Regularization of the spectral problem for the monolayer graphene with the separable in the angular momentum representation singular potential of defect

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The electronic states in the monolayer graphene with the short-range perturbation asymmetric with respect to the band index are analized. The study was made for the separable in the angular momentum representation potential basing on the (2+1)-dimensional Dirac equation. The characteristic equation for bound and resonance states obtained in the present paper is compared with one derived earlier for the same problem with different approach. The momentum representation approach used in the present paper allowed us to obtain the satisfactory regularization of the Hadamar incorrect boundary problem stemming from the potential singularity.

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I. INTRODUCTION

Transport theory in the presence of the resonances and theory of the optical absorption in graphene need nonperturbative analysis of electronic states. This makes it necessary to consider exactly solvable models of defects. One of them is the delta function potential. In the case of the two-band nonrelativistic problem for three-dimensional zero- and narrow-gap semiconductors described by the Dirac equation the problem of bound and resonance states was considered with a use of such potential in the paper [1]. The delta function is determined in this model on the circumference of the sphere of proper dimension. In the present case it is the circumference of circle. This potential has no singularity at $r = 0$ and is separable in the angular momentum representation. This potential is sepable in the angular momentum representation. We take into account possible difference of the perturbation matrix elements calculated on wave functions of the upper and lower bands that is equivalent to consideration of both potential and mass perturbations. Such asymmetry with respect to the band index can be induced by the local shift of sublattices in the vicinity of the point defect. The aim of the present work is a regularization of this incorrect in Hadamar's sence problem.

II. BASIC EQUATIONS

During the last years much attention was paid to the problem of the electronic spectrum of graphene (see a review [2]). Two-dimensional structure of it and a presence of the cone points in the electronic spectrum make actual a comprehensive study of the external fields effect on the spectrum and other characteristics of the electronic states described by the Dirac equation in the 2+1 space-time. Short-range potential impurities in graphene were considered in works [3], [4], [5]. In our works [6], [7], a new model of the short-range impurities in graphene was considered taking into account possible local shift of sublattices. This means that the perturbation must be generically described by a Hermitian matrix. We considered it in the diagonal representation. We do not take into account the inter-valley transitions. The characteristic equation for the bound states wasderived in [6] within the framework of this model. It was understood that singularity of the delta-potential induces a problem of incorrectness of the boundary problem that made some regularization necessary. The present work is just dedicated to one possible way of regularization of this Hadamar incorrect problem. Notwithstanding a presence of this difficulty, the delta potential is extremely popular particularly for use in electronic kinetics and, therefore, deserves thorough analysis.

The Dirac equation describing electronic states in graphene reads

$$\left(-i\hbar v_F \sum_{\mu=1}^{2} \gamma_\mu \partial_\mu - \gamma_0 \left(m + \delta m\right) v_F^2\right)\psi = \left(E - V\right)\psi, \tag{1}$$

where v_F is the Fermi velocity of the band electrons, γ_μ are the Dirac matrices

$$\gamma_0 = \sigma_3, \ \gamma_1 = \sigma_1, \ \gamma_2 = \sigma_2, \tag{2}$$

σ_i are the Pauli matrices, $2mv_F{}^2 = E_g$ is the electronic bandgap, $\psi(\mathbf{r})$ is the two-component spinor:

$$\psi(\mathbf{r}) = \begin{pmatrix} f(\mathbf{r}) \\ g(\mathbf{r}) \end{pmatrix}. \tag{3}$$

. The electronic gap can appear in the graphene monatomic film lying on the substrate because of the sublattices mutual shift [8]. The spinor structure takes into account the two-sublattice structure of graphene. $\delta m(\mathbf{r})$ and $V(\mathbf{r})$ are the local perturbations of the mass (gap) and the chemical potential. A local mass perturbation can be induced by defects in a graphene film or in the substrate [8]. We consider here the delta function model of the perturbation:

$$\delta m(\mathbf{r}) = -b\delta(r - r_0), \ \ V(\mathbf{r}) = -a\delta(r - r_0), \tag{4}$$

that can be re-written in the form of the band-asymmetric potential

$$V_1(\mathbf{r}) = V_1^0 \delta(r - r_0), \ \ V_2(\mathbf{r}) = V_2^0 \delta(r - r_0). \tag{5}$$

The parameters V_1^0, V_2^0 , a and b are related as follows

$$V_1^0 = -(a + b), \ \ V_2^0 = -(a - b). \tag{6}$$

Here r and r_0 are respectively the polar coordinate radius and the perturbation radius. Such short-range perturbation was used in the (3+1)-Dirac problem for narrow-gap and zero-gap semiconductors in [1]. The perturbation forms the diagonal matrix

$$diag(V_1^0, V_2^0) \tag{7}$$

The delta function perturbation is the simplest solvable short-range model. Finite radius r_0 plays a role of the regulator and is necessary in order to exclude deep states of the atomic energy scale. The finite perturbation radius r_0 leads to the quasi-momentum space form-factor proportional to the Bessel function that justifies our neglect of transitions between the Brillouin band points K and K' [1].

Let us introduce the two-dimensional Fourier representation of the two-component wave function (3:

$$f(\mathbf{r}) = \int \frac{dp_x dp_y}{(2\pi)^2} e^{i\mathbf{k}\mathbf{r}} f_{\mathbf{p}}, \ \ g(\mathbf{r}) = \int \frac{d^2p}{(2\pi)^2} e^{i\mathbf{k}\mathbf{r}} g_{\mathbf{p}}, \tag{8}$$

with the Fourier-components $f_{\mathbf{p}}$ and $g_{\mathbf{p}}$ determined by the inverse Fourier transforms:

$$f_{\mathbf{p}} = \int dx dy e^{-i\mathbf{k}\mathbf{r}} f(\mathbf{r}), \ \ g_{\mathbf{p}} = \int dx dy e^{-i\mathbf{k}\mathbf{r}} g(\mathbf{r}) \tag{9}$$

The inverse transform can be written as a combination of the Hankel transform and the angular Fourier series [9]:

$$f_{\mathbf{p}} \equiv f(p, \theta) = \sum_{n=-\infty}^{\infty} i^n e^{in\theta} f_n(p), \ \ g_{\mathbf{p}} \equiv g(p, \theta) = \sum_{n=-\infty}^{\infty} i^n e^{in\theta} g_n(p) \tag{10}$$

$$f_n(p) = \int_0^\infty dr r f_n(r) J_n(pr), \ \ g_n(p) = \int_0^\infty dr r g_n(r) J_n(pr) \tag{11}$$

where $f_n(r)$ is the angular Fourier component:

$$f(r, \theta) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} f_n(r) e^{in\theta}, \ \ g(r, \theta) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} g_n(r) e^{in\theta} \tag{12}$$

Making the Fourier transform of the Dirac equation (1), we consider preliminary two terms of it, which can be considered as rather complicated. The kinetic term reads

$$-i\left(\widehat{\sigma}_x \partial_x + \widehat{\sigma}_y \partial_y\right)\psi\left(\mathbf{r}\right) = \left(\begin{array}{c}\left(\widehat{p}_x + i\widehat{p}_y\right)g\left(\mathbf{r}\right)\\\left(\widehat{p}_x - i\widehat{p}_y\right)f\left(\mathbf{r}\right)\end{array}\right). \tag{13}$$

Therefore, we can write for the upper and lower components of the kinetic term in the momentum representation

$$\left(\begin{array}{c}\left(p_x + ip_y\right)g\left(\mathbf{p}\right)\\\left(p_x - ip_y\right)f\left(\mathbf{p}\right)\end{array}\right) = \left(\begin{array}{c}pe^{i\theta}g\left(p,\theta\right)\\pe^{-i\theta}f\left(p,\theta\right)\end{array}\right) \tag{14}$$

Substituting (10) into (14), we obtain:

$$\left(\begin{array}{c}+i\sum_{n=-\infty}^{\infty}i^n e^{in\theta}g_{n+1}\left(p\right)\\-i\sum_{n=-\infty}^{\infty}i^n e^{in\theta}f_{n-1}\left(p\right)\end{array}\right) \tag{15}$$

The potential Fourier transform $V_i\left(\mathbf{p}\right)$ can be expanded into a series in the case of the circular symmetry:

$$V_i\left(|\mathbf{p} - \mathbf{p}'|\right) = \pi \sum_{n=-\infty}^{\infty} e^{in\theta} \cdot V_i^n\left(p,p'\right), \tag{16}$$

$$V_i^n\left(p,p'\right) = \int_0^{\infty} dr \cdot r J_n\left(pr\right) V_i\left(r\right) J_n\left(p'r\right) \tag{17}$$

where $J_n\left(pr\right)$ is the Bessel function, $i = 1,\ \ 2$. Thus we obtain the integral equations:

$$\left(E - m\right)f_j\left(p\right) + ipg_j\left(p\right) - \int dp' \cdot p'f_j\left(p'\right)V_1^j\left(p',p\right) = 0, \tag{18}$$

$$\left(E + m\right)g_j\left(p\right) - ipf_j\left(p\right) - \int dp' \cdot p'g_j\left(p'\right)V_2^j\left(p',p\right) = 0, \tag{19}$$

where we have put $n = j - 1/2$, where j is the pseudospin quantumnumber, $j = \pm 1/2,\ \pm 3/2\ldots$. In opposite to the relativistic theory, this quantum number has nothing to do with the real spin and indicates a degeneracy in the biconic Dirac point. These equations have a symmetry:

$$f_j \leftrightarrow g_j,\ E \to -E,\ j - 1/2 \to j + 1/2,\ a \to -a. \tag{20}$$

We have introduced the notations:

$$f_{n=j-1/2} \equiv f_j,\ \ g_{n=j+1/2} \equiv g_j \tag{21}$$

Zero-radius [10] and separable potentials [11] are popular in the nonrelativistic scattering theory. However, the Dirac equation is extremely sensitive to a singularity of the potential [12]. The singularity of the delta function potential can be regulated putting the delta function to the circular support (4) [1]

Substituting (7) into (16) we obtain the separable in the angular momentum-momentum modulus representation potential:

$$V_i^j\left(p,p'\right) = v_i^j\left(p\right)v_i^j\left(p'\right), \tag{22}$$

where

$$v_1^j\left(p\right) = \sqrt{r_0 V_1^0}J_{j-1/2}(pr_0),\quad v_2^j\left(p\right) = \sqrt{r_0 V_2^0}J_{j+1/2}(pr_0), i = 1, 2 \tag{23}$$

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Equations (18), (19) become degenerate and can be written as follows:

$$\left(E - m\right)f_j\left(p\right) + ipg_j\left(p\right) - v_1^j\left(p\right)\int_0^{\infty}dp'p'f_j\left(p'\right)v_1^j\left(p'\right) = 0, \tag{24}$$

$$\left(E + m\right)g_j\left(p\right) - ipf_j\left(p\right) - v_2^j\left(p\right)\int_0^{\infty}dp'p'g_j\left(p'\right)v_2^j\left(p'\right) = 0. \tag{25}$$

III.   CHARACTERISTIC EQUATION

Introducing the functions

$$F_j(E) = \int_0^\infty dp\, p f_j(p)\, v_1^j(p), \quad G_j(E) = \int_0^\infty dp\, p g_j(p)\, v_2^j(p), \quad R(p) = \left(p^2 + m^2 - E^2\right)^{-1},$$
(26)

we obtain the homogeneous algebraic equations set for F and G:

$$F_j\left(1 + (E+m)\int_0^\infty dp\, p R(p)\left(v_1^j(p)\right)^2\right) - iG_j\int_0^\infty dp\, p^2 R(p)\, v_1^j(p)\, v_2^j(p) = 0,$$
(27)

$$iF_j\int_0^\infty dp\, p^2 R(p)\, v_1^j(p)\, v_2^j(p) + G_j\left(1 + (E-m)\int_0^\infty dp\, p R(p)\left(v_2^j(p)\right)^2\right) = 0.$$
(28)

The solvability condition for this equations set gives the characteristic equation:

$$\left[1 + (m+E)\int_0^\infty dp\, p R(p)\left(v_1^j(p)\right)^2\right]\cdot\left[1 + (m-E)\int_0^\infty dp\, p R(p)\left(v_2^j(p)\right)^2\right]$$
$$= \left[\int_0^\infty dp\, p^2 R(p)\, v_1^j(p)\, v_2^j(p)\right]^2.$$
(29)

Using the well known formula [13]

$$\int_0^\infty dx\, \frac{x^{\mu-\nu+2n+1}}{x^2 + z^2} J_\mu(bx)\, J_\nu(cx) = (-1)^n\, z^{\mu-\nu+2n} I_\nu(x)\, K_\mu(x)$$

we write it in the form:

$$\left[1 + (m+E)\, r_0 V_1^0 I_{j-1/2}(\kappa r_0)\, K_{j-1/2}(\kappa r_0)\right]\left[1 + (m-E)\, V_2^0 I_{j+1/2}(\kappa r_0)\, K_{j+1/2}(\kappa r_0)\right]$$
$$= (m+E)(m-E) V_1^0 V_2^0 r_0^2 I_{j-1/2}^2(\kappa r_0)\, K_{j+1/2}^2(\kappa r_0),$$
(30)

where $\kappa^2 = \left(m^2 - E^2\right)$, $I_n(x)$, $K_n(x)$ are the modified Bessel functions. Making use of the identity [14]

$$I_\nu(x)\, K_{\nu+1}(x) + I_{\nu+1}(x)\, K_\nu(x) = 1/x,$$
(31)

we obtain the characteristic equation:

$$\kappa\left[I_{l-1/2}(\kappa r_0)\, K_{j+1/2}(\kappa r_0) + I_{j+1/2}(\kappa r_0)\, K_{j-1/2}(\kappa r_0)\right] + (m+E) V_1^0 I_{j-1/2}(\kappa r_0)\, K_{j-1/2}(\kappa r_0) +$$
$$(m-E) V_2^0 I_{j+1/2}(\kappa r_0)\, K_{j+1/2}(\kappa r_0) = 0.$$
(32)

Using the relations (6), we can write the characteristic equation in the form:

$$\kappa\left[I_{j-1/2}(\kappa r_0)\, K_{j+1/2}(\kappa r_0) + K_{j-1/2}(\kappa r_0)\, I_{j+1/2}(\kappa r_0)\right] =$$

$$\left[(m-E)(a-b)\, I_{j+1/2}(\kappa r_0)\, K_{j+1/2}(\kappa r_0) + (a+b)(m+E) I_{j-1/2}(\kappa r_0)\, K_{j-1/2}(\kappa r_0)\right].$$
(33)

This equation has to be compared with one derived using the different approach in [7]:

$$p\left(J_{j-1/2}(pr_0)\, H_{j+1/2}^{(1)}(pr_0) - J_{j+1/2}(pr_0)\, H_{j-1/2}^{(1)}(pr_0)\right)$$
$$= \frac{\tan\left(\sqrt{a^2 - b^2}\right)}{\sqrt{a^2 - b^2}}\left[\sqrt{\frac{E-m}{E+m}}(a-b)\, J_{j+1/2}(pr_0)\, H_{j+1/2}^{(1)}(pr_0) + \sqrt{\frac{E+m}{E-m}}(a+b)\, J_{j-1/2}(pr_0)\, H_{j-1/2}^{(1)}(r_0)\right], \quad (34)$$

where $H_n^{(1)}(z)$ is Hankel's function, $p = \sqrt{E^2 - m^2}$. Making the analytic continuation from the case of the band states with $E^2 > m^2$ to the opposite one of bound states $E^2 < m^2$ we obtain the equation

$$\kappa \left[I_{j-1/2}\left(\kappa r_0\right) K_{j+1/2}\left(\kappa r_0\right) + K_{j-1/2}\left(\kappa r_0\right) I_{j+1/2}\left(\kappa r_0\right) \right] =$$

$$\frac{\tan\left(\sqrt{a^2 - b^2}\right)}{\sqrt{a^2 - b^2}} \left[(m - E)(a - b) I_{j+1/2}\left(\kappa r_0\right) K_{j+1/2}\left(\kappa r_0\right) + (a + b)(m + E) I_{j-1/2}\left(\kappa r_0\right) K_{j-1/2}\left(\kappa r_0\right) \right]. \qquad (35)$$

We see that the only distinction between the formulae (33) and (35) is a presence of the factor

$$T(a, b) = \frac{\tan\left(\sqrt{a^2 - b^2}\right)}{\sqrt{a^2 - b^2}} \qquad (36)$$

in the equation derived in [7]. They are identical in the limit

$$a^2 - b^2 \longrightarrow 0, \quad T(a, b) \longrightarrow 1. \qquad (37)$$

This limit can be reached near the lines $a^2 - b^2 = 0$, or when a and b are small. The reason of this distinction is the following. The delta function potential in the Dirac equation creates a boundary problem, which is incorrect in the Hadamar sense [15]. Such a problem needs a regularization. Distinct regularization procedures were used in the present work and in [7]. Singular feature of the potential was preserved in [7], a regularization was carried out due to very special join of partial solutions, while in the present work, a regularization took place due to the Fourier transform smoothing property. In particular, the potential takes the separable form with the nonlocal kernel $v_i^j(p) = \sqrt{r_0 V_i^0} J_{j+1/2}(p r_0)$ (see eq. (23)). Just this nonlocality plays the role of regularizator. Equations (33) and (35) have asymptotically similar solutions , when (37) is valid. Their sets of solutions are quite different outside this region of parameters a and b. Moreover, equation (35) has significantly richer set of solutions, than equation (33) [7] due to periodicity of tangent present in (36). We come to conclusion that the rich set of solutions given by (35) is the artifact of the zero-support interaction. Besides, the annular well model analyzed in [16] does not reproduce all of this rich set of solutions even in the limit of zero radius. Therefore, the equation obtained in the present work can be considered as a correctly regularized one.

IV. CONCLUSION

Non-relativistic problem of the electronic spectrum described by the Dirac equation is considered in the case of the two-component short-range perturbation potential with a help of the Fourier transforming. This approach is shown to make regularized the incorrect in the Hadamar sense problem.

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