Bound electron states in the monolayer gapped graphene with the short-range impurities

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1. Introduction

The Dirac equation is a fundamental base of the relativistic field theory. However, it is an important model in the non-relativistic solid state theory as well. Superconductors with d-pairing [1], the Cohen–Blount two-band model of narrow-gap semiconductors [2,3], electronic spectrum of the carbon tubes form an incomplete list of the non-relativistic applications of this equation. During the last two years extremely much attention was payed to the problem of the electronic spectrum of graphene (see for the review [5]).

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. We consider in this work the bound states of the 2 + 1 gapped Dirac equation due to the short-range perturbation. The pristine graphene is gapless, but violation of symmetry can be triggered by the substrate or be developed dynamically. Notice that “short-range” stands here for the symmetry violation can be induced by defects in the graphene film or in the substrates [9]. We consider here the delta function model of the perturbation:

\[ \delta m(r) = -\delta \delta(r - r_0), \quad V(r) = -a\delta(r - r_0), \]

where \( r \) and \( r_0 \) are respectively the polar coordinate radius and the perturbation radius. Such short-range perturbation (and the equivalent form \( \text{diag}(V_1, V_2)\delta(r - r_0) \) with \( -V_1 = \frac{a}{1 + b}, -V_2 = \frac{a}{1 - b} \)) was used in the (3 + 1)-Dirac problem for narrow-gap and zero-gap semiconductors in [3]. The two-dimensional Dirac problem with the scalar short-range perturbation (2) (but without the mass perturbation) was considered in [10]. The obtained there characteristic equation for the discrete spectrum energy contains one mistake. We correct it here and take account of the mass perturbation \( \delta m(r) \).

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Abstract

Bound electron states in impure graphene with the massive Dirac spectrum are considered. Short-range perturbations for defect and impurities of the types “local chemical potential” and “local gap” are taken into account.

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1. Introduction

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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. We consider in this work the bound states of the 2 + 1 gapped Dirac equation due to the short-range perturbation. The pristine graphene is gapless, but violation of symmetry can be triggered by the substrate or be developed dynamically. Notice that “short-range” stands here for the symmetry violation can be induced by defects in the graphene film or in the substrates [9]. We consider here the delta function model of the perturbation:

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Let us present the two-component spinor in the form
\[
\psi_j(r, t) = \frac{\exp(-iEt)}{\sqrt{r}} \begin{pmatrix} f_j(r) \exp[(i - 1/2)\phi] \\ g_j(r) \exp[(i + 1/2)\phi] \end{pmatrix},
\]
where \( j \) is the pseudospin quantum number; \( j = \pm 1/2, \pm 3/2, \ldots \).

In the opposite to the relativistic theory, this quantum number has nothing to do with the real spin and indicates the degeneracy in the biconic Dirac point. The upper \( f_j(r) \) and \( g_j(r) \) components of the spinor satisfy the equations
\[
\frac{dg_j}{dr} + \frac{j}{r} g_j - (E - m) f_j = (a + b)\delta(r - r_0)f_j, \\
\frac{df_j}{dr} + \frac{j}{r} f_j - (E + m)g_j = (a - b)\delta(r - r_0)g_j.
\]
These equations have a symmetry:
\[
f_j \rightarrow g_j, \quad E \rightarrow -E, \quad j \rightarrow -j.
\]

Let us introduce the function \( \varphi_j(r) = f_j/g_i \). It satisfies the equation:
\[
\frac{1}{(a + b)\varphi_j^2 + (a - b)} \left[ \frac{d\varphi_j}{dr} - \frac{2j}{r} \varphi_j - E(\varphi_j^2 + 1) \right] + \delta(r - r_0) = 0.
\]
Integrating in the vicinity of \( r = r_0 \)
\[
\varphi_{j(r_0 + \epsilon)} = \frac{a + b}{a - b} \varphi_{j(r_0 - \epsilon)} - 1,
\]
we obtain the matching condition
\[
\arctan\left( \frac{\varphi_j^* \sqrt{a + b}}{\sqrt{a - b}} \right) - \arctan\left( \frac{\varphi_j^* \sqrt{a + b}}{\sqrt{a - b}} \right) = \sqrt{a^2 - b^2},
\]
where \( \varphi_j^* \equiv \varphi_j(r_0 - \epsilon), \varphi_j^* \equiv \varphi_j(r_0 + \epsilon), a^2 > b^2 \). The upper and lower component matching condition resulting from (9) reads
\[
\begin{pmatrix} f_j^+ \\ g_j^+ \end{pmatrix} = \hat{A} \begin{pmatrix} f_j^- \\ g_j^- \end{pmatrix},
\]
where the matrix \( \hat{A} \)
\[
\begin{pmatrix} \cos \sqrt{a^2 - b^2} & -\sin \sqrt{a^2 - b^2} \\ \sin \sqrt{a^2 - b^2} & \cos \sqrt{a^2 - b^2} \end{pmatrix}
\]
is orthogonal for \( b = 0 \). It transmutes into the matrix
\[
\begin{pmatrix} \cos \sqrt{b^2 - a^2} & -\sin \sqrt{b^2 - a^2} \\ \sin \sqrt{b^2 - a^2} & \cos \sqrt{b^2 - a^2} \end{pmatrix},
\]
when \( a^2 - b^2 < 0 \).

The general solution can be found solving the second-order equation obtained by excluding one of the spinor components from the equation set (4), (5) in the domains \( 0 < r < r_0 \) and \( r > r_0 \):
\[
\frac{d^2f_j}{dr^2} + \left[ E^2 - m^2 - j(j - 1)/r^2 \right] f_j = 0.
\]
This equation is related to the Bessel one. Its general solution reads
\[
f_j = C_1\sqrt{r}J_{j-1/2}(kr) + C_2\sqrt{r}K_{j-1/2}(kr),
\]
where \( x^2 = m^2 - E^2 \), \( I_n(z) \) and \( K_n(z) \) are the modified Bessel functions. The constant \( C_2 = 0 \) in the domain \( 0 < r < r_0 \), while \( C_1 = 0 \) in the domain \( r > r_0 \). Expressing the \( g_j \)-component using (5), we can write
\[
\varphi_j^+ = \frac{m + E'}{m - E} J_{j-1/2}(kr_0), \\
\varphi_j^- = \frac{m + E}{m - E'} K_{j-1/2}(kr). 
\]

Applying the matching condition (9) to the expressions (16), (15) we obtain the characteristic equation for the bound state energy levels:
\[
k \begin{pmatrix} J_{j-1/2}(kr_0) & J_{j+1/2}(kr_0) \\ K_{j+1/2}(kr_0) & K_{j-1/2}(kr_0) \end{pmatrix}
\]
\[
= \frac{\tan(\sqrt{a^2 - b^2})}{\sqrt{a^2 - b^2}} \left[ (m - E)(a - b) \\
+ (a + b)(m + E) \frac{J_{j-1/2}(kr_0) K_{j-1/2}(kr_0)}{J_{j+1/2}(kr_0) K_{j+1/2}(kr_0)} \right]
\]
where \( a^2 - b^2 > 0 \). This equation turns to the characteristic equation obtained in [10], for \( b = 0 \) apart from the mistakenly omitted terms in the right-hand side of (17). In the opposite case of \( a^2 - b^2 < 0 \) we have
\[
k \begin{pmatrix} J_{j-1/2}(kr_0) & J_{j+1/2}(kr_0) \\ K_{j+1/2}(kr_0) & K_{j-1/2}(kr_0) \end{pmatrix}
\]
\[
= \frac{\tan(\sqrt{b^2 - a^2})}{\sqrt{b^2 - a^2}} \left[ -(m - E)(b - a) \\
+ (b + a)(m + E) \frac{J_{j-1/2}(kr_0) K_{j-1/2}(kr_0)}{J_{j+1/2}(kr_0) K_{j+1/2}(kr_0)} \right].
\]
We write these equations in another form making the symmetry (6) manifest:
\[
k \begin{pmatrix} J_{j-1/2}(kr_0) & J_{j+1/2}(kr_0) \\ K_{j+1/2}(kr_0) & K_{j-1/2}(kr_0) \end{pmatrix}
\]
\[
= \frac{\tan(\sqrt{b^2 - a^2})}{\sqrt{b^2 - a^2}} \left[ -(m - E)(b - a) \\
+ (b + a)(m + E) \frac{J_{j-1/2}(kr_0) K_{j-1/2}(kr_0)}{J_{j+1/2}(kr_0) K_{j+1/2}(kr_0)} \right].
\]

3. Analysis of the characteristic equation and numerical results

Making use of the Bessel functions limiting forms for small arguments [11]
\[
I_{\nu}(z) \sim (z/2)^\nu, \quad K_\nu(z) \sim -\ln z,
\]
\[
K_{\nu}(z) \sim \frac{1}{2} \Gamma(\nu)(z/2)^{-\nu},
\]
we can obtain a simple relation describing the asymptotic behaviour of the energy level, where the perturbation power approaches zero:
\[
E = m - \frac{r_0^2}{2r_0^2} \exp\left( -\frac{r_0}{m + (a + b)} \right).
\]
where \( m = m^{-1} \) (in units with \( h = \hbar = 1 \), \( a + b > 0 \). This result conforms the well known general property of the two-dimensional quantum systems: a threshold for creation of the bound state is absent; the point \( a + b = 0 \) is the essentially singular point of the function \( E = E(a + b) \). One can see that the function \( E(a) \) approaches the point \( E = -m \) at some large enough value of \( a > 0 \).

Making use of the Bessel function asymptotic behaviour [11],
Graphical solution of the characteristic equation (17). It illustrates three various possibilities for different $a$ magnitudes $(0.93; 1.23; 1.53)$ and fixed $b = -1$: M: one energy eigenvalue; N: two energy eigenvalues; P: no energy eigenvalues within the gap.

In Fig. 2, the electron bound state energy is presented as a function of the potential amplitude for the angular momentum quantum number values $j = 1/2$, $\rho_0 = 1$, and $b = 0$. Inspecting this plot one can see that our analytic solution (21) perfectly approximates approaching of the bound state energy value the upper band bottom, when $b$ approaches zero.

In Fig. 3, the bound state energy is presented as a function of the mass perturbation amplitude $b$ for $a = 0$, $\rho_0 = 1$, $j = 1/2$. Points M, N, P correspond to eigenvalues depicted in Fig. 1.

In Fig. 4, the electron bound state energy is presented as a function of the potential amplitude for the angular momentum quantum number $j = 1/2$, $\rho_0 = 1$, and $b = -1$. We see that the energy dependence on $a$ is non-monotonic function, but approaching the upper band bottom takes place similarly to the case of $b = 0$. Points M, N, P correspond to eigenvalues depicted in Fig. 1.

Distribution of the bound states number in the $(a,b)$ plane for $j = 1/2$ is depicted in Fig. 5. Points M, N, P stand respectively for one, two and zero crossings shown in Fig. 1. It is seen from our figures that simultaneous existence of two bound states is possible within the narrow segment in the plane $(a,b)$. 

$I_\nu(z) \sim (2\pi z)^{-1/2} \exp z, \quad K_\nu(z) \sim \left( \frac{\pi}{2z} \right)^{1/2} \exp(-z),$

and Eq. (18), we can see that the function $E(b)$ approaches the point $E = 0$, when $\frac{\rho_0}{r} = 1$ is large enough and $b \to \infty$.

Graphical solution of the characteristic equation (17) is presented in Fig. 1. It illustrates three various possibilities for different $a$ magnitudes $(0.93; 1.23; 1.53)$ and fixed $b = -1$: M stands for one eigenvalue; N stands for two eigenvalues; P stands for absence of eigenvalues within the gap.

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4. Conclusion

In conclusion, we considered the bound electron states for the two-dimensional Dirac equation with the short-range perturbation. The short-range perturbation is approximated by the delta function $\delta(r - r_0)$ with different amplitudes in the upper and lower bands. We found the characteristic equation for the discrete energy levels. Energy levels behaviour in dependence on the perturbation amplitudes was investigated both analytically and numerically. The structure of our characteristic equations allows us to make the following general conclusions. The energy spectrum is a periodic function of $a$ for $b = 0$. In the case of finite value of $a$ and $b \to \infty$, $\tanh(\sqrt{b^2 - a^2}) \to 1$ and, therefore, $E \to \text{const}$. Notice that the bound states energy levels obtained in the case of the vanishing parameter $b$ are in the qualitative correspondence to the energy levels deduced from the scattering amplitude poles calculated in [12]. The obtained results can be useful for understanding of the graphene electron properties.

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