FUNCTIONAL INTEGRAL METHOD IN QUANTUM FIELD THEORY OF DIRAC FERMIONS AND PLASMONS IN GRAPHENE

Nguyen Duc Duoc Phan [1,2], Van Hau Tran [1,2], Van Hieu Nguyen [1,2] and Toan Thang Nguyen [3]

[1] Institute of Materials Science, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Hanoi, Vietnam;
[2] University of Engineering and Technology, Vietnam National University in Hanoi, 144 Xuan Thuy, Hanoi, Vietnam;
[3] Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Hanoi, Vietnam.
Email: ntthang@iop.vast.ac.vn

ABSTRACT

The purpose of present work is to elaborate the functional integral method in quantum field theory of Dirac fermions and plasmons in Dirac fermion gas of a graphene single layer at vanishing absolute temperature. The starting point to be assumed as the fundamental principle of the theory is the explicit expression of the action functional of this system. The efficient mathematical tool to be used in the study is the generating functional containing the Grassmann parameters anticommuting with the Dirac fermion field operators. The analytical expression of the generating functional of free Dirac fermion system is exactly derived and efficiently used in the study of 2n-point Green functions of free Dirac fermions. Then the celebrated Hubbard - Stratonovich transformation is applied to rewrite the functional integral of interacting system of Dirac fermions in a new form expressing in terms of a scalar Hermitian quantum field describing the collective excitations in the interacting Dirac fermion gas, and the relationship between these collective excitations and plasmons in graphene is established.

Keywords: Functional integral, Dirac fermions, collective excitations, plasmons,

INTRODUCTION

The discovery of graphene by Novoselov, Geim et al [1] has opened a new period in the development of condensed matter physics and materials science. Soon after this discovery a large number of basic and applied research works on graphene and graphene-based nanostructures has been performed. In the dynamical processes where the spin degree of freedom of electrons plays no role and therefore can be ignored, electrons can be considered as spinless fermions. In this case the quantum motion of charge carriers in single-layer graphene can be described by 2-component wave function satisfied Dirac equations in (2+1)-dimensional space-time and, therefore, they are called Dirac fermions [1]. The Dirac fermions exhibit many interesting properties, in particular, the collective charge density oscillatons so called the plasmon. Recently the plasmon in graphene has attracted a significant attention of both experimental and theoretical studies due to it's importance in fundamental research and technological applications. In particular, the strong coupling between the graphene plasmon modes and other charged particles or light is expected to have high potential to design the next generation nanoelectronic devices, operating from terahertz to infrared frequencies.

The frequently applied method for the theoretical study of interaction processes between Dirac fermions as well as between Dirac fermions and the electromagnetic field is the perturbation theory with the use of Green functions . The 2-point Green functions of Dirac fermions in graphene may be studied by means of the conventional canonical quantization method of quantum field theory. However, the most universal and efficient method in quantum field theory is the functional integral method.

The purpose of this report is to present the basics of functional integral method in quantum field theory of Dirac fermion system in a graphene single layer and to construct the mathe matical tools for the study of plasmons in graphene extending the method proposed in [2,3]. As an example, we apply the above formalism in the special and simplest non-trivial case to get the dispersion relation of plasmon at vanishing absolute tempreture in graphene single layer at Fermi level $E_F = 0$.

Due to the space limit in the following we only sketch the general features of the method. For the detail one refers to the original papers [4,5]. We adopt the same notations as in Refs. [4,5].

MODEL AND FORMALISM

Quantum fields of Dirac fermions with momenta in the neighbours of two inequevalent Dirac points **K** and **K′** of the first Brillouin zone are described by two 2-component field operators $\psi^K(x)$ and $\psi^{K'}(x)$. The Hamiltonian of corresponding free Dirac fermions are

$$H^K = v_F \boldsymbol{\tau}\left(-\mathrm{i}\boldsymbol{\nabla}\right), \quad H^{K'} = v_F \boldsymbol{\tau}^*\left(-\mathrm{i}\boldsymbol{\nabla}\right), \tag{1}$$

Introducing 4-component spinor field

$$\psi = \begin{pmatrix} \psi^K \\ \psi^{K'} \end{pmatrix} \tag{2}$$

we can write Hamiltonian (1) in 4×4 matrix form:

$$H = \begin{pmatrix} H^K & 0 \\ 0 & H^{K'} \end{pmatrix} \tag{3}$$

The key mathematical tool of the functional integral method in quantum field theory of interacting system of Dirac fermions is following functional integral [2]

$$Z^{\psi} = \int [D\psi][D\bar{\psi}] \exp\left\{\mathrm{i} I\left[\psi;\bar{\psi}\right]\right\} \tag{4}$$

where the total action functional of the system of Dirac fermions in the presence of their Coulomb V(x-y) interaction:

$$I\left[\psi,\bar{\psi}\right] = \int \mathrm{d}x \bar{\psi}(x)\left[\mathrm{i}\frac{\partial}{\partial x_0} - H\right]\psi(x) - \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}y \bar{\psi}(x)\psi(x)V(x-y)\bar{\psi}(y)\psi(y) \tag{5}$$

The 2n-point Green function of 2n component of Dirac fermions are defined as follows:

$$G_{\alpha_1\alpha_2\ldots\alpha_n\beta_n\beta_2\beta_1}(x_1,x_2\ldots x_n;y_n\ldots y_2,y_1) = \frac{1}{Z^{\psi}}\int\left[D\psi\right]\left[D\bar{\psi}\right]\exp\{iI[\psi;\bar{\psi}] \times \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n)\bar{\psi}_{\beta_n}(y_n)\ldots\bar{\psi}_{\beta_2}(y_2)\bar{\psi}_{\beta_1}(y_1).$$

The efficient mathematical tool for the study Green functions of Dirac fermion fields is the generating functional

$$Z^{\psi}\left[\eta,\bar{\eta}\right] = \int\left[D\psi\right]\left[D\bar{\psi}\right]\exp\left\{\mathrm{i}\int \mathrm{d}x\left[\bar{\psi}(x)\eta(x)+\bar{\eta}(x)\psi(x)\right]\right\} \times \exp\left\{\mathrm{i}I[\psi;\bar{\psi}]\right\}. \tag{6}$$

where we introduce 4-component Grassmann variables $\eta(x)$ and $\bar{\eta}(x)$ anticommuting with both Dirac fermion fields $\psi(x)$ and $\bar{\psi}(x)$

It can be showed that in the general case of the 2n-point Green function we have formula:

$$G_{\alpha_1\alpha_2\ldots\alpha_n\beta_n\ldots\beta_2\beta_1}(x_1,x_2\ldots x_n;y_n\ldots y_2,y_1) = \frac{1}{Z_0^{\psi}}\frac{\delta^{2n}Z_0^{\psi}[\eta,\bar{\eta}]}{\delta\bar{\eta}_{\alpha_1}(x_1)\delta\bar{\eta}_{\alpha_2}(x_2)\ldots\delta\bar{\eta}_{\alpha_n}(x_n)\delta\eta_{\beta_n}(y_n)\ldots\delta\eta_{\beta_2}(y_2)\delta\eta_{\beta_1}(y_1)}\Bigg|_{\eta=\bar{\eta}=0} \tag{7}.$$

For the case of free Dirac fermions one can get explicit formula of the generating functional:

$$Z_0^{\psi}[\eta,\bar{\eta}] = Z_0^{\psi}\exp\left\{-\mathrm{i}\int \mathrm{d}x\int \mathrm{d}y\ \bar{\eta}(x)S(x,y)\eta(y)\right\} \tag{8}$$

where the matrix elements $S_{\alpha\beta}^{K,K'}(x,y)$ of 4×4 block diagonal matrix functions S(x,y) are

$$S^{K,K'}(x,y) = \frac{1}{2\pi}\int \mathrm{d}\omega e^{-i\omega(x_0-y_0)} \frac{1}{(2\pi)^2}\int \mathrm{d}\mathbf{k}\sum_{\sigma}\tilde{S}_{\sigma}(\omega,\mathbf{k})u_{\mathbf{k}\sigma}^{K,K'}(\mathbf{x})u_{\mathbf{k}\sigma}^{K,K'}(\mathbf{y})^{+} \tag{9}$$

with

$$\tilde{S}_{\sigma}(\omega,\mathbf{k}) = \frac{1-n_{\sigma}(\mathbf{k})}{\omega - E_{\sigma}(\mathbf{k})+\mathrm{i}0} + \frac{n_{\sigma}(\mathbf{k})}{\omega - E_{\sigma}(\mathbf{k})-\mathrm{i}0}. \tag{10}$$

$u_{\mathbf{k}\pm}^{K}(\mathbf{x})$ and $u_{\mathbf{k}\pm}^{K'}(\mathbf{x})$ are the 2-component wave

functions of free Dirac fermions with momentum $\mathbf{k}$ in the neighbors of Dirac points $\mathbf{K}$ and $\mathbf{K}'$ in graphene, respectively, and energies $E_{\pm}(\mathbf{k}) = \pm v_F k$.

In the case of the interacting Dirac fermions the functional integrals (4) and (5) contain a bilinear expression of the density $\bar{\psi}(x)\psi(x)$ of Dirac fermions due to the Coulomb interaction term . In order to get rid of this four - field term we use the famous Hubbard – Stratonovich transformation introducing a Hermitian scalar field. As the result we rewrite the functional integral Z^{ψ} of the interacting Dirac fermions in the form linearized with respect to the Dirac fermion density :

$$Z^{\psi} = \frac{1}{Z_0^{\varphi}} \int [D\varphi] \exp\left\{ \frac{i}{2} \int dx \int dy \varphi(x) V(x-y) \varphi(y) \right\}$$
$$\times \int [D\psi] \int [D\bar{\psi}] \exp\left\{ i \int dx \bar{\psi}(x) \left[i \frac{\partial}{\partial x_0} - H \right] \psi(x) \right\}$$
$$\times \exp\left\{ -i \int dx \int dy \bar{\psi}(x) \psi(x) V(x-y) \varphi(y) \right\}. \quad (11)$$

Expanding the exponential function

$$\exp\left\{ -i \int dx \int dx' \bar{\psi}(x) \psi(x) V(x-x') \varphi(x') \right\}$$

into functional power series of the function $\bar{\psi}(x)\psi(x)u(x-x')\varphi(x')$, we obtain following functional integral of the Hermitian scalar field $\varphi(x)$ describing the collective excitations of the spinless Dirac fermion gas in graphene at vanishing absolute temperature

$$Z^{\varphi} = Z_0 \int [D\varphi] \exp\{iI[\varphi]\}, \quad (12)$$

where Z_0 is an arbitrary constant and $I[\varphi]$ has the form of a series

$$I[\varphi] = \sum_{n=1}^{\infty} I^{(n)}[\varphi], \quad (13)$$

$$I^{(1)}[\varphi] = -\int dx \int dx' \left\langle \bar{\psi}^{K}(x)\psi^{K}(x) + \bar{\psi}^{K'}(x)\psi^{K'}(x) \right\rangle_0 V(x-x')\varphi(x'), \quad (14)$$

$$I^{(2)}[\varphi] = \frac{1}{2} \int dx \int dy \varphi(x) V(x-y) \varphi(y)$$
$$+ \frac{i}{2} \int dx \int dx' \int dy \int dy' V(x-x') V(y-y') \varphi(x') \varphi(y')$$
$$\times \left[S^{K}_{\alpha\beta}(x,y) S^{K}_{\beta\alpha}(y,x) + S^{K'}_{\alpha\beta}(x,y) S^{K'}_{\beta\alpha}(y,x) \right], \quad (15)$$

and so on. The Hermitian scalar field $\varphi(x)$ describes collective excitation in the interacting system of Dirac fermions. Using Eqs.(12) –(15) we can carry out the perturbative study of this collective field, which is related with the plasmons in graphene.

QUANTUM FIELD OF PLASMONS IN GRAPHENE

In the second order approximation of functional (12) with respect to the Hermitian scalar field $\varphi(x)$ the functional integral of the system becomes

$$Z^{\varphi} = Z_0 \int [D\varphi] \exp\{iI_0[\varphi]\}, \quad (16)$$

Denote $\varphi_0(x)$ is the scalar field $\varphi(x)$ corresponding to the extremum value of $I_0[\varphi]$, which is determined by the variational equation

$$\left. \frac{\delta I_0[\varphi]}{\delta \varphi(x)} \right|_{\varphi(x)=\varphi_0(x)} = 0. \quad (17)$$

The fluctuation of $\varphi(x)$ around the background $\varphi_0(x)$ is described by the difference

$$\xi(x) = \varphi(x) - \varphi_0(x). \quad (18)$$

Then the functional integral (16) becomes

$$Z^{\varphi} = \exp\{iI_0[\varphi_0]\} Z^{\xi}, \quad (19)$$

Z^{ξ} being the functional integral of the fluctuation field $\xi(x)$

$$Z^{\xi} = Z_0 \int [D\xi] \exp\{iI_2[\xi]\}, \quad (20)$$

The functional $I_2[\xi]$ has the following formula

$$I_2[\xi] = \frac{1}{2} \frac{1}{2\pi} \quad (21)$$
$$\int d\omega \frac{1}{(2\pi)^2} \int d\mathbf{k} \tilde{\xi}(\omega, \mathbf{k}) \tilde{V}(\mathbf{k}) \left[1 + \tilde{W}(\omega, \mathbf{k}) \right] \tilde{\xi}(-\omega, -\mathbf{k}).$$

where

$$\tilde{W}(\omega, \mathbf{k}) = \tilde{V}(\mathbf{k}) \frac{1}{(2\pi)^2} \int d\mathbf{k}' \frac{1}{(2\pi)^2} \int d\mathbf{l}' \quad (22)$$
$$\times (2\pi)^2 \delta(\mathbf{k} + \mathbf{k}' - \mathbf{l}') \frac{2v_F(k'+l')}{v_F^2(k'+l')^2 - \omega^2} \left\{ 1 - \cos[\theta(\mathbf{k}') - \theta(\mathbf{l}')] \right\}$$

with $\theta(\mathbf{k}) = arctg \frac{k_y}{k_x}$ (23)

Because of the complicated form of the Eqs.(21)-(22), there does not exist a simple analytical calculation method enabling to establish the differential equation for the quantum field of plasmons in graphene, in

contrast to the case of plasmons in electron gas. Therefore we consider a special case with $\omega^2 \ll v_F^2 k^2$ and the long wavelength limit $(k \to 0)$, when we can elaborate the analytical calculation method by extending the reasoning presented in Refs. [2,3].

Introducing new functions:

$$\tilde{\lambda}(\omega,\mathbf{k}) = \mathrm{i}\tilde{\xi}(\omega,\mathbf{k})\frac{\tilde{V}(\mathbf{k})^{1/2}}{\omega} \tag{24}$$

from (21) we obtain a functional containing $\tilde{\lambda}(\omega,\mathbf{k})$

$$I_2[\lambda] = \frac{1}{2}\frac{1}{2\pi}\int \mathrm{d}\omega \frac{1}{(2\pi)^2}\int \mathrm{d}\mathbf{k}\tilde{\lambda}(\omega,\mathbf{k})\left[\omega^2 - \tilde{U}(\mathbf{k})\right]\tilde{\lambda}(-\omega,-\mathbf{k}) \tag{25}$$

where

$$\tilde{U}(\mathbf{k}) = \tilde{V}(\mathbf{k})\frac{1}{(2\pi)^2}\int \mathrm{d}\mathbf{k}'\frac{1}{(2\pi)^2}\int \mathrm{d}\mathbf{l}'(2\pi)^2\delta(\mathbf{k}+\mathbf{k}'-\mathbf{l}') \times 2v_F(k'+l')\left\{1-\cos\left[\theta(\mathbf{k}')-\theta(\mathbf{l}')\right]\right\}. \tag{26}$$

From (26) we get the expression of the functional in terms of the quantum field $\lambda(x)$ with Fourier components $\tilde{\lambda}(\omega,\mathbf{k})$

$$I_2[\lambda] = \frac{1}{2}\int \mathrm{d}x_0 \int \mathrm{d}\mathbf{x}\left[\frac{\partial\lambda(x_0,\mathbf{x})}{\partial x_0}\right]^2 - \frac{1}{2}\int \mathrm{d}x_0 \int \mathrm{d}\mathbf{x}\int \mathrm{d}\mathbf{x}'\lambda(x_0,\mathbf{x})U(\mathbf{x}-\mathbf{x}')\lambda(x_0,\mathbf{x}'), \tag{27}$$

where

$$U(\mathbf{x}-\mathbf{x}') = \frac{1}{(2\pi)^2}\int \mathrm{d}\mathbf{k}e^{-\mathrm{i}\mathbf{k}(\mathbf{x}-\mathbf{x}')}\tilde{U}(\mathbf{k}), \tag{28}$$

The appearance of nonlocal term containing function $U(\mathbf{x}-\mathbf{x}')$ is the peculiarity of the quantum field $\lambda(x)$ of plasmons in graphene. The physical origin of this term is the extended structure of the quasiparticles which are the quanta of collective excitations in the system of interacting Dirac fermions in graphene. From the principle of extremum action $\frac{\delta I_2[\lambda]}{\delta\lambda(x_0,\mathbf{x})} = 0$ we derive following differential equation for the quantum field $\lambda(x)$ of graphene plasmons in the region with $\omega^2 \ll v_F^2 k^2$:

$$\frac{\partial^2\lambda(x_0,\mathbf{x})}{\partial x_0^2} + \int \mathrm{d}\mathbf{x}'U(\mathbf{x}-\mathbf{x}')\lambda(x_0,\mathbf{x}') = 0. \tag{29}$$

In terms of the Fourier components $\tilde{\lambda}(\omega,\mathbf{k})$ of $\lambda(x)$ and Fourier components $\tilde{U}(\mathbf{k})$ of $U(\mathbf{x}-\mathbf{x}')$ Eq.(30) gives the explicit formula of plasmon frequency as a function of its wave vector

$$\omega = \left(4\pi n\right)^{1/4}\left(e^2 v_F k\right)^{1/2}, \tag{30}$$

where n is the density of Dirac fermions in grapheme, that is compatible with the result of Ref. [6] obtained by RPA method.

CONCLUSION

In this work we have presented the basics of functional integral method for the study of interacting system of spinless Dirac fermion gas in a graphene single layer. The functional integral of the system may be expressed in terms of a Hermitian scalar field describing collective oscillations in this system. We have applied the functional integral method in studying plasmons in graphene at vanishing absolute temperature and at Fermi level $E_F = 0$. We have investigated the relationship of the scalar fluctuation field with the quantum field of plasmons in graphene and derived the differential equation for the quantum field of plasmons in graphene. Using this equation we established the relation between frequency and wave vector of plasmons in the long wavelength limit.

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References

[1] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 *Rev. Mod. Phys.* **81** 109-162

[2] Nguyen V H and Nguyen B H 2012 *Adv. Nat. Sci.: Nanosci. Nanotechnol.* **3** 035009

[3] Nguyen V H and Nguyen B H 2015 *Adv. Nat. Sci: Nanosci. Nanotechnol.* **6** 023001

[4] Phan N D D, Nguyen N D, Tran V H, Nguyen T T and Nguyen V H 2017 *Adv. Nat. Sci.: Nanosci. Nanotechnol.* **8** 035018

[5] Phan N D D, Tran V H 2017 Accepted for publication *Adv. Nat. Sci.: Nanosci. Nanotechnol.*

[6] Das Sarma S and Hwang E H 2009 *Phys. Rev. Lett.* **102** 206412.

BIOGRAPHY

The work presented some results obtained by Academician Nguyen Van Hieu with his students.

1. **Nguyen Van Hieu:** Professor, Academician (Former USSR and Third World), Lenin Prize (Former USSR) and Ho Chi Minh prize, author of hundreds papers published in the international ISI scientific journals on high energy physics - elementary particle and condensed matter theory. He was the founding director of the Institute of Physics (VAST) and the president of VAST. He was the first who twenty years ago urged the physics society in Vietnam to start the research on nanoscience, nanotechnology and application.
2. **Nguyen Toan Thang:** Ph.D (1982-supervisor: Academician Nguyen Van Hieu), professor (1996), high rank researcher of Institute of Physiscs (VAST), author and coauthor of some hundred papers published in the national and international journal on the theory of semiconductors, high Tc superconcuctors, strongly correlated electron systems, frustrated magnets, low dimensional systems…
3. **Phan Nguyen Duc Duoc:** Ph.D student.
4. **Tran Van Hau:** Ph.D student.