EXCITONIC INSTABILITY AND GAP GENERATION IN MONOLAYER GRAPHENE

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We analyze the excitonic instability in graphene by solving the Bethe–Salpeter equation for the electron-hole bound state. In the supercritical regime, we show that this equation has a tachyon in its spectrum. We argue that the excitonic instability is resolved through the formation of an electron-hole condensate leading to the gap (mass) generation in the quasiparticle spectrum. Such a gap could be observed in a free standing clean graphene.

1. Introduction

Graphene is an atomically thin layer of carbon atoms densely packed in a honeycomb crystal lattice. Although theoretically considered long time ago [1], graphene became an active area of research only recently after the experimental fabrication [2] of this material and due to a variety of its unusual electronic properties, among them metallic conductivity in the limit of no carriers and the half-integer quantum Hall effect [3, 4].

At low energies, the quasiparticle excitations in graphene are described by the massless Dirac equation and have a relativistic-like dispersion $E = \pm \hbar v_{\rm F} |\mathbf{k}|$, where $v_{\rm F} \approx 10^6 m/s$ is the Fermi velocity, and \mathbf{k} is the quasiparticle wave vector. This fact brings an exciting connection between graphene and quantum electrodynamics (QED).

The Coulomb interaction between the electrons in graphene retains its long-range character in view of the vanishing of the static polarization function as $q \to 0$ [5]. The large value of the coupling constant $\alpha = e^2/\hbar v_{\rm F} \sim 1$ means that a strong attraction takes place between electrons and holes in graphene, and this resembles strongly coupled QED, thus providing an opportunity for studying the strong coupling phase experimentally at a condensed matter laboratory. Given the strong attraction, one may expect an instability in the excitonic channel in graphene with a subsequent quantum phase transition to a phase with gapped quasiparticles that may turn graphene into an insulator. This semimetal-insulator transition in graphene is widely discussed now in the literature [6, 8] since the first study of the problem in

Refs. [9, 10]. The gap opening is similar to the chiral symmetry breaking phenomenon that occurs in strongly coupled QED and was studied in the 1970s and 1980s [11–15]. In fact, the predicted strong coupling phase of QED, like other QED effects not yet observed in the nature (Klein tunneling, Schwinger effect, etc.), has a chance to be tested in graphene.

In the present paper, we solve the Bethe–Salpeter (BS) equation for the electron-hole bound state in graphene and demonstrate that, for a strong enough coupling constant, there are tachyon states with imaginary energy $(E^2 < 0)$. The presence of tachyons signals that the normal state of a freely standing graphene is unstable. In fact, the tachyon instability can be viewed as the field theory analog of the "fall into the center" phenomenon, and the critical coupling α_c is an analog of the critical coupling constant $Z_c e^2/\hbar v_{\rm F}$ in the problem of the Coulomb center [16, 17]. However, in view of the manybody character of the problem, the way of curing the instability in graphene (like in QED [12]) is quite different from that in the case of the supercritical Coulomb center. Since the coupling constant in a freely standing graphene $\alpha \approx 2.19$ is larger than the critical value 1/2 in the Coulomb center problem, the quasielectron in graphene has the supercritical Coulomb charge. This leads to the production of an electron-hole pair, the hole is coupled to the initial quasielectron forming a bound state, but the emitted quasielectron has again a supercritical charge. Thus, the processes of creation of pairs and formation of bound states lead to the formation of an exciton (chiral) condensate in the stable phase, and, as a result, the quasiparticles acquire a gap. The exciton condensate formation resolves the problem of instability, hence a gap generation should take place in a free standing graphene making it an insulator.

2. Bethe-Salpeter Equation

The signs of the excitonic instability can already be seen in the spectrum of the Coulomb center problem, where resonances appear for a large enough charge [16–18].

In this section, we will study the BS equation for an electron-hole bound state and show that it has a tachyon in the spectrum in the supercritical regime. The excitonic instability plays a role similar to that of the Cooper instability in a normal metal that leads to the gap generation in superconductors. Indeed, according to [19], the BS equation for an electron-electron bound state in the normal state of a metal has a solution with imaginary energy, i.e. a tachyon. This means that the normal state is unstable, and a phase transition to the superconducting state takes place.

For the description of the dynamics in graphene, we will use the same model as in Refs. [9, 10], in which the electromagnetic (Coulomb) interaction between quasiparticles is three-dimensional in nature while they are confined to a two-dimensional plane. The excitations of low-energy quasiparticles in graphene are conveniently described in terms of a four-component Dirac spinor $\Psi_a^T = (\psi_{KAa}, \psi_{KBa}, \psi_{K'Ba}, \psi_{K'Aa})$ which combines the Bloch states with spin indices a = 1, 2 on the two different sublattices (A, B) of the hexagonal graphene lattice and with momenta near the two nonequivalent valley points (K, K') of the two-dimensional Brillouin zone. In what follows, we treat the spin index as a "flavor" index with N_f components, $a = 1, 2, ..., N_f$; then $N_f = 2$ corresponds to a graphene monolayer, while $N_f = 4$ is related to the case of two decoupled graphene layers interacting solely via the Coulomb interaction.

The action describing graphene quasiparticles interacting through the Coulomb potential has the form

$$S = \int dt d^2x \overline{\Psi}_a(t, \mathbf{r}) \left(i \gamma^0 \partial_t - i v_F \gamma \nabla \right) \Psi_a(t, \mathbf{r}) -$$

$$-\frac{1}{2}\int dtdt'd^2rd^2r'\overline{\Psi}_a(t,{\bf r})\gamma^0\Psi_a(t,{\bf r})\times$$

$$\times U_0(t - t', |\mathbf{r} - \mathbf{r}'|) \overline{\Psi}_b(t', \mathbf{r}') \gamma^0 \Psi_b(t', \mathbf{r}'), \tag{1}$$

where $\overline{\Psi} = \Psi^{\dagger} \gamma^0$, and the 4×4 Dirac γ -matrices $\gamma^{\mu} = \tau^3 \otimes (\sigma^3, i\sigma^2, -i\sigma^1)$ furnish a reducible representation of the Dirac algebra in 2+1 dimensions. The Pauli matrices τ, σ act in the subspaces of the valleys (K, K') and sublattices (A, B), respectively. The other two γ -matrices we use are $\gamma^3 = i\tau_2 \otimes \sigma_0, \gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3 = \tau_1 \otimes \sigma_0$ (σ_0 is the 2×2 unit matrix).

The bare Coulomb potential $U_0(t, |\mathbf{r}|)$ takes the simple form:

$$U_0(t, |\mathbf{r}|) = \frac{e^2 \delta(t)}{\kappa} \int \frac{d^2 k}{2\pi} \frac{e^{i\mathbf{k}\mathbf{r}}}{|\mathbf{k}|} = \frac{e^2 \delta(t)}{\kappa |\mathbf{r}|}.$$
 (2)

However, the polarization effects considerably modify this bare Coulomb potential, and the interaction will be

$$U(t, |\mathbf{r}|) = \frac{e^2}{\kappa} \int \frac{d\omega}{2\pi} \int \frac{d^2k}{2\pi} \frac{\exp(-i\omega t + i\mathbf{k}\mathbf{r})}{|\mathbf{k}| + \Pi(\omega, \mathbf{k})},$$
 (3)

where κ is the dielectric constant due to a substrate, and the polarization function $\Pi(\omega, \mathbf{k})$ is proportional (within the factor $2\pi/\kappa$) to the time component of the photon polarization function. Correspondingly, the Coulomb propagator has the form

$$D(\omega, |\mathbf{q}|) = \frac{1}{|\mathbf{q}| + \Pi(\omega, |\mathbf{q}|)}.$$
 (4)

We use the one-loop polarization function in the static approximation, where it is given by the expression [5]

$$\Pi(\omega = 0, \mathbf{k}) = \frac{\pi e^2 N_f}{4\kappa \hbar v_F} |\mathbf{k}|. \tag{5}$$

In general, the static polarization operator must have the form $\Pi(0, |\mathbf{q}|) = |\mathbf{q}| F(\alpha, N_f)$ due to dimensional reasons. However, its exact form is not known, and we will use the one-loop approximation in the present paper.

The continuum effective theory described by action (1) possesses the $U(2N_f)$ symmetry. However, as was pointed out in Ref. [20] (see also Refs. [21, 22]), it is not exact for the Lagrangian on the graphene lattice. In fact, there are small on-site repulsion interaction terms which break the $U(2N_f)$ symmetry.

In order to analyze the excitonic instability, we consider the BS equation for the electron-hole bound state,

$$\left[S^{-1}(q + \frac{1}{2}P)\chi(q, P)S^{-1}(q - \frac{1}{2}P) \right]_{\alpha\beta} =$$

$$= \frac{i\alpha}{(2\pi)^2} \int d^3k \, D(|\mathbf{q} - \mathbf{k}|) \left[\gamma^0 \chi(k, P) \gamma^0 \right]_{\alpha\beta}, \tag{6}$$

where $k = (k_0, \mathbf{k})$, α, β are spinor indices, $\chi(q, P)$ is the BS amplitude in the momentum space,

$$\chi_{\alpha\beta}(q,P) = \int d^3x \, e^{iqx} \langle 0|T\Psi_{\alpha}\left(\frac{x}{2}\right)\overline{\Psi}_{\beta}\left(-\frac{x}{2}\right)|P\rangle, \quad (7)$$

 $q = (q_0, \mathbf{q}), P = (P_0, \mathbf{P}), \mathbf{q}$ and \mathbf{P} are the relative and total momenta, respectively, and

$$S(p) = \frac{\gamma^0 p_0 - \gamma \mathbf{p} + \Delta}{p_0^2 - \mathbf{p}^2 - \Delta^2 + i\delta}$$

is the quasiparticle propagator with a gap Δ (the gap Δ is zero in non-interacting graphene; however, it may

be generated due to the strong Coulomb interaction). In what follows, we put $\hbar = v_{\rm F} = 1$.

Accounting for the static vacuum polarization by massless fermions, Eq. (5), we get Eq. (6), where the following replacements are made:

$$\alpha \to \frac{\alpha}{1 + \pi \alpha N_f / 4} \equiv 2\lambda, \quad D(|\mathbf{q} - \mathbf{k}|) \to \frac{1}{|\mathbf{q} - \mathbf{k}|}.$$

Further, introducing the function

$$\widehat{\chi}(q,p) = S^{-1}(q + \frac{1}{2}P)\chi(q,P)S^{-1}(q - \frac{1}{2}P)$$

with p=P/2, the BS equation can be equivalently rewritten as follows:

$$\widehat{\chi}(q,p) = \frac{2i\lambda}{(2\pi)^2} \int \frac{d^3k}{|\mathbf{q} - \mathbf{k}|} \gamma^0 S(k+p) \widehat{\chi}(k,p) S(k-p) \gamma^0.$$

In general, $\widehat{\chi}$ can be expanded in 16 independent matrix structures. In view of the experience in QED [12], we expect a gap generation in graphene in the supercritical regime. Then the spin-valley U(4) symmetry will be broken (see, e.g. [9,10]), which leads to the appearance of massless Nambu–Goldstone bosons in the spectrum. Similarly to QED [12], these Nambu–Goldstone bosons are transformed into tachyons if they are considered on the wrong vacuum state without a gap generation. In the present paper, we will consider only matrix structures of $\widehat{\chi}$ connected with the γ^5 matrix

$$\widehat{\chi}(q) = \chi_5(q)\gamma^5 + \chi_{05}(q)q^i\gamma^i\gamma^0\gamma^5, \quad \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3, (9)$$

where $\chi_5(q)$ and $\chi_{05}(q)$ are coefficient functions. We will see in the next section that it is enough to consider only χ_5 in order to describe a Nambu–Goldstone excitation in the massive state. However, we retain the function χ_{05} because it is necessary in the study of tachyons. In principle, there could be tachyons in different channels which describe different ways of breaking the $U(2N_f)$ symmetry. The real pattern of a symmetry breaking is defined by solving the gap equations for various kinds of order parameters and by determining which of them corresponds to the global energy minimum of the system. For simplicity, we consider only the channel described by the wave function (9) which can be treated analytically.

2.1. Tachyon states

Let us firstly show that, for $\lambda > \lambda_c$, there is a tachyon in the spectrum of the Bethe–Salpeter equation in the

massless theory $\Delta = 0$ and determine the critical value λ_c . For the study of a tachyon, we can set $\mathbf{p} = 0$, however, should keep nonzero p_0 . One can check that ansatz (9) is consistent for Eq. (8) and leads to a coupled system of equations for the functions $\chi_5(q)$ and $\chi_{05}(q)$. Since Eq. (8) implies that $\hat{\chi}(q, p)$ does not depend on q_0 , we can integrate then over k_0 by using the integrals

$$i\int_{-\infty}^{\infty} \frac{dk_0}{\pi} \frac{c_1 + c_2 k_0 + c_3 k_0^2}{((k_0 - p_0)^2 - \mathbf{k}^2 + i\delta) ((k_0 + p_0)^2 - \mathbf{k}^2 + i\delta)} =$$

$$= \frac{c_1 + c_3(p_0^2 - \mathbf{k}^2)}{2|\mathbf{k}| (p_0^2 - \mathbf{k}^2)},$$

where $\delta \to +0$. We obtain the following system of integral equations:

$$\chi_5(\mathbf{q}) = \lambda \int \frac{d^2k}{2\pi} \frac{\mathbf{k}^2 \left(\chi_5(\mathbf{k}) + p_0 \chi_{05}(\mathbf{k})\right)}{|\mathbf{q} - \mathbf{k}| |\mathbf{k}| \left(\mathbf{k}^2 - p_0^2\right)},\tag{10}$$

$$\chi_{05}(\mathbf{q}) = \lambda \int \frac{d^2k}{2\pi} \frac{\mathbf{qk} \left(\mathbf{k}^2 \chi_{05}(\mathbf{k}) + p_0 \chi_5(\mathbf{k}) \right)}{\mathbf{q}^2 |\mathbf{q} - \mathbf{k}| |\mathbf{k}| \left(\mathbf{k}^2 - p_0^2 \right)}.$$
 (11)

We assume that $\chi_5(\mathbf{q})$ and $\chi_{05}(\mathbf{q})$ depend only on $q = |\mathbf{q}|$. Then we can integrate over the angle and arrive at a system of integral equations with kernels depending on the elliptic integrals K(x) and E(x). Approximating the elliptic integrals by their asymptotic at $x \ll 1$,

$$K(x) \simeq \frac{\pi}{2} \left(1 + \frac{x^2}{4} \right), E(x) \simeq \frac{\pi}{2} \left(1 - \frac{x^2}{4} \right),$$
 (12)

we find

$$\chi_5(q) = \lambda \int_0^q \frac{k^2 dk}{q(k^2 - p_0^2)} \left(\chi_5(k) + p_0 \chi_{05}(k)\right) +$$

$$+\lambda \int_{q}^{\Lambda} \frac{kdk}{k^2 - p_0^2} \left(\chi_5(k) + p_0 \chi_{05}(k) \right), \tag{13}$$

$$\chi_{05}(q) = \frac{\lambda}{2} \int_{0}^{q} \frac{k^2 dk}{q^3 (k^2 - p_0^2)} \left(k^2 \chi_{05}(k) + p_0 \chi_5(k) \right) +$$

$$+\frac{\lambda}{2} \int_{q}^{\Lambda} \frac{dk}{k(k^2 - p_0^2)} \left(k^2 \chi_{05}(k) + p_0 \chi_5(k) \right). \tag{14}$$

Here, we also introduced a finite ultraviolet cutoff Λ which could be taken to be of order π/a , where a is a characteristic lattice size, a=2.46 Å for graphene, or of the size of the energy band, $\Lambda=t/v_{\rm F}$, where t=2.4 eV in graphene.

These equations are equivalent to the system of differential equations

$$\chi_5'' + \frac{2}{q}\chi_5' + \lambda \frac{\chi_5 + p_0 \chi_{05}}{q^2 - p_0^2} = 0, \tag{15}$$

$$\chi_{05}^{"} + \frac{4}{q}\chi_{05}^{'} + \frac{3\lambda}{2} \frac{q^2\chi_{05} + p_0\chi_5}{q^2(q^2 - p_0^2)} = 0$$
 (16)

with the following boundary conditions:

$$q^2 \chi_5' \Big|_{q=0} = 0, \quad (q \chi_5(q))' \Big|_{q=\Lambda} = 0,$$
 (17)

$$q^4 \chi'_{05} \Big|_{q=0} = 0, \quad (q^3 \chi_{05}(q))' \Big|_{q=\Lambda} = 0.$$
 (18)

The system of differential equations (16) can be reduced to one equation of the fourth order, whose solutions are given in terms of the generalized hypergeometric functions ${}_{4}F_{3}(q^{2}/p_{0}^{2})$ with the corresponding boundary conditions [18]. However, since we seek for the solution with $p_{0} \rightarrow 0$, it is simpler to analyze directly system (16). In this regime, the system decouples

$$\chi_5'' + \frac{2}{q}\chi_5' + \lambda \frac{\chi_5}{q^2 - p_0^2} = 0, \tag{19}$$

$$\chi_{05}^{"} + \frac{4}{q}\chi_{05}^{"} + \frac{3\lambda}{2}\frac{\chi_{05}}{q^2 - p_0^2} = 0, \tag{20}$$

where we keep p_0 in the denominators, because it regularizes singularities for $q \to 0$.

Obviously, Eqs. (19) and (20) are differential equations for the hypergeometric function F(a, b; c; z) [25]. The solutions that satisfy the infrared boundary conditions are

$$\chi_5 = C_1 F\left(\frac{1+\gamma}{4}, \frac{1-\gamma}{4}; \frac{3}{2}; \frac{q^2}{p_0^2}\right),\tag{21}$$

$$\chi_{05} = C_2 F\left(\frac{3(1+\tilde{\gamma})}{4}, \frac{3(1-\tilde{\gamma})}{4}; \frac{5}{2}; \frac{q^2}{p_0^2}\right),\tag{22}$$

where $\gamma = \sqrt{1-4\lambda}$ and $\tilde{\gamma} = \sqrt{1-2\lambda/3}$. Using the asymptotic of the hypergeometric functions, one may

easily check that the ultraviolet boundary conditions for the function χ_5 can be satisfied only for $\lambda > 1/4$. Therefore, 1/4 is the critical coupling for the approximation we used above. The UV boundary condition for the function χ_{05} can be satisfied for the values of $\lambda > 3/2$ but not for $\lambda < 3/2$. Therefore, for $1/4 < \lambda < 3/2$, we take a trivial solution $\chi_{05} = 0$, and we are left only with the equation for the function χ_5 . Knowing the function χ_5 , we then solve the inhomogeneous equation (16) for χ_{05} . In this way, we find that the function $\chi_{05} \sim p_0$. The critical value $\lambda_c = 1/4$ coincides with the critical coupling constant found in [10], where the same approximation for the kernel was made. In the supercritical regime, $\gamma = i\omega$, $\omega = \sqrt{4\lambda - 1}$, and the function $\chi_5(q)$ behaves asymptotically as

$$\chi_5(q) \sim q^{-1/2} \cos\left(\sqrt{\lambda - 1/4} \ln q + \text{const}\right).$$
 (23)

Such oscillatory behavior is typical of the phenomenon known in quantum mechanics as the collapse ("fall into the center") phenomenon: in this case, the energy of a system is unbounded from below, and there is no ground state. Zeros of the wave function of the bound state signify the existence of the tachyon states with imaginary energy p_0 , $\text{Im}p_0^2 < 0$. Indeed, the UV boundary condition for χ_5 leads to the equation

$$\frac{(1+i\omega)\Gamma\left(1+\frac{i\omega}{2}\right)\Gamma\left(\frac{1-i\omega}{4}\right)\Gamma\left(\frac{5-i\omega}{4}\right)}{(1-i\omega)\Gamma\left(1-\frac{i\omega}{2}\right)\Gamma\left(\frac{1+i\omega}{4}\right)\Gamma\left(\frac{5+i\omega}{4}\right)}\left(-\frac{\Lambda^2}{p_0^2}\right)^{i\frac{\omega}{2}}=1. \tag{24}$$

If λ tends to 1/4 from the above, i.e. $\omega \to 0$, then we find the following tachyon solution:

$$p_0^2 = -\Lambda^2 \exp\left(-\frac{4\pi n}{\omega} - \delta\right), \ \delta \approx 7.3, \ n = 1, 2, \dots$$
(25)

Thus, we see that the strongest instability, i.e., the smallest negative value of p_0^2 is given by the solution for the function χ_5 with n=1. The tachyon states play here the role of the quasistationary states in the problem of a supercritical Coulomb center. In fact, the tachyon instability can be viewed as the field theory analog of the "fall into the center" phenomenon and the critical coupling α_c is an analog of the critical coupling $Z_c\alpha$ in the problem of a Coulomb center.

The solution for the tachyon energy p_0^2 has a characteristic essential singularity of the kind $1/\sqrt{\lambda-\lambda_c}$ in the exponent. It can be argued that this behavior reflects a scale invariance in the problem under consideration and

keeps its form for any approximation which does not introduce a new scale parameter except the cutoff [26].

Finally, since chiral symmetry is spontaneously broken, there must exist Nambu–Goldstone excitations in the stable phase, where a quasiparticle gap arises. Let us show that the BS equation (8) indeed admits such solutions. To see this, according to [12], we set $p_0 = \mathbf{p} = 0$. Then, Eq. (8) has a solution of the form $\chi(q,0) = \chi_5(q,0)\gamma_5$, for which we obtain the equation

$$\chi_5(q,0) = \frac{\lambda}{2\pi} \int \frac{d^2k}{|\mathbf{q} - \mathbf{k}|} \frac{\chi_5(k,0)}{\sqrt{\mathbf{k}^2 + \Delta^2(k)}}$$
 (26)

or, after integrating over the angle,

$$\chi_5(q,0) = \lambda \int_0^{\Lambda} \frac{dk \, k \chi_5(k,0)}{\sqrt{k^2 + \Delta^2(k)}} \mathcal{K}(q,k)$$
 (27)

with the kernel

$$K(q,k) = \frac{2}{\pi} \left[\frac{\theta(q-k)}{q} K\left(\frac{k}{q}\right) + \frac{\theta(k-q)}{k} K\left(\frac{q}{k}\right) \right]. \tag{28}$$

On the other hand, the equation for a gap function obtained in Ref. [10] has the form

$$\Delta(q) = \Delta_0 + \lambda \int_0^{\Lambda} \frac{dk \, k \Delta(k)}{\sqrt{k^2 + \Delta^2(k)}} \mathcal{K}(q, k), \tag{29}$$

where we included also a bare gap Δ_0 for the further analysis. One can see that Eq. (27) has the solution $\chi_5(q,0) = C\Delta(q)$, if the gap function $\Delta(q)$ satisfies Eq. (29) with $\Delta_0 = 0$, and C is a constant. Thus, the wave function $\chi_5(q,0)$ describes a gapless Nambu–Goldstone excitation. Solving the BS equation at nonzero p_0, \mathbf{p} , one can obtain a dispersion law $p_0 \sim |\mathbf{p}|$ for a Nambu–Goldstone excitation.

3. Gap Generation

We now study the gap generation in graphene and show that it resolves the excitonic instability.

The equation for a quasiparticle gap in graphene is given by Eq. (29) above. For the zero bare gap $\Delta_0 = 0$, Eq. (29) admits a nontrivial solution which bifurcates from the trivial one at $\lambda = \lambda_c$, where the critical coupling $\lambda_c = 0.2285$. To find this critical point, we neglect the terms that are quadratic or higher orders in the gap function. It must be emphasized that this is *not* an approximation: it is a precise manner to locate the critical

point by applying the bifurcation theory. Hence, the bifurcation equation amounts to a linearization of Eq. (29) with respect to the gap function. The result reads

$$\Delta(p) = \lambda \int_{0}^{\infty} dq \, \Delta(q) \, \mathcal{K}(p, q). \tag{30}$$

Note that the ultraviolet cutoff Λ has been taken to infinity, which is appropriate at the bifurcation point [7]. Since the equation is scale invariant, it is solved by

$$\Delta(p) = p^{-\gamma} \tag{31}$$

with the condition that the exponent γ satisfies the transcendental equation

$$1 = \frac{2\lambda}{\pi} \int_{0}^{1} dx \left[x^{-\gamma} + x^{\gamma - 1} \right] K(x). \tag{32}$$

This equation defines roots γ for any value of the coupling λ . Bifurcation occurs when two of the roots in the interval (0,1) become equal. Numerically, we find that this happens when $\gamma=1/2$. For this value, the integral in Eq. (32) is exactly evaluated [29]), and we find the critical value

$$\lambda_c = \frac{4\pi^2}{\Gamma^4(1/4)} \approx 0.23. \tag{33}$$

For $\lambda > \lambda_c$, the roots become complex indicating that the oscillatory behavior of the gap function takes over the non-oscillatory one. The condition $\lambda = \lambda_c$ determines the critical line in the plane (α, N_f) ,

$$\alpha_c = \frac{4\lambda_c}{2 - \pi N_f \lambda_c} \tag{34}$$

(compare with Eq.(28) in [10]). A dynamical gap is generated only if $\alpha > \alpha_c$. The critical value $N_{\rm crit} \approx 2.8$, which corresponds to $\alpha = \infty$. Since the number of "flavors" $N_f = 2$ for graphene, the critical coupling is estimated to be $\alpha_c \approx 1.62$ in the considered approximation. Since the "fine structure" constant $\alpha \approx 2.19$ for a free standing graphene, the dynamical gap will be generated. For graphene on a SiO₂ substrate, the dielectric constant $\epsilon \approx 2.8$ and $\alpha \approx 0.78$, i.e., the system is in the subcritical regime. The values of α_c are rather large, which indicates that a weak-coupling approach is quantitatively inadequate for the problem of the gap generation in a free standing graphene. Certainly, both $1/N_f$ corrections and improving the instantaneous approximation

can vary the critical coupling. Therefore, it is instructive to compare our analytical results with those of lattice Monte Carlo studies [6]. They obtained $\alpha_c = 1.08 \pm 0.05$ for $N_f = 2$ and $N_{\rm crit} = 4.8 \pm 0.2$ for $\alpha = \infty$, i.e., the ratio of the factors ≈ 1.5 comparing to our analytical findings.

The above analysis is adequate precisely at the critical coupling, i.e., at the bifurcation point of the original nonlinear equation. To get insight into analytical solutions of Eq. (29), we approximate the kernel $\mathcal{K}(p,q)$ by its asymptotic values at $p \ll q$ and $p \gg q$:

$$\mathcal{K}(p,q) = \frac{\theta(p-q)}{p} + \frac{\theta(q-p)}{q}.$$
 (35)

This allows us to reduce the nonlinear integral equation (29) to the second-order nonlinear differential equation

$$\left(p^2 \Delta'(p)\right)' + \lambda \frac{p\Delta(p)}{\sqrt{p^2 + \Delta^2(p)}} = 0 \tag{36}$$

with the infrared (IR) and ultraviolet (UV) boundary conditions

$$p^2 \Delta'(p) \Big|_{p=0} = 0,$$
 (37)

$$(p\Delta(p))'\Big|_{p=\Lambda} = \Delta_0. \tag{38}$$

Equation (36) possesses a scale invariance, i.e., if $\Delta(p)$ is a solution, then $\kappa\Delta(p/\kappa)$ is also a solution. The scale invariance is broken by the UV boundary condition only.

The order parameter is given by

$$\langle 0|\bar{\psi}\psi|0\rangle = -\lim_{x\to 0} \langle 0|T\psi(x)\bar{\psi}(0)|0\rangle =$$

$$= -\frac{N_f}{\pi} \int_0^{\Lambda} \frac{dp p \Delta(p)}{\sqrt{p^2 + \Delta^2(p)}} = \frac{N_f}{\pi \lambda} p^2 \Delta'(p) \Big|_{p=\Lambda}, \tag{39}$$

where we used Eq. (36) in the last equality. One can easily find the solutions of Eq. (36) in two asymptotic regions. For $p \ll \Delta(p)$,

$$\Delta(p) = C_1 + \frac{C_2}{p} \tag{40}$$

due to the IR boundary condition (37), $C_2 = 0$, and $\Delta(p) \simeq C_1$ for $p \ll \Delta(p)$. For $p \gg \Delta(p)$,

$$\Delta(p) \simeq C_3 p^{-\gamma_+} + C_4 p^{-\gamma_-}, \quad \gamma_{\pm} = \frac{1}{2} \pm \sqrt{\lambda - \lambda_c}. \quad (41) \quad u'' + 3u' + (2 + \lambda)u = 0$$

However, in order to find a solution of Eq. (29), one needs to show that there exists a solution of the differential equation (36) connecting the asymptotics $\Delta(p) \simeq const$ in the infrared region, $p \to 0$, with asymptotics given by Eq. (41) at large momenta. To this end, let us define

$$\Delta(p) = e^t u(t + t_0), \quad t = \ln p. \tag{42}$$

Then the function u(t) satisfies the differential equation

$$u'' + 3u' + 2u + \lambda \frac{u}{\sqrt{1+u^2}} = 0. {(43)}$$

The IR boundary condition implies

$$e^{2t}(u'+u)\Big|_{t=-\infty} = 0.$$
 (44)

We require that $e^t u(t) \to 1$ as $t \to -\infty$, since all other solutions for $\Delta(p)$ are obtained by varying the constant t_0 . With this normalization, the infrared scale is given by $\Delta(0) = e^{-t_0}$ for the general solution.

The dependence of the integral equation (29) on the bare gap Δ_0 now becomes an ultraviolet boundary condition for the differential equation. It is

$$e^{t_{\Lambda}}(u'(t_{\Lambda}+t_0)+2u(t_{\Lambda}+t_0))=\Delta_0.$$
(45)

This condition determines the parameter $t_0 = -\ln \Delta(0)$ as a function of the coupling constant λ , the bare gap Δ_0 , and the cutoff Λ .

Equation (43) can be rewritten in the form

$$u'' + 3u' = -\frac{d}{du}V(u) \tag{46}$$

or,

$$\left(\frac{1}{2}(u')^2 + V(u)\right)' = -3(u')^2,\tag{47}$$

where

$$V(u) = u^2 + \lambda \sqrt{1 + u^2}. (48)$$

This is the equation for a particle of unit mass moving in a potential V under a friction proportional to the velocity. Since V(u)>0, the "energy" $\frac{1}{2}(u')^2+V(u)$ reaches its minimum at u=0. Hence, the particle moves toward u=0 damped by the friction. The asymptotic behavior in this regime is described by the linearized equation

$$u'' + 3u' + (2 + \lambda)u = 0 \tag{49}$$

and depends on the coupling constant λ . For the weak coupling $\lambda < \lambda_c = 1/4$,

$$u(t) \to \frac{Ae^{-3t/2}}{\sqrt{\lambda - \lambda_c}} \sin\left[\sqrt{\lambda - \lambda_c} (t + \delta)\right], \quad t \to \infty, \quad (50)$$

$$u(t) \to \frac{Be^{-3t/2}}{\sqrt{\lambda_c - \lambda}} \sinh\left[\sqrt{\lambda_c - \lambda} (t + \delta')\right], \quad t \to \infty,$$
(51)

where the constants A, B, δ , and δ' are functions of the coupling constant λ .

At a weak coupling, there are no nontrivial solutions satisfying the UV boundary condition for $\Delta_0 = 0$. For a strong coupling, the UV boundary condition (45) with $\Delta_0 = 0$ admits the infinite number of solutions for $\Delta(0)$ corresponding to different solutions of the equation

$$u'(t_{\Lambda} + t_0) + 2u(t_{\Lambda} + t_0) =$$

$$= \frac{A\sqrt{\lambda}}{\sqrt{\lambda - \lambda_c}} e^{-3(t_{\Lambda} + t_0)/2} \sin\left(\theta + \phi\right) = 0, \tag{52}$$

where $\phi = \arctan\left(2\sqrt{\lambda - \lambda_c}\right)$,

$$\theta = \sqrt{\lambda - \lambda_c} \left(t_{\Lambda} + t_0 + \delta \right) = \sqrt{\lambda - \lambda_c} \ln \left(\frac{e^{\delta} \Lambda}{\Delta(0)} \right). \quad (53)$$

Hence, the solution is given by $\theta = \pi n - \phi$ or

$$\Delta(0) = \Lambda e^{\delta} \exp\left(-\frac{\pi n - \phi}{\sqrt{\lambda - \lambda_c}}\right), \quad n = 1, 2, \dots$$
 (54)

Only the solution without nodes, n=1, corresponds to the ground-state solution, since it generates the largest fermion gap and, hence, has the lowest energy for the ground state. The critical coupling $\lambda_c=1/4$ is a bifurcation point of the integral equation (29). Physically, it corresponds to the point of a continuous phase transition of the infinite order. According to the discussion in the previous section, the critical coupling λ_c is closely related to the "fall into the center" phenomenon in quantum mechanics. A similar situation takes place in strong coupling QED4 [12], where the phase transition is also of the infinite order in the ladder approximation (and, more generally, in the quenched approximation where fermions loops are neglected [26]). The dimensionless correlation length

$$\xi = \frac{\Lambda}{\Delta(0)} \sim \exp\left(\frac{\pi}{\sqrt{\lambda - \lambda_c}}\right) \tag{55}$$

exponentially grows when $\lambda \to \lambda_c$. That is the behavior inherent in the Berezinskii–Kosterlitz–Thouless phase transition. Note, however, that considering the finite size of graphene samples should transform this phase transition into a second-order one (as it was shown for QED3 in Ref. [27]).

3.1. Excitonic condensate and critical exponents

The order parameter is calculated to be

$$\langle \bar{\psi}\psi \rangle = -\frac{N_f A}{\pi \lambda^{3/2}} \Lambda^{1/2} \Delta^{3/2}(0). \tag{56}$$

For a nonzero bare gap $\Delta_0 \neq 0$, we obtain the equation for $\Delta(0)$,

$$\Delta_0 = \frac{A\sqrt{\lambda}}{\sqrt{\lambda_c - \lambda}} \frac{\Delta^{3/2}(0)}{\sqrt{\Lambda}} \sin\left(\theta + \phi\right),\tag{57}$$

and the expression for the order parameter

$$\langle \bar{\psi}\psi \rangle = \frac{N_f A}{\pi \sqrt{\lambda(\lambda - \lambda_c)}} \Lambda^{1/2} \Delta^{3/2}(0) \sin(\phi - \theta).$$
 (58)

Let us write $\theta + \phi = \pi - \epsilon$, where ϵ goes to zero when $\Delta_0 \to 0$ and $\lambda \to \lambda_c$. Then the above equations are rewritten as

$$\Delta_0 = \frac{A\sqrt{\lambda}}{\sqrt{\lambda - \lambda_c}} \frac{\Delta^{3/2}(0)}{\sqrt{\Lambda}} \sin \epsilon, \tag{59}$$

(54)
$$\langle \bar{\psi}\psi \rangle = -\frac{N_f \Lambda}{\pi \lambda} \left[\frac{|2\lambda - 1|}{2\lambda} \Delta_0 + A \frac{\Delta^{3/2}(0)}{\sqrt{\Lambda}} \frac{\cos \epsilon}{\sqrt{\lambda}} \right].$$
 (60)

In such a form, the equations are convenient for finding the critical exponents near the phase transition point λ_c . We define the critical exponents in a standard way [28]:

$$\xi = \frac{\Lambda}{\Delta(0)} \sim (\lambda - \lambda_c)^{-\nu}, \quad \frac{\langle \bar{\psi}\psi \rangle}{\Lambda^2} \sim (\lambda - \lambda_c)^{-\beta}, \quad (61)$$

$$\chi = \frac{\partial \langle \bar{\psi}\psi \rangle}{\partial \Delta_0} \Big|_{\Delta_0 = 0} \sim (\lambda - \lambda_c)^{-\gamma}, \lambda \to \lambda_c, \tag{62}$$

$$\langle \bar{\psi}\psi\rangle\Big|_{\lambda=\lambda_c} \sim \Delta_0^{1/\delta}, \quad \Delta_0 \to 0.$$
 (63)

The exponents are assumed to obey the following hyperscaling relations in arbitrary dimensions D, if the theory of second-order phase transitions is applicable:

$$2\beta + \gamma = D\nu, \quad 2\beta\delta - \gamma = D\nu, \tag{64}$$

$$\frac{\delta - 1}{\delta + 1} = \frac{2 - \eta}{D}, \quad \beta = \nu \frac{D - 2 + \eta}{2}.$$
 (65)

Here, the exponent η describes the behavior of the correlation function

$$\langle \bar{\psi}\psi(r)\bar{\psi}\psi(0)\rangle\Big|_{\lambda=\lambda_c} \propto r^{-D+2-\eta}, \quad r\to\infty.$$
 (66)

From Eq. (60), we find

$$\langle \bar{\psi}\psi \rangle \Big|_{\lambda=\lambda_c} = -\frac{4N_f\Lambda}{\pi} \left[\Delta_0 + \frac{2A\Delta^{3/2}(0)}{\sqrt{\Lambda}} \right],$$
 (67)

and, in view of Eq. (57),

$$\Delta(0) \sim \left(\frac{\Delta_0}{\ln(\Lambda/\Delta_0)}\right)^{2/3},\tag{68}$$

the critical exponent $\delta = 1$. Then the hyperscaling relations imply

$$\eta = 2, \quad \gamma = 0, \quad \beta = \frac{3\nu}{2}. \tag{69}$$

The infinite-order phase transition with the correlation length (55) formally corresponds to the limit

$$\beta = \frac{3\nu}{2} \to \infty. \tag{70}$$

Certainly, the infinite-order phase transition is quite different from that studied in the lattice simulations [6], where the phase transition was found to be of the second order with the critical exponents $\delta \sim 2.3, \beta \sim 0.8, \gamma \sim 1(N_f=2)$. One of the reasons for such a difference might be a finite size of the lattice which changes the order of the phase transition [23, 24, 27]. Another reason could be that one should take residual lattice interactions into account, i.e., the present analysis has to be further refined by incorporating effective four-fermion terms. The corresponding analysis will be postponed for a separate publication.

4. Conclusion

In this paper, we have studied excitonic instabilities in graphene which arise at a strong Coulomb coupling. Considering the many-body problem of strongly interacting gapless quasiparticles in graphene, we have showed that the Bethe–Salpeter equation for an electronhole bound state contains a tachyon in its spectrum in the supercritical regime $\alpha > \alpha_c$ and found the critical constant $\alpha_c = 1.62$ in the static random phase approximation. The tachyon states play a role of quasistationary states in the problem of the supercritical Coulomb

center and necessitate the rearrangement of the ground state and the formation of the exciton condensate.

We have calculated the critical coupling $\alpha_c = 1.62$ and found the critical indices for the order parameter $\langle \bar{\psi}\psi \rangle$ for the excitonic condensation $\delta = 1, \eta = 2, \gamma = 0, \beta =$ ∞ . These values should be compared with $\alpha_c = 1.08$ and $\delta \sim 2.3, \gamma \sim 1, \beta \sim 0.8$ found in Monte Carlo simulations [6]. The obtained value of α_c is rather large, which indicates that the ladder approximation is not quantitatively good enough for the problem of excitonic instability and gap generation in a freely standing graphene. Certainly, both higher-order corrections and improving the instantaneous approximation can vary the value of critical coupling. The discrepancy of the critical indices can be explained through the necessity of the careful calculation of the finite-size lattice effects and taking residual lattice interactions into account, which leads to effective four-fermion interactions. It is essential that a ground state rearrangement at the strong coupling is connected with the "fall into the supercritical Coulomb center" phenomenon. This implies that a rearrangement in graphene with the large Coulomb interaction is very plausible for a strong enough coupling even if one goes beyond the ladder approximation. The physical picture of instabilities in graphene is quite similar to that elaborated earlier in strongly coupled QED [11, 12, 15] (see, also, [13, 14]). In QED, the ladder approximation is not reliable quantitatively as well, because the critical coupling constant for chiral symmetry breaking is of order of 1. However, the main results of the ladder approximation survive when all diagrams with exchanges by photons are included (the so-called quenched approximation without fermion loops) [26]. Further, the existence of the critical point is exactly proved in the lattice version of QED [30]. We note also that, in the presence of an external magnetic field, the critical coupling reduces to zero (the magnetic catalysis phenomenon [31]), so that the gap generation takes place already in the weak coupling regime.

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ЕКСИТОННА НЕСТАБІЛЬНІСТЬ ТА ГЕНЕРАЦІЯ ІЦІЛИНИ В ОДНОШАРОВОМУ ГРАФЕНІ

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Резюме

За допомогою рівняння Бете-Солпітера для електрондіркового зв'язаного стану досліджено проблему екситонної нестабільності в графені. Показано, що для надкритичної константи зв'язку спектр має тахіонні розв'язки. Екситонна нестабільність приводить до формування електрон-діркового конденсату та щілини у спектрі квазічастинок. Ця щілина може бути спостережена у графені без домішок.