene create two dimensional (planar) relativistic atoms and molecules where electron dynamics is described by the Dirac equation.
- If the charge of the impurity exceeds critical value bound state energy levels approach the boundary of continuum and diving can also occur.
- This allows one to realize pair production phenomena with one or more charged impurities.
- Since coupling constant is such systems is much larger than fine structure constant, the critical charge needed for pair production is also quite small (compared to 3D system, i.e. 170).

Screening Charged Impurities and Lifting the Orbital Degeneracy in Graphene by Populating Landau Levels

Adina Luican-Mayer,[1] Maxim Kharitonov,[1] Guohong Li,[1] Chih-Pin Lu,[1] Ivan Skachko,[1] Alem-Mar B. Gonçalves,[1] K. Watanabe,[2] T. Taniguchi,[2] and Eva Y. Andrei[1,*]

[1]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*

[2]*Advanced Materials Laboratory, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*

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We report the observation of an isolated charged impurity in graphene and present direct evidence of the close connection between the screening properties of a 2D electron system and the influence of the impurity on its electronic environment. Using scanning tunneling microscopy and Landau level spectroscopy, we demonstrate that in the presence of a magnetic field the strength of the impurity can be tuned by controlling the occupation of Landau-level states with a gate voltage. At low occupation the impurity is screened, becoming essentially invisible. Screening diminishes as states are filled until, for fully occupied Landau levels, the unscreened impurity significantly perturbs the spectrum in its vicinity. In this regime we report the first observation of Landau-level splitting into discrete states due to lifting the orbital degeneracy.

10 MAY 2013 VOL 340 SCIENCE www.sciencemag.org

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.

Planar relativistic two center system

Hamiltonian:

$$H = (-i\partial_x)\sigma_x + (-i\partial_y)\sigma_y + \Delta\sigma_z + V.$$

Potential:

$$V(x,y) = \frac{p/d}{\sqrt{(x+d/2)^2+y^2}} - \frac{p/d}{\sqrt{(x-d/2)^2+y^2}},$$

Planar relativistic atom

$$(h = v_F = m = 1)$$

$$\left[(-i\partial_x)\sigma_x + (-i\partial_y)\sigma_y - \frac{Z\alpha}{\sqrt{x^2 + y^2}} \right] \psi = E\psi$$

Ground state energy $E_0 = \sqrt{1 - 4Z^2\alpha^2}$

Energy levels:

$$E_n = \left[1 + \frac{Z^2\alpha^2}{\left(n + \sqrt{\left(l + \frac{1}{2} \right)^2 - Z^2\alpha^2} \right)} \right]^{-\frac{1}{2}}$$

Relativistic Method of Linear Combination of Atomic Orbitals (LCAO)

$$\left[\vec{\alpha}\vec{p} + \beta - \frac{Z\alpha}{r_1} - \frac{Z\alpha}{r_2}\right]\psi = E\psi$$

$$\psi(r_1, r_2) = A\phi_1(r_1) + B\phi_2(r_2)$$

$\phi(r)$ - one center Coulomb wave function

Relativistic Method of Linear Combination of Atomic Orbitals (LCAO)

$$E(R) = \langle \psi | H | \psi \rangle$$

$$A = B = \frac{1}{\sqrt{2(1+s)}}$$

$$s = \langle \phi_1 | \phi_2 \rangle$$

$$|\psi > = [\varphi, \chi >$$

V.I. Matveev, D.U. Matrasulov, H.Yu. Rakhimov. Phys. At. Nuclei **63**(2000) 318

Planar relativistic two center system

Hamiltonian:

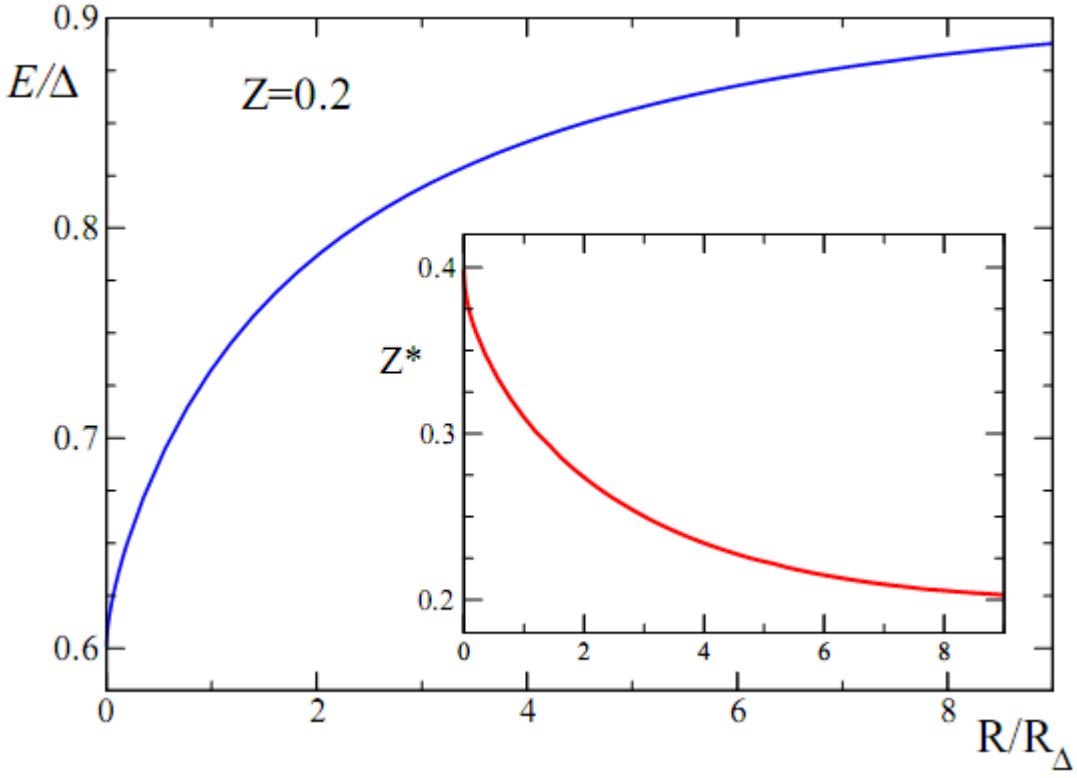
$$H = H_0 - Z_{\text{eff}} \left(\frac{1}{r_1} + \frac{1}{r_2} \right) - \frac{\delta Z_1}{r_1} - \frac{\delta Z_2}{r_2},$$

Condition:

$$\det \begin{pmatrix} H_{11} - E & H_{12} - SE \\ H_{21} - SE & H_{22} - E \end{pmatrix} = 0,$$

D. Klopfer, A. De Martino, D. Matrasulov, and R. Egger. Eur. Phys. J. B 87, 187 (2014).

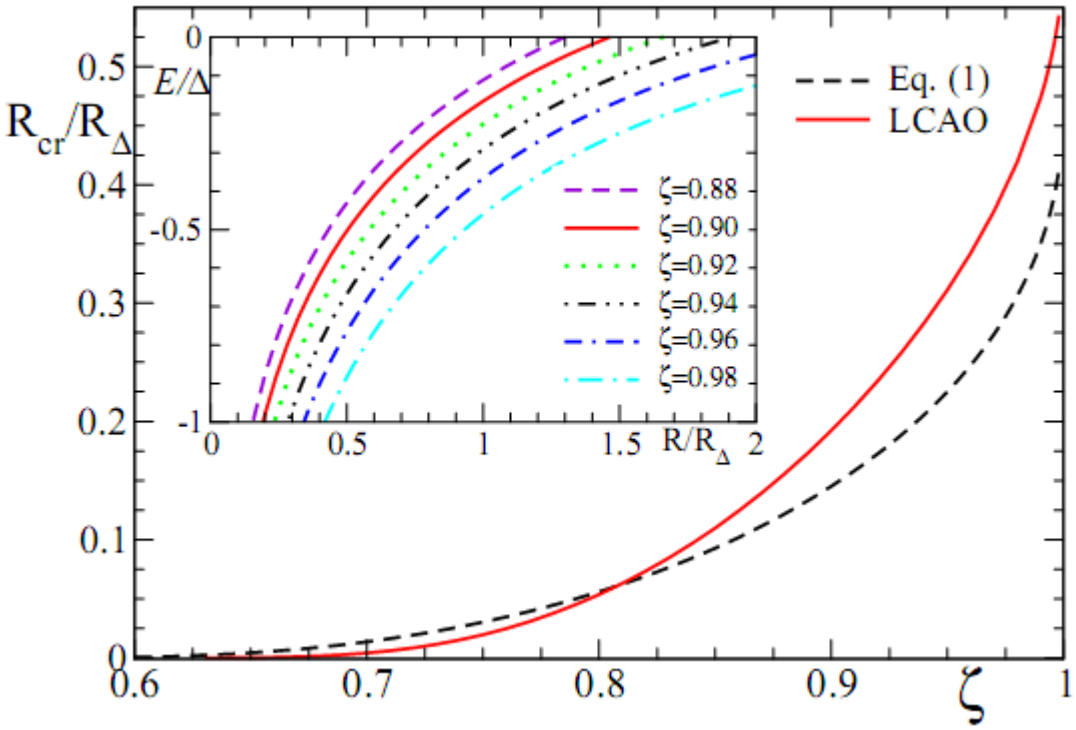
Planar relativistic two center system



Main panel: LCAO result for the ground-state energy, E, vs impurity distance R (which is given in units of $R_\Delta = \hbar v_F/\Delta$), for the two-center potential with $Z_1 = Z_2 = Z = 0.2$. Inset: Optimal choice for the variational parameter, $Z_{\rm eff} = Z^*$, determining the LCAO ground state, as a function of R.

D. Klopfer, A. De Martino, D. Matrasulov, and R. Egger. Eur. Phys. J. B 87, 187 (2014).

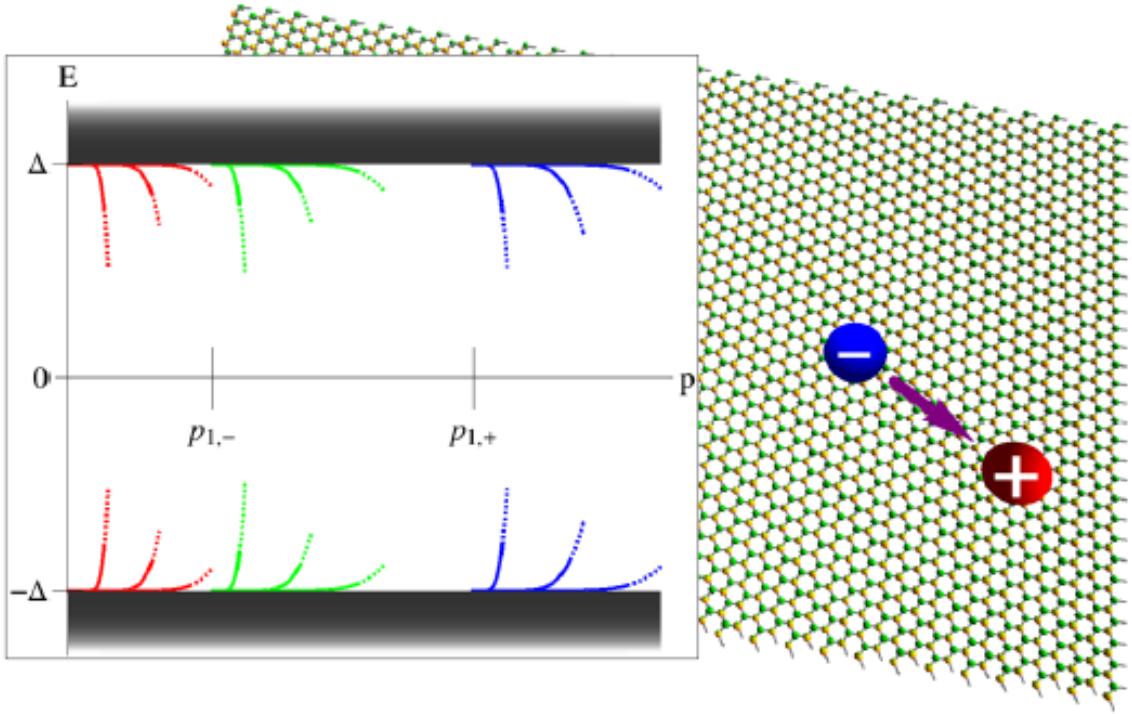
Planar relativistic two center system



Main panel: Critical distance $R_{\rm cr}$ vs $\zeta = Z/Z_c$, for the symmetric two-center problem. The red curve gives the LCAO result, and the black curve is the corresponding asymptotic matching result (1). Inset: LCAO ground state energy vs R, for various ζ. Once $E(R)$ reaches $-\Delta$, the level "dives" into the lower continuum and turns supercritical.

D. Klopfer, A. De Martino, D. Matrasulov, and R. Egger. Eur. Phys. J. B 87, 187 (2014).

Dipole type impurities in graphene



A. De Martino, D. Kloepfer, D. Matrasulov, R. Egger Phys.Rev.Lett., 112, 186603 (2014)

Relativistic electron-dipole system

PHYSICAL REVIEW A VOLUME 60, NUMBER 5 NOVEMBER 1999

Eigenvalue problem for the relativistic electric-dipole system

D. U. Matrasulov* and V. I. Matveev
Heat Physics Department, Uzbek Academy of Sciences, 28 Katartal Street, 700135 Tashkent, Uzbekistan

M. M. Musakhanov
Theoretical Physics Department, Tashkent State University, Tashkent 700095, Uzbekistan
(Received 16 March 1999)

The two-center Coulomb problem (with opposite signs of charges) for the Dirac equation is solved by the method of matching the logarithmic derivatives of the asymptotic solutions. The formulas for the near continuum-state energy term of a relativistic electric-dipole system are obtained analytically. Two cases are considered: $Z<137$ and $Z>137$. The Dirac equation for $Z>137$ is solved by the usual method of a cutoff potential at small distances. [S1050-2947(99)10108-2]

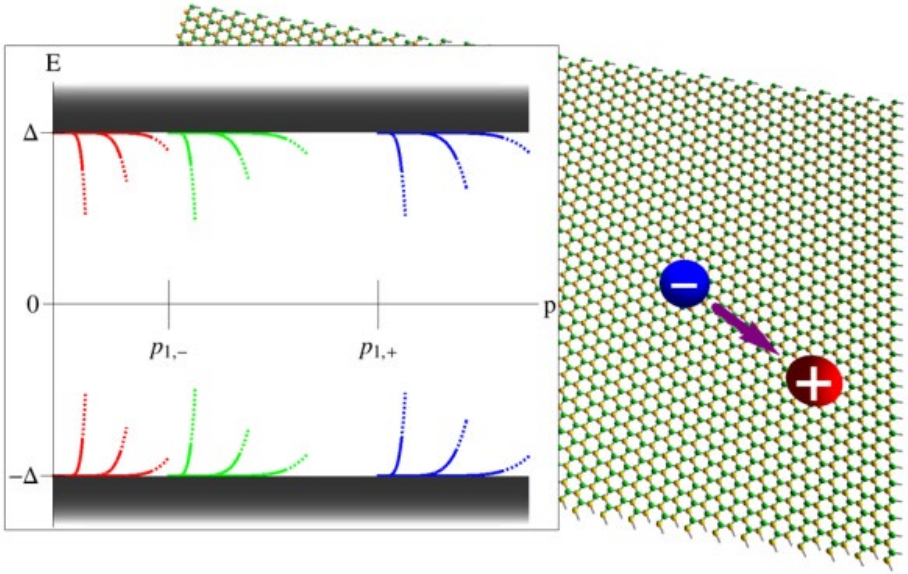
Relativistic electron-dipole system

$$V(r_1, r_2) = \frac{Z\alpha}{r_1} - \frac{Z\alpha}{r_2} = \frac{Z\alpha}{\sqrt{\left(x + \frac{d}{2}\right)^2 + y^2}} - \frac{Z\alpha}{\sqrt{\left(x - \frac{d}{2}\right)^2 + y^2}}$$

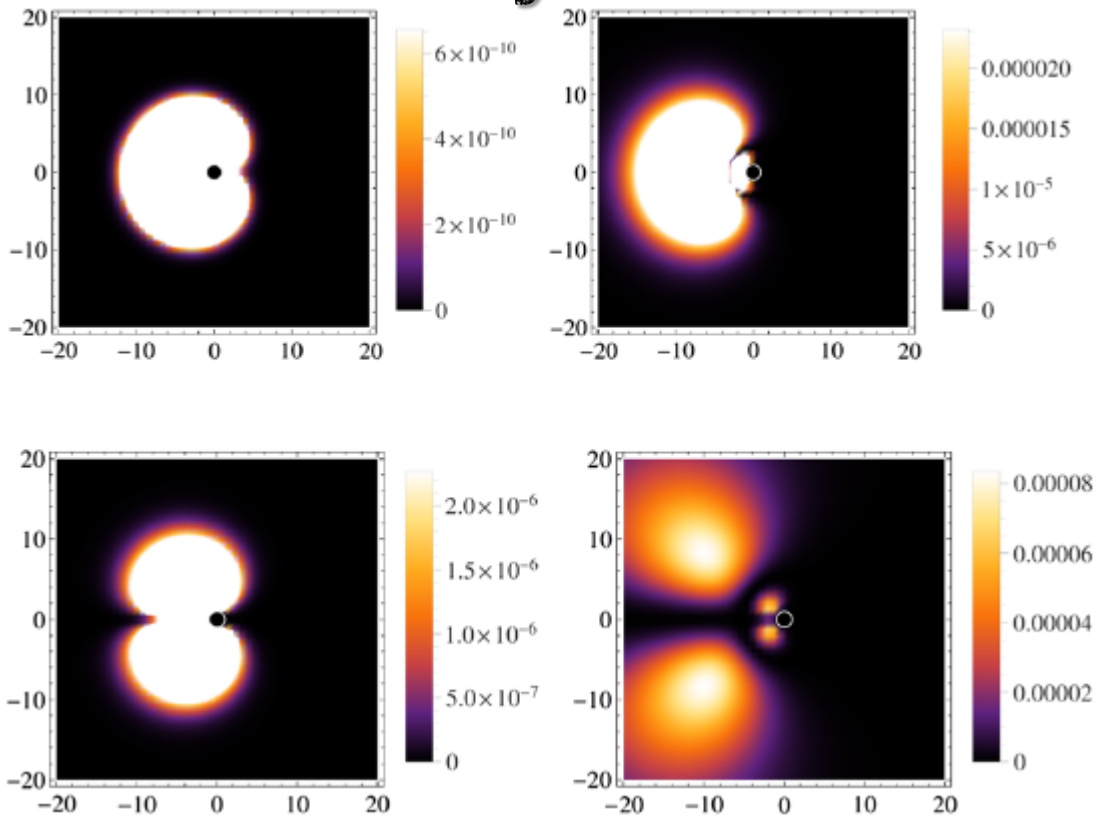
$$\begin{bmatrix} V + m & e^{-i\theta}\left(-i\partial_r - \frac{1}{r}\partial_\theta\right) \\ e^{i\theta}\left(-i\partial_r + \frac{1}{r}\partial_\theta\right) & V - m \end{bmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ \chi \end{pmatrix}$$

Electric-Dipole-Induced Universality for Dirac Fermions in Graphene

Alessandro De Martino,[1] Denis Klöpfer,[2] Davron Matrasulov,[3] and Reinhold Egger[2]
[1]*Department of Mathematics, City University London, London EC1V 0HB, United Kingdom*
[2]*Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany*
[3]*Turin Polytechnic University in Tashkent, 17 Niyazov Street, 100095 Tashkent, Uzbekistan*



Dipole type impurities in graphene
Density of states



Density of states for planar relativistic electron-dipole system.

A. De Martino, D. Kloepfer, D. Matrasulov, R. Egger Phys.Rev.Lett., 112, 186603 (2014)

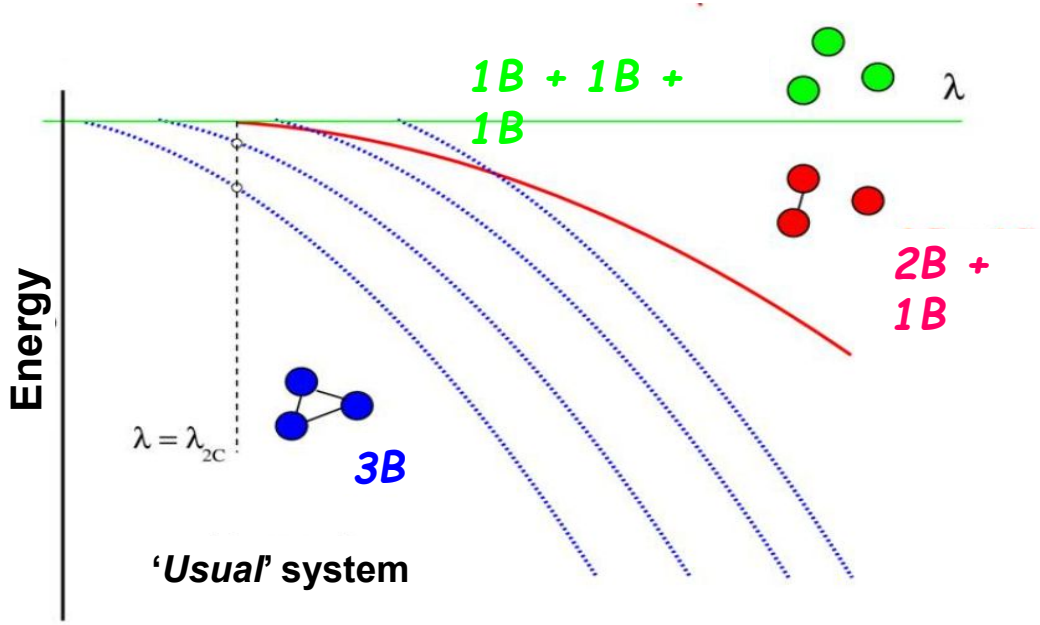
Efimov effect

Efimov effect first discovered by V. Efimov in 1970 is one of the most intriguing phenomena in the physics of few body systems. This effect appears in 3-body systems in 3-dimensional space, which interact through short-range pair-potentials. It is always possible to tune the couplings of the interactions in such a way that none of the particle pairs has a negative energy bound state, but at least two pairs have a resonance at zero energy. In this case the 3-body system exhibits an infinite sequence of bound levels, where the energy of the n-th level decreases exponentially with n.

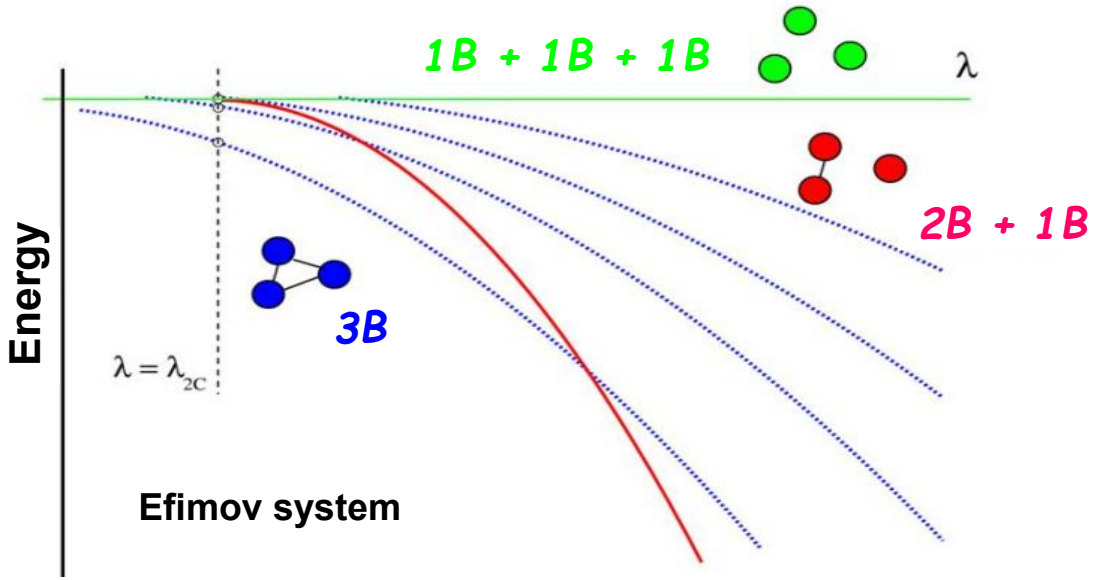
Efimov effect

$V_{3B}(R_1,R_2,R_3) = \Sigma \lambda V_{2B}(R_i)$

3B bound states *appear* through the ***2B*** threshold as λ increases

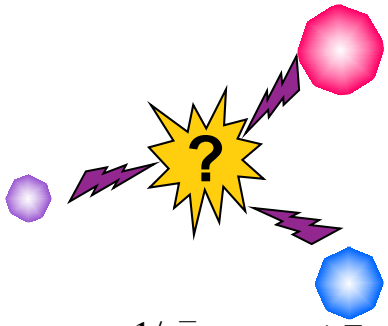


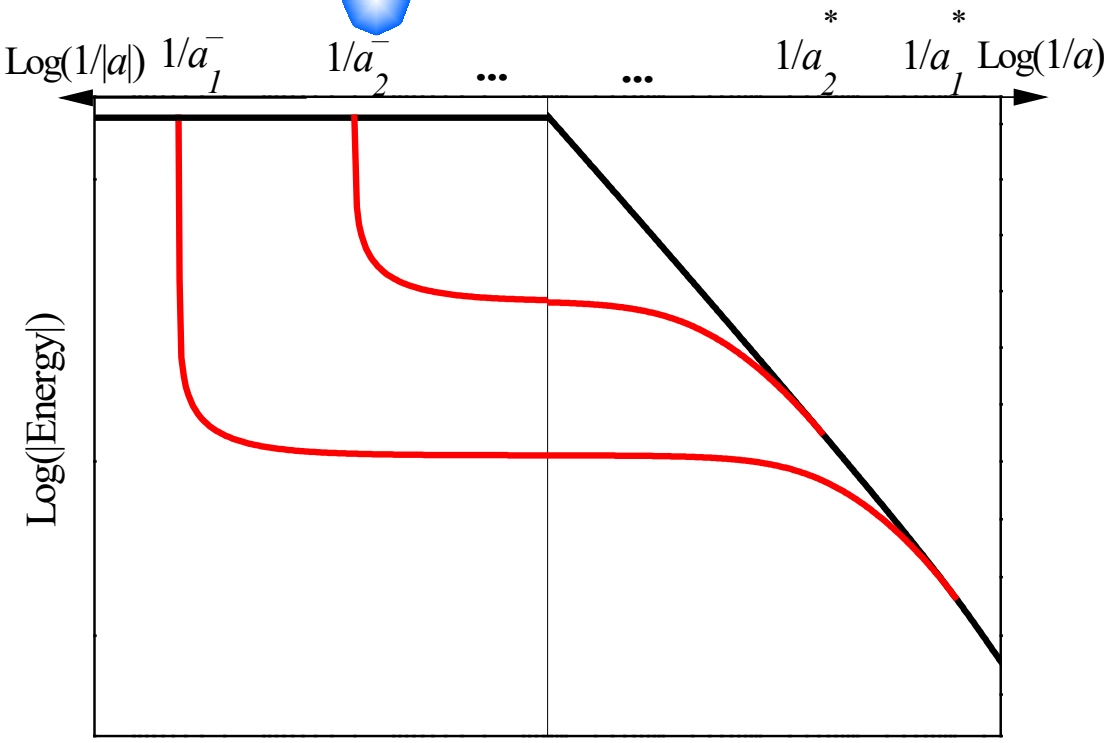
3B bound states *disappear* through the ***2B*** threshold as λ increases



Efimov effect

Efimov effect





$$\frac{E_{n+1}}{E_n} = Exp(-2\pi / s_0)$$

$$E_1 \approx -\frac{\hbar^2}{Mr_0^2}$$

$$s_0 \approx 1.00624$$

Efimov effect in electron-dipole system

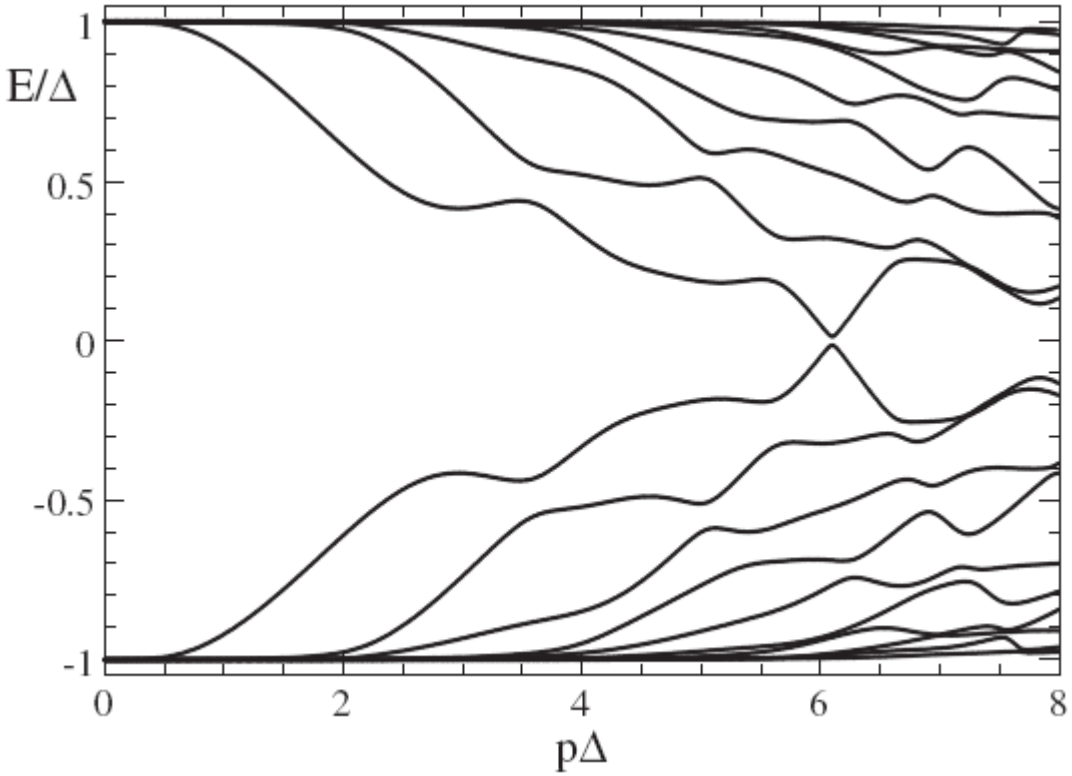
Bound states of the planar relativistic electron-dipole system obey the scaling hierarchy (*n = 1, 2, . . .)*

$$\frac{\varepsilon_{n+1}}{\varepsilon_n} = \exp\left(-\frac{2\pi}{s_{j,k}}\right),$$

with the numbers ($P > P_{j,\kappa}$)

$$s_{j,k} \cong \begin{cases} \sqrt{2P\Delta}, & (j,k) = (0,+), \\ 0.956\sqrt{(P - P_{j,k})\Delta}, & j > 0. \end{cases}$$

Efimov effect in electron-dipole system



Bound state spectrum vs dipole moment

A. De Martino, D. Kloepfer, D. Matrasulov, R. Egger Phys.Rev.Lett., 112, 186603 (2014)

SUMMARY & OUTLOOK

- ✓Supercritical states appearing in relativistic quantum mechanics near the Dirac sea can be studied with charged impurities in graphene which create (artificial) relativistic 2D atoms and molecules;
- ✓For equal nuclear charges of slightly subcritical value, one can induce a transition to the supercritical regime by reducing the distance R between the Coulomb centers below a critical value
- ✓The electric dipole problem for 2D Dirac fermions exhibits rich physics that could be probed by STM spectroscopy in graphene
- ✓The Efimov-like scaling of the bound state energies, with the gap edges as accumulation points, suggests that electrons can be captured (and, thus, confined) by a dipole potential.

Challenges:

- ✓Boundary effects (Atom-in-box system)
- ✓Finite size effects
- ✓Dynamical supercritical phenomena

COLLABORATORS

- ✓Reinhold Egger (Heinrich-Heine-Universität Düsseldorf)
- ✓Alessandro De Martino (City University London, London)
- ✓Denis Kloepfer (Heinrich-Heine-Universität Düsseldorf)