GRAPHENE AND QUANTUM ELECTRODYNAMICS

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A single atomic layer of carbon, graphene, has the low-energy "relativistic- like" gapless quasiparticle excitations which in the continuum approximation are described by quantum electrodynamics in 2+1 dimensions. The Dirac-like character of charge carriers in graphene leads to several unique electronic properties which are important for applications in electronic devices. We study the gap opening in graphene following the ideas put forward by P. I. Fomin for investigation of chiral symmetry breaking and particle mass generation in quantum field theory.

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1. INTRODUCTION

Graphene, a one-atom-thick sheet of crystalline carbon with atoms packed in the honeycomb lattice, is a remarkable system with many unusual properties that was fabricated for the first time 8 years ago [1]. Graphene is the building block for many forms of carbon allotropes, for example, graphite is obtained by the stacking of graphene layers that is stabilized by weak van der Waals forces, carbon nanotubes are formed by graphene wrapping, and fullerenes can also be obtained from graphene by replacing several hexagons into pentagonsand heptagons.

The ability to sustain huge ($> 10^8 \mathrm{A/cm}^2$) electric currents and a very high electron mobility, $\mu \sim 2{\cdot}10^5 \mathrm{cm}^2/\mathrm{Vs}$ for suspended graphene, make graphene a promising candidate for applications in electronic devices such as nanoscale field effect transistors. Its thermal conductivity $\sim 5 \cdot 10^3 \mathrm{W/mK}$ is larger than for carbon nanotubes or diamond. Graphene is optically transparent: it absorbs $\pi\alpha \approx 2.3\%$ of white light ($\alpha = 1/137$ – fine structure constant) that can be important for making liquid crystal displays. It is the strongest material ever tested with stiffness 340 N/m. Because of this graphene remains stable and conductive at extremely small scales of order several nanometers.

Theoretically, it was shown long time ago [2] that quasiparticle excitations in graphene have a linear dispersion at low energies and are described by the massless Dirac equation in 2+1 dimensions. The observation of anomalous integer quantum Hall effect in graphene [3, 4] is in perfect agreement with the theoretical predictions [5]–[7] and became a direct experimental proof of the existence of gapless Dirac quasiparticles in graphene. In the continuum limit, graphene model on a honeycomb lattice, with both on-site and nearest-neighbor repulsions,maps onto a 2+1-dimensional field theory of Dirac fermions interacting through the Coulomb potential plus, in general, some residual short-range interactions represented by local four-fermion terms.

The vanishing density of states at the Dirac points ensures that the Coulomb interaction between the electrons in graphene retains its long-range character due to vanishing of the static polarization function when the wave vector $\vec{q} \to 0$. The large value of the "fine-structure" coupling constant $\alpha_g = e^2/\hbar v_F \sim 1$ ($v_F \approx 10^6$ m/s is the Fermi velocity) means that a strong attraction takes place between electrons and holes in graphene at the Dirac points. For graphene on a substrate with the effective coupling $\alpha_g/\kappa \ll 1$, κ being a dielectric constant, the system is in a weak-coupling regime and exhibits semimetallic properties due to the absence of a gap in the electronic spectrum. All the currently proposed applications of graphene are based on that fact. Much less is known about suspended graphene where the coupling constant is large.In fact, suspended graphene provides a condensed-matter analog of strongly coupled quantum electrodynamics (QED) intensively studied by P.I. Fomin and collaborators in the 1970s and 1980s. [8, 9]. The dynamics of the vacuum in QED leads to many peculiar effects not yet observed in nature. Some QED-like effects such as zitterbewegung (trembling motion), Klein tunneling, Schwinger pair production, supercritical atomic collapse and symmetry broken phase with a gap at strong coupling have a chance to be tested in graphene. In fact, graphene could be used as a bench-top particle-physics laboratory,allowing us to investigate the fundamental interactions of matter(recently, the Klein tunneling and supercritical atomic collapse in graphene were observed experimentally, see papers [10] and [11], respectively).

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2. DYNAMICAL MASS GENERATION IN QUANTUM FIELD THEORY

Proposals that electron-electron interactions in graphene could generate an electronic gap were investigated and actually preceded the discovery of graphene [12, 13]. The gap opening in graphene is an analogue of the phenomenon of dynamical mass generation which is studied in quantum field theory since the Nambu-Jona-Lasinio (NJL) paper in 1961 [14] The Lagrangian of the NJL model//

$$L = \bar{\Psi} i\gamma^{\mu}\partial_{\mu}\Psi + \frac{G}{2}\left[(\bar{\Psi}\Psi)^2 + (\bar{\Psi} i\gamma_5\Psi)^2\right] \quad (1)$$

is invariant under ordinary phase and chiral transformations,

$$\begin{array}{ll} \Psi \to e^{i\alpha}\Psi, & \bar{\Psi} \to \bar{\Psi}e^{-i\alpha}, \\ \Psi \to e^{i\alpha\gamma_5}\Psi, & \bar{\Psi} \to \bar{\Psi}e^{-i\alpha\gamma_5}, \end{array} \quad (2)$$

and the chiral invariance forbids the mass generation in perturbation theory. The self-consistent Hartree-Fock equation for a mass (Λ is a cutoff),

$$\frac{4\pi^2 m}{G\Lambda^2} = m - \frac{m^3}{\Lambda}\ln\left(1 + \frac{m^2}{\Lambda^2}\right) \quad (3)$$

has a nontrivial solution $m \neq 0$ if the coupling constant exceeds some critical value, $G > G_c = \frac{4\pi^2}{\Lambda^2}$, leading to a nontrivial chiral condensate $< \bar{\Psi}\Psi > \neq 0$.

In QED the problem of a mass generation starts since the work by V. Weisskopf [15] who calculated for the first time the one-loop correction to the bare electron mass m_0,

$$m = m_0 + \frac{3\alpha}{2\pi} m_0 \ln\left(\frac{\Lambda}{m}\right) \quad (4)$$

The total electron mass m vanishes for $m_0 = 0$. On the other hand, solving the self-consistent equation for the mass,

$$m = m_0 + \frac{3\alpha}{2\pi} m \ln\left(\frac{\Lambda}{m}\right) \quad (5)$$

one gets a nontrivial solution,

$$m = \Lambda \exp\left(-\frac{3\pi}{2\alpha}\right), \quad (6)$$

even for zero bare electron mass $m = 0$. This solution, called the superconducting-type solution because of its nonanalytical dependence on the coupling α, was thoroughly studied in the works by P. I. Fomin (see review [16] and the references therein) using the Schwinger-Dyson equations for the electron and photon propagators and for the vertex function. The solution (6) should be compared to the solution for a quasiparticle gap in the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity,

$$\Delta = \omega_D \exp(-\frac{2}{g\nu_F}), \quad (7)$$

where ω_D is the Debye frequency, g the electron-phonon coupling constant, and ν_F is the density of states on the Fermi surface. In the BCS theory the gap in the quasiparticle spectrum is generated for any value of the coupling constant. The physical reason for zero value of the critical coupling constant in the BCS theory is connected with the presence of the Fermi surface.

More refined study of the Schwinger-Dyson equation for the fermion propagator in QED (Fig. 1), leads in the ladder approximation to the solution [17],

$$m \simeq \Lambda \exp\left(-\frac{\text{const}}{\sqrt{\alpha - \alpha_c}}\right), \quad (8)$$

where the critical coupling constant is of order one, $\alpha_c \sim 1$ Note the essentially nonanalytical dependence of the mass on the coupling constant α. Such a behavior of a mass remains valid in more refined approximation when fermions loops are neglected but all diagrams with crossed photon lines are taken into account (the so-called quenched approximation). Taking into account the vacuum polarization [18] changes the result to

$$m \simeq \Lambda(\alpha - \alpha_c)^{\beta}, \quad \alpha \gtrsim \alpha_c, \quad \beta \lesssim \frac{1}{2}. \quad (9)$$

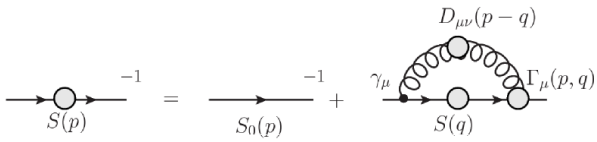

Fig.1. *The Schwinger-Dyson equation for the fermion propagator*

The solution (8) for the dynamical electron mass combines features of a superconducting gap(nonanalytical dependence on the coupling constant) and of the NJL gap (the presence of a critical coupling).

The presence of a magnetic field makes the situation even more interesting. It was shown in Ref. [19] that a magnetic field catalyzes the gap generation for gapless fermions in relativistic-like systems, and even the weakest attraction leads to the formation of a symmetry-breaking condensate and a gap generation. For example, in the four-dimensional NJL model in an external magnetic field the gap (mass) is generated at any coupling constant [20]:

$$\Delta \simeq \sqrt{|eB|}\exp(-\frac{1}{2\nu_0 G}), \quad (10)$$

where B is the strength of a magnetic field and $\nu_0 = |eB|/4\pi^2$ is the density of states at the lowest Landau level (compare with a superconducting gap).This phenomenon is called magnetic catalysis and its main features are model independent. The essence of the magnetic catalysis is that the dynamics of the electrons in a magnetic field, B,corresponds effectively to a theory with spatial dimension reduced by two units (note a close similarity with the role of

the Fermi surface in the BCS theory) if their energy is much less than the Landau gap $\sqrt{|eB|}$. The zero-energy Landau level, which plays, in fact, the role of the Fermi surface, has a finite density of states and this is the key ingredient of magnetic catalysis. The magnetic catalysis plays an important role in quantum Hall effect studies in graphene where it is responsible for lifting the degeneracy of the Landau levels.

3. LOW-ENERGY EFFECTIVE THEORY OF GRAPHENE

The electronic band structure of graphene close to the Fermi level forms the basis of the low-energy effective theory of graphene. This band structure is a reflection of the hexagonal arrangement of the carbon atoms. As was shown by P. Wallace [2], the two-dimensional graphene honeycomb lattice has two atoms per unit cell and its tight-binding band structure consists of conduction and valence bands. The energy spectrum of electrons as a function of a wave vector has the form

$$E(\vec{k}) = \pm t\sqrt{1 + 4\cos\frac{\sqrt{3}k_x a}{2}\cos\frac{k_y a}{2} + 4\cos^2\frac{k_y a}{2}}\,, \tag{11}$$

where $t \approx 2.8$ eV is nearest-neighbor hopping energy (hopping between different sublattices), in the tight-binding lattice Hamiltonian, $a = 2.46$ Å is the lattice constant. The two bands touch each other and cross the Fermi level, corresponding to zero chemical potential $\mu = 0$, in six K points located at the corners of the hexagonal 2D Brillouin zone, but only two of them, say K, $K' = (\pm\frac{4\pi}{3\alpha}, 0)$, are nonequivalent. Low-energy excitations near two nonequivalent K-points have a linear dispersion, $E(\vec{k}) = \pm\hbar v_F|\vec{k}|$ where $\hbar = h/2\pi$ is the Planck constant, $v_F = \sqrt{3}ta/2\hbar \approx 10^6$ m/s is the Fermi velocity which is only 300 times less the velocity of light. Electron states at each K-point are described by the spinor,

$$\Psi_{K\sigma} = \begin{pmatrix} \Psi_{KA\sigma} \\ \Psi_{KB\sigma} \end{pmatrix},$$

which consists of electron wave functions on atoms A, B of two sublattices, $\sigma = \pm$ describes the real spin, and satisfies the massless Dirac equation,

$$\left(\hbar\gamma^0 i\partial_t + \hbar v_F(i\gamma^1\partial_x + i\gamma^2\partial_y)\right)\Psi_{K\sigma}(x,y) = 0. \tag{12}$$

Two-dimensional Dirac gamma matrices are given in terms of the Pauli matrices $\gamma^\mu = (\tau_3, i\tau_2, -i\tau_3), \mu = 0, 1, 2$. Spinors at two K-points can be combined into one four-dimensional Dirac spinor

$$\Psi_\sigma = (\Psi_{KA\sigma}, \Psi_{KB\sigma}, \Psi_{K'A\sigma}, \Psi_{K'B\sigma})^T,$$

which satisfies the Dirac equation (12) but with 4x4 gamma matrices $\gamma^\mu = \tilde{\tau}_3 \otimes (\tau_3, i\tau_2, -i\tau_3)$ (the Pauli matrix $\tilde{\tau}_3$ acts in the space of two K-points). The four-component spinor structure accounts for quasiparticle excitations of sublattices A and B around the two Dirac points (valleys) in the band structure.

Taking into account the Coulomb interaction between quasiparticles we come at the effective low-energy theory described by the QED-like action (the spin index is omitted)

$$S = \int dtd^3r\left\{\frac{1}{2}(\partial_i A_0)^2 - A_0 j_0 + \left[\bar{\Psi}(t,r)(\hbar\gamma^0 i\partial_t + \hbar v_F i\gamma^i\partial_i - \Delta_0)\Psi(t,r)\right]\delta(z)\right\}, \tag{13}$$

where $j_0 = e\bar{\Psi}(t,r)\gamma^0\Psi(t,r)\delta(z)$ is the charge density. Note that the electric field, described by the scalar potential A_0 and responsible for interparticle interaction, propagates in a three-dimensional space, while fermion fields, describing electron- and hole-type quasiparticles, are localized on two-dimensional planes. This is a typical example of the so-called brane world models studied last years in high energy physics.Integration over z-coordinate leads to the standard nonlocal Coulomb interaction for quasiparticles in a plane. In Eq. (13) we included also a bare gap Δ_0 which can be generated due to the interaction with a substrate [21]. In the presence of this term the dispersion law for quasiparticles takes the form $E(\vec{k}) = \pm\sqrt{(\hbar v_F\vec{k})^2 + \Delta_0^2}$ and two zones are separated by $2\Delta_0$. For $\Delta_0 = 0$ the continuum effective theory described by the action (13) possesses the large "flavor" U(4) symmetry in the spin-valley space. In the next section we will study the dynamical symmetry breaking of this symmetry and generation of a quasiparticle gap due to the Coulomb interaction when the bare gap is zero.

4. GAP GENERATION AND SEMIMETAL-INSULATOR PHASE TRANSITION IN GRAPHENE

In pristinegraphenean analog of the fine-structure constant $\alpha_g \gtrsim 1$. Given the strong attraction, one may expect an instability in the excitonic channel (electron-hole pairing) with subsequent quantum phase transition to a phase with gapped quasiparticles that may turn graphene into an insulator. In graphene sheets deposited on a substrate,such a transition is effectively inhibited due to the screening of the Coulomb interaction by the dielectric ($\alpha_g \to \alpha_g/\kappa$). This semimetal-insulator transition in graphene is widely discussed now in the literature since the first study of the problem in Refs. [12, 13].

As is well known, in the BCS theory the Bethe-Salpeter (BS) equation for an electron-electron bound state in the normal state of metal has a solution with imaginary energy, i.e., a tachyon. This means that normal state is unstable and a phase transition to the superconducting state takes place.

In order to analyze excitonic instability in graphene, we consider the BS equation for an electron-hole bound state. In the random phase approximation, the BS equation for an amputed bound-

state wave function reads

$$\chi_{\alpha\beta}(q,P) = \frac{i\alpha_g}{(2\pi)^2}\int d^3k D(k_0,|\vec{q}-\vec{k}|)\times \\ \times\left[\gamma^0 S(q+\frac{P}{2}\chi(k,P)S(k-\frac{P}{2})\gamma^0\right]_{\alpha\beta}, \quad (14)$$

where $q=(q_0,\vec{q})$, $P=(P_0,\vec{P})$ are relative and total energies-momenta of bound electron and hole. The Coulomb propagator has the form

$$D(\omega,\vec{q}) = \frac{1}{|\vec{q}|+\Pi(\omega,\vec{q})}, \quad (15)$$

and the one-loop polarization function is

$$\Pi(\omega,\vec{q}) = \frac{\pi e^2}{2\kappa}\frac{\vec{q}^2}{\sqrt{(\hbar v_F\vec{q})^2-\omega^2}}, \quad (16)$$

which in the instantaneous approximation reduces to $\Pi(\omega,\vec{q}) = \pi\alpha_g|\vec{q}|/2\kappa$. We consider the following ansatz for the matrix structure of the wave function of an excitonic bound state,

$$\chi(q,P) = \chi_5(q,P)\gamma^5 + \chi_{05}(q,P)\vec{q}\vec{\gamma}\gamma^0\gamma^5\,. \quad (17)$$

In the random phase approximation with static polarization function, i.e., $\Pi(\omega=0,\vec{q})$, we find an analytical solution with pure imaginary energy (tachyon) if the coupling constant α_g exceeds some critical value α_{gc} (for details, see Ref. [22]):

$$P_0^2 = -4\Lambda^2\exp\left(-\frac{4\pi n}{\sqrt{4\lambda-1}}+\delta\right), \delta\approx 7.3, \quad (18)$$
$$\lambda>\lambda_c=\frac{1}{4}, \quad \lambda=\frac{\alpha_g}{2+\pi\alpha_g}, \quad n=1,2,...$$

In the instantaneous approximation $\alpha_{gc}=2.33$, while more accurate numerical treatment gives $\alpha_{gc}=1.62$. In the supercritical regime the wave function $\chi_5(\vec{q})$ as a function of a relative momentum behaves asymptotically as

$$\chi_5(|\vec{q}|)\sim|\vec{q}|^{-1/2}\cos\left(\sqrt{\lambda-\frac{1}{4}}\ln\left(\frac{|\vec{q}|}{|P_0|}\right)+\text{const}\right).$$

Such oscillatory behavior is typical for the phenomenon known in quantum mechanics as the "fall into the center" (collapse): in this case the energy of a system is unbounded from below and there is no ground state. Nodes of the wave function of the bound state signify the existence of the tachyon states with imaginary energy P_0.

To find a stable ground state we solved a gap equation which in the random phase approximation with static polarization has the form [23],

$$\Delta(P) = \lambda\int_0^\Lambda \frac{q\Delta(q)\mathrm{K}(p,q)}{\sqrt{q^2+(\Delta(q)/v_F)^2}}\,.dq \quad (19)$$

Here the symmetric kernel of the equation is

$$\mathrm{K} = \frac{2}{\pi}\frac{1}{p+q}K\left(\frac{2\sqrt{pq}}{p+q}\right),$$

and $K(x)$ is the complete elliptic integral of the first kind. The nontrivial solution for the momentum dependent gap function $\Delta(p)$ exists if the coupling $\lambda>1/4$ ($\alpha_{gc}>1.62$ and its value at $p=0$ (gap itself) is given by

$$\Delta(p=0) = \Lambda v_F\exp\left(-\frac{\pi}{\sqrt{\lambda-1/4}}\right). \quad (20)$$

The essentially nonanalytical dependence of the gap (20) on the coupling constant corresponds to a continuous phase transition of infinite order. Such a behavior is inherent for the Berezinskii-Kosterlitz-Thouless phase transition, or the conformal phase transition, and is related to the scale invariance of the problem under consideration. Note, however, that taking into account the finite size of graphene samples should turn this phase transition into a second-order one.

In the case of frequency dependent polarization function (dynamical screening) the critical constant is lower, $\alpha_{gc}=0.92$. A dynamical gap is generated only if $\alpha_g>\alpha_{gc}$. Since for suspended clean graphene the fine-structure constant $\alpha_g=2.19$ is supercritical, the dynamical gap will be generated making graphene an insulator. Note that for graphene on SiO_2 substrate, the dielectric constant κ=2.8 and $\alpha_g=0.78$, i.e., the system is in the subcritical regime. The value of α_{gc} is rather large that implies that a weak-coupling approach might be quantitatively inadequate for the problem of the gap generation in suspended clean graphene. Therefore, it is instructive to compare our analytical results to lattice MonteCarlo studies, [24] where $\alpha_{gc}=1.08\pm0.05$ that is rather close to our analytical findings.

Additional short-range four-fermion interactions were also included in the continuum model to account for the lattice simulation results [23]. In spite of being small, the induced local interactions can play a significant role in the critical behavior observed in lattice simulations.Instead of a critical point, we obtained the critical line in the plane of electromagnetic, α, and four-fermion, $\tilde{g}$, coupling constants (Fig. 2), and found a second-order phase transition separating zero gap and gapped phases with critical exponents close to those found in lattice calculations.

We expect that the form of the critical curve in graphene can be checked in further lattice simulations.

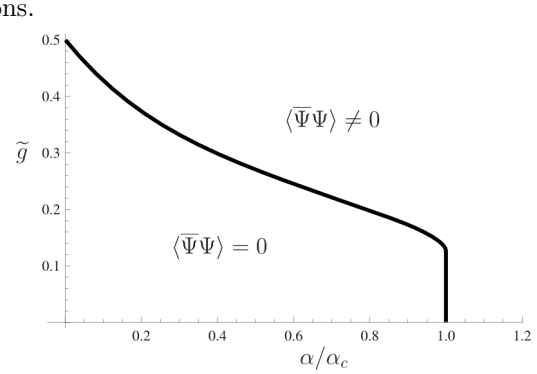

Fig.2. *Phase diagram*

5. CONCLUSIONS

We studied in this paper an intriguing possibility that spontaneous formation of excitons, electron-hole bound states, and the concomitant formation of excitonic condensate which breaks chiral symmetry, may turn graphene into a Mott insulator. The insulator phase of graphene with gapped quasiparticles is in line with the strong coupling phase of QED studied by P.I. Fomin and his collaborators in the 70s and 80s. The strong coupling phase of QED was searched in heavy ion collisions in GSI-Darmstadt in the 80s. Various sharp lines were observed in energy spectra of electron-positron and photon-photon emitted back-to-back with kinetic energies near 350 keV. Suggested explanation was that the correlated signals corresponded to the decay of a neutral particle produced in the collision, and that particle is naturally present in strong coupling phase of QED (tightly bound electron-positron pairs). [25] However, later on the Darmstadt experiments have faded.

The spontaneous gap generation and insulator phase in graphene(strong coupling phase of graphene) have been predicted [12, 13] before graphene was fabricated in the laboratory. So far, however experimentally there has been no conclusive evidence that semimetal-insulator transition of suspended monolayer graphene occurs at low temperature. [26] In this respect, it has been already suggested that the growth of the Fermi velocity,when approaching the charge neutrality point [23, 27], makes the effective interaction strength smaller than a critical value, thus preventing a gap generation.Certainly, this problem worth of further studying, both theoretically and experimentally.

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ГРАФЕН И КВАНТОВАЯ ЭЛЕКТРОДИНАМИКА

В.П. Гусынин

Одноатомный слой углерода, графен, обладает низкоэнергетическими безщелевыми квазичастичными возбуждениями, которые в континуальном приближении описываются квантовой электродинамикой в размерности $2+1$. Дираковский характер заряженных носителей в графене приводит ко многим уникальным электронным свойствам, имеющим важное значение для применений в электронных устройствах. Мы исследуем открытие щели в графене, следуя идеям, предложенным П.И. Фоминым для исследования нарушения киральной симметрии и генерации масс частиц в квантовой теории поля.

ГРАФЕН І КВАНТОВА ЕЛЕКТРОДИНАМІКА

В.П. Гусинін

Одноатомний шар вуглецю, графен, має низькоенергетичні безщілинні квазічастинкові збудження, які в континуальному наближенні описуються квантовою електродинамікою в розмірності 2+1. Діраківський характер заряджених носіїв у графені призводить до багатьох унікальних електронних властивостей, що мають важливе значення для застосувань в електронних пристроях. Ми досліджуємо відкриття щілини в графені, слідуючи ідеям, запропонованим П.І. Фоміним для дослідження порушення киральної симетрії і генерації мас частинок у квантовій теорії поля.