Theory of Green functions of free Dirac fermions in graphene

Van Hieu Nguyen1,2, Bich Ha Nguyen1,2 and Ngoc Dung Dinh1

1 Advanced Center of Physics and Institute of Materials Science, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay District, Hanoi, Vietnam
2 University of Engineering and Technology, Vietnam National University, 144 Xuan Thuy, Cau Giay District, Hanoi, Vietnam

E-mail: nvhieu@iop.vast.ac.vn

Received 10 November 2015
Accepted for publication 8 December 2015
Published 12 February 2016

Abstract
This work is the beginning of our research on graphene quantum electrodynamics (GQED), based on the application of the methods of traditional quantum field theory to the study of the interacting system of quantized electromagnetic field and Dirac fermions in single-layer graphene. After a brief review of the known results concerning the lattice and electronic structures of single-layer graphene we perform the construction of the quantum fields of free Dirac fermions and the establishment of the corresponding Heisenberg quantum equations of these fields. We then elaborate the theory of Green functions of Dirac fermions in a free Dirac fermion gas at vanishing absolute temperature \( T = 0 \), the theory of Matsubara temperature Green functions and the Keldysh theory of non-equilibrium Green functions.

Keywords: Dirac fermions, Heisenberg quantum equation of motions, Green functions

Classification numbers: 2.01, 3.00, 5.15

1. Introduction

In the comprehensive review [1] on the rise of graphene as the emergence of a new bright star ‘on the horizon of materials science and condensed matter physics’, Geim and Novoselov have remarked exactly that, as a strictly two-dimensional (2D) material, graphene ‘has already revealed a cornucopia of new physics’. It is the physics of graphene and graphene-based nanosystems, including graphene quantum electrodynamics (GQED). In the language of another work by Novoselov et al [2], GQED (‘resulting from the merger’ of the traditional quantum field theory with the dynamics of Dirac fermions in graphene) would ‘provide a clear understanding’ and a powerful theoretical tool for the investigation of a huge class of physical processes and phenomena taking place in the rich world of graphene-based nanosystems and their electromagnetic interaction processes. This work is the first step in the establishment of the basics of graphene quantum electrodynamics: the construction of the theory of Green functions of free Dirac fermions in graphene.

Since throughout the present work we often use knowledge of the lattice structure of graphene as well as expressions of the wave functions of Dirac fermions with the wave vectors near the corners of the Brillouin zones of the graphene lattice, first we present a brief review of this knowledge in section 2. In the subsequent section 3, the explicit expressions of the quantum field of free Dirac fermions in graphene and the corresponding Heisenberg quantum equations of motion are established. Section 4 is devoted to the study of Green functions of Dirac fermions in a free Dirac fermion gas at vanishing absolute temperature \( T = 0 \). The theory of Matsubara temperature Green functions of free Dirac fermions is presented in section 5, and the content of section 6 is the Keldysh theory of non-equilibrium Green functions. The conclusion and discussions are presented in section 7. The unit system with \( c = \hbar = 1 \) will be used.
2. Definitions and notations

According to the review [3] on the electronic properties of graphene, each graphene single layer is a 2D lattice of carbon atoms with the hexagonal structure presented in figure 1(a). It consists of two interpenetrating triangular sublattices with the lattice vectors

\[ \mathbf{l}_1 = \frac{a}{2}(3, \sqrt{3}), \quad \mathbf{l}_2 = \frac{a}{2}(3, -\sqrt{3}) \]

(1)

where \( a \) is the distance between the two nearest carbon atoms \( a \approx 1.42 \). The reciprocal lattice has the following lattice vectors

\[ \mathbf{k}_1 = \frac{2\pi}{3a}(1, \sqrt{3}), \quad \mathbf{k}_2 = \frac{2\pi}{3a}(1, -\sqrt{3}) \]

(2)

Vectors \( \mathbf{l}_i \) and \( \mathbf{k}_i \) satisfy the condition

\[ \mathbf{k}_i \cdot \mathbf{l}_j = 2\pi \delta_{ij} \]

(3)

The first Brillouin zone (BZ) is presented in figure 1(b). Two inequivalent corners \( K \) and \( K' \) with the coordinate vectors

\[ \mathbf{K} = \frac{3\pi}{2a} \left(1, \frac{1}{\sqrt{3}}\right), \quad \mathbf{K}' = \frac{3\pi}{2a} \left(1, -\frac{1}{\sqrt{3}}\right) \]

(4)

are called the Dirac points. Each of them is the common vertex of two consecutive cone-like energy bands of Dirac fermions.

The corners of all BZs in the reciprocal lattice form a new hexagonal lattice of the points equivalent to the Dirac points \( K \) and \( K' \) in the first BZ (figure 2). This new hexagonal lattice also consists of two interpenetrating triangular sublattices with the lattice vectors

\[ \mathbf{l}'_1 = \frac{3\pi}{a}(1, 0), \quad \mathbf{l}'_2 = \frac{3\pi}{a} \left(1, \frac{\sqrt{3}}{2}\right) \]

(5)

As an example let us consider the sublattice of all points equivalent to the corner \( K \). They form a triangular lattice with the natural parallelogram elementary cell drawn in the left part of figure 3. For avoiding the presence of four equivalent corners in each natural parallelogram elementary cell, in the sequel we shall use the symmetric Wigner–Seitz elementary cell drawn in the right part of figure 3 instead of the parallelogram one. The wave vector \( \mathbf{k} \) is called to be near the corner \( K \) if it is contained inside the symmetric Wigner–Seitz elementary cell around this corner. With respect to the sublattice of all points equivalent to the corner \( K' \) we also have a similar result. We chose the length unit such that the area of elementary cell is equal to 1.
3. Quantum field of free Dirac fermions

In order to establish explicit expressions of the quantum field of free Dirac fermions it is necessary to have formulae of the wave functions of these quasiparticles. Denote \( \Phi_{k, \pm}^{K} (r) \) the wave function of the state with the wave vector \( k \) near the Dirac points \( K \) or \( K' \) and the energy \( E \). It was known that

\[
\begin{align*}
\Phi_{k, \pm}^{K} (r) &= e^{ikr} \varphi_{k, \pm}^{K} (r), \\
\Phi_{k, \pm}^{K'} (r) &= e^{iK' r} \varphi_{k, \pm}^{K'} (r),
\end{align*}
\]

(6)

where \( \varphi_{k, \pm}^{K} (r) \) are the solutions of the 2D Dirac equations

\[
\begin{align*}
v_F (i \tau \nabla) \varphi_{k, \pm}^{K} (r) &= E \varphi_{k, \pm}^{K} (r), \\
v_F (i \tau \nabla) \varphi_{k, \pm}^{K'} (r) &= E \varphi_{k, \pm}^{K'} (r),
\end{align*}
\]

(7)

(8)

where two components \( \tau_1 \) and \( \tau_2 \) of vector matrix \( \tau \) are two matrices

\[
\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\]

Equations (7) and (8) both have two solutions corresponding to two eigenvalues

\[
E_{\pm}(k) = \pm v_F k, \quad k = |k| = \sqrt{k_x^2 + k_y^2},
\]

(9)

and two eigenfunctions

\[
\begin{align*}
\varphi_{k, \pm}^{K} (r) &= e^{ikr} u_{\pm}^K (k), \\
u_{\pm}^K &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta(k)/2} \eta, \\ \pm e^{i\theta(k)/2} \eta', \end{pmatrix}, \\
\varphi_{k, \pm}^{K'} (r) &= e^{iK' r} u_{\pm}^{K'} (k), \\
u_{\pm}^{K'} &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta(k)/2} \eta, \\ \pm e^{-i\theta(k)/2} \eta', \end{pmatrix},
\end{align*}
\]

(10)

(11)

(12)

where

\[
\theta(k) = \arctan \left( \frac{k_y}{k_x} \right).
\]

(13)

\( \eta \) and \( \eta' \) are two arbitrary phase factors \( |\eta| = |\eta'| = 1 \). The quantum field of free Dirac fermions in the hexagonal graphene lattice has the expression

\[
\Psi(r, t) = e^{iKr} \bar{\psi}^{K} (r, t) + e^{iK'r} \bar{\psi}^{K'} (r, t)
\]

(14)

with the following expansion of \( \psi^{K, K'} (r, t) \):

\[
\psi^{K, K'} (r, t) = \frac{1}{\sqrt{N}} \sum_{k} \sum_{\pm} e^{i(E_{\pm}(k) - E_k)t} u_{\pm}^{K} (k) a^{K, K'} (k),
\]

(15)

where \( a^{K, K'} \) is the destruction operator of the Dirac fermion with the wave function being the plane wave whose wave vector \( k \) satisfies the periodic boundary condition for a very large square graphene lattice containing \( N \) elementary cells.

Note that the role of the electron spin was omitted and electrons are considered as the spinless fermions. Two-component wave functions (11) and (12) are not the usual spinors (Pauli spinors) in the three-dimensional (3D) physical space with the Cartesian coordinate system. Being the spinors with respect to the rotations in some fictive 3D Euclidean space, they are similar to the isospinor called nucleon \( N \) with proton \( p \) and neutron \( n \) as its two components

\[
N = \begin{pmatrix} P \\ n \end{pmatrix}
\]

in nuclear physics [4] and elementary particle physics [5–8]. In order to distinguish the spinors (11) and (12) from the usual Pauli spinors let us call them Dirac spinors, quasi-spinors or pseudo-spinors. It is worth investigating the symmetry with respect to the rotations in the above-mentioned fictive 3D Euclidean space.

The Hamiltonian of the quantum field of free Dirac fermions is

\[
H_0 = v_F \int d^3r \{ \bar{\psi}^{K} (r, t) (-i \tau \nabla) \psi^{K} (r, t) + \bar{\psi}^{K'} (r, t) (-i \tau \nabla) \psi^{K'} (r, t) \}.
\]

(16)

From the expansion formula (15) and the canonical anticommutation relations between destruction and creation operators \( a^{K, K'} \) and \( (a^{K, K'})^\dagger \) it follows that Dirac equations

\[
\begin{align*}
\frac{i}{\hbar} \frac{\partial \bar{\psi}^{K} (r, t)}{\partial t} &= v_F (-i \tau \nabla) \psi^{K} (r, t), \\
\frac{i}{\hbar} \frac{\partial \bar{\psi}^{K'} (r, t)}{\partial t} &= v_F (-i \tau \nabla) \psi^{K'} (r, t),
\end{align*}
\]

(17)

(18)

can be rewritten in the form of the Heisenberg quantum equation of motion

\[
\frac{i}{\hbar} \frac{\partial \bar{\psi}^{K, K'} (r, t)}{\partial t} = [-H_0, \bar{\psi}^{K, K'} (r, t)].
\]

(19)

Consider now the free Dirac fermion gas at vanishing absolute temperature \( T = 0 \). In this case it is convenient to work in the electron hole formalism. Denote \( E_F \) the Fermi level and \( |G\rangle \) the state vector of the ground state of the Dirac fermion gas in which all levels with energies larger than \( E_F \) are empty and all those with energies less than \( E_F \) are fully occupied. The ground state \( |G\rangle \) is expressed in terms of the Dirac fermion creation operators and the state vector \( |0\rangle \) of the vacuum

\[
|G\rangle = \sum_{E_k, E_{k'}} \langle a_{k, K'}^{\dagger} a_{k, K}^{\dagger} \rangle |0\rangle.
\]

(20)

With respect to the ground state \( |G\rangle \) the destruction/creation operator \( a_{k, K'}^{\dagger} / (a_{k, K}^{K'})^{\dagger} \) of the Dirac fermion with energy less than \( E_F \) becomes the creation/destruction operator of the Dirac hole in the corresponding state with the momentum and energy which will be specified in each separate case. Since the reasonings for the states with wave vectors \( k \) near \( K \) and \( K' \) are the same, until the end of this section we shall omit the indices \( K \) and \( K' \) in the notations of field operators, destruction and creation operators as well as of the wave functions for simplifying the formulæ.
These are three different cases depending on the position of the Fermi level $E_F$ (figure 4).

Case 1: $E_F = 0$ (figure 4(a))

All levels with energies $E_i(k)$ are empty and all those with energies $E_x(k)$ are occupied. We set

$$ E_x(k) = E_x(k), \quad u_x(k) = u(k), \quad a_{k+} = a_k, $$

$$ E_x(k) = -E_x(k), \quad u_x(k) = v(-k), \quad a_{k-} = b_k^+ $$

and obtain

$$ \Psi(r, t) = \frac{1}{\sqrt{N_k}} \sum_k \{ e^{i[kr - E_i(k)t]} u(k)a_k + e^{-i[kr - E_i(k)t]} v(k)b_k^+ \}. \quad (21) $$

Case 2: $E_F > 0$ (figure 4(b))

All states with energies $E_x(k) > E_F$ are empty and for them we set

$$ E_x(k) = E_F + E_x(k), \quad a_{k+} = a_k, \quad u_x(k) = u(k). $$

All states with energies $E_x(k) < E_F$ are occupied and for them we set

$$ E_x(k) = E_F - E_x^{(1)}(k), \quad a_{k+} = b_k^{(1)+}, \quad u_x(k) = v^{(1)}(-k). $$

All states with energies $E_x(k)$ are occupied and for them we set

$$ E_x(k) = E_F - E_x^{(2)}(k), \quad a_{k+} = b_k^{(2)+}, \quad u_x(k) = v^{(2)}(-k). $$

In this case we obtain

$$ e^{iE_Ft} \Psi(r, t) = \frac{1}{\sqrt{N_k}} \sum_k \{ e^{i[kr - E_x^{(2)}(k)t]} u^{(2)}(k)a_k^{(2)} + \theta [E_x(k) - E_F] e^{i[kr - E_x^{(1)}(k)t]} u^{(1)}(k)b_k^{(1)+} + e^{-i[kr - E_x^{(2)}(k)t]} v^{(2)}(k)b_k^{(2)+} \}. \quad (22) $$

Case 3: $E_F < 0$ (figure 4(c))

All states with energies $E_x(k)$ are empty and for them we set

$$ E_x(k) = E_F + E_x^{(2)}(k), \quad a_{k+} = a_k^{(2)}, \quad u_x(k) = u^{(2)}(k). $$

All states with energies $E_x(k) > E_F$ are also empty and for them we set

$$ E_x(k) = E_F + E_x^{(1)}(k), \quad a_{k+} = a_k^{(1)}, \quad u_x(k) = u^{(1)}(k). $$

All states with energies $E_x(k) < E_F$ are occupied and for them we set

$$ E_x(k) = E_F - E_x(k), \quad a_{k+} = b_k^+, \quad u_x(k) = v(-k). $$

In this case we obtain

$$ e^{iE_Ft} \Psi(r, t) = \frac{1}{\sqrt{N_k}} \sum_k \{ e^{i[kr - E_x^{(2)}(k)t]} u^{(2)}(k)a_k^{(2)} + \theta [E_x(k) - E_F] e^{i[kr - E_x^{(1)}(k)t]} u^{(1)}(k)b_k^{(1)+} + e^{-i[kr - E_x(k)t]} v(k)b_k^{(2)+} \}. \quad (23) $$

Instead of the quantum fields $\Psi(r, t)$ we use the new ones

$$ \tilde{\Psi}(r, t) = e^{iE_Ft} \Psi(r, t). \quad (24) $$

From formulae (20)–(23) it follows that the new fields (24) satisfy the new Heisenberg quantum equation of motion

$$ i \frac{\partial \tilde{\Psi}(r, t)}{\partial t} = -[H'_0, \tilde{\Psi}(r, t)] \quad (25) $$

where

$$ H'_0 = \sum_k \{ E_x(k) a_k^+ a_k + E_x(k) b_k^+ b_k \}. \quad (26) $$
in the case 1 with $E_F = 0$,
\[
H_0' = \sum_k \{ \theta [E_x(k) - E_F] E_z(k) a_k^+ a_k \\
+ \theta [E_F - E_x(k)] E_z^{(1)}(k) b_{k_1}^{(1)*} b_k^{(1)} \}
+ E_z^{(2)}(k) b_k^{(2)*} b_k^{(2)}
\]  
(27)

in the case 2 with $E_F > 0$, and
\[
H_0' = \sum_k \{ E_x^{(2)}(k) a_k^{(2)+} a_k^{(2)} \\
+ \theta [E_x(k) - E_F] E_z^{(1)}(k) a_{k_1}^{(1)+} a_k^{(1)} \\
+ \theta [E_F - E_x(k)] E_z(k) b_k^{(1)*} b_k^{(1)} \}
\]  
(28)
in the case 3 with $E_F < 0$.

4. Green functions of Dirac fermions in the free Dirac fermion gas at $T = 0$

Green functions of Dirac fermions in the free Dirac fermion gas at $T = 0$ are defined by the following formulae
\[
\Delta_{\alpha \beta}^K(r - r', t + t') = -i \langle G | T [\hat{\Psi}_\alpha^K(r, t) \hat{\Psi}_\beta^K(r', t')^+] | G \rangle,
\]  
(29)

and
\[
\Delta_{\alpha \beta}^{K'}(r - r', t + t') = -i \langle G | T [\hat{\Psi}_\alpha^{K'}(r, t) \hat{\Psi}_\beta^{K'}(r', t')^+] | G \rangle.
\]  
(30)

Using the Heisenberg quantum equation of motion (25) as well as the equal-time canonical anticommutation relations between the quantum field operators $\Psi_\alpha^K(r, t)$ and $\Psi_\beta^{K'}(r', t')$, we derive the following inhomogeneous differential equations for these Green functions
\[
i \frac{\partial}{\partial t} \Delta_{\alpha \beta}^K(r - r', t + t') - v_F (-i \tau \nabla)_{\alpha \beta} \Delta_{\alpha \beta}^K(r - r', t + t') = \delta_{\alpha \beta} \delta(t + t') \delta(r - r')
\]  
(31)

and
\[
i \frac{\partial}{\partial t} \Delta_{\alpha \beta}^{K'}(r - r', t + t') - v_F (-i \tau \nabla)_{\alpha \beta} \Delta_{\alpha \beta}^{K'}(r - r', t + t') = \delta_{\alpha \beta} \delta(t + t') \delta(r - r').
\]  
(32)

Explicit expressions of Green functions (29) and (30) depend on the position of the Fermi level $E_F$. For simplifying formulae let us omit again the indices $K$ and $K'$ until the end of this section. Depending on the value of $E_F$ there exist three different cases. In the first case with $E_F = 0$ the operator $\hat{\Psi}_\alpha(r, t)$ is expressed in terms of the components $u_{\alpha}^{(1)}(k)$ and $v_{\alpha}(k)$ by means of formula (21), in the second case with $E_F > 0$ it is expressed in terms of the components $u_{\alpha}^{(2)}(k)$, $v_{\alpha}^{(1)}(k)$ and $v_{\alpha}(k)$ by means of formula (22), while in the third case with $E_F < 0$ it is expressed in terms of the components $u_{\alpha}^{(2)}(k)$, $u_{\alpha}^{(1)}(k)$ and $v_{\alpha}(k)$ by means of formula (23).

Introduce the Fourier transformation of Green functions (29) and (30)
\[
\Delta_{\alpha \beta}(r, t) = \frac{1}{N_c} \sum_{k} \frac{1}{2\pi} \int d\omega \tilde{\Delta}_{\alpha \beta}(k, \omega).
\]  
(33)

It is straightforward to derive the expressions of $\tilde{\Delta}_{\alpha \beta}(k, \omega)$ in all three cases. In the first case with $E_F = 0$ we obtain
\[
\tilde{\Delta}_{\alpha \beta}(k, \omega) = \frac{u_{\alpha}^{(1)}(k) u_{\beta}^{(1)}(k)^*}{\omega - E_x(k) + i0} + \frac{v_{\alpha}(k) v_{\beta}(k)^*}{\omega + E_x(k) - i0}
\]  
(34)

In the second case with $E_F > 0$ we have
\[
\tilde{\Delta}_{\alpha \beta}(k, \omega) = \frac{u_{\alpha}^{(2)}(k) u_{\beta}^{(2)}(k)^*}{\omega - E_x(k) + i0} + \frac{v_{\alpha}^{(1)}(k) v_{\beta}^{(1)}(k)^*}{\omega + E_x(k) - i0}
\]  
(35)

while in the third case with $E_F < 0$
\[
\tilde{\Delta}_{\alpha \beta}(k, \omega) = \frac{u_{\alpha}^{(2)}(k) u_{\beta}^{(2)}(k)^*}{\omega - E_x(k) + i0} + \frac{v_{\alpha}^{(1)}(k) v_{\beta}^{(1)}(k)^*}{\omega + E_x(k) - i0} + \frac{v_{\alpha}(k) v_{\beta}(k)^*}{\omega + E_x(k) - i0}.
\]  
(36)

5. Matsubara temperature Green functions of Dirac fermions in the free Dirac fermion gas

Let us study the free Dirac fermion gas in the equilibrium state at a non-vanishing temperature $T_{\text{temp}}$. Instead of formulae (29) and (30) now we have the following definition of Green functions of Dirac fermions:
\[
\Delta_{\alpha \beta}^K(r - r', t + t') = -i \frac{\text{Tr} [e^{-\beta H_F} T [\hat{\Psi}_\alpha^K(r, t) \hat{\Psi}_\beta^K(r', t')^+]]}{\text{Tr} [e^{-\beta H_F}]}.
\]  
(37)

and
\[
\Delta_{\alpha \beta}^{K'}(r - r', t + t') = -i \frac{\text{Tr} [e^{-\beta H_F} T [\hat{\Psi}_\alpha^{K'}(r, t) \hat{\Psi}_\beta^{K'}(r', t')^+]]}{\text{Tr} [e^{-\beta H_F}]}.
\]  
(38)

where
\[
\beta_T = \frac{1}{k_B T_{\text{temp}}},
\]  
(39)
and $\delta_B$ is the Boltzmann constant. Note that formula (38) can be obtained from formula (37) by means of the replacement $K \rightarrow K'$. Field operators $\psi^K_{\alpha}(r, t)$ and $\psi^{K'}_{\alpha}(r, t)^+$ are obtained from the corresponding operators at $t = 0$ by means of the action of the time translation operator $e^{iH_0t}$, namely

$$\psi^{K,K'}_{\alpha}(r, t) = e^{iH_0t}\psi^{K,K'}_{\alpha}(r, 0)e^{-iH_0t}$$  (40)

and

$$\psi^{K,K'}_{\alpha}(r, t)^+ = e^{iH_0t}\psi^{K,K'}_{\alpha}(r, 0)^+e^{-iH_0t}.$$  (41)

Following Matsuraba [9] and Abrikosov et al [10] we consider $t$ as an imaginary variable and set $t = -i\tau$, where $\tau$ is a real variable. Instead of $t$-dependent field operators (40) and (41) we introduce corresponding $\tau$-dependent ones

$$\psi^K_{\alpha}(r, \tau)_M = e^{iH_0\tau}\psi^K_{\alpha}(r, 0)^+e^{-iH_0\tau}$$  (42)

and

$$\hat{\psi}^{K,K'}_{\alpha}(r, \tau)_M = e^{iH_0\tau}\psi^{K,K'}_{\alpha}(r, 0)^+e^{-iH_0\tau}.$$  (43)

They obey the Heisenberg equation of motion

$$\frac{\partial\psi^K_{\alpha}(r, \tau)_M}{\partial \tau} = [H_0, \psi^K_{\alpha}(r, \tau)_M],$$

$$\frac{\partial\psi^{K,K'}_{\alpha}(r, \tau)_M}{\partial \tau} = [H_0, \psi^{K,K'}_{\alpha}(r, \tau)_M].$$  (44)

From this common form it is easy to derive concrete forms of the differential equations for different fields $\psi^K_{\alpha}(r, \tau)_M, \hat{\psi}^{K,K'}_{\alpha}(r, \tau)_M$ and $\hat{\psi}^K_{\alpha}(r, \tau)_M$. We obtain

$$\frac{\partial\psi^K_{\alpha}(r, \tau)_M}{\partial \tau} = -[v_F(-i\tau\nabla) - E_F\delta_{\alpha\gamma}]\psi^K_{\gamma}(r, \tau)_M,$$  (45)

$$\frac{\partial\psi^{K,K'}_{\alpha}(r, \tau)_M}{\partial \tau} = -[v_F(-i\tau\nabla) - E_F\delta_{\alpha\gamma}]\psi^{K,K'}_{\gamma}(r, \tau)_M,$$  (46)

$$\frac{\partial\psi^{K,K'}_{\alpha}(r, \tau)_M}{\partial \tau} = -[v_F(-i\tau\nabla) - E_F\delta_{\alpha\gamma}]\psi^{K,K'}_{\gamma}(r, \tau)_M.$$  (47)

The Matsuraba temperature Green functions of Dirac fermions are defined by the following formula

$$\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M = \langle T_T[\psi^K_{\alpha}(r, \tau)_M\hat{\psi}^{K}_{\beta}(r', \tau')_M]\rangle$$

$$= Tr\{e^{-\beta H_0}\gamma_T[\psi^K_{\alpha}(r, \tau)_M\hat{\psi}^{K}_{\beta}(r', \tau')_M]\}$$

(48)

and a similar one obtained from this formula after the replacement $K \rightarrow K'$, where $T_T$ denotes the operation of ordering the product of operators along the decreasing direction of the real variable $\tau$ (the ‘chronological product’ with respect to the real ‘time’ variable), for example

$$T_T[\hat{\psi}^K_{\alpha}(r, \tau)_M\hat{\psi}^{K'}_{\beta}(r', \tau')_M] = \theta(\tau - \tau')\hat{\psi}^{K'}_{\alpha}(r', \tau')_M - \theta(\tau' - \tau)\hat{\psi}^K_{\beta}(r, \tau)_M.$$ (49)

From homogeneous differential equations (45) and (46) for the field operators $\psi^K_{\alpha}(r, \tau)_M$ and $\psi^{K,K'}_{\alpha}(r, \tau)_M$ it follows that corresponding inhomogeneous differential equations for the Green functions $\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M$ and $\Delta^{K'}_{\alpha\beta}(r - r', \tau - \tau')_M$ are:

$$\frac{\partial\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M}{\partial \tau} + [v_F(-i\tau\nabla) - E_F\delta_{\alpha\gamma}]\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M = \delta_{\alpha\beta}\delta(r - r')\delta(\tau - \tau'),$$

$$\frac{\partial\Delta^{K'}_{\alpha\beta}(r - r', \tau - \tau')_M}{\partial \tau} + [v_F(-i\tau\nabla) - E_F\delta_{\alpha\gamma}]\Delta^{K'}_{\alpha\beta}(r - r', \tau - \tau')_M = \delta_{\alpha\beta}\delta(r - r')\delta(\tau - \tau').$$

(50)

(51)

Now let us derive the explicit expressions of the Green functions $\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M$ and $\Delta^{K'}_{\alpha\beta}(r - r', \tau - \tau')_M$. Since the reasonings and calculations do not depend on the presence of the indices $K$ and $K'$, we shall omit both these indices until the end of this section. There are three different cases depending on the position of the Fermi level $E_F$. By means of standard calculations we obtain following result in the case $1$ with $E_F = 0$:

$$\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M = \frac{1}{N_e}\sum_{k}e^{ik(r - r')}[\theta(\tau)\hat{\psi}^K_{\alpha}(r, \tau)_M\hat{\psi}^{K}_{\beta}(r', \tau')_M + \theta(\tau)\hat{\psi}^{K}_{\alpha}(r', \tau')_M\hat{\psi}^K_{\beta}(r, \tau)_M].$$

(52)

It is straightforward to extend this result to other cases with non-vanishing $E_F$. In the case 2 with $E_F > 0$ we have

$$\Delta^{K}_{\alpha\beta}(r - r', \tau - \tau')_M = \frac{1}{N_e}\sum_{k}e^{ik(r - r')}\left\{\theta(\tau)\hat{\psi}^K_{\alpha}(r, \tau)_M\hat{\psi}^{K}_{\beta}(r', \tau')_M + \theta(\tau)\hat{\psi}^{K}_{\alpha}(r', \tau')_M\hat{\psi}^K_{\beta}(r, \tau)_M\right\}.$$ (53)
Similarly, in the case 3 with $E_F < 0$ the result is

\[
\Delta_{\alpha\beta}(r - r', \tau) = \frac{1}{N_c} \sum_k e^{ik(r-r')} \left[ \theta(\tau)e^{-\frac{i}{\beta}E_{\nu}^{(k)}} - \theta(-\tau)e^{\frac{i}{\beta}E_{\nu}^{(k)}} \right] \times u_{\alpha}^{(1)}(k)u_{\beta}^{(2)}(k)^* + \theta[E_F - E_{\nu}^{(k)}] \frac{v_{\alpha}(-k)v_{\beta}(-k)^*}{i\varepsilon_n - E_{\nu}^{(1)}(k)}
\]

6. Keldysh non-equilibrium Green functions of Dirac fermions in the free Dirac fermion gas

With the purpose of extending the Green function theory for application to the study of non-equilibrium physical processes and phenomena in quantum systems, Keldysh [11] has developed the theory of Green functions of quantum fields depending on the complex time $z = t + i\tau$, where $t$ and $\tau$ are the real and imaginary components of $z$. These new Green functions were briefly called non-equilibrium Green functions. In the definition of Green functions of complex time-dependent field operators it was proposed to define the ‘extended chronological ordering’ $T_C$ of two complex variables $z$ and $\bar{z}$ as the ordering along some contour $C$ passing through these two points in the complex plane. Thus the Keldysh non-equilibrium Green functions of Dirac fermions in the free Dirac fermion gas are defined as follows [12–14]:

\[
\Delta^{K,K}_{\alpha\beta}(r, r' ; z - z') = -i\langle \bar{T}_C \{ \Psi_{\alpha}^K(r, z)\Psi_{\beta}^K(r', z') \rangle \}
\]

\[
= -\frac{Tr \{ e^{-\beta H_0}T_C [ \Psi_{\alpha}^K(r, z)\Psi_{\beta}^K(r', z') ] \}}{Tr \{ e^{-\beta H_0} \}}
\]

where complex time-dependent field operators $\Psi_{\alpha}^{K,K'}(r, z)c$ and $\Psi_{\alpha}^{K,K'}(r, z)c$ have the form

\[
\Psi_{\alpha}^{K,K'}(r, z)c = e^{iH_0t}\Psi_{\alpha}^{K,K'}(r, 0)c e^{-iH_0}\]

They satisfy the Heisenberg quantum equation of motion

\[
\frac{i}{\hbar} \frac{\partial \Psi_{\alpha}^{K,K'}(r, z)c}{\partial z} = \left[ H_0, \Psi_{\alpha}^{K,K'}(r, z)c \right],
\]

From this common form it is easy to derive concrete forms of the differential equations for different fields $\Psi_{\alpha}^{K}(r, z)c$, $\Psi_{\alpha}^{K,K'}(r, z)c$ and $\Psi_{\alpha}^{K,K'}(r, z)c$. We obtain

\[
\frac{i}{\hbar} \frac{\partial \Psi_{\alpha}^{K}(r, z)c}{\partial z} = \left[ V_F ( -i\tau \nabla )_{\alpha\gamma}, -E_F \delta_{\alpha\gamma} \right] \Psi_{\gamma}^K( r, z)c
\]

\[
\frac{i}{\hbar} \frac{\partial \Psi_{\alpha}^{K,K'}(r, z)c}{\partial z} = \left[ V_F ( -i\tau \nabla )_{\alpha\gamma}, -E_F \delta_{\alpha\gamma} \right] \Psi_{\gamma}^{K,K'} ( r, z)c
\]

\[
\frac{i}{\hbar} \frac{\partial \Psi_{\alpha}^{K,K'}(r, z)c}{\partial z} = \left[ V_F ( -i\tau \nabla )_{\alpha\gamma}, -E_F \delta_{\alpha\gamma} \right] \Psi_{\gamma}^{K,K'} ( r, z)c
\]
For the application of Keldysh non-equilibrium Green functions to the study of physical quantum processes and phenomena it is convenient to choose the contour $C$ to consist of four parts
\[ C = C_1 \cup C_2 \cup C_3 \cup C_4, \]
where $C_1$ being the part of the straight line over and infinitely close to the real axis from some point $t_0 + i0$ to infinity $+\infty + i0$, $C_2$ being the part of the straight line under and infinitely close to the real axis from infinity $+\infty - i0$ to the point $t_0 - i0$, $C_3$ and $C_4$ being the segments $[t_0 - i0, t_0 - i0+i\gamma]$ and $[+\infty + i0, +\infty - i0]$ (Figure 5). The contributions of the segment $[+\infty + i0, +\infty - i0]$ to all physical observables are negligibly small, because of its vanishing length. Therefore this segment plays no role, and the contour $C$ can be considered to consist of only three parts $C_1$, $C_2$ and $C_3$. When both variables $z$ and $z'$ belong to the line $C_1$, the functions (60) and (61) are the quantum statistical average of the usual chronological products of the quantum field operators $\Psi^K (r, t)$ and $\bar{\Psi}^K (r, t)$ in the Heisenberg picture over a statistical ensemble. When both variables $z$ and $z'$ belong to the line $C_3$, the functions (60) and (61) are reduced to the Matsubara temperature Green function.

In the study of stationary physical processes one often used the complex time-dependent Green functions of the form (60) and (61) in the limit $t_0 \to -\infty$. Because the interaction must satisfy the 'adiabatic hypothesis' and vanish at this limit, the segment $C_3$ also gives no contribution. In this case the contour $C$ can be considered to consist of only two lines $C_1$ and $C_2$, and each of the complex time-dependent Green functions (60) and (61) effectively becomes a set of four functions of real variables $t$ and $t'$. For example, Green function (60) is equivalent to the set four functions
\[ \Delta^K_{\alpha\beta}(r - r', t - t'), \]
\[ \Delta^K_{\alpha\beta}(r - r', t - t')_{11} = -i \{ \theta (t' - t) \langle \Psi^K_{\alpha}(r, t + i0) \times \bar{\Psi}^K_{\beta}(r', t' + i0) \rangle - \theta (t' - t) \langle \bar{\Psi}^K_{\beta}(r', t' + i0) \Psi^K_{\alpha}(r, t + i0) \rangle \}, \]
\[ \Delta^K_{\alpha\beta}(r - r', t - t')_{12} = i \{ \langle \bar{\Psi}^K_{\beta}(r', t' - i0) \Psi^K_{\alpha}(r, t + i0) \rangle - \langle \Psi^K_{\alpha}(r, t - i0) \bar{\Psi}^K_{\beta}(r', t' + i0) \rangle \}, \]
\[ \Delta^K_{\alpha\beta}(r - r', t - t')_{21} = -i \{ \langle \bar{\Psi}^K_{\beta}(r', t' - i0) \Psi^K_{\alpha}(r, t + i0) \rangle - \langle \Psi^K_{\alpha}(r, t - i0) \bar{\Psi}^K_{\beta}(r', t' + i0) \rangle \}, \]
\[ \Delta^K_{\alpha\beta}(r - r', t - t')_{22} = -i \{ \theta (t' - t) \langle \bar{\Psi}^K_{\beta}(r', t' - i0) \Psi^K_{\alpha}(r, t - i0) \rangle - \langle \theta (t' - t) \Psi^K_{\alpha}(r, t - i0) \bar{\Psi}^K_{\beta}(r', t' - i0) \rangle \}. \]

They satisfy following differential equations:
\[ i \frac{\partial \Delta^K_{\alpha\beta}(r - r', t - t')_{11}}{\partial t} = -[\mathbf{V} (-i\mathbf{\tau})]_{\alpha\beta} - E_\beta \delta_{\alpha\gamma}, \]
\[ i \frac{\partial \Delta^K_{\alpha\beta}(r - r', t - t')_{12}}{\partial t} = -[\mathbf{V} (-i\mathbf{\tau})]_{\alpha\beta} - E_\beta \delta_{\alpha\gamma}, \]
\[ i \frac{\partial \Delta^K_{\alpha\beta}(r - r', t - t')_{21}}{\partial t} = -[\mathbf{V} (-i\mathbf{\tau})]_{\alpha\beta} - E_\beta \delta_{\alpha\gamma}, \]
\[ i \frac{\partial \Delta^K_{\alpha\beta}(r - r', t - t')_{22}}{\partial t} = -[\mathbf{V} (-i\mathbf{\tau})]_{\alpha\beta} - E_\beta \delta_{\alpha\gamma}. \]

For the set of four functions $\Delta^K_{\alpha\beta}(r - r', t - t')_{ij}$, with $i, j = 1, 2$, we have the definition obtained from formulae (68)–(71) and four differential equations obtained from equations (72)–(75) after the replacement $K \to K'$ and $\mathbf{\tau} \to \mathbf{\tau}'$. Since in the sequel all reasonings and calculations do not depend on the indices $K$ and $K'$, we shall omit them for simplifying the expressions.

It is straightforward to derive the explicit expressions of four Green functions $\Delta^K_{\alpha\beta}(r - r', t - t')_{ij}$ and obtain following result:
In the case 1 with $E_\beta = 0$
\[ \Delta^K_{\alpha\beta}(r - r', t - t')_{11} = \frac{i}{N} \sum_{k \neq 0} \mathbf{e}^{iE_k(t-t') \mathbf{v}_k} u_{\alpha}(k) u_{\beta}(k)^* \times [\theta (t' - t) - n_{\mathbf{v}}(k)] + \mathbf{e}^{iE_k(t-t') \mathbf{v}_k} u_{\alpha}(-k) u_{\beta}(-k)^* \times [n_{\mathbf{v}}(-k) - \theta (t' - t)], \]
where

\[ n_e(k) = \frac{e^{-\beta E_k}}{1 + e^{-\beta E_k}} \]

and

\[ n_h(-k) = \frac{e^{-\beta E_k}}{1 + e^{-\beta E_k}}. \]

In the case 2 with \( E_F > 0 \) we have

\[
\Delta_{\alpha\beta}(\mathbf{r}' - \mathbf{r}, t - t')_{11} = -\frac{i}{N_e} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}' - i\mathbf{k} \cdot \mathbf{r}} \left\{ \theta(E_F - E_F) e^{-iE_k(t-t')} \right. \\
\times u_{\alpha}(k) u_{\beta}(k)^* [\theta(t-t') - n_e(k)] \\
+ \theta(E_F - E_F) e^{iE_k(t-t')} v_{\alpha}^{(1)}(-k) v_{\beta}^{(1)}(-k)^* \\
\times [n_h^{(1)}(-k) - \theta(t-t')] \\
+ e^{iE_2(t-t')} v_{\alpha}^{(2)}(-k) v_{\beta}^{(2)}(-k)^* \\
\times [n_h^{(2)}(-k) - \theta(t-t')],
\]

(78)

\[
\Delta_{\alpha\beta}(\mathbf{r}' - \mathbf{r}, t - t')_{22} = -\frac{i}{N_e} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}' - i\mathbf{k} \cdot \mathbf{r}} \left\{ \theta(E_F - E_F) e^{-iE_k(t-t')} \\
\times u_{\alpha}(k) u_{\beta}(k)^* [\theta(t-t') - n_e(k)] \\
+ \theta(E_F - E_F) e^{iE_k(t-t')} v_{\alpha}^{(1)}(-k) v_{\beta}^{(1)}(-k)^* \\
\times [n_h^{(1)}(-k) - \theta(t-t')] \\
+ e^{iE_2(t-t')} v_{\alpha}^{(2)}(-k) v_{\beta}^{(2)}(-k)^* \\
\times [n_h^{(2)}(-k) - \theta(t-t')],
\]

(80)

In the case 3 with \( E_F < 0 \) the result is

\[
\Delta_{\alpha\beta}(\mathbf{r}' - \mathbf{r}, t - t')_{11} = -\frac{i}{N_e} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}' - i\mathbf{k} \cdot \mathbf{r}} \left\{ \theta(E_F - E_F) e^{-iE_k(t-t')} \\
\times u_{\alpha}(k) u_{\beta}(k)^* [\theta(t-t') - n_e(k)] \\
+ \theta(E_F - E_F) e^{iE_k(t-t')} v_{\alpha}^{(1)}(-k) v_{\beta}^{(1)}(-k)^* \\
\times [n_h^{(1)}(-k) - \theta(t-t')] \\
+ e^{iE_2(t-t')} v_{\alpha}^{(2)}(-k) v_{\beta}^{(2)}(-k)^* \\
\times [n_h^{(2)}(-k) - \theta(t-t')],
\]

(84)

\[
\Delta_{\alpha\beta}(\mathbf{r}' - \mathbf{r}, t - t')_{22} = -\frac{i}{N_e} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}' - i\mathbf{k} \cdot \mathbf{r}} \left\{ \theta(E_F - E_F) e^{-iE_k(t-t')} \\
\times u_{\alpha}(k) u_{\beta}(k)^* [\theta(t-t') - n_e(k)] \\
+ \theta(E_F - E_F) e^{iE_k(t-t')} v_{\alpha}^{(1)}(-k) v_{\beta}^{(1)}(-k)^* \\
\times [n_h^{(1)}(-k) - \theta(t-t')] \\
+ e^{iE_2(t-t')} v_{\alpha}^{(2)}(-k) v_{\beta}^{(2)}(-k)^* \\
\times [n_h^{(2)}(-k) - \theta(t-t')],
\]

(85)

\[
\Delta_{\alpha\beta}(\mathbf{r}' - \mathbf{r}, t - t')_{12} = -\frac{i}{N_e} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}' - i\mathbf{k} \cdot \mathbf{r}} \left\{ \theta(E_F - E_F) e^{-iE_k(t-t')} \\
\times u_{\alpha}(k) u_{\beta}(k)^* [\theta(t-t') - n_e(k)] \\
+ \theta(E_F - E_F) e^{iE_k(t-t')} v_{\alpha}^{(1)}(-k) v_{\beta}^{(1)}(-k)^* \\
\times [1 - n_h^{(1)}(-k)] \\
+ e^{iE_2(t-t')} v_{\alpha}^{(2)}(-k) v_{\beta}^{(2)}(-k)^* \\
\times [1 - n_h^{(2)}(-k)]},
\]

(86)
\[ \Delta_{\alpha\beta}(r - r', t - t')_{21} = \frac{1}{N_{k}} \sum_{k} e^{i(kr - r'k)} \{ e^{-iE_{k}(t - t')} u_{\alpha}^{(1)}(k)u_{\beta}^{(2)}(k) \}
\times [1 - n_{e}^{(2)}(k)] + \theta(E_{+} - E_{F})e^{-iE_{k}(t - t')} u_{\alpha}^{(1)}(k)u_{\beta}^{(1)}(k) \]
\times [1 - n_{e}^{(1)}(k)] + \theta(E_{-} - E_{F})e^{iE_{k}(t - t')} n_{\alpha}(k)v_{\beta}^{(1)}(-k) \] (87)

The Keldysh Green functions (76)–(87) have the Fourier expansion of the form
\[ \Delta_{\alpha\beta}(k, \omega)_{ij} = \frac{1}{N_{k}} \sum_{k} \frac{1}{2\pi} \int e^{i(kr - r')} \Delta_{\alpha\beta}(r', t') \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (88)

It is straightforward to derive the expressions of \( \Delta_{\alpha\beta}(k, \omega)_{ij} \) in all three cases. In the first case with \( E_{F} = 0 \) we obtain
\[ \Delta_{\alpha\beta}(k, \omega)_{11} = u_{\alpha}(k)u_{\beta}(k)^{*} \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (89)

\[ \Delta_{\alpha\beta}(k, \omega)_{22} = u_{\alpha}(k)u_{\beta}(k)^{*} \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (90)

In the second case with \( E_{F} > 0 \) we have
\[ \Delta_{\alpha\beta}(k, \omega)_{11} = \theta(E_{+} - E_{F})u_{\alpha}(k)u_{\beta}(k)^{*} \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (91)

\[ \Delta_{\alpha\beta}(k, \omega)_{22} = u_{\alpha}(k)u_{\beta}(k)^{*} \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (92)

while in the third case with \( E_{F} < 0 \)
\[ \Delta_{\alpha\beta}(k, \omega)_{11} = - \frac{2\pi}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (93)

\[ \Delta_{\alpha\beta}(k, \omega)_{22} = \theta(E_{+} - E_{F})u_{\alpha}(k)u_{\beta}(k)^{*} \]
\times \frac{1}{\omega - E_{k} + i0} - 2\pi\delta(\omega - E_{k})n_{e}(k) \] (94)
In this paper we have presented the theory of the three most commonly used types of Green functions of Dirac fermions in a free Dirac fermion gas of single-layer graphene: real-time Green functions at vanishing absolute temperature \( T = 0 \), imaginary-time Matsubara temperature Green functions and complex-time Keldysh non-equilibrium Green functions. In all three cases the expressions of corresponding Green functions were explicitly established. In the theoretical study of all quantum dynamical processes taking place in single-layer graphene it is necessary to use the expressions of corresponding Green functions established in the present work. However, for the comprehensive study of quantum dynamical processes with the participation of Dirac fermions in graphene it remains to study the interaction of Dirac fermions with photons as well as with phonons. We shall continue to study these topics. In particular, in the subsequent work we shall elaborate the quantum field theory of the interaction between the quantized electromagnetic field and the Dirac fermions in graphene, the second step in the establishment of the basics of GQED.

Acknowledgment

The authors would like to express their deep gratitude to the Vietnam Academy of Science and Technology for the support.

References

[1] Geim A K and Novoselov K S 2007 Nature Mater. 6 183
[2] Novoselov K S, Geim A K, Morozov S V, Jiang D, Katsnelson M I, Grigorieva I V, Dubonos S V and Firsov A A 2005 Nature 438 197
[3] Castro Neto A H, Guinea F, Peres NMR, Novoselov K S and Geim A K 2009 Rev. Mod. Phys. 81 109
[4] Blatt J M and Weisskopf V F 1979 Theoretical Nuclear Physics (New York: Springer)
[5] Weinberg S 1995 The Quantum Theory of Fields vol 1 Foundation (Cambridge: Cambridge University Press)
[6] Gross F 1993 Relativistic Quantum Mechanics and Field Theory (New York: Wiley)
[7] Brown L S 1992 Quantum Field Theory (Cambridge: Cambridge University Press)
[8] Sterman G 1993 An Introduction to Quantum Field Theory (Cambridge: Cambridge University Press)
[9] Matsubara T 1995 Prog. Theor. Phys. 14 351
[10] Abrikosov A A, Gorkov L P and Dzyaloshinski I E 1963 Methods of Quantum Field Theory in Statistical Physics (New York: Prentice-Hall)
[11] Keldysh L V 1965 Sov. Phys.—JETP 20 1018
[12] Kapusta J I 1989 Finite Temperature Field Theory (Cambridge: Cambridge University Press)
[13] Le Bellac M 1996 Thermal Field Theory (Cambridge: Cambridge University Press)
[14] Umezawa H, Matsumoto H and Tachiki M 1982 Thermofield Dynamics and Condensed States (Amsterdam: North-Holland)