Two-dimensional zero-gap electronic states at a magnetic field

S.A. Ktitorov and Yu.V. Petrov
Ioffe Physico-Technical Institute of the Russian Academy of Sciences

This work was firstly published in 1986 [?]. No real two-dimensional object with the zero-gap quasi-relativistic spectrum was known in that time. Such an object is well known now: this is graphene. That is why we decided to present it again as an e-print in a slightly modified form.

A density of the two-dimensional zero-gap electronic states at the quantizing magnetic field in the presence the Gaussian random potential has been calculated. The problem is reduced to zero-dimensional spinor field theory using the holomorphic supersymmetric representation. The calculated density of states in the case of the mass perturbation has a delta function peak in the Dirac point. This peak smears due to the potential perturbation.

I. INTRODUCTION

A supersymmetry formalism for calculation of the two-dimensional Schrödinger electronic density of states (EDOS) in the presence of the random potential was developed in [1]. The problem was formulated in terms of the path integrals. The supersymmetric holomorphic representation [2], [4] was used to project the state onto the lower Landau level. The problem was reduced to the zero-dimensional field theory after averaging over the random potential distribution. The EDOS was calculated exactly. This result was in accord with one obtained in [4] for the case of the Gaussian white noise distribution.

This approach is generalized in this work to the case of the zero-gap semiconductor with the quasirelativistic spectrum described by the Dirac equation in the vicinity of the bands crossing point, zero-gap semiconductors of the first kind (ZGSC-I) [5].

The random background field is created by the distribution short-range impurities of two kinds: (i) impurities shifting the conduction and valence bands edges synchronously, i.e. shifting the chemical potential (potential impurities), and (ii) impurities shifting the bands edges in the opposite directions, i.e. modulating the gap width (chemical impurities). Such situation can be realized in IV-VI semiconductors solid solutions, where the band gap can be made varying temperature, pressure and composition. The spatial fluctuations of the composition play a role of the chemical perturbation, while the random violations of stoichiometry play a role of the potential perturbation. Small correlation radius of the random potential stems from the extremely strong lattice polarization in IV-VI semiconductors: the Coulomb tail $e^2/\epsilon r$ can be neglected, when $\epsilon>400$. In the two-dimensional systems like graphene a potentials shifting the chemical potential and modulating the mass (gap) appear because the Kolmogorov matrix elements of the short-range impurity potential are not equal generically for the upper and lower bands.

A character of the EDOS is in accord with [1] in the case of Coulomb impurities. In the case of the chemical impurities there is a delta function singularity in the centre of the band. Simultaneous effect of the chemical and Coulomb perturbations smears this singularity, when chemical perturbation dominates. When intensities of these perturbations are equal, EDOS is similar to one obtained in [1].

II. HOLOMORPHIC REPRESENTATION FOR ZGSC-I

Electronic states in ZGSC-I with impurities at the quantizing magnetic field are described by the two-band Hamiltonian [6]:

$$\hat{H}=\hat{H}_0 + \hat{V}(r),$$

$$\hat{H}_0 = s\alpha \left( \hat{p} - \frac{e}{c} A \right)$$

where $\alpha$ is the Dirac matrix, $s$ is the Fermi velocity, $V(r)$ is the potential of impurities. We choose the axial gauge for the magnetic field potential: $A = \frac{1}{2} H \times r$, $H \parallel e_y$. The spectrum of the operator [2] is well known [2]. Let us construct the relativistic holomorphic representation. It is carried out by functions of the following form:

$$\Psi_j(x, y) = \exp \left[ -\varsigma \xi \right] u_j(\varsigma),$$
where \( \zeta = (x + iy)/2l_H, \bar{\zeta} = (x - iy)/2l_H, l_H^2 = eH/hc \) is the magnetic length, \( j \) is the spinor index, \( u_j(\zeta) \) is a holomorphic function of the variable \( \zeta \) in the Fock-Bargmann space [3]. We can make use of the close relation between the holomorphic representation and the Glauber coherent state representation [8]. The wave functions of a holomorphic function of the variable \( \zeta \) where \( u \) acting in the Fock space. Their commutators read:

\[
\left[ \zeta, \bar{\zeta} \right] = 1, \quad [\zeta, \bar{\zeta}] = 0.
\]

III. FUNCTIONAL INTEGRAL REPRESENTATION FOR GREEN’S FUNCTIONS

Our goal in this section is to derive a general expression for EDOS for the quasirelativistic states of the lower Landau band of a two-dimensional system at the random impurity field. We follow to the approach developed in [11] generalizing it to the quasirelativistic system. A general expression for EDOS reads:

\[
\rho(E) = -\frac{1}{\pi S} \text{Im} \text{Tr} \int dxdy \langle G(E + i0; r = r') \rangle,
\]

where \( G(E + i0; r, r') \) is a one-particle Green’s function; trace is taken on the spinor indices, \( S \) is the surface area; the angle brackets indicate averaging on the random potential configurations. The Green function can be presented by the functional integral:

\[
G_{\alpha j, \alpha' j'} (E + i0; r, r') = -iZ^{-1} \int D\varphi D\varphi^\ast \varphi_{\alpha j} (r) \varphi_{\alpha' j'}^\ast (r') \exp \left[ i \int dxdy \varphi_{\alpha j}^\ast (r) \left( E - \tilde{H} + i0 \right) \varphi_{\alpha j} (r) \right].
\]
\[ Z = \int D\varphi D\varphi^* \exp \left[ i \int dx dy \varphi^*_{\alpha j}(r) \left( E - \hat{H} + i0 \right) \varphi_{\alpha j}(r) \right], \] (13)

where \( \hat{H} \) is determined by (11). The impurity potential is given by the formulae:

\[ V(r) = V_1(r) + \sigma_1 V_2(r), \quad \langle V_i(r) \rangle = 0, \quad \langle V_i(r) V_j(r') \rangle = \lambda_{ij} \delta(r - r'). \] (14)

Here \( V_1(r) \) is a screened Coulomb potential, \( V_2(r) \) is a mass (gap) modulating perturbation; \( \sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \) is the Pauli matrix.

Let us define a supervector belonging to the zero Landau level subspace:

\[ \Phi = \begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \quad \psi_j = \exp(-i \zeta) v_j(\zeta), \quad \Phi = (\varphi^*, \psi), \] (15)

where \( v_j(\zeta) \) is the Grassmann variable. Then the averaged Green function reads in terms of the supervectors:

\[ G_{ij} = -i \int D\Phi D\Phi u_i(\zeta) u^*_j(\zeta) \exp(-i\zeta) \exp(iS_{\text{hol}}), \] (16)

where the effective action reads

\[ S_{\text{hol}} = E \int d\zeta d\bar{\zeta} \exp(-i\zeta/2) \Phi \bar{\Phi} + \int d\zeta d\bar{\zeta} \exp(-i\zeta) \left[ \lambda_1 (\Phi \Phi) + \lambda_2 (\bar{\Phi} \sigma_1 \Phi)^2 \right]. \] (17)

Here \( \lambda_1 \) and \( \lambda_2 \) are intensities of the impurity correlators (14). It is seen from (17) that varying of the free action with respect to \( \Phi \) gives the equation for the Landau gapless zero-band; in the two-dimensional case it is a zero-energy state

\[ \mathcal{H}_0 \Phi = 0. \] (18)

Following (11), we introduce the holomorphic superfields:

\[ \chi_i = u_i(\zeta) + \frac{1}{\sqrt{2}} \theta_i v_i(\zeta), \quad \bar{\chi}_i = u^*_i(\bar{\zeta}) + \frac{1}{\sqrt{2}} \bar{\theta}_i (\zeta) \bar{\phi}_i, \] (19)

where \( \theta_i, \bar{\theta}_i \) are Grassmannian algebra generators. The effective action presented in terms of the superfields \( \chi_i \) is supersymmetric similarly to the Schroedinger case (11). i.e. it is invariant under the magnetic translation group (translation \( \times \) gauge transformation) for the Dirac electron (11) and the superspace rotation group:

\[ S = i 2\pi l_H^2 \int d\theta d\bar{\theta} d\zeta d\bar{\zeta} \exp \left[ -\frac{1}{2} (\zeta \bar{\zeta} + \theta \bar{\theta}) \right] \chi_i \bar{\chi}_i - \] 
\[ 2\pi l_H^2 \int d\theta d\bar{\theta} d\zeta d\bar{\zeta} \exp \left[ \frac{1}{2} (\zeta \bar{\zeta} + \theta \bar{\theta}) \right] \left[ \lambda_1 (\chi_i \bar{\chi}_i)^2 + \lambda_2 (\bar{\chi}_i \sigma_1 \chi_i)^2 \right], \] (20)

\[ \chi_i(z, \theta) = \chi_i(z - a, \theta - \omega) \exp \left\{ -\frac{1}{2} \left[ z a^* + \theta \bar{z} + \frac{1}{2} (|a|^2 + |\omega|^2) \right] \right\}, \]

\[ \delta z = \omega \theta, \quad \delta \theta = \omega z. \] (21)

Substituting (20) into (12) and calculating the Green function perturbatively we can see that the superspace Gaussian integral equals unity in all orders, while the corrections to the bare Green function are nothing but the zero-dimensional spinor \( \lambda \varphi^4 \) field theory symmetry coefficients. The total Green function can be written as a ratio of ordinary Riemannian integrals; the resulting formula differs from the derived in (11) one only by the spinor structure presence.
IV. EDOS CALCULATION

A general formula for calculation of the EDOS for ZGSC-I at the quantizing magnetic field in the presence of the random impurity field reads:

\[
\rho(E) = \frac{1}{2\pi S} \text{Im} \frac{\partial}{\partial \epsilon} \log \int_0^\infty dx dy \exp \left[ i \alpha \epsilon (x+y) - \alpha \lambda_1 (x+y)^2 - \alpha \lambda_2 (x-y)^2 \right],
\]

where \( \alpha = 2\pi l_H^2 \), \( x = |u_1|^2 \), \( y = |u_2|^2 \), \( u_i \) are spinor components, \( \epsilon = E + i0 \). Notice that the total number of unperturbed states per the unit area resulting from (22) is twice larger, than in the one-band case \( \int_0^\infty dE \rho_{0H}(E) = 1/2\pi l_H^2 \). We will show below by the direct calculation that a presence of the chemical impurities modulating the mass (gap) leads to the singularity of EDOS at \( E = 0 \). Assuming \( \lambda_1 << \lambda_2 \) we can one of the integrals:

\[
\rho(E) = \frac{1}{2\pi S} \text{Im} \frac{\partial}{\partial \epsilon} \log \int_0^\infty dx \exp (2i\alpha x) \text{erf} \left( x \sqrt{\alpha \lambda_2} + \frac{\epsilon}{2} \sqrt{\alpha / \lambda_1} \right) + \int_0^\infty dE \exp (2i\alpha x) \text{erf} \left( x \sqrt{\alpha \lambda_2} + \frac{\epsilon}{2} \sqrt{\alpha / \lambda_1} \right)
\]

We have neglected the term \( 4\alpha \lambda_2 x^2 \) in the exponent since convergence of the integral at the upper limit is guarantied by the complementary error function \( \text{erf} c(x) \to 0 \) at \( x \to \infty \) within the domain \( |\arg z| < \pi/4 \). The integral in (22) can be calculated exactly \(^{10}\):

\[
\rho(E) = \sqrt{2/\lambda_1} \frac{\pi}{4\pi l_H^2} \exp \left( -\epsilon^2 / \lambda_1 \right) + \exp \left( \frac{\pi}{2} \right) (\exp (\epsilon / \lambda) F(\epsilon) \left( 1 - \lambda_2 / 2\epsilon^2 \right) - \frac{\lambda}{2\epsilon} (\exp (\epsilon / \lambda) F(\epsilon)) + \right)
\]

\[
\left( \left( \sqrt{\pi / 2} \right) \exp \left( -\epsilon^2 / \lambda_1 \right) - \frac{\lambda}{2\epsilon} \exp (\epsilon / \lambda) F(\epsilon) \right)^2 + [F(\epsilon)]^2
\]

\[
\frac{1}{2\pi l_H^2} \delta(E),
\]

where \( \epsilon = \frac{E \sqrt{\alpha / \lambda_2}}{\lambda} \), \( \lambda = \sqrt{\lambda_1 / \lambda_2} \), \( F(x) = \exp \left( -x^2 \right) \int_0^x dt \exp t^2 \).

Let us consider some limiting cases. If \( \lambda_2 = 0 \), i.e. chemical impurities modulating the mass (gap) are absent, we can simplify (24):

\[
\rho(E) = \sqrt{2/\lambda_1} \frac{\pi}{4\pi l_H^2} \exp \left( \frac{\eta^2}{\lambda_1} \right) + \exp \left( \frac{\pi}{2} \right) \left( \frac{\exp (\epsilon / \lambda)}{\sqrt{\pi}} \right)^2,
\]

where \( \eta = \frac{E \sqrt{\alpha / \lambda_1}}{\lambda} \).

Taking account of the delta-correlated chemical impurities only \( \lambda_1 = 0 \), \( \lambda_2 \neq 0 \) gives a delta function peak at \( E = 0 \) on the smooth background:

\[
\rho(E) = \sqrt{\pi / 2\lambda_2} \frac{\pi}{\pi l_H^2} \left( \frac{\pi}{2} \delta(\epsilon) + \exp (\epsilon^2 / \sqrt{\pi}) \right),
\]

Notice that in the case of \( \lambda_1 = \lambda_2 = w / 8 \) we obtain EDOS similar to obtained in (22), but with the additional facto 2:

\[
\rho(E) = \sqrt{2\pi / w} \frac{2}{\pi l_H^2} \exp \left( \nu^2 / \sqrt{\pi} \right) \left( 1 + \frac{\exp (\epsilon^2 / \sqrt{\pi})}{\sqrt{\pi}} \right)^2,
\]

\[
\nu = E \sqrt{\alpha / w}.
\]

In the limit of the Coulomb impurity correlator low intensity at \( 4\lambda_1 / \alpha^2 E^2 << 4\lambda_2 / \alpha \) and assuming \( E \to 0 \),we obtain from (24):

\[
\rho(E) = \sqrt{2\pi / \lambda_1} \frac{1}{8\pi l_H^2} \sqrt{\pi} \exp (\epsilon^2) \left( \frac{\exp (\epsilon^2)}{\sqrt{\pi}} + \left[ \frac{\exp (\epsilon^2 / \sqrt{\pi})}{\sqrt{\pi}} \right]^2 \right).
\]
It is seen that the peak width is proportional to \( \sqrt{\frac{2\lambda_1}{\alpha}} \). When \( E^2 \gg 4\lambda_2/\alpha \gg 4\lambda_1/\alpha \), we have a result similar to obtained in (??) and (??) for the one-band semiconductor:

\[
\rho(E) = \sqrt{2l_H E^2} \exp\left(\frac{-\pi l_H E^2 / 2\lambda^2}{4\lambda_2^{3/2}}\right). \tag{29}
\]

Such asymptotic was obtained in [11] by the semi-classical quantization approach.

Narrow peak appear in the strongly irregular semiconductors with the Lorentz distribution. The effective action takes the form \( S = -\lambda x \). This gives a generalization of the Lloyd model [12] to the zero-gap semiconductor. The EDOS takes the form

\[
\rho(E) = \frac{1}{2\pi^2 l_H^2} \left[ \frac{\Lambda_+}{\Lambda_+^2 + E^2} + \frac{\Lambda_-}{\Lambda_-^2 + E^2} \right], \tag{30}
\]

where \( \Lambda_{\pm} = \lambda_1 \pm \lambda_2 \). When \( \Lambda_- \to 0 \) (close values of intensities), the peak width tends to zero.

\[\text{V. DISCUSSION}\]

In the absence of dynamic interaction the action (20) is invariant with respect to the supersymmetry transformations. It is doubly degenerate (apart from the usual Landau degeneracy in the magnetic field): \( E = 0 \). Impurities do not violate the supersymmetry that results in appearing of the delta-peak. Possible physical realization: surface states, states in the supersymmetric interface in the heterojunction of mutually inverted narrow-gap semiconductors [13], and, now the most interesting, graphene.

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