Pis'ma v ZhETF, vol. 95, iss. 3, pp. 168 – 174 © 2012 February 10

Fermi point in graphene as a monopole in momentum space

M. A. Zubkov[1)]

Institute of Theoretical and Experimental Physics, 117259 Moscow, Russia

Submitted 19 December 2011

We consider the effective field theory of graphene monolayer with the Coulomb interaction between fermions taken into account. The gauge field in momentum space is introduced. The position of the Fermi point coincides with the position of the corresponding monopole. The procedure of extracting such monopoles during lattice simulations is suggested.

1. Introduction. Graphene is a unique $(2+1)$-dimensional nonrelativistic system that shares common properties with relativistic quantum field theory. In particular, in the effective field theory of graphene the massless Dirac spinors appear [1–4]. When the Coulomb interaction is taken into account, the effective Lorentz symmetry is broken. The phase structure of the model may be changed when the external conditions are changed (that may lead, say, to the change of Fermi velocity $v_{\rm F}$) [5–9]. Change of the phase structure of the model must be accompanied with the deformation of the momentum space topology [10, 11]. Therefore, it is important to investigate various topological invariants in momentum space of the effective field model.

In general in $3D$ the Fermi points are not topologically stable [10]. This is because $\pi_2(GL(N,C))=0$ for $N\geq 2$. The $N\times N$ Green function in momentum space belongs to $GL(N,C)$. That's why topological triviality of mapping $S_2\to GL(N,C)$ does not allow topological stability of the Green function's poles in general case. However, if a certain symmetry is present that reduces the size of the space of the Green functions, the topological stability becomes possible [11, 7]. In particular, the $3D$-model of graphene monolayer has such a symmetry that effectively reduces space of the Green functions considerably. As a result, the topological invariant $\mathcal{N}_2$ appears. This invariant is expressed through Green function at zero frequency $\omega=0$ and is an integral over the closed contour $\mathcal{C}$ around Fermi point in the plane of $2D$ momenta $\mathbf{p}$ (see, for example, [11]). The important advantage of the existence of this invariant is that the pole of the Green function cannot disappear without a phase transition. It is worth mentioning, however, that this construction is less natural than that of the invariant $\mathcal{N}_3$ of $4D$-theory [10]. This is because only the structure of $\omega=0$ plane in momentum space is reflected by $\mathcal{N}_2$. Moreover, the given construction was introduced when Coloumb interaction between quasiparticles is neglected, and in the case, when these interactions are present, it requires an additional investigation.

In this paper we extend the construction of $\mathcal{N}_2$ to the effective field model of graphene in such a way that the topological invariant is written as an integral over the surface in $3D$ momentum space $(\omega,\mathbf{p})$. In the form presented here this invariant works also for the case, when the Coulomb interaction is present. We show that when the Green function is smooth enough, our construction can be reduced to the original construction of $\mathcal{N}_2$. In addition, we present the definition of the gauge field in momentum space such that the positions of the corresponding monopoles coincide with the positions of the poles or zeros of the Green function. This construction is intended mainly to be used during lattice simulations. We also suggest the procedure of extraction the monopoles in momentum space for the lattice discretization with staggered fermions.

2. The field theoretical effective model for grapheme. The low energy effective model of graphene may be derived [1–3] starting from the simple nonrelativistic Hamiltonian that describes the interactions of electrons that belong to neighbor Carbon atoms. The carbon atoms of graphene form a honeycomb lattice with two sublattices A and B (or the triangular form). Further we denote the lattice spacing by a. Let us introduce vectors that connect a vertex of the sublattice A to its neighbors (that belong to the sublattice B): $\mathbf{l}_1=(-a,0)$, $\mathbf{l}_2=(a/2,a\sqrt{3}/2)$, $\mathbf{l}_3=(a/2,-a\sqrt{3}/2)$. The Hamiltonian has the form

$$H=-t\sum_{\alpha\in A}\sum_{j=1}^{3}\Big[\psi^\dagger(\mathbf{r}_\alpha)\psi(\mathbf{r}_\alpha+\mathbf{l}_j)+ + \psi^\dagger(\mathbf{r}_\alpha+\mathbf{l}_j)\psi(\mathbf{r}_\alpha)\Big], \quad (1)$$

Here t is the hopping parameter, operator $\psi^\dagger$ creates electrons at the points of the lattice.

Let us define two electron fields in momentum space that correspond to two sublattices:

[1)] e-mail: zubkov@itep.ru

$$\psi_A(\mathbf{k}) = \frac{1}{V}\sum_{\alpha\in A}\psi(r_\alpha)e^{-i\mathbf{k}(r_\alpha+\mathbf{l}_1)},$$
$$\psi_B(\mathbf{k}) = \frac{1}{V}\sum_{\beta\in B}\psi(r_\beta)e^{-i\mathbf{k}r_\beta}. \quad (2)$$

Here V is the number of points in the sublattice A. The Brillouin zone is a hexagon with opposite sides identified. There are two different vertices of the hexagon that are denoted K_+, K_-. Quasiparticle energy vanishes at these points. We expand ψ around K_+, K_-, denote $\psi^{\pm}_{A,B}(\mathbf{q}) \equiv \psi_{A,B}(K_\pm+\mathbf{q})$ and introduce the 4-component field $\psi = \left(\psi^+_A, \psi^+_B, \psi^-_A, \psi^-_B\right)^{\mathrm{T}}$.

At low energy the effective field theory appears. Taking the Fourier transform from $\mathbf{q}$ to the coordinate space we come to the field – theoretic formulation of the model:

$$H = \int d^2x\psi^\dagger(\mathbf{x})\hat{D}\psi(\mathbf{x}), \quad (3)$$

where $\hat{D}$ has the form of the usual Dirac operator taken on the $2D$ hypersurface $x_3 = 0$: $\hat{D} = -iv_F\gamma^0\gamma^a\partial_a$, $a = 1,2$, where $v_{\mathrm{F}} = (3ta)/2$ is the Fermi velocity (that is about 1/300). Here, γ are the gamma-matrices in the representation to be specified below. Let us remind that we started from the nonrelativistic Hamiltonian and completely disregarded spin degrees of freedom. Now we take them into account adding a new index to the field ψ. We assume it has two spin components. In hamiltonian (3) gamma-matrices act on the pseudospin index while the true spin operator does not enter the Hamiltonian.

We consider the interaction between quasiparticles due to the photon exchange (A is the $3+1$ electromagnetic field). Let us perform the Wick rotation, the rescaling of time, and gauge fields: $t \to ix^4/v_{\mathrm{F}}$ $A^0 \to i\sqrt{v_{\mathrm{F}}}A^4$, $\bar{A} \to \frac{1}{\sqrt{v_{\mathrm{F}}}}\bar{A}$.

Further we denote $g = e/\sqrt{v_{\mathrm{F}}}$. Therefore, the analogue of the fine structure constant is $\alpha_{\mathrm{F}} = \alpha/v_{\mathrm{F}} \sim \sim 300/137 \sim 2$. We also introduce Euclidean Dirac matrices that satisfy $\{\Gamma_i,\Gamma_j\} = 2\delta_{ij}$:

$$\Gamma^4 = \begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}, \qquad \Gamma^1 = \begin{pmatrix}-\sigma_1 & 0\\ 0 & -\sigma_1\end{pmatrix},$$
$$\Gamma^2 = \begin{pmatrix}-\sigma_2 & 0\\ 0 & \sigma_2\end{pmatrix}, \quad \Gamma^3 = \begin{pmatrix}0 & -\sigma_2\\ -\sigma_2 & 0\end{pmatrix},$$
$$\Gamma^5 = \begin{pmatrix}0 & -i\sigma_2\\ i\sigma_2 & 0\end{pmatrix}, \quad i\Gamma^3\Gamma^5 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$
$$\bar{\psi} = \psi^+\Gamma^4. \quad (4)$$

We introduce finite temperature T via taking an integral over x^4 within the interval $[0, v_{\mathrm{F}}/T]$ and adopting the periodic in x^4 boundary conditions. The chemical potential is assumed to be equal to zero. Due to $v_{\mathrm{F}} \sim 1/300 \ll 1$ the fluctuations of A_a are suppressed and we neglect them in the functional integral. We arrive at the partition function:

$$Z = \int D\bar{\psi}D\psi DA\exp\Big\{-\frac{1}{2}\int d^4x(\partial_I A_4)^2 -$$
$$-\int d^3x\bar{\psi}^A[(\partial_4 - igA_4)\Gamma^4 + \partial_a\Gamma^a]\psi_A\Big\},$$
$$a = 1,2;\ I,J = 1,2,3. \quad (5)$$

Here index $A = 1,2$ belongs to the spin degrees of freedom.

3. Green functions. It is worth mentioning that the Green function has to be considered in a certain gauge. The gauge freedom of the system corresponds to the transformation $A_4 \to A_4 + \partial_4\alpha(x^4)$, $\psi \to e^{i\alpha}\psi$. We may fix this gauge freedom via implying a certain gauge fixing condition. For example we may choose the condition $A_4(x^4,\mathbf{z}) = 0$ for a certain $3D$-position $\mathbf{z}$. The model at finite temperature, i.e., with periodic boundary conditions along x^4 should be considered with care. When the system is considered in lattice regularization, the value of A_4 on a certain point $(x^4_0,\mathbf{z})$ must not be fixed. This choice of the gauge might appear to break general properties of the Green functions (see Appendix) as it introduces the selected point in plane $x-y$. We may instead fix another gauge minimizing the functional $\int A_4^2 d^4x$ with respect to the gauge transformations. Further we imply that the given gauge is fixed and the gauge fixing condition is inserted into the functional measure over A_4.

Fermion Green function has the form:

$$\mathbf{G} = \langle\psi^\dagger_x\psi_y\rangle = \frac{1}{Z}\int D\psi^\dagger D\psi DA\psi^\dagger_x\psi_y \times$$
$$\times\exp\Big\{-\frac{1}{2}\int d^4x(\partial_I A_4)^2 - \int d^3x\bar{\psi}[(\partial_4 - igA_4)\Gamma^4 +$$
$$+\partial_a\Gamma^a\psi]\Big\},\quad a = 1,2;\ I,J = 1,2,3. \quad (6)$$

In order to reveal the $3D$ nature of the system let us consider the following representation of the spinor field:

$$\psi \equiv \begin{pmatrix}\chi_+\\ \sigma_2\chi_-\end{pmatrix}. \quad (7)$$

In terms of χ_+ and χ_- the Green functions are:

$$\mathcal{G}_{\pm\pm} = \frac{1}{Z}\int D\chi^\dagger D\chi DA\chi^\dagger_\pm(x)\chi_\pm(y) \times$$
$$\times\exp\Big\{-\frac{1}{2}\int d^4x(\partial_I A_4)^2 -$$
$$-\int d^3x\chi_-{}^\dagger\sigma_3[(\partial_4 - igA_4)\sigma_3 - \partial_1\sigma_1 - \partial_2\sigma_2]\chi_- -$$
$$-\int d^3x\chi_+{}^\dagger\sigma_3[(\partial_4 - igA_4)\sigma_3 - \partial_1\sigma_1 - \partial_2\sigma_2]\chi_+\Big\}. \quad (8)$$

We have, obviously, $\mathcal{G}_{++} = \mathcal{G}_{--} = \mathcal{G}$. At the same time $\mathcal{G}_{\pm\mp} = \langle\chi^\dagger_\pm(x)\chi_\mp(y)\rangle = 0$. We also imply that the Green function is diagonal in spin index. That's why $\mathcal{G}$ can be understood as the 2×2-matrix. On the language of $\chi_\pm$ different Γ_3 chiralities correspond to the states with $\chi_+ = \pm\chi_-$. Different Γ_5 chiralities correspond to the states with $\chi_+ = \pm i\chi_i$, $i\Gamma_3\Gamma_5$ chiralities correspond to $\chi_\pm = 0$. In momentum space the 2×2-matrix $\mathcal{G}$ can be expressed as

$$\mathcal{G}(\omega,\mathbf{p}) = \int d^3x\mathcal{G}(0,x)e^{i\omega x^4 + i(\mathbf{px})} = \\ = i[g_0(\omega,\mathbf{p}) + g_a(\omega,\mathbf{p})\sigma^a]\sigma_3,\ a = 1,2,3. \tag{9}$$

Here vectors $\mathbf{p},\mathbf{x}$ are two component.

Direct calculation gives

$$\mathcal{G} = \frac{1}{Z}\int DA\exp\Big[-\frac{1}{2}\int d^4x(\partial_I A_4)^2\Big]\times \\ \times\,\mathrm{Det}^2\Big[i(\partial_4 - igA_4)\sigma_3 - i\partial_1\sigma_1 - i\partial_2\sigma_2\Big]\times \\ \times\frac{i}{i(\partial_4 - igA_4)\sigma_3 - i\partial_1\sigma_1 - i\partial_2\sigma_2}\sigma_3. \tag{10}$$

Operator $Q = i[\partial_4 - igA_4]\sigma_3 - i[\partial_1]\sigma_1 - i[\partial_2]\sigma_2$ is Hermitian for any real A_4. That's why we come to the conclusion that the operator $i\mathcal{G}\sigma_3$ is also Hermitian. This means that the functions $g_a(\omega,\mathbf{p}), a = 0,1,2,3$ are real. As a results $-i\mathcal{G}\sigma_3$ belongs to $u(2)$. Considering symmetries of the Green function, we come to the following form of $\mathcal{G}$ (see Appendix):

$$g_0(\omega,\mathbf{p}) = 0,\quad g_3(\omega,\mathbf{p}) = \tilde{f}\Big(\omega,|\mathbf{p}|^2\Big), \\ \mathbf{g}(\omega,\mathbf{p}) = \mathbf{p}\tilde{h}\Big(\omega^2,|\mathbf{p}|^2\Big), \\ \tilde{f}\Big(\omega,|\mathbf{p}|^2\Big) = -\tilde{f}\Big(-\omega,|\mathbf{p}|^2\Big). \tag{11}$$

That's why $i\mathcal{G}\sigma_3 \in \mathrm{su}(2)$. If in addition, the scale invariance is not broken (in particular, $T = 0$), and the functions $\tilde{f},\tilde{h}$ are smooth enough, we have the further simplification:

$$g_3(\omega,\mathbf{p}) = \frac{\omega}{\omega^2 + |\mathbf{p}|^2} f\Big(\frac{\omega^2}{|\mathbf{p}|^2}\Big), \\ \mathbf{g}(\omega,\mathbf{p}) = \frac{\mathbf{p}}{\omega^2 + |\mathbf{p}|^2} h\Big(\frac{\omega^2}{|\mathbf{p}|^2}\Big). \tag{12}$$

4. Topological invariant at $\omega = 0$. In some publications (see, for example, [11]) the following expression has been considered that is shown to be a topological invariant both with and without external magnetic field when the interaction with A_4 is switched off:

$$\mathcal{N}_2 = \frac{1}{4\pi i}\mathrm{Tr}\,\sigma_3\int_{\mathcal{C}}\mathcal{G}d\mathcal{G}^{-1}. \tag{13}$$

Here contour $\mathcal{C}$ around the Fermi point (the pole of $\mathcal{G}$) is taken in the $\omega = 0$ plane. For the noninteracting fermions we have $\mathcal{N}_2 = 1$. Further, if the interactions are introduced, the Green function is changed: $\mathcal{G}\to\mathcal{G}+\delta\mathcal{G}$. If the interactions are such that $\{\delta\mathcal{G}(0,\mathbf{p}),\sigma_3\} = 0$, then $\delta\mathcal{N}_2 = 0$. This means that $\mathcal{N}_2 = 1$ until the phase transition is encountered. For example, if the external magnetic field in z-direction is introduced we have $\{\delta\mathcal{G}(0,\mathbf{p}),\sigma_3\} = 0$ (see, for example, [12]). At a first look, it is not obvious, that with the Coulomb interaction turned on $\mathcal{N}_2$ remains the topological invariant.

However, using the above mentioned symmetry considerations we rewrite this function in the absence of external fields as follows:

$$\mathcal{N}_2 = -\frac{1}{4\pi i}\mathrm{Tr}\sigma_3\int_{\mathcal{C}}\frac{[dg_3\sigma_3 + (d\mathbf{g},\sigma)][g_3\sigma_3 + (\mathbf{g},\sigma)]}{g_3^2 + \mathbf{g}^2} = \\ = \frac{1}{2\pi}\int_{\mathcal{C}}\frac{\epsilon_{ab}n^a dn^b}{1 + g_3^2/\mathbf{g}^2}, \tag{14}$$

where $n^1 = p^1/\sqrt{[p^1]^2 + [p^2]^2}$, $n^2 = p^2/\sqrt{[p^1]^2 + [p^2]^2}$, and it is implied that $\tilde{h}(0,\mathbf{p}^2)\neq 0$. As it was mentioned above, when the functions g_a are smooth enough, we have $g_3(0,\mathbf{p}) = 0$ and, therefore, again $\mathcal{N}_2 = 1$. This means that the pole of the Green function (the Fermi point) is topologically stable if the symmetries considered above take place.

5. Topological invariant in space $(\omega,\mathbf{p})$. Below we generalize the construction of the topological invariant $\mathcal{N}_2$ considered above. The resulting construction uses the Green function defined on the surface that encloses the Fermi point in $\omega{-}\mathbf{p}$-space. The considered construction also works for nonzero $g_3(0,\mathbf{p})$. Let us define the function in momentum space

$$\mathcal{H} = \frac{\mathcal{G}\sigma_3}{\sqrt{\frac{1}{2}\mathrm{Tr}\,(\mathcal{G}\sigma_3)^2}}. \tag{15}$$

We can express $\mathcal{H}$ through the functions g_a mentioned above: $\mathcal{H} = n_a\sigma_a$, $n_a = g_a/|g|$, $|g| = \sqrt{g_a g_a}$, $a = 1,2,3$. Now let us consider the following integral over closed surface Σ in momentum space such that $\mathcal{G}$ does not have poles on Σ:

$$\mathcal{N}_2 = \frac{1}{16\pi i}\mathrm{Tr}\int_\Sigma \mathcal{H}\,d\mathcal{H}\wedge d\mathcal{H} = \\ = \frac{1}{8\pi}\epsilon_{abc}\int_\Sigma n^a\,dn^b\wedge dn^c. \tag{16}$$

The given expression (16) for the invariant $\mathcal{N}_2$ is, obviously, reduced to (13) in the case, when $g_3(0,\mathbf{p}) = 0$. Without interactions and without external magnetic field $\mathcal{G}$ has the pole at $\mathbf{p} = \omega = 0$ that corresponds to the

Fermi point. In this case $n_3(\omega, \mathbf{p}) = \omega/\sqrt{\omega^2 + \mathbf{p}^2}$, $\mathbf{n}(\omega, \mathbf{p}) = \mathbf{p}/\sqrt{\omega^2 + \mathbf{p}^2}$, and $\mathcal{N}_2 = 1$ for any surface that encloses the pole. When the interaction with the electromagnetic field is turned on, the value of $\mathcal{N}_2$ for the surface that encloses this pole remains equal to unity until a phase transition is encountered. The important advantage of the given formulation is that we already do not need the condition $g_3(0, \mathbf{p}) = 0$ to be satisfied. We only need $g_0 = 0$. The situation, when $g_0 = 0$ and $g_3(0, \mathbf{p}) \neq 0$ may appear in the other $(2+1)$-systems or even in the effective field model of graphene for the inhomogenious gauge or when some of the symmetries are broken dynamically.

6. Fermi point as a monopole. As it was explained above, $\tilde{\mathcal{G}} = -i\mathcal{G}\sigma_3 \in su(2)$ out of the region, where $\mathcal{G}$ has poles. We can diagonalize $\tilde{\mathcal{G}}$ via $SU(2)/U(1)$ transformations:

$$\tilde{\mathcal{G}} = V^{\dagger}(\sqrt{g_3^2 + \mathbf{g}^2}\sigma_3)V, \tag{17}$$

V is defined up to the $U(1)$ transformation $V \to e^{\alpha\sigma_3}V$. That's why here $V \in SU(2)/U(1) \sim S_2$. We can choose V to be smooth on the surface Σ except for a small vicinity Ω of a certain point. We have $\pi_2[SU(2)/U(1)] = Z$. Actually the invariant $\mathcal{N}_2$ is equal to the degree of the mapping $S_2 \to SU(2)/U(1)$:

$$\begin{aligned}\mathcal{N}_2 &= \frac{1}{16\pi i}\mathrm{Tr}\int_{\Sigma-\Omega} V^{\dagger}\sigma_3 V d[V^{\dagger}\sigma_3 V] \wedge d[V^{\dagger}\sigma_3 V] = \\ &= -\frac{1}{4\pi i}\mathrm{Tr}\int_{\Sigma-\Omega} \sigma_3 dV \wedge dV^{\dagger} = \\ &= -\frac{1}{4\pi i}\mathrm{Tr}\int_{\Sigma-\Omega} \sigma_3 d[V dV^{\dagger}] = \\ &= \frac{1}{4\pi i}\mathrm{Tr}\int_{\partial\Omega} \sigma_3 V dV^{\dagger}.\end{aligned} \tag{18}$$

Now we define the gauge field in momentum space $\mathcal{B} = -iVdV^{\dagger}$, $\mathcal{B}$ is smooth everywhere except for the string ended at the position of the pole of $\mathcal{G}$. The field strength of $\mathcal{B}$ vanishes everywhere except for the mentioned string. The position of the string (but not the positions of its ends) can be changed by the $U(1)$ transformations $V \to e^{\alpha\sigma_3}V$. The third component of the gauge field $B = \frac{1}{2}\mathrm{Tr}\,\mathcal{B}\sigma_3$ is the $U(1)$ field. The position of the corresponding Dirac monopole coincides with the pole (or zero) of $\mathcal{G}$. The position of the Fermi point without interactions coincides with the position of the monopole constructed of B in momentum space. The position of the antimonopole coincides with the zero of $\mathcal{G}$ (placed at the infinity). Monopole and antimonopole are connected by the Dirac string. This pattern cannot disappear until the phase transition is encountered.

7. $\mathcal{N}_2$ in $4D$ notations. In $4D$-notations Green function (6) has the form:

$$\mathbf{G} = \begin{pmatrix} \mathcal{G} & 0 \\ 0 & \sigma_2\mathcal{G}\sigma_2 \end{pmatrix} = i\begin{pmatrix} \tilde{\mathcal{G}} & 0 \\ 0 & -\sigma_2\tilde{\mathcal{G}}\sigma_2 \end{pmatrix}\Gamma_4. \tag{19}$$

Again, we define the function in momentum space: $\mathbf{H} = \frac{-i\mathbf{G}\,\Gamma_4}{\sqrt{1/4 - \mathrm{Tr}\,(\mathbf{G}\,\Gamma_4)^2}}$. We can express $\mathbf{H}$ through three real functions g_a mentioned above: $\mathbf{H} = -n_1\Gamma_1 - n_2\Gamma_2 + n_3\Gamma_4$, $n_a = g_a/|g|$, $|g| = \sqrt{g_a g_a}$, $a = 1, 2, 3$. Now the topological invariant can be expressed as

$$\begin{aligned}\mathcal{N}_2 &= \frac{1}{32\pi}\mathrm{Tr}\int_{\Sigma} \mathbf{H}\,d\mathbf{H} \wedge d\mathbf{H}\,\Gamma_3\Gamma_5 = \\ &= \frac{1}{8\pi}\epsilon_{abc}\int_{\Sigma} n^a\,dn^b \wedge dn^c.\end{aligned} \tag{20}$$

We denote $\tilde{\mathbf{G}} = -i\mathbf{G}\Gamma_4$, $\tilde{\mathbf{G}}$ can be diagonalized via the $SO(4)/[SU(2) \otimes U(1)]$ transformations:

$$\tilde{\mathbf{G}} = \mathbf{V}^{\dagger}(\sqrt{g_3^2 + \mathbf{g}^2}\Gamma_4)\mathbf{V}. \tag{21}$$

Here $\mathbf{V} = \begin{pmatrix} V & 0 \\ 0 & \sigma_2 V\sigma_2 \end{pmatrix}$, V can be chosen in the form:

$$V = \exp\Big[\frac{i(n_2\sigma_1 - n_1\sigma_2)\arccos n_3}{2\sqrt{1 - n_3^2}}\Big]. \tag{22}$$

8. Momentum space topology of lattice regularized model. Staggered fermions are unique for the graphene monolayer because in this regularization the doublers of the one-component fermion play the role of the components of two Dirac spinors. This regularization has been used in practical numerical simulations of the considered model [9, 13]. However, the additional doublers ever appear in lattice propagator as it will be explained below. Staggered fermion variables Ψ are obtained via the spin diagonalization: $\psi_x = \Gamma_1^{x_1}\Gamma_2^{x_2}\Gamma_3^{x_3}\Gamma_4^{x_4}\Psi_x$. Here always $x_3 = 0$. In terms of Ψ the free fermion action has the form:

$$\begin{aligned}S = \sum_x \Big(m\,\bar{\Psi}_x\Psi_x + \\ + \frac{1}{2}\sum_{i=1,\dots,4}[\bar{\Psi}_x\alpha_{xi}\Psi_{x+\hat{i}} - \bar{\Psi}_{x+\hat{i}}\alpha_{xi}\Psi_x]\Big), \\ \alpha_{xi} = (-1)^{x_1+\dots+x_{i-1}}.\end{aligned} \tag{23}$$

We keep the only component of Ψ. As a result the doublers play the role of the components of the two original spinors. In order to reconstruct the original spinor and flavor indices of the fermions we consider the lattice with even number of lattice spacings in each direction. Let us subdivide the lattice into the blocks consisted of elementary cubes. We denote the coordinates of the blocks by y_i. Therefore, the coordinates of the lattice sites are $x_i = 2y_i + \eta_i, \eta_i = 0, 1$. We define the new fields [14]:

$$[\Phi_y]^{\alpha}_a = \frac{1}{8}\sum_{\eta}[\Gamma_1^{\eta_1}\Gamma_2^{\eta_2}\Gamma_4^{\eta_4}]^{\alpha}_a \Psi_{2y+\eta}. \qquad (24)$$

Here index $\alpha = 1, ..., 4$ is the spinor index while $a = 1, ..., 4$ is the flavor index. Matrices Φ have 4×4 components. But not all of these components are independent. We have the following constraint on Φ: $\Gamma_3\Gamma_5\Phi_y\Gamma_5\Gamma_3 = \Phi_y$. There exists the representation of gamma-matrices such that the matrices Φ have the form: $\Phi = \left(\begin{array}{cc} A & 0 \\ 0 & B \end{array}\right)$. That's why we have two flavors of positive $i\Gamma_3\Gamma_5$ chirality and two flavors of negative $i\Gamma_3\Gamma_5$ chirality that is two flavors of 4-component Dirac spinors. Without interactions in terms of Φ the propagator in momentum representation (of the blocked lattice) has the form [14]:

$$\tilde{\mathbf{G}} = -i\langle\bar{\Phi}\Phi\rangle = \Big\{\sum_a \Gamma_a \frac{1}{2}\sin k_a - i\Big[m - \sum_a \frac{1}{2}(1-\cos k_a)\Gamma_5\otimes T_5 T_i\Big]\Big\}^{-1}. \qquad (25)$$

Here $T_i = \Gamma_i^T$ acts on the flavor indices while Γ-matrices act on the Dirac indices. Momenta k are $k_1 = \frac{2\pi K_1}{N_x/2}$, $k_2 = \frac{2\pi K_2}{N_y/2}$, $k_4 = \frac{2\pi K_4+\pi}{N_t/2}$, $K_1, K_2, K_4 \in Z$. In this regularization the mass term is necessarily added. At the end of the calculation one must set $m = 0$. This Green function turns to the form (19) with $\mathcal{G}$ in the form (9) in the continuum limit at $m = 0$. For $m = 0$ the only pole of the Green function at $p = 0$ appears. The fermion doublers do not have such poles. However, zeros of the functions g_a, $a = 1, 2, 4$ appear at $p_a = \pi k_a$, $k_a \in Z$. At any value of m vector n mentioned above has the following components: $n_a = g_a/\sqrt{g_a g_a}$, $g_1 = i\mathrm{Tr}\,\mathbf{G}\,\Gamma_4\Gamma_1/4$, $g_2 = i\mathrm{Tr}\,\mathbf{G}\,\Gamma_4\Gamma_2/4$, $g_3 = -i\mathrm{Tr}\,\mathbf{G}/4$. Without interactions we have $n_a = \frac{\sin k_a}{\sqrt{\sum_a \sin^2 k_a}}$. From this expression we obtain 4 monopole – antimonopole pairs in momentum space placed in the positions of the fermion doublers. For the surface that encloses any of these points of the Brillouin zone we obtain the values $\mathcal{N}_2 = \pm 1$. This demonstrates that the lattice formulation does not eliminate monopole in momentum space corresponding to the physical pole of the Green function. However, this formulation also gives monopoles that correspond to the unphysical doublers.

When the interaction is switched on the practical prescription for the calculation of the vector n is $n_a(k) = g_a(k)/\sqrt{g_a(k)g_a(k)}$, $a = 1, 2, 4$ with

$$g_a(k) = \frac{i}{16N_1^2N_2^2N_t^2}\sum_{y,z} e^{ik(z-y)}\sum_{\eta,\eta'}(-1)^{\eta_1+\ldots+\eta_{a-1}} \times \delta(\eta'_i - [\eta_i + \delta_{ia}]\mathrm{mod}\,2)\langle G(2y+\eta, 2z+\eta')\rangle. \qquad (26)$$

Here $\langle G(2y+\eta, 2z+\eta')\rangle$ is the staggered fermion one-component propagator in the external field averaged over the configurations of the $U(1)$ gauge field A_4 and over the pseudofermion configurations (the latter give the fermion determinant in the averaging over gauge fields).

Using expression (22) we may calculate the value of $V \in SU(2)/U(1)$ at any point of the momentum space lattice. Next, we may define the $U(1)$ gauge field B at any link of this momentum lattice via the following equation:

$$\left(\begin{array}{cc} \cos\phi\, e^{iB_{xy}} & \sin\phi\, e^{i\chi} \\ -\sin\phi\, e^{-i\chi} & \cos\phi\, e^{-iB_{xy}} \end{array}\right) = V_x V_y^{\dagger}. \qquad (27)$$

The position of the monopole is given by $j = \frac{1}{2\pi}{}^*d[dB\,\mathrm{mod}\,2\pi]$. We expect that the pattern described above with 4 monopole - antimonopole pairs in momentum space will remain until a phase transition is encountered.

9. Conclusions and discussion. In this paper we extend the construction of the topological invariant $\mathcal{N}_2$ to $\omega - \mathbf{p}$-space. The suggested construction works for the case when the Coulomb interaction between the quasiparticles is present. We also construct the gauge field in momentum space that has vanishing field strength everywhere except for the poles and zeros of the Green function (and the strings that connect them). The positions of poles and zeros themselves coincide with the positions of monopoles extracted from the given gauge field.

The 8×8 Green functions of the fermion quasiparticles are reduced to (2×2)-matrices, and even further, to the elements of su(2). These matrices can be represented as $i\mathcal{G}\sigma_3 = g_3\sigma_3 + \mathbf{g}_a\sigma_a$ with real $g_3, \mathbf{g}_a$. The constructed topological invariant catches zeros and poles of $\mathcal{G}$. If interactions are absent, $\mathcal{N}_2 = 1$. When the Coulomb interaction is turned on, the equation $\mathcal{N}_2 = 1$ holds until the phase transition is encountered. This means that the pole in $\mathcal{G}$ cannot disappear until the phase transition occurs.

The system may be transferred to various phases, where different symmetries of the initial system are broken. There may appear different fermion condensates [5–9]. The phase structure of the effective field model of graphene is still unknown. Topology of momentum space must have the relation to this phase structure. The constructed invariant $\mathcal{N}_2$ and the monopoles in momentum space have direct connection only to the phase that includes the noninteracting system. The transition to the other phas(es) may be accompanied with the change of $\mathcal{N}_2$. The transition between the new phases may have connection to the other topological invariants. In particular, the topological invariants for the $2+1$ gapped systems enter the expression for the quantized Hall conductivity [10, 12, 15, 16]. Also it is worth mentioning that in the presence of the finite chemical potential the Fermi surface appears that is related to the invariant $\mathcal{N}_1$ [10].

The construction presented here is intended for the use mainly in lattice simulation of the effective field theory of graphene at vanishing chemical potential and in the absence of external fields (for the review of recent numerical investigations of the model see [6, 9, 13] and references therein). We expect that the phase transition(s) may take place to the phase(s), where chiral symmetry of the noninteracting system is broken [7] in a certain way. The transition to the new phase must lead to the change of the momentum space topology. The behavior of the monopoles in momentum space constructed here are expected to be related intimately to the mechanism of the phase transition(s) and to the nature of the new phase(s). Their investigation may also be important for the understanding of the role of doublers in various lattice discretizations of the Fermion systems.

The author kindly acknowledges private communication with G.E. Volovik, and discussions with members of the lattice ITEP group M.I. Polikarpov, P. Buividovich, V.I. Zakharov, O. Pavlovsky, M. Ulybyshev. This work was partly supported by RFBR grants # 09-02-00338, 11-02-01227, by Grant for Leading Scientific Schools 679.2008.2. This work was also supported by the Federal Special-Purpose Programme 'Cadres' of the Russian Ministry of Science and Education, by Federal Special-Purpose Programme # 07.514.12.4028.

10. Appendix. Let us denote $\bar{\chi} = \chi^\dagger \sigma_3$. Then we introduce new function $\tilde{\mathcal{G}}$ as $\mathcal{G} = i\tilde{\mathcal{G}}\sigma_3$ and represent it in the following form:

$$i\tilde{\mathcal{G}}(x)=\frac{1}{Z}\int D\bar{\chi}D\chi DA\bar{\chi}(0)\chi(x)\exp\Big\{-\frac{1}{2}\int d^4x[\partial_I A_4]^2 - \int d^3x\bar{\chi}([\partial_4 - igA_4]\sigma_3 - [\partial_1]\sigma_1 - [\partial_2]\sigma_2)\chi\Big\}. \quad (28)$$

We consider severar cases, when the transformational properties of the action leads to symmetries of the Green function.

Let us consider the following transformation $\chi \to i\sigma_2[\bar{\chi}]^{\mathrm{T}}$, $\bar{\chi} \to -i\chi^{\mathrm{T}}\sigma_2, A_4(x) \to A_4(-x)$ (remind that χ and $\bar{\chi}$ are independent anticommuting variables), $x \to -x$. Using this transformation we obtain:

$$\begin{aligned} S_f &= \int d^3x\bar{\chi}([\partial_4 - igA_4]\sigma_3 - [\partial_1]\sigma_1 - [\partial_2]\sigma_2)\chi \to \\ &\to \int d^3x\chi^{\mathrm{T}}\sigma_2([-\partial_4 - igA_4]\sigma_3 + [\partial_1]\sigma_1 + [\partial_2]\sigma_2)\sigma_2\bar{\chi}^{\mathrm{T}} = \\ &= \int d^3x\chi^{\mathrm{T}}([\partial_4 + igA_4]\sigma_3 - [\partial_1]\sigma_1 + [\partial_2]\sigma_2)\bar{\chi}^{\mathrm{T}} = \\ &= \int d^3x\bar{\chi}([\partial_4 - igA_4]\sigma_3 - [\partial_1]\sigma_1 - [\partial_2]\sigma_2)\chi. \end{aligned} \quad (29)$$

Measure over $\chi_\pm$ and the gauge field action are also invariant under this transformation. As a result we obtain

$$\begin{aligned} \tilde{\mathcal{G}}_{ab}(x) &= \langle\bar{\chi}_a(0)\chi_b(x)\rangle = \epsilon_{ac}\epsilon_{bd}\langle\chi_c(0)\bar{\chi}_d(-x)\rangle = \\ &= \epsilon_{ac}\langle\bar{\chi}_d(-x)\chi_c(0)\rangle\epsilon_{db} = \\ &= \epsilon_{ac}\langle\bar{\chi}_d(0)\chi_c(x)\rangle\epsilon_{db} = -[\sigma_2\tilde{\mathcal{G}}^T(x)\sigma_2]_{ab}. \end{aligned} \quad (30)$$

This implies $g_0(\omega,\mathbf{p}) = -g_0(\omega,\mathbf{p}) = 0$, $g_3(\omega,\mathbf{p}) = g_3(\omega,\mathbf{p})$, and $\mathbf{g}(\omega,\mathbf{p}) = \mathbf{g}(\omega,\mathbf{p})$.

Analogue of CP-transformation corresponds to $\chi \to \sigma_1[\bar{\chi}]^{\mathrm{T}}$, $\bar{\chi} \to -\chi^{\mathrm{T}}\sigma_1$, $\mathbf{x} \to -\mathbf{x}, A_4(x_4,\bar{x}) \to -A_4(x_4,-\bar{x})$. In a similar way we obtain:

$$\begin{aligned} S_f &= \int d^3x\bar{\chi}([\partial_4 - igA_4]\sigma_3 - [\partial_1]\sigma_1 - [\partial_2]\sigma_2)\chi \to \\ &\to \int d^3x\chi^{\mathrm{T}}\sigma_1([-\partial_4 - igA_4]\sigma_3 - [\partial_1]\sigma_1 - [\partial_2]\sigma_2)\sigma_1\bar{\chi}^{\mathrm{T}} = \\ &= \int d^3x\chi^{\mathrm{T}}([\partial_4 + igA_4]\sigma_3 - [\partial_1]\sigma_1 + [\partial_2]\sigma_2)\bar{\chi}^{\mathrm{T}} = \\ &= \int d^3x\bar{\chi}([\partial_4 - igA_4]\sigma_3 - [\partial_1]\sigma_1 - [\partial_2]\sigma_2)\chi. \end{aligned} \quad (31)$$

That's why

$$\begin{aligned} \tilde{\mathcal{G}}_{ab}(x) &= \langle\bar{\chi}_a(0)\chi_b(x)\rangle = -\sigma^1_{ac}\sigma^1_{bd}\langle\chi_c(0)\bar{\chi}_d(x_4,-\bar{x})\rangle = \\ &= \sigma^1_{ac}\langle\bar{\chi}_d(x_4,-\bar{x})\chi_c(0)\rangle\sigma^1_{db} = \\ &= \sigma^1_{ac}\langle\bar{\chi}_d(0)\chi_c(-x_4,\bar{x})\rangle\sigma^1_{db} = \\ &= [\sigma_1\tilde{\mathcal{G}}^T(-x_4,\bar{x})\sigma_1]_{ab}. \end{aligned} \quad (32)$$

The Fourier transformation gives

$$\tilde{\mathcal{G}}(\omega,\mathbf{p}) = \sigma_1\tilde{\mathcal{G}}^{\mathrm{T}}(-\omega,\mathbf{p})\sigma_1. \quad (33)$$

Therefore, $g_0(\omega,\mathbf{p}) = g_0(-\omega,\mathbf{p})$, $g_3(\omega,\mathbf{p}) = -g_3(-\omega,\mathbf{p})$, and $\mathbf{g}(\omega,\mathbf{p}) = \mathbf{g}(-\omega,\mathbf{p})$.

Rotation of the (1), (2) plane corresponds to the transformation $\chi \to e^{i\phi\sigma_3/2}\chi$, and $\mathbf{x} \to e^{i\phi\sigma_2}\mathbf{x}$ with the angle ϕ. We have:

$$\tilde{\mathcal{G}}(\omega,\mathbf{p}) = e^{-i\phi\sigma_3/2}\tilde{\mathcal{G}}(\omega, e^{i\phi\sigma_2}\mathbf{p})e^{i\phi\sigma_3/2}. \quad (34)$$

This implies $g_0(\omega,\mathbf{p}) = g_0(\omega, e^{i\phi\sigma_2}\mathbf{p})$, $g_3(\omega,\mathbf{p}) = g_3(\omega, e^{i\phi\sigma_2}\mathbf{p})$, and $\mathbf{g}(\omega,\mathbf{p}) = e^{-i\phi\sigma_2}\mathbf{g}(\omega, e^{i\phi\sigma_2}\mathbf{p})$.

All mentioned above allow to derive the general form of $\mathcal{G}$:

$$g_0(\omega,\mathbf{p}) = 0, \quad g_3(\omega,\mathbf{p}) = \tilde{f}\Big(\omega, |\mathbf{p}|^2\Big),$$
$$\mathbf{g}(\omega,\mathbf{p}) = \mathbf{p}\tilde{h}\Big(\omega^2, |\mathbf{p}|^2\Big). \qquad (35)$$

Here $\tilde{f}$ is odd as a function of ω.

---

1. G. W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984).
2. P. R. Wallace, Phys. Rev. **71**, 622 (1947).
3. A. H. Castro Neto, F. Guinea, N. M. R. Peres et al., Rev. Mod. Phys. **81**, 109 (2009).
4. I. V. Fialkovsky and D. V. Vassilevich, *Quantum Field Theory in Graphene*, talk at QFEXT 11, arXiv:1111.3017.
5. D. T. Son, Phys. Rev. B **75**, 235423 (2007); arXiv:cond-mat/0701501.
6. Y. Araki, Annals Phys. **326**, 1408 (2011); arXiv:1010.0847.
7. V. P. Gusynin, S. G. Sharapov, and J. P. Carbotte, Int. J. Mod. Phys. B **21**, 4611 (2007); arXiv:0706.3016.
8. G. W. Semenoff, . *Ch. Symmetry Breaking in Graphene, Proceedings of the Nobel Symposium on Graphene and Quantum Matter*, arXiv:1108.2945.
9. J. E. Drut and T. A. Lahde, Phys. Rev. B **79**, 165425 (2009); arXiv:0901.0584.
10. G. E. Volovik, *The Universe in a Helium Droplet*, Clarendon Press, Oxford, 2003.
11. G. E. Volovik, in *Quantum Analogues: From Phase Transitions to Black Holes and Cosmology* (eds. W. G. Unruh and R. Schutzhold), Springer Lecture Notes in Physics 718/2007, p. 31; cond-mat/0601372.
12. Y. Hatsugai, *Topological aspect of graphene physics*, Proceedings for HMF-19, arXiv:1008.4653.
13. W. Armour, S. Hands, and C. Strouthos, Phys. Rev. B **81**, 125105 (2010); arXiv:0910.5646.
14. I. Montvay and G. Munster, *Quantum Fields on a Lattice*, Cambridge University press, 1994.
15. Y. Hatsugai, T. Fukui, and H. Aoki, *Topological analysis of the quantum Hall effect in graphene: Dirac–Fermi transition across van Hove singularities and the edge vs bulk quantum numbers*, arXiv:cond-mat/0607669.
16. E. V. Gorbar, V. P. Gusynin, V. A. Miransky, and I. A. Shovkovy, Phys. Rev. B **78**, 085437 (2008); arXiv:0806.0846.
17. G. E. Volovik, Pis'ma v ZhETF **91**, 61 (2010); JETP Lett. **91**, 55 (2010); arXiv:0912.0502.