Transition of Graphene on a Substrate to a Semimetallic State

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Graphene on a substrate has been shown to exhibit a transition, depending on the substrate material, from a zero-gap semiconductor state to a semimetallic state. The ground-state energy of the electron (hole) gas has been calculated within the random-phase approximation.

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1. INTRODUCTION

A monolayer of carbon atoms that form a perfect hexagonal lattice (graphene) has such a band structure that the energy gap is equal to zero in three \( K \) and three \( K' \) points of the Brillouin zone [1]. The Schrödinger equation in the \( \mathbf{k} \cdot \mathbf{p} \) approximation has the form [2]

\[
\hat{H}_0 F(\mathbf{r}) = \varepsilon F(\mathbf{r}), \tag{1}
\]

where the quantity \( \varepsilon = \frac{3}{2} \gamma a_0 \approx 9.84 \times 10^7 \text{ cm/s} \) is similar to the Kane matrix element for the rate of interband transitions in the Dirac model [3], \( \gamma \approx 3 \text{ eV} \) is the band parameter numerically equal to the overlap integral of atomic orbitals that participate in the chemical bonds of carbon atoms in graphene, \( a_0 = 1.44 \text{ Å} \) is the interatomic distance in the graphene lattice, \( \sigma = (\sigma_1, \sigma_2) \) are the Pauli matrices, \( \mathbf{k} = (k_x, k_y) \), \( \mathbf{k}' = (k_x', -k_y') \), \( k_{x,y} = -i \partial_{x,y} \), and \( \hbar = 1 \).

The unitary transformation \( \hat{U}_1 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \) reduces the Hamiltonian \( \hat{H}_0 \) to the form

\[
\hat{H}_0' = \hat{U}_1 \hat{H}_0 \hat{U}_1^\dagger = \begin{pmatrix} u \sigma \cdot \mathbf{k} & 0 \\ 0 & -u \sigma \cdot \mathbf{k}' \end{pmatrix}, \tag{3}
\]

where the quantity \( u = \frac{3}{2} \gamma a_0 \approx 9.84 \times 10^7 \text{ cm/s} \) is similar to the Kane matrix element for the rate of interband transitions in the Dirac model [3], \( \gamma \approx 3 \text{ eV} \) is the band parameter numerically equal to the overlap integral of atomic orbitals that participate in the chemical bonds of carbon atoms in graphene, \( a_0 = 1.44 \text{ Å} \) is the interatomic distance in the graphene lattice, \( \sigma = (\sigma_1, \sigma_2) \) are the Pauli matrices, \( \mathbf{k} = (k_x, k_y) \), \( \mathbf{k}' = (k_x', -k_y') \), \( k_{x,y} = -i \partial_{x,y} \), and \( \hbar = 1 \).

The corresponding equation with the transformed wavefunction \( \varphi(\mathbf{r}) = \hat{U}_1 F(\mathbf{r}) \) is equivalent to a pair of Weyl equations. In quantum electrodynamics (QED), the Weyl equation describes neutrino, a massless spin-1/2 particle. Since the particles were assumed to be spinless when deriving Eq. (1), Novoselov [1] introduced the notion of pseudospin. As correctly mentioned in [5], a complete model should include an \( 8 \times 8 \) matrix Hamiltonian due to the twofold valley degeneracy, twofold pseudospin degeneracy, and twofold spin degeneracy. The \( 8 \times 8 \) Hamiltonian may be reduced to the \( 4 \times 4 \) Hamiltonian given by Eq. (3) if the Fermi momentum is determined in the spin-unpolarized state of the particles. In this case, the degeneracy multiplicity is \( \nu = \nu_{e,h} = 2 \) (\( \nu_{e,h} \) is the valley degeneracy of the conduction band or the valence band).

To obtain the Dirac equation, let us perform another unitary transformation \( \hat{U}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ I & -I \end{pmatrix} \)

\[
\hat{H}_0'' = \hat{U}_2 \hat{H}_0' \hat{U}_2^\dagger = \begin{pmatrix} 0 & u \sigma \cdot \mathbf{k} \\ u \sigma \cdot \mathbf{k} & 0 \end{pmatrix} \equiv u \alpha \cdot \mathbf{k}, \tag{4}
\]

where \( \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \) are the Dirac matrices. Thus, the charge carriers in graphene are described in the framework of the zero-gap (\( \Delta = 0 \)) Dirac model. The use of the Dirac equation as a \( 4 \times 4 \) matrix equation in the two-dimensional system is justified because the \( 4 \times 4 \) and \( 2 \times 2 \) matrix representations may be equally used in the case of two spatial dimensions [6]. This allows us to apply the diagram technique of QED to the case of the two-dimensional system of Dirac fermions (graphene).

In this work, it is shown that graphene on a substrate may undergo a transition from a zero-gap semiconductor state to a semimetallic state, depending on the substrate material. The transition occurs at \( \alpha^* \approx 1 \), where \( \alpha^* = \frac{e^2}{\kappa_{c,ff} \hbar} \) is the analog of the fine-structure constant, whose numerical value depends on the relative permittivity \( \epsilon_{1,2} \) of the media surrounding the graphene and \( \kappa_{c,ff} \approx \frac{4 \pi e^2}{2} \), similar to a thin film [7].
2. GROUND-STATE ENERGY  
(GENERAL CONSIDERATION)

To determine whether the zero-gap semiconductor phase of graphene is stable with respect to the transition to another phase, one has to calculate the ground-state energy of the electron (hole) gas that appears in graphene when the electric field is applied. The ground-state energy per particle is the sum of the three terms

\[ E_{gs} = E_{kin} + E_{exch} + E_{corr}. \]

Here, the average kinetic energy is given by the expression \( E_{kin} = \frac{3}{2} \nu p_F \) because, according to Eq. (1), the dispersion relation of the charge carriers is linear near the \( K \) and \( K' \) points of the Brillouin zone: \( \epsilon_p = \pm u |p| \) (+ and \( - \)correspond to electrons and holes, respectively), \( p_F = \sqrt{2 \pi n_{2D}/\nu} \) is the Fermi momentum, \( n_{2D} \) is the areal density of particles, and \( \nu \) is the abovementioned degeneracy multiplicity. If the Fermi level \( \epsilon_F \) lies above \( \epsilon = 0 \), the charge carriers in the system are only the conduction electrons with a number of valencies \( \nu_e = 2 \); if \( \epsilon_F < 0 \), then the charge carriers are holes with \( \nu_h = 2 \). The position of the Fermi level may be changed by applying the electric field [1]. Both cases are obviously equivalent in the Dirac model. Below, we will consider the case of electrons for definiteness.

The exchange energy is given by the diagram (see Fig. 1)

\[ E_{exch} = -\frac{\nu}{2n_{2D}} \int \frac{d^2p d\epsilon d^2k d\omega}{(2\pi)^3} S \{ \gamma^\mu(p, \epsilon; k, \omega) \}
\times G(p, \epsilon) \gamma^\nu G(k, \omega) \frac{\delta}{\delta \mu} \delta_{\mu k} \delta_{\omega 0}(p - k, \epsilon - \omega), \]

where the photon propagator is \( D^{(0)}_{\mu \nu}(p - k, \epsilon - \omega) \approx V(p - k) \delta_{\mu \nu} \delta_{\omega 0} \) (we neglect the photon poles whose contributions to the integral with respect to the frequencies \( \epsilon \) and \( \omega \) are on the order of \((u/c)^2 \sim 10^{-5}\) each, i.e., small compared to the contribution of the Green’s function poles), \( V(q) = \frac{2\pi \epsilon_q}{\kappa_{eff} |q|} \) is the Coulomb law in the two-dimensional case.

The correlation energy is given by the formula \(^2\)

\[ E_{corr} = \frac{1}{2n_{2D}} \int \frac{d^2k d\omega}{(2\pi)^3} \frac{1}{\lambda} \delta \left[ -\lambda \nu V(k) \Pi_{44}(k, i\omega) + \lambda \nu V(k) \Pi_{44}(k, i\omega) \right]. \]

The polarization operator \( \Pi^{(0)}_{44}(k, i\omega) \) in the lowest order in the interaction (see Fig. 2) is calculated from the zero-approximation Green’s functions \(^9\)

\[ G^{(0)}(p, \epsilon) = -\frac{u}{(\epsilon_p - \epsilon - i\delta_+)(\epsilon_p + \epsilon - i\delta_+)} \]

\(^2\) Formula (7) is derived in the nonrelativistic case and is the sum of the ring diagrams of all orders (as the most divergent diagrams). The situation in the relativistic case is similar; therefore, the same formula with the corresponding polarization operators is used here.

\(^9\) The polarization operator \( \Pi^{(0)}_{44}(k, i\omega) \) given by the diagram in Fig. 3 is a renormalized quantity with respect to \( \Pi^{(0)}_{44}(k, i\omega) \) due to the Coulomb interaction.

3. RENORMALIZATION PROCEDURE

The relation for the constant \( u = \frac{3}{2}\gamma a_0 \) was obtained analytically by linearizing the dispersion relation in the vicinity of the \( K \) and \( K' \) points of the Brillouin zone. The dispersion relation was, in turn, found by solving the Schrödinger equation with the Hamiltonian in the tight-binding approximation. However, the interaction between particles as the interaction in a many-body system is disregarded in this approximation. Thus, the constant \( u \) must be renormalized taking into account the Coulomb interaction. The renormalized value of \( u \), generally speaking, depends on the electron density.
The problem is strictly formulated as a problem of solving the system of integral equations for the exact Green’s function $G(p, \varepsilon)$, exact photon propagator $D_{\mu\nu}(q, \Omega)$, and vertex function $\Gamma(p, \varepsilon; p', \varepsilon')$ (as well as for the polarization operator and self-energy). The approximate solution of the equations is possible, but seems too lengthy. We use here the renormalization theory developed in QED. In fact, the exact Green’s function, photon propagator, and vertex function are replaced by the respective quantities in the lowest order in the interaction multiplied by the renormalizing constants.

We proceed from two assumptions:

(i) the charge coincides with the physically observed charge (ignoring the environment)

\begin{equation}
    e = e_0;
\end{equation}

(ii) the effective mass of particles remains equal to zero; i.e., the Coulomb interaction does not open a gap until the transition point to the semimetallic state

\begin{equation}
    \Delta \equiv 0.
\end{equation}

The gap opening is energetically unfavorable \[11\], which is confirmed in experiments.

Let us quote the known relations of the renormalization theory

\begin{equation}
    \Gamma^\mu = Z_1 \gamma^\mu,
\end{equation}

\begin{equation}
    G = Z_2^{-1} G^{(0)},
\end{equation}

\begin{equation}
    D_{\mu\nu} = Z_3^{-1} D_{\mu\nu}^{(0)}.
\end{equation}

According to the renormalization theory, the charge satisfies the relation \[12\]

\begin{equation}
    e = Z_1^{-1} Z_2 Z_3^{1/2} e_0.
\end{equation}

Taking into account Eq. (10) and the Ward identity $Z_1 = Z_2$, we obtain $Z_3 = 1$, which was assumed in Eq. (6). The Green’s function satisfies the relation

\begin{equation}
    G = G^{(0)} + G^{(0)} \Sigma G
\end{equation}

with the formal solution

\begin{equation}
    G^{-1} = G^{(0)-1} - \Sigma,
\end{equation}

where $G^{(0)-1} = -\hat{\mu} \hat{p}$. Therefore, it should be expected that the inclusion of the interaction results in the renormalization of $u$, the only parameter in the dispersion relation, taking into account Eq. (11). Looking for the self-energy in the form\[3\]

\begin{equation}
    \Sigma(p, \varepsilon) = Au\hat{p},
\end{equation}

we obtain

\begin{equation}
    G^{-1}(p, \varepsilon) = -u^*\hat{p},
\end{equation}

where $u^* = (1 + A)u$ is the renormalized $u$ value. The self-energy is given by the expression (see Fig. 4)

\begin{equation}
    \Sigma(p, \varepsilon) = i \int \frac{d^3q d\Omega}{(2\pi)^3} \Gamma^\nu(p - q, \varepsilon - \Omega; p, \varepsilon) G(p - q, \varepsilon - \Omega) \times \gamma^n D_{\mu\nu}(q, \Omega).
\end{equation}

\[\text{Fig. 4. Self-energy.}\]

Taking into account Eqs. (12) and (13) and the Ward identity, we come to

\begin{equation}
    \Sigma(p, \varepsilon) = i \int \frac{d^3q d\Omega}{(2\pi)^3} \gamma^n G^{(0)}(p - q, \varepsilon - \Omega) \gamma^\nu D_{\mu\nu}^{(0)}(q, \Omega).
\end{equation}

After simple calculations (see below), we obtain

\begin{equation}
    A = \alpha^* I \left( \frac{|p|}{p_F} \right),
\end{equation}

\begin{equation}
    I(x) = \frac{\pi}{2} \int_0^{\pi/2} \ln \left( \frac{1}{2} + \frac{1}{2} \sqrt{1 - x^2 \sin^2 \varphi} \right) d\varphi,
\end{equation}

i.e., the renormalized dispersion relation has the form

\begin{equation}
    \varepsilon^*_p = \pm u |p| \left( 1 + \alpha^* I \left( \frac{|p|}{p_F} \right) \right).
\end{equation}

Self-Energy Calculation

Evaluating the pole integral with respect to $\Omega$ in Eq. (21), we obtain the expressions for the imaginary and real part, which will be considered separately:

\begin{equation}
    Re \Sigma(p) = -\int \frac{d^3q}{(2\pi)^3} \frac{u\gamma^1(p_1 - q_1)}{2\pi p - q} V(q) \theta(|p - q| - p_F),
\end{equation}

\begin{equation}
    Im \Sigma(p) = -\int \frac{d^3q}{(2\pi)^3} \frac{u\gamma^2(p_2 - q_2)}{2\pi p - q} V(q) \theta(|p - q| - p_F)
    + \frac{1}{2} u\gamma^0 \int \frac{d^3q}{(2\pi)^3} V(q) \theta(|p - q| - p_F).
\end{equation}

Let $p$ be directed along $q_\alpha$, then $p_1 = p$ and $p_2 = 0$. Integral (25) is the difference between two integrals (with $p_1$ and $q_1$ in their numerators), both diverging at $q \gg p$. Let us expand the integrand of the integral with $q_1$ in the series to the $\sim p/q^2$ term, which gives

\begin{equation}
    \frac{\alpha^*}{4} u\gamma^1 \ln \frac{q_c}{p_F},
\end{equation}

where the upper momentum cutoff $q_c \simeq 2\pi/3\sqrt{3}a_0$ is introduced, which is on the order of the half-distance between the neighboring $K$ and $K'$ points of the Brillouin zone (it is the momentum at which the linear dispersion relation breaks down).

To evaluate the integral with $p_1$, let us introduce the dimensionless variable $z = \frac{p_F p}{\sqrt{3} p F}$. By taking the integral with respect to $z$, the integral with respect to the angle is reduced to the form

\begin{equation}
    I(z) = \frac{\alpha^*}{4\pi} u\gamma^1 \int_0^{2\pi} d\varphi \ln \left( \frac{z + \sqrt{1 + z^2}}{z_0 + \sqrt{1 + z_0^2}} \right),
\end{equation}

\[\text{3}\]

\[\text{Below, we show that } \Sigma \text{ is independent of the frequency } \varepsilon \text{ and } \Sigma(p) = Au\gamma^1 p, \text{ which does not, however, influence Eq. (19), because } p_0 \text{ at } p_4 = ip_0 \text{ should be replaced by } \varepsilon/u^*.\]
where
\[ z_0 = \frac{\sqrt{p_F^2 - p^2 \sin^2 \varphi}}{p \sin \varphi}, \quad z_c = \frac{q_c - p \cos \varphi}{p \sin \varphi}. \]

Taking into account that \( z_c \gg 1 \), we may write
\[ -\frac{\alpha^*}{4\pi} u\gamma^\dagger p \int_0^{2\pi} d\varphi \ln \left( z_c + \sqrt{1 + z_c^2} \right) \]
\[ \approx -\frac{\alpha^*}{2} u\gamma^\dagger p \ln \frac{q_c}{p_F} + \frac{\alpha^*}{4\pi} u\gamma^\dagger p \int_0^{2\pi} d\varphi \ln \frac{y}{\sin \varphi}. \]

Combining all these integrals together, we obtain the real part in the form
\[ Re\Sigma(p) = -\frac{\alpha^*}{4} u\gamma^\dagger p \ln \frac{q_c}{p_F} + \]
\[ + \frac{\alpha^*}{\pi} u\gamma^\dagger p \int_0^{\pi/2} d\varphi \ln \left( \frac{1}{2} + \frac{1}{2} \sqrt{1 - \left( \frac{p}{p_F} \right)^2 \sin^2 \varphi} \right). \]

The first term in Eq. (27) must be disregarded due to the following reasons:
(i) \( q_c \gg p_F \), and \( \ln \frac{q_c}{p_F} \) may be arbitrarily large at an arbitrarily small \( p_F \); the renormalization coefficient for \( u \) becomes negative and, thereby, the further calculation of the ground-state energy \( E_{gs} \) is senseless;
(ii) the corresponding contribution to the coefficient \( A \) is independent of the particle momentum; one may expect that the particles with \( p \to 0 \) are insensitive to the renormalization of \( u \) and the particles with \( p \to p_F \) are the most sensitive to this renormalization. Thus, the condition \( A(0) = 0 \) must be fulfilled.

The integration with respect to the angle in the first integral in Eq. (26) yields zero; the non-zero contribution is
\[ Im\Sigma(p) = -\frac{\alpha^*}{2} \gamma^\dagger q_c - \frac{\alpha^*}{\gamma} \gamma^\dagger E \left( \frac{p}{p_F} \right) u p_F, \]
\[ (28) \]
where \( E(x) \) is the complete elliptic integral of the second kind. The first term is removed by the requirement \( Im\Sigma_{Reg}(0) = 0 \), i.e.,
\[ Im\Sigma_{Reg}(p) = \frac{\alpha^*}{\pi} \left[ \pi - E \left( \frac{p}{p_F} \right) \right] \gamma^\dagger u p_F, \]
which represents the momentum-dependent shift of the frequency \( \varepsilon \) in the renormalized Green’s function
\[ G^{-1}(p, \varepsilon) = -(1 + A)u \gamma^\dagger p - i \left\{ \gamma^\dagger \varepsilon + Im\Sigma_{Reg}(p) \right\}. \]

However, the shift is a slowly varying function of the momentum and, therefore, may be replaced by its average value, i.e., by the constant by which the integration with respect to the frequency may be shifted when calculating the diagrams. Thus, the shift may be disregarded and we arrive at the result given by Eqs. (22) and (23).

4. GROUND-STATE ENERGY

The average kinetic energy is now equal to
\[ E_{kin} = \frac{2}{3} up_F + \]
\[ + \frac{2\alpha^*}{\pi} up_F \int_0^{\pi/2} \frac{d\varphi}{\pi} \left( \frac{1}{2} + \frac{1}{2} \sqrt{1 - x^2 \sin^2 \varphi} \right) \]
\[ \approx \left[ \frac{2}{3} - 0.0342\alpha^* \right] up_F, \]
\[ (29) \]
Hence, the contribution of the renormalization is \( \lesssim 0.1 \); the respective contribution to the exchange and correlation energies is expected to be of the same order of magnitude (or even smaller). Therefore, to simplify further calculations, it reasonable to retain the linear form of the dispersion relation by averaging Eq. (22) in \( |p| \) and replacing \( u^* \) with \( \bar{\pi}^* = (1 + A)u \), where
\[ A = \frac{\alpha^*}{\pi} \int_0^{1} \int_0^{\pi/2} \frac{d\varphi}{\pi} \left( \frac{1}{2} + \frac{1}{2} \sqrt{1 - x^2 \sin^2 \varphi} \right) \]
\[ \approx -0.0269\alpha^*. \]
\[ (30) \]
The renormalization of Eq. (6) for the exchange energy results in the equality \( E_{exch} = Z_2^{-1} E_{exch}^{(0)} \), where \( E_{exch}^{(0)} \) is the exchange energy calculated with the non-renormalized Green’s function, photon propagator, and vertex function:
\[ E_{exch}^{(0)} = -\frac{\alpha^*}{2\pi} up_F, \]
\[ (31) \]
where
\[ J = \int_0^{1} \int_0^{\pi/2} \frac{d\varphi}{\pi} \left( \frac{1 + \cos \chi}{{\sqrt{x^2 + y^2 - 2xy \cos \chi}}} \right) = \frac{8}{3} \left( \mathcal{G} + \frac{1}{2} \right), \]
with \( \mathcal{G} = 0.915965 \ldots \) being the Catalan’s constant.

The correlation energy may be calculated in the second order of the perturbation theory. The corresponding diagrams are renormalized by the factor \( Z_2^{-2} \); thus, \( E_{cor} = Z_2^{-2} E_{exch}^{(0)}. \)

The further calculation with the use of the asymptotic expressions for the polarization operator in the lowest order in the interaction at low and high transferred momenta leads to the expression
\[ E_{cor}^{(0)} = -\alpha^* \int_0^2 \frac{d\nu}{128\pi} \left( \frac{3\pi}{8} - \frac{25}{27} - \frac{1}{27\nu} \right) up_F. \]
\[ (32) \]
The final result for the ground-state energy reads
\[ E_{gs} = \left[ \sqrt{2\pi} \left( \frac{2}{3} - 0.0342\alpha^* \right) - \frac{8}{3\sqrt{2\pi}} \frac{(\mathcal{G} + \frac{1}{2})}{3} \right] up_F. \]
5. TRANSITION TO A SEMIMETALLIC STATE

It is seen from Eq. (33) that the coefficient of \( u (n_{2D} / \nu)^{1/2} \) changes its sign at \( \alpha^* \approx 1.0204 \) for \( \nu = 2.5 \). When this coefficient is negative, the creation of electron–hole pairs in the system of the two-dimensional massless Dirac fermions becomes favorable taking into account that the absolute value of the ground-state energy is a monotonically increasing function of the particle density. This behavior is a manifestation of the system instability with respect to the Coulomb interaction. In this case, a phase transition occurs.

As mentioned above, the gap opening is energetically unfavorable; therefore, this is a transition from a zero-gap semiconductor state to a semimetallic one. Remarkably, the transition occurs depending on the \( \alpha^* \) value, which in turn depends on the substrate permittivity. Thus, the substrate material determines whether graphene has semiconductor or semimetallic properties. It is also seen that the spin-unpolarized state with \( \nu = 2 \) is energetically more favorable at a positive value of the ground-state energy, whereas the spin-polarized state with \( \nu = 1 \) is more favorable at the opposite sign. As a result, the additional transition to the spin-polarized state occurs simultaneously with the transition to the semimetallic state.

The closeness of the parameter \( \alpha^* \) to unity indicates that there is a close analogy between the case under consideration and the instability of the Coulomb field of the charge \( Z = 137 \) in QED with respect to the spontaneous creation of electron–positron pairs (the fine-structure constant effectively approaches unity). It is possible that the exact value of \( \alpha^* \), at which the described transition occurs, is actually equal to unity and the insignificant deviation of \( \alpha^* \) from unity obtained in this work is due to the inaccuracy of the approximation used.

6. POSSIBLE EXPERIMENTAL OBSERVATIONS

According to the experiments, the \( \alpha^* \) value depends on the substrate material. For instance, \( \kappa_{eff} = 5 \) and \( \alpha^* \approx 0.44 \) for the SiO\(_2\) substrate and \( \kappa_{eff} = 3 \) and \( \alpha^* \approx 0.73 \) [13] for the SiC substrate, but the condition \( \alpha^* \approx 1 \), which corresponds to \( \kappa_{eff} \approx 2 \), is required for the transition.

Formally, \( \kappa_{eff} = 1 \) in a vacuum and graphene must be a semimetal. The overlap of the valence band

\[
\times \frac{\alpha^*}{1 - 0.0269\alpha^*} \frac{\nu}{64\sqrt{2\pi}} \left( \frac{3\pi}{8} - \frac{25}{27} - \frac{1}{27\nu} \right) \times \frac{\alpha^*^2}{(1 - 0.0269\alpha^*)^2} u \left( \frac{n_{2D}}{\nu} \right)^{1/2}.
\]

(33)

conduction band in the semimetallic state may be estimated as [11]

\[
\delta E \approx \left( b - \frac{1}{b} \right) u p_F,
\]

(34)

where \( b = \alpha^*\alpha_{0}^* \), which is only meaningful at \( \alpha^* > \alpha_{0}^* \). It follows from Eq. (34) that \( \delta E \sim n_{2D}^{1/2} (p_F = \sqrt{2\pi n_{2D}}) \). Electrons and holes may appear as charge carriers in graphene at \( T = 0 \) when it is situated on a substrate and the electric field is applied (the electric field effect). In this case, the concentration of the charge carriers is proportional to the applied voltage, \( n_{2D} \propto V \) [1]. In the absence of a substrate, \( n_{2D} = 0 \) and \( \delta E = 0 \) and graphene in a vacuum remains a zero-gap semiconductor. Thus, a substrate material with a sufficiently small \( \kappa_{eff} \) value should be found. It could be, e.g., a substrate with regularly spaced pin holes or some metamaterials. The application of an electric field is unnecessary for the appearance of charge carriers in graphene in the case of the second-type contact of graphene with the substrate, i.e., when the \( \varepsilon = 0 \) level of graphene does not lie in the band gap of the substrate material.

7. DISCUSSION

The main qualitative result of this work is the presence of the phase transition from a zero-gap semiconductor to a semimetal in the two-dimensional case at \( \alpha^* \approx 1 \). The zero-gap semiconductor phase is stable at \( \alpha^* \leq 1 \), which is an analog of the stability criterion for the system of three-dimensional non-relativistic fermions

\[
\frac{1}{\varepsilon_{tot}(q, 0)} \leq 1,
\]

where \( \varepsilon_{tot}(q, 0) \) is the statistical limit of the total di-electric function.

A semimetal–semiconductor transition in disordered degenerate semiconductors was studied by Fradkin [14]. The HgTe (III–V semiconductors) and SnTe (IV–VI semiconductors) alloys, as well as the twodimensional graphite, i.e., graphene, were considered as the examples of such systems. The transition appears due to the scattering of the charge carriers on a random potential and is caused by the carrier localization, but the Coulomb and spin–orbit interactions were disregarded in the model. In this work, the influence of the disorder in graphene on its transport properties is not considered, but it is shown that the inclusion of the Coulomb interaction leads to a qualitatively similar result.

\footnote{There is also a purely technological difficulty in performing the experiment with graphene suspended in a vacuum: the presence of a large number of defects such as vacancies and local ruptures is possible. It is not excluded that the graphene film is bent, creating a geometric potential. If all of these difficulties were overcome, electrons could be “sputtered” onto graphene, the necessity of the substrate as a source of the charge carriers disappears, and the semimetallic state of graphene becomes possible.}

\footnote{When \( \alpha^* \) exceeds unity by an infinitesimal value, the system becomes unstable. However, at the exact equality \( \alpha^* = 1 \), \( E_{gap} \equiv 0 \) should be expected and the system still remains stable.}

\footnote{For \( \nu = 1 \), we obtain \( \alpha_{01}^* \approx 1.0214 \) and \( \alpha_{01}^* > \alpha_{02}^* \), which is important if the transition is approached from the \( \alpha^* < 1 \) side. In this case, the transition from the spin-unpolarized phase to the spin-polarized one occurs due to the charge sign of \( E_{gap} \).}

\footnote{A spin factor of 2 is already taken into account in the formula for \( p_F \). Thus, in our notation, \( \nu \) should be replaced by \( \nu_{c,h} / 2 \) in the spin-polarized case without changing the formulas.
Abrikosov and Beneslavskii [15] considered the case of a Fermi point, a single-point touching of the conduction and valence bands at $\varepsilon_F = 0$. In this case, the Fermi energy does not enter the Green’s function and the subsequent calculations were performed at $p_F \equiv 0$, which is essentially different from the problem considered in this work, namely, graphene on a substrate with a non-zero concentration of charge carriers, i.e., $p_F \neq 0$.

8. CONCLUSIONS

In this work, the ground-state energy of an electron (hole) gas was calculated including the renormalization of the quantity $u$. The stability of a zero-gap semiconductor phase with respect to the transition to a semimetallic state was analyzed on the basis of the calculation. The condition of the transition appearance was obtained in the form $\alpha^* \simeq 1$. Possible systems for the experimental observation were pointed out.

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