Analytical study of bound states in graphene nano-ribbons and carbon nanotubes: the variable phase method and the relativistic Levinson theorem

D. S. Miserev$^1$$^2$

$^1$School of Physics, University of New South Wales, Sydney, Australia and
$^2$Rzhанов Institute of Semiconductor Physics, Siberian Branch, Russian Academy of Sciences, pr. Akademika Lavrenteva 13, Novosibirsk, 630090 Russia

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The problem of localized states in 1D systems with the relativistic spectrum, namely, graphene stripes and carbon nanotubes, has been analytically studied. The bound state as a superposition of two chiral states is completely described by their relative phase. The criteria of bound states appearance have been obtained based on the variable phase method (VPM) and the relativistic Levinson theorem developed via the VPM. The problem of bound states is reduced to the analysis of singularities of some vector field where the Levinson theorem appears as the Poincare indices theorem for closed trajectories of this field. The reduction of the VPM equation to the non-relativistic and semi-classical limits has been done. The limit of the small momentum $p_y$ of the transverse quantization is applicable to arbitrary integrable potential. In this case the only confined mode is predicted.

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INTRODUCTION

Graphene, carbon nanotubes and topological insulators has attracted keen attention for intensive theoretical and experimental research in recent years. The uniqueness of these quantum materials towards the fundamental physics consists in the opportunity to observe QED effects with the big coupling constant $g = e^2/\hbar c \approx 1$, where $s \approx c/300$ is the Fermi velocity, $\varepsilon$ is an average dielectric constant of environment (for instance, for graphene sheet on the substrate with the dielectric constant $\varepsilon_s$ one can obtain $\varepsilon = (1 + \varepsilon_s)/2$). Such effects as the atomic collapse and pair production in the supercritical potentials $^1$, $^2$, the Adler-Bell-Jackiw anomaly (the chiral anomaly) $^3$–$^5$ have been intensively studied. The Klein tunnelling of electrons in the gated graphene $^6$–$^10$ reveals the complete suppression of the backscattering.

The present work is related to the general theoretical study of the confined electronic states in graphene nano-ribbons or single-walled carbon nanotubes affected by the longitudinal electric field. Omitting the inter-valley scattering, the author considers the electron behaviour near one of two independent Dirac points where electrons are well-described by the Dirac-Weyl hamiltonian $^1$ in the one-particle approach.

I propose a convenient technique to analyse bound states analytically for the 2D Dirac-Weyl equation with a 1D potential $U(x)$. It refers to the variable phase method (VPM) developed generally by P. M. Morse and W. P. Allis $^6$, V. V. Babikov $^7$, F. Calogero $^8$ and others $^9$–$^{21}$. The wave function is expressed as a linear combination of two Weyl fermions and the phase between them is considered as a desired phase function for the VPM to be applied. Then, the reduction to the non-relativistic and semi-classical limits is demonstrated. Later on, I consider one more limiting case of the $\delta$-potential which is applicable to any integrable potentials at sufficiently small momentum $p_y \ll 1/d$ of the transverse quantisation ($d$ is the characteristic width of the potential).

Developed herein VPM allows one to formulate the relativistic analogue of the Levinson theorem $^2$. The relativistic Levinson theorem for the Dirac equation was formulated in 3D by M. Klaus $^2$ for central potentials, K. Hayashi $^{23}$ and R. L. Warnock $^{24}$ as a relation between zeroes of the vertex function and particle poles of the total amplitude. This problem has been considered in two dimensions with the compact supported central potential $^{25}$. D. P. Clemence $^{26}$ thoroughly investigated the Levinson theorem for the Dirac equation with a 1D potential which satisfies the condition $\int_{-\infty}^{\infty} U(x)(1 + |x|) dx < \infty$ via the scattering matrix approach taking into account the half-bound states. The particular case of the relativistic Levinson theorem for the symmetric 1D potentials has been studied by Q. Lin $^{27}$ with additional restriction for the potential to be a compact supported function, A. Calogero and N. Dombey $^{28}$ for potentials of definite sign, Z. Ma et al. $^{30}$ with the similar condition as in $^{27}$. The developed herein method permits one to prove the Levinson theorem with the minimal restriction $\int_{-\infty}^{\infty} U(x) dx < \infty$ which significantly broadens the result obtained by D. P. Clemence. For example, my results are applicable to so-called top-gate potential $^{23}$ which asymptotics are expected to be realistic for the gated graphene structures $^{31}$. Afterwards, a graphic interpretation of the Levinson theorem together with the corresponding numerical method that does not involve solving any differential equations numerically is considered.
THEORETICAL MODEL

Near conic points, electrons in graphene with the gated potential \( U(x) \) are described by the Dirac-Weyl Hamiltonian:

\[
\hat{H} = s \sigma \hat{p} + U(x) = s \sigma_x \hat{p}_x + s \sigma_y \hat{p}_y + U(x)
\]  

(1)

where \( s \) is the Fermi velocity, \( \sigma = (\sigma_x, \sigma_y) \) are Pauli matrices, \( \hat{p} = -i \hbar \nabla \). Henceforth, it is assumed that the potential decays at infinity. Further calculations are executed in the dimensionless variables: \( \hbar = s = 1 \). It is also assumed \( p_y > 0 \) where \( p_y \) is the quantized transverse momentum of quasi-1D systems such as graphene nanoribbons and single-walled carbon nanotubes where for nanotubes \( y = r \phi \), \( r \) is the radius, \( \phi \) is the cyclic variable.

The spectrum of the free-particle Hamiltonian is linear on the momentum: \( E = \pm \sqrt{p_x^2 + p_y^2} \). The negative-energy states correspond to the hole’s description according to the conventional views.

The stationary wave function can be represented in a symmetric form:

\[
\Psi = \frac{e^{ip_y y}}{\sqrt{4W}} \left( g(x) + p_y^{-1} g'(x) \right) e^{i \int (E-U(\zeta)) d\zeta}
\]  

(2)

via the axillary function \( g(x) \) [14]:

\[
g''(x) + 2i(E-U(x))g'(x) - p_y^2 g(x) = 0
\]  

(3)

where \( E \) is the electron energy, \( W \) is the normalization coefficient.

Eq. [2] represents an equivalent statement of the problem described by the Hamiltonian [11]. Here, I deal with electronic states of zero current along \( x \)-direction and apply it to the analysis of confined states.

Zero flow \( j_x = \Psi^\dagger(x) \sigma_x \Psi(x) = 0 \) along \( x \)-direction yields the restriction on the function \( g(x) \):

\[
|g(x)| = |p_y^{-1} g'(x)|.
\]  

(4)

The first consequence is that \( g(x) \) and hence the electron density of confined states \( \rho(x) = \Psi^\dagger(x) \Psi(x) = |g(x)|^2/W \) vanishes nowhere except infinity.

Separating modulus and phase \( g(x) = Re^{i\phi} \), I arrive at the condition:

\[
(\Phi')^2 + (R'/R)^2 = p_y^2,
\]  

(5)

which concedes the following substitution:

\[
\begin{aligned}
\Phi'(x) &= p_y \sin \Omega(x) \\
R'/R &= p_y \cos \Omega(x)
\end{aligned}
\]  

(6)

where the function \( \Omega(x) \) is the solution of the first-order differential equation:

\[
\Omega'(x) = 2(U(x) - E) - 2p_y \sin \Omega(x).
\]  

(7)

Thereby, I receive desirable equation for the VPM to be employed.

Considering bound states, I set the boundary conditions for the function \( \Omega(x) \):

\[
\begin{aligned}
\Omega(x \to +\infty) &= \pi + \arcsin \frac{E}{p_y} + 2\pi n \\
\Omega(x \to -\infty) &= -\arcsin \frac{E}{p_y}.
\end{aligned}
\]  

(8)

These conditions provide the exponential decay of the density \( \rho(x) \sim R^2(x) \) at infinity as it follows from (3), \( n \) being an integer.

To reveal the physical meaning of the function \( \Omega(x) \), I use the following representation of the wave function:

\[
\Psi(x, y) = \frac{e^{ip_y y}}{\sqrt{4W}} \left( \frac{1}{1} + e^{i\Omega} \left( \frac{1}{-1} \right) \right) R(x)e^{-i\Omega/2}.
\]  

(9)

Hence, confined state appears as a linear combination of two chiral (Weyl) states and is completely described by the phase between them. Another form of Eq. [9] refers to the spin with the polar angle \( \Omega \) and the azimuthal angle \(-\pi/2\):

\[
\Psi(x, y) = \frac{R(x)e^{ip_y y}}{\sqrt{W}} \left( \cos \frac{\Omega}{2} \right)
\]  

(10)

LIMITING CASES FOR THE PHASE FUNCTION

Non-relativistic limit

To be more specific, consider the non-relativistic limit for electrons: \( E = p_y + \varepsilon \), \( \varepsilon = -k^2/2p_y \) where \( k, U(x), 1/d \ll p_y, d \) is the width of the potential. Boundary conditions [13] for \( \Omega(x) \) take the form: \( \Omega(-\infty) = -\pi/2 + k/p_y, \Omega(+\infty) = -\pi/2 - k/p_y + 2\pi n, n \) being an integer. Suppose then \( \Omega(x) \sim -\pi/2 + \delta \Omega \) where \( \delta \Omega \ll 1 \) almost everywhere. Given assumption is violated only when \( \Omega' \sim p_y \) which corresponds to \( \delta \Omega \sim 1 \). The behaviour of the phase function \( \Omega(x) \) in this region does not depend on the potential because \( U(x) \ll p_y \). Notice that the width of this region \( \delta \Omega \sim 1/p_y \ll d \) is small in the non-relativistic limit. Hence, the expansion of the initial equation [7] results in the Riccati equation:

\[
\delta \Omega' = 2(U(x) - \varepsilon) - p_y \delta \Omega^2,
\]  

(11)

where \( \psi(x) = \exp(p_y \int \delta \Omega(x) dx) \) satisfies the 1D Schrodinger equation for a non-relativistic particle with mass \( p_y \). The function \( \delta \Omega(x) \) tends to the infinity in zeroes of the wave function \( \psi(x) \).

Semi-classical limit

Let me rewrite Eq. [7] in the dimensional quantities:

\[
\hbar \Omega' = \frac{2}{s} (U(x) - E) - 2p_y \sin \Omega,
\]  

(12)
where $s$ is the Fermi velocity. In the semi-classical limit $h \to 0$ the elimination of the left-hand part of this equation yields:

$$\sin \Omega = \frac{U(x) - E}{sp_y}. \tag{13}$$

This approximation is solvable in the real-valued functions when $|U(x) - E| < sp_y$ which conforms to the case of the non-classical motion where the wave function decays. In breakpoints $x_i$ when $U(x_i) - E = -\mu sp_y$ I define $\Omega(x_i) = -\mu \pi/2, \mu = \pm 1$ is definite for each region of motion.

In the regions of classical motion where the wave function is oscillatory shaped, $\Omega(x)$ is a complex function, namely, $\Omega(x) = -\mu \pi/2 + i \delta \Omega$:

$$\cosh \delta \Omega(x) = -\mu \frac{U(x) - E}{sp_y} = \left| \frac{U(x) - E}{sp_y} \right|. \tag{14}$$

Eq. (14) has two solutions $\pm \delta \Omega$ (for definiteness, I set $\delta \Omega > 0$). Corresponding amplitude of the wave function $R_{\pm}(x)$ is determined from Eq. (6):

$$R_{\pm}(x) \sim \exp \left( \pm \frac{py}{h} \int \sinh \delta \Omega(x) \, dx \right).$$

According to the definition, it is required for the function $R(x)$ to be real-valued. It means that I have to consider a linear combination of corresponding functions $g_{\pm}(x) = R_{\pm}(x)e^{i\Phi_{\pm}(x)}$ where

$$\Phi_{\pm}(x) = -\mu \int \left| \frac{U(x) - E}{s} \right| \frac{dx}{h} = \int \frac{U(x) - E}{s} \frac{dx}{h},$$

as it follows from Eq. (6) and $\Phi$ is the same for two different solutions of Eq. (14). Finally:

$$R(x) \sim \cos \left( \int p_x \frac{dx}{h} + \phi_0 \right) \tag{15}$$

where the semi-classical momentum $p_x = py \sinh \delta \Omega(x) = \sqrt{(E - U(x)^2)/s^2 - p^2_y}$ is introduced. The phase $\phi_0$ is defined by the matching conditions.

Hence, the Bohr-Sommerfeld quantisation takes the form:

$$\int p_x \, dx = 2 \pi \hbar (n + \gamma) \tag{16}$$

where $n \gg 1$ is an integer, $\gamma \sim 1$ is defined from the matching conditions in the turning points, for example, $\gamma = 1/2$ for smooth potentials. The semi-classical approximation is valid when $\hbar py U'(x) \ll sp^2_y$.

**Limit of small $p_y$ or delta-potential limit**

From now on, let me suppose $U(x)$ be an integrable function. The limit considered here is characterized by the only condition $p_y d \ll 1$, i.e. the scale of the wave function should be much longer then the width of the potential. Notice that this limit is valid for any integrable potential and does not require the potential to be $\delta$-like as long as the transverse quantisation momentum $p_y$ is sufficiently small. The reason why I named this limit as the delta-potential limit is described below. Integrating Eq. (7) and applying the boundary conditions (8), one can find the total variance of the phase function $\Delta \Omega = \Omega(+\infty) - \Omega(-\infty)$:

$$\Delta \Omega = 2 \arcsin \frac{E}{py} + 2 \pi \left( n + \frac{1}{2} \right) = 2 G + O(p_y d), \tag{17}$$

where $G = \int_{-\infty}^{+\infty} U(x) \, dx < \infty$; the integer $n$ is exactly determined unless $G$ is a multiple of $\pi$. This approximation is obviously valid if $G \sim 1$ or, especially if $G > 1$.

Consider the case $G \ll 1$ more thoroughly. It involves $\Omega(x) = -\arcsin(E/py) + \delta \Omega(x)$ with $\delta \Omega(x) \ll 1$. Notice that the given definition of $\delta \Omega(x)$ does not coincide with the function $\delta \Omega(x)$ in the non-relativistic formula (11). The expansion of Eq. (7) gives:

$$\delta \Omega'(x) = 2 U(x)' - 2k \delta \Omega(x) - E \delta \Omega^2(x). \tag{18}$$

The non-linear term $\delta \Omega^2$ can be neglected if $k \sim E$ or $k \gg E$. In this case, one can find exactly that:

$$\delta \Omega(x) = 2 \int_{-\infty}^{x} U(x') e^{2k(x' - x)} \, dx'.$$

Integrating then Eq. (18) I arrive at:

$$\Delta \Omega = 2 G - 2k \int_{-\infty}^{\infty} \delta \Omega(x) \, dx = 0.$$  

This result means that in the case $G \ll 1$ and $p_y d \ll 1$ the energy of the bound state approaches to the boundaries of the continuous spectrum $E \approx \pm p_y$ or equivalently $k \ll p_y$ corresponding to the non-relativistic equation (11). Indeed, it is sufficient to pick out a perfect square in the left-hand side of (18) and replace $\delta \Omega \to \delta \Omega - k/E$ where such substitution does not violate the condition $\delta \Omega \ll 1$ after which the non-relativistic equation (11) is obtained. The difference from the non-relativistic limit is that $p_y \to 0$ which provides $\delta \Omega \ll 1$ without exceptions as long as $G \ll 1$ at arbitrary relation between $U(x)$ and $p_y$.

One can easily show that in this limit for electrons (and analogically for holes) $\Delta \Omega = -2k/p_y = 2G + O(k^2d/p_y)$ where $k^2d/p_y \ll k/p_y$ and thereby I receive that $\Delta \Omega = 2G + O(G^2 \cdot p_y d)$ for the case of small $G$. Summing up I conclude:

$$\arcsin \frac{E}{py} \approx G - \pi \left( n + \frac{1}{2} \right) \tag{20}$$

for arbitrary finite parameter $G$ as soon as $p_y d \ll 1$. 

The discrete spectrum in the $\delta$-potential limit possesses only one energy level except for the situations when $G$ is an integer of $\pi$ and there are no confined states in the whole energy interval $E \in (-p_y, p_y)$:

\[
\begin{cases}
E = p_y \cos G, \quad G \in (2\pi n - \pi, 2\pi n) \\
E = -p_y \cos G, \quad G \in (2\pi n, 2\pi n + \pi).
\end{cases}
\]

However, there are three possibilities for the case $G = \pi n$, $n$ is an integer: potential possesses two shallow discrete levels near the boundaries of the continuum or one such energy level or none. This situation requires additional analysis and depends on the concrete potential.

The obtained spectrum \[21\] exactly coincides with the spectrum of the $\delta$-potential $U(x) = G \delta(x)$ which is considered in Appendix A. This correspondence serves as the reason for considered limit to be referred to the delta-potential limit in spite of the absence of any restrictions for the potential except the integrability. It yields the universality of this limit for any integrable potentials as soon as $p_y \ll 1/d$ where $d$ is the effective potential width (not the width of the wave function!). Notice that as it was maintained in papers \[32, 33\], the $\delta$-potential by itself concedes some ambiguities in the solutions. I proved in Appendix A the definiteness of the solution for this problem. Moreover, the direct integration of the Eq. \[17\] in the vicinity of $\delta$-peak yields $\Delta \Omega = 2G$ in the full agreement with the limiting case \[17\].

For example, the considered limit allows one to find the restriction on the potential strength $G$ which requires the zero-energy confined state $E = 0$:

\[
G = \pi \left( n + \frac{1}{2} \right), \quad (22)
\]

$n$ is an integer. Zero-energy confined modes and their importance in possible construction of 1D gated structures (waveguides) were discussed thoroughly in the paper \[31\] where the analytical solution for the case of the gate potential $V(x) = -U_0 / \cosh(x/d)$ is provided. Taking into account that $G = -\pi U_0 d$ I receive the condition of existence of zero-energy modes in the limit of small $p_y$:

\[
U_0 d = n + \frac{1}{2}
\]

where it is substituted $n \to -n - 1$ in Eq. \[22\]. These simple calculations exactly coincide with those derived from the analytical solution.

The bound states in the potential $V(x) = -U_0 / \cosh(x/d)$ for non-zero energy have been analytically studied in the recent paper \[34\]. One of the main statements of this paper is that there is a threshold value of the potential strength $G = \pi U_0 d > \pi/2$ for confined states to appear which contradicts to the non-relativistic limit and the limit of $\delta$-potential that are developed herein. Unconditionally, the considered potential easily acknowledges both of these limits which do prejudice the contents of the paper \[34\].

Some results of the paper \[35\] where the VPM is developed also (D. A. Stone et al. considered another phase function which satisfies a more complex equation) contradict my approach. In particular, they manifest that confined zero-energy modes are possible for arbitrary small power-law decaying potentials. I suppose that they made a mistake due to some difficulties of the convergence of their VPM equation because the restriction \[22\] analytically obtained here does not permit any integrable potential being arbitrarily small to possess zero-energy modes. Moreover, there is a mistake in the wave function asymptotics for exponentially decaying potentials $U(x \to \pm \infty) \sim \exp(-|x|/d)$ at $x \to -\infty$ (at $x \to +\infty$ the asymptotics are correct) which caused the wrong statement that there are no confined states in such potentials as long as $p_y < 1/d$. However, it apparently contradicts the limit $p_y \ll 1/d$ which guaranties the only discrete energy level for every potential with $G \neq \pi n$, $n$ being an integer.

To compare my results with one more exactly solvable problem, let me consider the potential $V(x) = U_0 \exp(-|x|/d)$ which is solved in \[35\]. My model predicts zero-energy modes when $2U_0 d = \pi(n + 1/2)$, in particular, the minimal value of the potential strength $(U_0 d)_{\text{min}} = \pi/4$ which exactly corresponds to the numerical result obtained by D. A. Stone et al. \[35\].

Due to the simplicity of this method, let me calculate the condition of zero modes existence for so-called top-gate potential $V_t(x)$ (see reference \[31\]):

\[
V_t(x) = \frac{U_0}{2} \ln \left( \frac{x^2 + (h_2 - h_1)^2}{x^2 + (h_2 + h_1)^2} \right)
\]

where parameters $h_1 < h_2$ depend on geometry of the gate electrodes. Namely, $h_1$ is a width of the insulator between the graphene plane and so-called back-gate electrode, $h_2$ is a distance between top and back electrodes. Applying Eq. \[22\] one receives the condition of zero mode existence:

\[
U_0 h_1 = \frac{1}{2} \left( n + \frac{1}{2} \right) \geq \frac{1}{4}.
\]

Notice that this condition does not depend on the parameter $h_2$ which determines the distance of the top electrode from the graphene sheet.

Hence, the $\delta$-potential limit is a powerful tool to study one-particle confined states in arbitrary integrable 1D gate potentials in graphene and it should be included in the analysis of bound states for concrete configuration of the gate potential to avoid possible misconceptions.
In this section, I formulate the oscillation theorem in terms of the phase function \( \Omega(x) \) as it has been done for the case of massive non-relativistic particles through the analysis of the scattering phase function \([16]\). Herein I suppose \( U(x) \) is an integrable function.

Let me consider two auxiliary solutions \( \Omega_{l,r}(x) \) (left and right separatrices) of Eq. (7) with the following boundary conditions:

\[
\begin{align*}
\Omega_l(x \to -\infty) &= \Omega_- = -\arcsin \frac{E}{p_y} \\
\Omega_r(x \to +\infty) &= \Omega_+ = \pi + \arcsin \frac{E}{p_y}.
\end{align*}
\] (24)

which exist for arbitrary energy \( |E| < p_y \). Separatrices are equivalent if conditions (24) are shifted to an integer of 2\( \pi \). Emphasize that \( \Omega_l(x) \equiv \Omega_- \) and \( \Omega_r(x) \equiv \Omega_+ \) in the absence of the potential: \( U(x) \equiv 0 \). Moreover, \( \Omega_l \) (\( \Omega_r \)) is unstable at negative (positive) infinity and asymptotically stable otherwise (exception is the separatrix degeneration described below). All other solutions of Eq. (7) are stable at both positive and negative infinities and come along asymptotes \( \Omega_+ (\Omega_-) \) at negative (positive) infinity.

From now on, set some integrable potential \( U(x) \). Comparing the conditions (24) on separatrices with the conditions (8) for confined states I arrive at the conclusion that the problem of the discrete spectrum could be reduced to the problem of the separatrix degeneration, namely, \( \Omega_l(x) \equiv \Omega_r(x) \). Degenerated separatrices represent the desirable solution for a bound state and corresponding parameter \( E \) is the discrete energy level in a given potential \( U(x) \).

Let me consider the behavior of separatrices, say \( \Omega_l(x) \), at continuous variation of the parameter \( E \). Define the full invariance of \( \Omega_l(x) \) as:

\[\Delta \Omega_l(E) = \Omega_l(x \to +\infty) - \Omega_l(x \to -\infty).\]

\(\Delta \Omega_l(E)\) is the bounded function in the segment \( |E| \leq p_y \) due to the integrability of the potential. Integrating Eq. (7) and taking into account the boundary condition for \( \Omega_l(x) \), one instantly arrives at the following relation:

\[\Delta \Omega_l(E) = 2G - 2p_y \int_{-\infty}^{\infty} (\sin \Omega_l(x) - \sin \Omega_l(-\infty)) dx, \] (25)

where \( G = \int_{-\infty}^{\infty} U(x) dx \). Substituting \( \Omega_l(x) = \Omega_- + \delta \Omega(x) \), one can find that \( \delta \Omega(x) \) satisfies Eq. (13) at \( x \to -\infty \) with the condition \( \delta \Omega(x \to -\infty) = 0 \). Omitting the quadratic term at any \( k \neq 0 \), I obtain the result (19) which involves that the integral in the right-hand side of Eq. (25) converges at \( x \to -\infty \) for every \(-p_y < E < p_y\). Actually, expanding \( p_y (\sin \Omega_l(x) - \sin \Omega_-) \approx k \cdot \delta \Omega(x) \) at \( x \to -\infty \), I finally receive:

\[k \int_{-\infty}^{x_0} \delta \Omega(x) dx = \int_{-\infty}^{x_0} U(x) dx - \frac{1}{2} \delta \Omega(x_0).\]

If \( k = 0 \) or equivalently \( E = \pm p_y \), the following expansion is valid:

\[p_y (\sin \Omega_l(x) - \sin \Omega_-) \approx \pm p_y, \delta \Omega^2(x)/2\]

where \( \delta \Omega(x) \) satisfies Eq. (11) with \( \varepsilon = 0 \). It indicates that \( \delta \Omega^2(x) \) vanishes, at least, as \( U(x) \) or faster which brings the proof of the boundedness of \( \Delta \Omega_l(E) \) at every \( |E| \leq p_y \).

The properties of the function \( \Delta \Omega_l(E) \) are given in the following:

**Theorem.** \( \Delta \Omega_l(E) \) is the piecewise constant function that undergoes finite jumps of \(-2\pi\) in the discrete energy levels \( E_d \):

\[|\Delta \Omega_l|_{E_d} = \Delta \Omega_l(E_d + 0) - \Delta \Omega_l(E_d - 0) = -2\pi.\]

For every \( E \neq E_d \), \( |E| < p_y \) \( \Delta \Omega_l(E) \) is the continuous function.

**Proof.** In order to find jumps of \( \Delta \Omega_l(E) \) at \( E = E_d \), let me consider the function \( \Omega_l(x) \) that corresponds to some discrete energy level \( E_d \) and, therefore, meets the conditions (8). Consider then separatrices \( \Omega_l(x, E_d + \varepsilon), \varepsilon \to 0 \) which declines from \( \Omega_l(x) \) slightly, at least, at \( x \to -\infty: \Omega_l(x, E_d + \varepsilon) = \Omega_l(x) + \delta \Omega_l(x) \). Expanding Eq. (7) and the boundary condition (24) for the separatrices \( \Omega_l \) to the first order of \( \varepsilon \), one can find:

\[
\begin{align*}
\delta \Omega_l' &= -2\varepsilon - 2p_y \cos \Omega_s \cdot \delta \Omega_l \\
\delta \Omega_l(x \to -\infty) &= -\varepsilon/k,
\end{align*}
\] (26)

where \( k = \sqrt{p_y^2 - E_d^2} \). The solution of the Cauchy problem (20) has the following form:

\[\delta \Omega_l(x) = -2\varepsilon \int_{-\infty}^{x} e^{2p_y \int_{y}^{x} \cos \Omega_s(y') dy'} dy.\] (27)

When \( x \to -\infty \) let me substitute \( p_y \cos \Omega_s(y') \) \( \to k = p_y \cos \Omega_s(-\infty) \) because \( y \leq y' \leq x \) and \( x \to -\infty \). Hence, one does get that at \( x \to -\infty: \delta \Omega_l \to -\varepsilon/k \).

According to my conceptions, \( \Omega_l(x) \) falls on the stable asymptote \( \Omega_- \) at \( x \to +\infty \) (Fig. 1) for arbitrarily small deviation \( \varepsilon \) from the exact energy of the confined state \( E_d \) (otherwise \( \Omega_l(x) \) coincides with \( \Omega_r(x) \) which is equivalent to the statement that \( E_d + \varepsilon \) is the exact discrete energy.
level which causes the contradiction). It involves $\delta \Omega_l(x)$ is not a small correction at $x \to +\infty$ even for infinitesimal $\varepsilon \neq 0$. Indeed, $p_y \cos \Omega_l(x) \to -k$ at $x \to +\infty$ which causes the exponential instability of the variation $\Omega^\prime_{l-2}$. Assume the substitution $p_y \cos \Omega_l(x) \approx -k$ is valid starting from some big positive point $x_0 \gg d$, $d$ is the width of the potential, and separate finite contribution to the integral $\Omega^{\prime\prime}_{l-2}$ at $y < x_0$ (which can be neglected at sufficiently small $\varepsilon$) and the divergent part at $y > x_0$, then at $x \gg x_0 \gg d$:

$$
\delta \Omega_l \to -2\varepsilon \int_{x_0}^{x} e^{-2k(y-x)} \, dy + O(\varepsilon) \approx -\frac{\varepsilon}{k} e^{2k(x-x_0)}.
$$

For sufficiently small $\varepsilon$ the correction $\delta \Omega_l(x)$ is still small even when $x \gg d$. Notice that in this case $\Omega_l(x)$ has almost reached the unstable asymptote $\Omega_\pm$. Hence, I will consider $\Omega_l(x \gg d)$ as a solution of Eq. (7) with the initial value $\Omega_l(x_0) = \Omega_\pm + \delta \Omega_l(x_0)$ at $x_0 \gg d$ where $U(x_0) \ll \delta \Omega_l(x_0)$ and $\Omega_l(x_0) - \Omega_\pm \ll \delta \Omega_l(x_0) < 1$. Under this circumstance, I conclude that $\Omega_l(x)$ falls on the nearest of the attractive asymptotes $\Omega_\pm$ at $x \to +\infty$. To determine the value of the gap I set only the sign of the variation $\delta \Omega_l(x_0)$ due to the instability of the asymptote $\Omega_\pm$ at $x \gg d$:

$$
\text{sign}(\delta \Omega_l) = -\text{sign}(\varepsilon)
$$

as it follows from Eq. (27). If the exact solution $\Omega_l(x)$ tends to some unstable asymptote $\Omega_\pm$, then $\Omega_l(x, E_d + \varepsilon)$ falls on the nearest asymptote $\Omega_- \leq (\Omega_\pm)$ below (above) this $\Omega_\pm$ when $\varepsilon > 0 \, (\varepsilon < 0)$, see Fig. 1. Thereby, the first statement of the theorem is proved: $|\delta \Omega_l|_{E_d} = -2\pi$.

To complete this proof, I have to verify that $\Delta \Omega_l(E)$ is the continuous function if $E$ does not belong to the discrete spectrum. Reductio ad absurdum. Let $\Delta \Omega_l(E)$ jump at some $E \neq E_d$, $|E| < p_y$. Since $E \neq E_d$ the separatrix $\Omega_l$ arrives at $x = +\infty$ along the stable at $x \to +\infty$ $\Omega_-$ asymptote. In contrast with the unstable solution $\Omega_s(x)$, the separatrix $\Omega_l(x)$ has the small variation $\delta \Omega_l(x, \varepsilon) = O(\varepsilon) \ll 1$ in the order of $\varepsilon$ at arbitrary $x$ even at $x \to +\infty$ because $\cos \Omega_l(x \to \pm \infty) = +k$ that provides the convergence of corresponding integral in Eq. (27) and thereby the continuity of $\Delta \Omega_l(E)$ at $E \neq E_d$. The fact that $\Omega_l(x)$ tends to $\Omega_-$ at $x \to +\infty$ involves that $\Delta \Omega_l(E) = 2\pi n, n$ is an integer. Which was to be proved.

Hence, the function $\Delta \Omega_l(E)$ plays the same role as the scattering phase in the non-relativistic theory. In other words, the theorem represents the relativistic Levinson theorem for the 2D Dirac equation with the 1D potential.

As a consequence, I arrive at the result which gives the total number of discrete energy levels at given $p_y$:

$$
N_d(p_y) = \frac{\Delta \Omega_l(p_y) - \Delta \Omega_l(-p_y)}{2\pi}.
$$

Actually, I can follow the number of discrete levels between any two given energies $|E_{1,2}| < p_y$:

$$
N_d(p_y, E_1, E_2) = \frac{|\Delta \Omega_l(E_2) - \Delta \Omega_l(E_1)|}{2\pi}.
$$

GEOMETRICAL INTERPRETATION OF THE RELATIVISTIC LEVINSON THEOREM

In order to apply the relativistic Levinson theorem and the consequences [23–26] I propose herein a simple approach to find the value of the function $\Delta \Omega_l(E)$ at the given parameter $E \in [-p_y, p_y]$. Thereto let me consider the following system:

$$
\begin{align*}
\Omega' &= 2(U(x) - E) - 2p_y \sin \Omega(x) \\
U'(x) &= G(U)
\end{align*}
$$

(30)

with the initial condition (24) for $\Omega_l(x)$. To define the function $G(U)$ I have to find the inverse function $U^{-1}(x)$ (or equivalently $x(U)$) on every interval of monotonicity $I_j$ of $U(x)$. Hence, I receive the autonomous system (20) for each of these intervals. Now, one is ready to determine the variance $\Delta \Omega_l(E)$ of the separatrix $\Omega_l(x)$ without solving Eq. (7) but just following the velocity fields:

$$
F_j(E) = \begin{pmatrix} U'(x) \\ \Omega'(x) \end{pmatrix} = \begin{pmatrix} G_j(U) \\ 2(U - E - 2p_y \sin \Omega) \end{pmatrix}
$$

(31)
induced by the system (30) which is autonomous on every interval \( I_j \). I assume that \( U(x) \) has the finite number of the intervals \( I_j, j = 1, \ldots, N \). Thus, \( U(x) \) is the monotonous function at \( x \to \pm \infty \). Notice that I have to match different pictures for adjacent intervals of monotonicity \( I_j, I_{j+1} \) to provide the continuity of the solutions of Eq. (7).

The asymptotes \( \Omega_{\pm} \) correspond to the stationary points \( (0, \Omega_{\pm}) \) of the vector fields \( \mathbf{F}_{1,N}(E) \) relating to the left and right infinite intervals of monotonicity \( I_1 \) and \( I_N \) for which \( G_{1,N}(0) = 0 \). If one moves along the positive direction of \( x \)-axis being on the interval \( I_1 \) or \( I_N \) streamlines flow into the point \( (0, \Omega_{-}) \) (drain) and flow out the point \( (0, \Omega_{+}) \) (source). When I follow only the separatrix \( \Omega_l(x) \) I have to slightly change the boundary condition (24) to come down from the stationary point \( (0, \Omega_{-}) \). Note that sufficiently small ambiguity in the initial condition and possible small errors in the matching conditions does not affect the result which follows from the piecewise-constant character of the function \( \Delta \Omega_l(E) \) (see the Theorem) and hence provides the error-resistant approach for the numerical calculations.

To make this picture clearer I give the following example. Consider the Lorentzian shaped potential \( U(x) = -U_0/(x^2 + 1) \) which does not acknowledge an exact analytical solution for the problem of bound states in the graphene devices. There are two intervals of monotonicity \( I_1 = (-\infty, 0) \) and \( I_2 = (0, +\infty) \) for the potential \( U(x) \). The inverse functions \( x_{1,2}(U) \) turn out to be calculated explicitly which yields for the functions \( G_{1,2}(U) \):

\[
G_n(U) = (-1)^n \frac{2U^2}{U_0} \sqrt{-\frac{U_0}{U} - 1}
\]

for the interval \( I_n, n = 1, 2, U \in (-U_0, 0) \).

From now on, set the parameters equal to \( p_y = 0.1, U_0 = 1 \). To find the number of confined modes I have to know the values of the function \( \Delta \Omega_l(E) \) only on the boundaries of the continuum \( E = \pm p_y \) where stationary points \( (0, \Omega_{-}) \) and \( (0, \Omega_{+}) \) merge. Pictures (Fig. 2,3) of the vector field \( \mathbf{F}_{1,2}(E = p_y) \) show the approximate trajectories \( (U, \Omega_l(x_{1,2}(U))) \) (red lines) for two intervals \( I_{1,2} \). I chose the point \( (U = -10^{-6}, \Omega = -\pi/2 + 0.05) \) as the initial condition for the trajectory \( (U, \Omega_l(x_{1}(U))) \) on the interval \( I_1 \). Matching trajectories corresponding to the intervals \( I_1 \) and \( I_2 \) (black points on Fig. 2,3) I finally obtain the variance \( \Delta \Omega_l(p_y) = -4\pi \). Analogically, drawing such pictures for \( E = -p_y \) I receive \( \Delta \Omega_l(p_y) = 0 \). Applying Eq. (28) one can find that considered potential possesses \( N_0(p_y) = 2 \) confined energy levels for \( p_y = 0.1 \).

There is no difference to apply the given approach in order to find graphically \( \Delta \Omega_l(E) \) for any other value of the energy parameter \( |E| \leq p_y \).

Pass on to the new variables \( X(U, \Omega) = (|U| + a) \cos \Omega, Y(U, \Omega) = (|U| + a) \sin \Omega, a > 0 \) is arbitrary para-
The initial condition for the separatrix $\Omega_l(x)$ yields $X_0 = a \cos \Omega_-$ and $Y_0 = a \sin \Omega_-$ for the interval $I_1$. If $|E| < p_y$, $E \neq E_d$, $E_d$ is the exact energy of the discrete level, $\Omega_l(x \to +\infty) = \Omega_- + 2\pi n$, $n$ is an integer which means that the trajectory corresponding to $\Omega_l(x)$ is closed in $(X,Y)$ plane. This is valid for $\Omega_r(x)$, as well. Meanwhile, all other solutions of the Eq. (7) are represented by an open trajectories because $\Omega_+ \neq \Omega_-$ for every $|E| < p_y$. Hence, the separatrices $\Omega_{l,r}(x)$ are the only solutions of the Eq. (7) which have closed trajectories in $(X,Y)$ plane for any $|E| < p_y$, $E \neq E_d$. For the boundaries $E = \pm p_y$ all trajectories are closed because $\Omega_+ = \Omega_-$. As it follows from aforesaid, $\Delta\Omega_l(E) = 2\pi n$ where $n$ is the number of full rotations of the closed trajectory corresponding to the separatrix $\Omega_l(x)$. In other words, $n$ is the Poincare index of this closed trajectory [36].

CONCLUSIONS

The variable phase method has been developed herein for the electrostatically confined 2D massless Dirac-Weyl particles such as electrons in graphene devices. The desirable phase function $\Omega(x)$ appears as the phase between two chiral states whose superposition yields the wave function of the confined state. Besides the well-known non-relativistic and semi-classical limits, it has been shown that confined states with small $p_y \ll 1/d$, $d$ being the width of the potential, are successfully described in so-called $\delta$-potential limit that is valid for every integrable potential $U(x)$ which possesses only one confined mode with given small $p_y$. Then, the relativistic Levinson theorem has been formulated and proved for the variance $\Delta\Omega_l(E)$ of the separatrix $\Omega_l(x)$ of Eq. (7). As a consequence of the theorem, the number of confined modes with given $p_y$ has been obtained. Finally, the geometrical approach to find the function $\Delta\Omega_l(E)$ has been suggested.

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APPENDIX A: UNAMBIGUOUS SOLUTION OF THE $\delta$-POTENTIAL

I found in the literature that the 2D Dirac-Weyl equation does not possess unambiguous solutions for the case of the local potential $U(x) = G\delta(x)$ [32, 33]. This problem arises from the fact that the wave function is discontinuous at $x = 0$ which results in the ambiguous integral of the type

$$\int_{-\epsilon}^{\epsilon} \delta(x)\theta(x) \, dx$$

which takes arbitrary value from the segment $[0,1]$, $\theta(x)$ is the Heaviside step function, $\epsilon \to +0$. This problem is passed round by A. Calogero et al. [3]. They represented the wave function $\Psi(x)$ as the $x$-ordered exponent (the analogue of the evolution operator) acting on the wave function in the initial point $x_0$. I cite herein the exact solution of Eq. (3) in order to demonstrate explicitly the absence of any ambiguities.

Let me start the consideration from Eq. (3):

$$g''(x) + 2i(E - G\delta(x))g'(x) - p_y^2 g(x) = 0.$$  \hspace{1cm} (32)

The function $g(x)$ appears to be continuous, $g'(x)$ is discontinuous at $x = 0$. Assume that $g'(\pm 0) \neq 0$ and divide this equation over the function $g'(x)$, $x \in I_\epsilon = (-\epsilon, \epsilon)$. Integrating then this equation over the interval $I_\epsilon$ and taking the limit $\epsilon \to +0$ I arrive at the correct matching condition:

$$\frac{g'(+0)}{g'(-0)} = e^{2iG}.$$  \hspace{1cm} (33)

If one is interested in the discrete spectrum of this problem one has to apply the condition (33) to the function $g(x) = g_0 e^{-iE_x e^{-k|x|}}$ which represents the common form of the continuous at $x = 0$ bounded solution of Eq. (32), $k = \sqrt{p_y^2 - E^2}$. This yields explicitly the spectrum [21]. The initial assumption $g'(\pm 0) \neq 0$ is obviously valid for such functions $g(x)$.

If one considers the scattering problem with definite $|E| > p_y$, the continuous function $g(x)$ has the following form:

$$g(x) = \begin{cases} Ae^{i\pi(k-E)} + Be^{-i\pi(k+E)}, & x < 0, \\
(A+B)e^{i\pi(k-E)}, & x > 0, \end{cases}$$

$$k = \sqrt{E^2 - p_y^2}. \quad \text{Applying the condition (33) one can receive the transmission coefficient:}$$

$$T = \left| 1 + \frac{B}{A} \right|^2 = \frac{k^2}{k^2 + p_y^2 \sin^2 G}.$$  

Finally, I have to check that the initial assumption $g'(\pm 0) \neq 0$ is not violated. $g'(\pm 0) \neq 0$ as far as $E \neq k$ when $p_y \neq 0$. Suppose then that $g'(0) = 0$ which leads to $A(k-E) = B(k+E)$ or equivalently $T = 4k^2/(k+E)^2$ which has no physical sense because the transmission coefficient $T$ has to be dependent on the parameter $G$ and satisfy the condition $T(G \to 0) = 0$. Hence, the unambiguous solution for the case of the $\delta$-potential is provided.
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