

ANALYTICAL STUDY OF BOUND STATES IN GRAPHENE NANORIBBONS AND CARBON NANOTUBES: THE VARIABLE PHASE METHOD AND THE RELATIVISTIC LEVINSON THEOREM

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The problem of localized states in 1D systems with a relativistic spectrum, namely, graphene stripes and carbon nanotubes, is studied analytically. The bound state as a superposition of two chiral states is completely described by their relative phase, which is the foundation of the variable phase method (VPM) developed herein. Based on our VPM, we formulate and prove the relativistic Levinson theorem. The problem of bound states can be reduced to the analysis of closed trajectories of some vector field. Remarkably, the Levinson theorem appears as the Poincaré index theorem for these closed trajectories. The VPM equation is also reduced to the nonrelativistic and semiclassical limits. The limit of a small momentum p_y of transverse quantization is applicable to an arbitrary integrable potential. In this case, a single confined mode is predicted.

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1. INTRODUCTION

Graphene, carbon nanotubes, and topological insulators have recently attracted keen attention as subjects of intensive theoretical and experimental research. The uniqueness of these quantum materials in fundamental physics consists in the opportunity to observe QED effects with a large coupling constant $g = e^2/s\hbar\varepsilon \sim 1$, where $s \approx c/300$ is the Fermi velocity and ε is the average dielectric constant of the environment (for instance, $\varepsilon = (1+\varepsilon_s)/2$ for a graphene sheet on a substrate with the dielectric constant ε_s). Effects such as the atomic collapse and pair production in supercritical potentials [1–7] and the Adler–Bell–Jackiw anomaly (the chiral anomaly) [8, 9] have been intensively studied. The Klein tunnelling of electrons in gated graphene [10–15] reveals the complete suppression of backscattering.

In this paper, we are concerned with the general theoretical study of confined electronic states in graphene nanoribbons or single-walled carbon nanotubes affected by a longitudinal electric field. Omitting the inter-valley scattering, we consider the electron behavior near one of two independent Dirac points where electrons are well described by Dirac–Weyl Hamiltonian (1) in the one-particle approach.

We 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 Morse and Allis [16], Babikov [17], Calogero [18], and others [19–21]. 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. A reduction to the nonrelativistic and semiclassical limits is then demonstrated. In what follows, we consider one more limit case, that of a δ-potential, which is applicable to any integrable potential at a sufficiently small transverse momentum p_y. Physically, this limit contains both the shallow quantum-well limit and the opposite limit of a strongly supercritical potential.

Our VPM allows formulating a relativistic analogue of the Levinson theorem [22]. The relativistic Levinson theorem for the Dirac equation was formulated in three dimensions by Klaus [23] for central potentials, and by Hayashi [24], and Warnock [25] as a relation be-

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tween zeroes of the vertex function and particle poles of the total amplitude. This problem has been considered in two dimensions with a compactly supported central potential [26]. Clemence [27] thoroughly investigated the Levinson theorem for the Dirac equation with a 1D potential that satisfies the condition $\int_{-\infty}^{\infty} U(x)(1+|x|)\,dx < \infty$ via the scattering matrix approach, taking the half-bound states into account. The particular case of the relativistic Levinson theorem for the symmetric 1D potentials has been studied by Lin [28] with the additional restriction for the potential to be a compactly supported function, Calogeracos and Dombey [29] for potentials of definite sign, and Ma et al. [30] with a condition similar to that in [27]. The method developed in this paper permits us to prove the Levinson theorem with the minimal restriction $\int_{-\infty}^{\infty} U(x)\,dx < \infty$, which significantly broadens the result obtained by Clemence. For example, our results are applicable to so-called top-gate potential (30), whose asymptotic form is expected to be realistic for gated graphene structures [31]. A geometric interpretation of the Levinson theorem and the corresponding numerical method for the analysis of integral curves of some vector field are also considered.

2. THEORETICAL MODEL

Near conic points, electrons in graphene with a gated potential $U(x)$ are approximately described by the Dirac–Weyl Hamiltonian

$$\hat{H} = s\boldsymbol{\sigma}\hat{\mathbf{p}} + U(x) = s\sigma_x\hat{p}_x + s\sigma_y\hat{p}_y + U(x), \qquad (1)$$

where s is the Fermi velocity, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ are Pauli matrices, and $\mathbf{p} = -i\hbar\boldsymbol{\nabla}$. 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 that $p_y > 0$, where p_y is the quantized transverse momentum of quasi-1D systems such as graphene nanoribbons and single-walled carbon nanotubes (for nanotubes, $y = r\phi$, where r is the radius and ϕ is a cyclic variable). The spectrum of the free-particle Hamiltonian is linear in 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

$$\Psi = \frac{\exp(ip_y y)}{\sqrt{4W}} \begin{pmatrix} g(x) + p_y^{-1}g'(x) \\ g(x) - p_y^{-1}g'(x) \end{pmatrix} \times \exp\left\{ i\int^{x} (E - U(\zeta))\, d\zeta \right\} \qquad (2)$$

in terms of the axillary function $g(x)$ introduced in [14]:

$$g''(x) + 2i\,(E - U(x))\,g'(x) - p_y^2 g(x) = 0, \qquad (3)$$

where E is the electron energy and W is the normalization coefficient. Equation (3) represents an equivalent statement of the problem described by Hamiltonian (1). In what follows, we deal with electronic states of zero current along the x direction.

We apply this condition to the analysis of confined states. A zero flow $j_x = \Psi^\dagger(x)\sigma_x\Psi(x) = 0$ along the x direction yields a restriction on the function $g(x)$:

$$|g(x)| = |p_y^{-1}g'(x)|. \qquad (4)$$

The first consequence is that $g(x)$ and hence the electron density of confined states $\rho(x) = \Psi^\dagger(x)\Psi(x) = |g(x)|^2/W$ vanish nowhere except infinity. Otherwise, it follows from (4) that $g(x_0) = g'(x_0) = 0$, where $|x_0| < \infty$ is some point, which yields $g(x) \equiv 0$.

Separating the modulus and phase by writing $g(x) = R\exp(i\Phi)$, we arrive at the condition

$$(\Phi')^2 + (R'/R)^2 = p_y^2, \qquad (5)$$

which admits the substitution

$$\begin{aligned} \Phi'(x) &= p_y \sin\Omega(x), \\ R'/R &= p_y\cos\Omega(x), \end{aligned} \qquad (6)$$

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

$$\Omega'(x) = 2\,(U(x) - E) - 2p_y\sin\Omega(x). \qquad (7)$$

Thereby, we arrive at the desired VPM equation. We emphasize here that Eq. (7) is valid for any quantum state with zero flow, not only for bound states.

Considering bound states, we have to set the boundary conditions for the function $\Omega(x)$:

$$\begin{aligned} \Omega(x\to+\infty) &= \pi + \arcsin\frac{E}{p_y} + 2\pi n, \\ \Omega(x\to-\infty) &= -\arcsin\frac{E}{p_y}. \end{aligned} \qquad (8)$$

For $E \in (-p_y, p_y)$, these conditions ensure the exponential decay of the density $\rho(x) \sim R^2(x)$ at infinity, as it follows from (6), with n being an integer.

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

$$\Psi(x,y) = \frac{e^{ip_y y}}{\sqrt{4W}} \left(\begin{pmatrix} 1 \\ 1 \end{pmatrix} + e^{i\Omega} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right) R(x) e^{-i\Omega/2}. \quad (9)$$

Hence, a 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 Ω and the azimuthal angle $-\pi/2$:

$$\Psi(x,y) = \frac{R(x)e^{ip_y y}}{\sqrt{W}} \begin{pmatrix} \cos\dfrac{\Omega}{2} \\ -i\sin\dfrac{\Omega}{2} \end{pmatrix}. \quad (10)$$

3. NONRELATIVISTIC LIMIT

We show that Eq. (7) can be reduced to a nonrelativistic equation. To be more specific, we consider the nonrelativistic limit for electrons:

$$E = p_y + \varepsilon,$$
$$\varepsilon = -k^2/2p_y,$$

where all energy scales are understood to be small compared with p_y: $k, U(x), 1/d \ll p_y$, and d is the characteristic width of the confinement. Boundary conditions (8) for $\Omega(x)$ take the form

$$\Omega(-\infty) = -\frac{\pi}{2} + \frac{k}{p_y}, \quad \Omega(+\infty) = -\frac{\pi}{2} - \frac{k}{p_y} + 2\pi n$$

with n being an integer.

We now suppose that $\Omega(x) = -\pi/2 + \delta\Omega$, where $\delta\Omega \ll 1$ almost everywhere. This assumption is violated only when $\Omega' \sim p_y$, which corresponds to $\delta\Omega \sim 1$. The behavior of the phase function $\Omega(x)$ in this region does not depend on the potential because $U(x) \ll p_y$. We note that the width of this region $\delta x \sim 1/p_y \ll d$ is small in the nonrelativistic limit. Hence, the expansion of the initial equation (7) results in the Riccati equation:

$$\delta\Omega' = 2(U(x) - \varepsilon) - p_y \delta\Omega^2, \quad (11)$$

where $\psi(x) = \exp\left(p_y \int \delta\Omega(x)\,dx\right)$ satisfies the 1D Schrödinger equation for a non-relativistic particle with the mass p_y. The function $\delta\Omega(x)$ tends to infinity at zeros of the wave function $\psi(x)$.

4. SEMICLASSICAL LIMIT

We rewrite Eq. (7) in terms of dimensional quantities:

$$\hbar\Omega' = \frac{2}{s}\left(U(x) - E\right) - 2p_y \sin\Omega, \quad (12)$$

where s is the Fermi velocity. In the semiclassical limit $\hbar \to 0$, neglecting the left-hand side of this equation yields

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

We show that Eq. (13) represents the usual semiclassical approach.

This approximation is solvable in terms of real-valued functions when $|U(x) - E| < sp_y$, which conforms to the case of nonclassical motion where the wave function decays. At the breakpoints x_i where $U(x_i) - E = -\mu s p_y$, we define $\Omega(x_i) = -\mu\pi/2$, where $\mu = \pm 1$ is fixed 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, $\Omega(x) = -\mu\pi/2 + i\delta\Omega$:

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

Equation (14) has two solutions $\pm\delta\Omega$ (for definiteness, we set the first solution $\delta\Omega \geq 0$). The corresponding amplitude of the wave function $R_\pm(x)$ is determined from Eq. (6):

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

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

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

as follows from Eq. (6), and Φ is the same for two different solutions of Eq. (14). Finally, the semiclassical amplitude is given by

$$R(x) \sim \cos\left(\int p_x\frac{dx}{\hbar} + \phi_0\right), \quad (15)$$

where the semiclassical momentum

$$p_x = p_y\sinh\delta\Omega(x) = \sqrt{\left(E - U(x)\right)^2/s^2 - p_y^2}$$

is introduced. The phase ϕ_0 is defined by the matching conditions.

Hence, the Bohr–Sommerfeld quantization takes the usual form

$$\oint p_x dx = 2\pi\hbar(n+\gamma), \qquad (16)$$

where $n \gg 1$ is an integer, and $\gamma \sim 1$ is defined from the matching conditions at the turning points, for example, $\gamma = 1/2$ for smooth potentials. The semiclassical approximation is valid when $\hbar p_y U'(x) \ll s p_x^3$.

5. DELTA-POTENTIAL LIMIT

Before we start, we emphasize that we do not require the confinement potential $U(x)$ to be δ-like. The reason why we call this limit the delta-potential limit is that under some conditions, the discrete spectrum and corresponding wave functions of any integrable potential are of the same analytic form as for the literal δ-potential, which is considered in Appendix.

In this section, we are interested in all possible cases where the nonlinear term in Eq. (7) can be neglected. This allows finding the spectrum and corresponding wave functions exactly. We formulate the following theorem.

Theorem. Let the potential $U(x)$ be an integrable function, d be the characteristic width of $U(x)$, and $p_y > 0$ be transverse momentum. We introduce the integral

$$G = \int\limits_{-\infty}^{\infty} U(x)\,dx = \pi(n_G + \delta n_G), \qquad (17)$$

where n_G is an integer and $\delta n_G \in [0,1)$; we also assume that $\delta n_G \neq 0$.

Let the condition

$$p_y d \ll \min\{\delta n_G, 1-\delta n_G\} \qquad (18)$$

hold. Then

a. The discrete spectrum contains only one level with an energy $E \in (-p_y, p_y)$:

$$E = (-1)^{n_G+1} p_y \cos G. \qquad (19)$$

b. If additionally $\int_{x_0}^{x} U(x')x'\,dx'$ converges as $x \to \to \pm\infty$ at some $|x_0| < \infty$, then the corresponding wave function takes form (10) with the phase function

$$\Omega(x) = -\arcsin\frac{E}{p_y} + 2\int\limits_{-\infty}^{x} U(x')\,dx'. \qquad (20)$$

Proof. We here mean $U(x)$ be integrable in the sense that the primitive integral

$$f_{x_0}(x) = \int\limits_{x_0}^{x} U(x')\,dx'$$

with some $|x_0| < \infty$ is defined for any $x \in (-\infty, +\infty)$ except maybe at a finite set of points and $f_{x_0}(x)$ is bounded function. We set the parameter $E \in \in (-p_y, p_y)$.

• Let $\Omega(x)$ be a physical solution with boundary conditions (8). Then the total variance of the phase function $\Delta\Omega = \Omega(+\infty) - \Omega(-\infty)$ is straightforward to obtain from (8):

$$\Delta\Omega = 2\arcsin\frac{E}{p_y} + 2\pi\left(n + \frac{1}{2}\right). \qquad (21)$$

On the other hand, the integration of Eq. (7) yields

$$\Delta\Omega = 2G + \mathfrak{K}, \qquad (22)$$

where n is an integer and we introduce the integral

$$\mathfrak{K} = \int\limits_{-\infty}^{\infty} 2(E + p_y \sin\Omega(x))\,dx. \qquad (23)$$

Convergence of $\mathfrak{K}$

We use Lemma 2 about the properties of solutions of Eq. (7) and rewrite $\mathfrak{K}$:

$$\mathfrak{K} = 2p_y \int\limits_{-\infty}^{\infty} (\sin\Omega(x) - \sin\Omega_\pm)\,dx.$$

We know from Lemma 2 that the physical solution corresponds to a degeneration of two separatrix families of Eq. (7). We consider the behavior of this physical solution as $x \to -\infty$, where we can represent it in the form

$$\Omega(x) = \Omega_- + \delta\Omega(x).$$

As $x \to -\infty$, $\delta\Omega(x)$ satisfies the approximate equation that follows directly from Eq. (7):

$$\delta\Omega'(x) \approx 2U(x) - 2k\delta\Omega(x),$$

where we took into account that $p_y \cos\Omega_- = k > 0$, $k = \sqrt{p_y^2 - E^2}$. The solution that satisfies the initial condition $\delta\Omega(-\infty) = 0$ is given by

$$\delta\Omega(x) = 2\int\limits_{-\infty}^{x} U(x')e^{-2k(x-x')}\,dx'. \qquad (24)$$

We use it to analyze the convergence of $\mathfrak{K}$ at $-\infty$. If $x \to -\infty$, we can use the expansion $p_y(\sin\Omega(x) - \sin\Omega_-) \approx k\delta\Omega(x)$. Then we obtain

$$2p_y \int\limits_{-\infty}^{x} (\sin\Omega(x') - \sin\Omega_-)\, dx' \approx \approx 2k \int\limits_{-\infty}^{x} \delta\Omega(x')\, dx' = 2\int\limits_{-\infty}^{x} U(x')\, dx' - \delta\Omega(x).$$

This proves the convergence of $\mathfrak{K}$ at $-\infty$ if $U(x)$ is an integrable function. We can prove the convergence at $+\infty$ similarly. Hence, $\mathfrak{K}$ converges.

Estimation of $\mathfrak{K}$

The convergence allows us to introduce some characteristic scale $D(\varepsilon)$, the diameter of the convergence domain of $\mathfrak{K}$. Mathematically, for any $\varepsilon > 0$, a number $0 < D(\varepsilon) < \infty$ exists such that

$$\left| \mathfrak{K} - 2p_y \int\limits_{-D(\varepsilon)/2}^{D(\varepsilon)/2} (\sin\Omega(x) - \sin\Omega_\pm)\, dx \right| < \varepsilon.$$

We consider only those cases where we can omit $\mathfrak{K}$ in Eq. (22). We then estimate it by the order of magnitude. As we can see from the convergence proof, the integrals $\mathfrak{K}$ and G converge simultaneously. Then

$$\mathfrak{K} \sim O(p_y d), \tag{25}$$

where d is a characteristic convergence length of the integral G or, as we mentioned in the statement of the theorem, the characteristic length of confinement.

Now we are ready to prove the theorem.

a. Combining Eqs. (21) and (22), we obtain

$$\arcsin\frac{E}{p_y} = \pi\left(\delta n_G + \frac{\mathfrak{K}}{2\pi} - \frac{1}{2} + n_G - n\right). \tag{26}$$

If condition (18) is satisfied, we can omit $\mathfrak{K}$ in Eq. (26). We can then set $n = n_G$ because $\arcsin x \in [-\pi/2, \pi/2]$, which finally gives

$$\arcsin\frac{E}{p_y} = \pi\left(\delta n_G - \frac{1}{2}\right).$$

This is equivalent to Eq. (19).

b. To obtain the wave function, we can naively neglect the influence of the non-linear term in Eq. (7). Then the approximate solution is

$$\Omega_0(x) = \Omega_- + 2\int\limits_{-\infty}^{x} U(x')\, dx',$$

which coincides with (20). But this approximation is valid when there is no divergence in the next correction of the order of $p_y d$. This correction can be estimated as

$$\Omega_1(x) = = -2p_y \int\limits_{-\infty}^{x} (\sin\Omega_0(x) - \sin\Omega_-)\, dx' + \Omega_1(-\infty),$$

where we assume that the integral converges. We check the convergence at $x \to -\infty$:

$$\Omega_1(x) \approx -2k \int\limits_{-\infty}^{x}\int\limits_{-\infty}^{x'} U(x'')\, dx'\, dx'' + \Omega_1(-\infty),$$

where the double integral reduces to $\int_{-\infty}^{x} U(x')x'\, dx'$, which means that we can use approximate wave function (20) only when $xU(x)$ is integrable. This is not surprising because for the convergence of $\mathfrak{K}$ with an integrable $U(x)$, we required the exponential decay of $\Omega(x)$ to Ω_- as $x \to -\infty$, as is shown in Eq. (24). This means that we cannot neglect the dependence of the wave function on k and hence we are not allowed to use approximate wave function (20) if $U(x)$ is integrable but $xU(x)$ is not. However, spectrum (19) is valid even if $xU(x)$ is nonintegrable but $U(x)$ is integrable and condition (18) is satisfied.

Physically, this limit can be understood as a supercritical regime for the confinement potential $U(x)$. Indeed, we imagine that $U(x)$ is a quantum well with the characteristic depth U_0 and width d. Then $\pi\delta n_G \lesssim G \sim U_0 d$ and condition (18) gives $U_0 \gg p_y$, which corresponds to the strong supercritical regime!

Hence, once condition (18) holds, we obtain

$$\arcsin\frac{E}{p_y} \approx G - \pi\left(n + \frac{1}{2}\right) \tag{27}$$

for any integrable potential.

□

We did not consider the cases $G = \pi n_G$, n_G is an integer, because they require a finer analysis than the one presented above.

Zero-energy states

We compare our results with some recent analytic work on graphene states. As an example, we consider the condition for the existence of confined modes with zero energy (exactly at the Dirac point). Zero-energy confined states and their importance in a possible construction of 1D gated structures (waveguides) were discussed thoroughly in [31].

In accordance with Eq. (27), we arrive at the desired restriction if Eq. (18) holds:

$$G = \pi \left(n + \frac{1}{2} \right) \tag{28}$$

with an integer n. This constraint means that we cannot have zero-energy confined states at an arbitrarily small potential strength G. However, at any $G \neq \pi n$, we have at least one bound state!

In [31], an analytic solution for zero-energy modes in the gate potential $V(x) = -U_0/\cosh(x/d)$, $U_0 > 0$, is given. Taking into account that $G = -\pi U_0 d$ in this case, we arrive at the condition for the existence of a zero-energy mode in the limit of small p_y:

$$U_0 d = n + \frac{1}{2},$$

where n is a nonnegative integer. Hence, we cannot have confined zero-energy modes if $|U_0 d| < 1/2$, which exactly coincides with the condition obtained analytically in [31].

A thorough analytic study of bound states in the potential

$$V(x) = -U_0/\cosh(x/d) \tag{29}$$

for nonzero energies has been done in recent paper [32]. The authors claim that there is a threshold value of the potential strength $G = \pi U_0 d > \pi/2$ for the first confined state to appear. We suppose that something essential is missed in [32] because this strong statement immediately contradicts the nonrelativistic limit and the limit of a δ-potential that are developed in this paper.

We now compare our VPM method with the one developed by Stone et al. [33]. They considered another phase function, which satisfies a more complex equation. One of the substantial points in their paper is that the zero-energy mode exists for arbitrarily small power-law decaying potentials (decaying faster than $1/x$). Again, this statement strongly contradicts Eq. (28). Moreover, their asymptotic analysis resulted in no bound states for potential (29) if $p_y < 1/d$. It apparently contradicts our δ-limit.

Finally, we consider the potential $V(x) = U_0 \times \exp(-|x|/d)$. The zero-energy mode condition was found analytically in [33], where the minimal potential strength is stated as $(U_0 d)_{min} = \pi/4$. Our model predicts zero-energy modes when $2U_0 d = \pi(n + 1/2)$, in excellent agreement with the analytic solution.

Due to the simplicity of our method, we can calculate the existence condition for the zero-energy mode for the so-called top-gate potential (see [31])

$$V_t(x) = \frac{U_0}{2} \ln \left(\frac{x^2 + (h_2 - h_1)^2}{x^2 + (h_2 + h_1)^2} \right), \tag{30}$$

where parameters $h_1 < h_2$ depend on geometry of the gate electrodes. Namely, h_1 is the width of the insulator between the graphene plane and the so-called back-gate electrode, and h_2 is the distance between the top and back electrodes. Using Eq. (28), we obtain the existence condition for the zero mode:

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

We note that this condition does not depend on the larger parameter h_2, which in our case determines the distance between electrodes.

Hence, the δ-potential limit is a simple and powerful tool to study one-particle confined states in arbitrary integrable 1D gate potentials in graphene stripes, and it should be included in the analysis of bound states for a concrete configuration of the gate potential to avoid possible misconceptions.

6. RELATIVISTIC LEVINSON THEOREM

In this section, we formulate the oscillation theorem in terms of the phase function $\Omega(x)$, as has been done in the case of massive non-relativistic particles through the analysis of the scattering phase function [16].

But before stating the main theorem, we give some properties of solutions of Eq. (7).

Lemma 1 (of continuity). Let $f_{x_0}(x) = \int_{x_0}^{x} U(x')\,dx'$, where $|x_0| < \infty$ is some constant. Let $f_{x_0}(x) \in C^k$, where k is a nonnegative integer, and C^k is the kth class of differentiability. Then every solution of Eq. (7) belongs to C^k.

Proof. By induction.

a. If $k = 0$, $f_{x_0}(x)$ is continuous function. This is equivalent to the condition $\int_x^{x+\epsilon} U(x')\,dx' \to 0$ as $\epsilon \to 0$ at arbitrary $x \in (-\infty, \infty)$. We then integrate Eq. (7) from x to $x + \epsilon$:

$$|\Omega(x+\epsilon)-\Omega(x)| = \left|2\int\limits_x^{x+\epsilon} U(x')\,dx' - \right.$$
$$\left. -\,2\int\limits_x^{x+\epsilon}(E+p_y\sin\Omega(x'))\,dx'\right| \le$$
$$\le 2\left|\int\limits_x^{x+\epsilon} U(x')\,dx'\right| + 2\epsilon(p_y+|E|) \to 0$$

which confirms the continuity of any solution of Eq. (7).

b. We assume that the statement of the lemma is true at all $k < n$, where n is a positive integer. Let $f_{x_0}(x) \in C^n$. We then prove the Lemma at $k = n$. We differentiate Eq. (7) $n-1$ times:

$$\Omega^{(n)}(x) = f_{x_0}^{(n)}(x) - 2(E + p_y\sin\Omega(x))^{(n-1)},$$

where $f_{x_0}^{(n)}(x)$ is continuous by the condition of the lemma, and $2(E+p_y\sin\Omega(x))^{(n-1)}$ is continuous by the induction hypothesis because it contains derivatives of $\Omega(x)$ not higher than $n-1$. Then $\Omega^{(n)}(x)$ is a continuous function, or $\Omega(x) \in C^{(n)}$.

□

We need to make one additional comment. If $f_{x_0}(x)$ is a piecewise-continuous function (which means that $U(x)$ has δ-like singularities at discontinuity points), then all solutions of Eq. (7) are piecewise-continuous with the same discontinuity points as in $f_{x_0}(x)$. In other words, the statement of Lemma 1 is valid even if $f_{x_0}(x)$ is a piecewise-continuous function.

Lemma 2 (of attractors and repellors) Let $U(x) \to \to 0$ as $x \to \infty$, and $E \in (-p_y, p_y)$. Then

a. All solutions of Eq. (7) at infinity tend to stationary points of the free motion equation (i. e., with a zero potential).

b. There are two families of stationary points:

$$\begin{aligned} \Omega_- &= -\arcsin\left(\frac{E}{p_y}\right) + 2\pi n, \\ \Omega_+ &= \arcsin\left(\frac{E}{p_y}\right) + 2\pi\left(n+\frac{1}{2}\right). \end{aligned} \tag{31}$$

c. Ω_+ (Ω_-) is an attractor (repellor) at $x \to -\infty$; Ω_+ (Ω_-) is a repellor (attractor) at $x \to +\infty$.

d. There are two types of separatrix solutions, which are defined by following Cauchy problems:

$$\begin{cases} \Omega_l(x\to-\infty) = \Omega_-, \\ \Omega_r(x\to+\infty) = \Omega_+. \end{cases} \tag{32}$$

We call $\Omega_l(x)$ ($\Omega_r(x)$) the left (right) separatrix.

e. The bound-state problem is equivalent to the degeneracy of two separatrix families Ω_l and Ω_r.

Proof. a. We first consider the free motion equation

$$\Omega'(x) = -2p_y\left(\sin\Omega(x) + \frac{E}{p_y}\right). \tag{33}$$

This equation has stationary points $\Omega(x) \equiv \text{const}$ if $\sin\Omega = -E/p_y$. Every solution of Eq. (33) tends to Ω_+ (Ω_-) as $x \to -\infty$ ($x \to +\infty$), where $\Omega_\pm$ are defined in (31). Moreover, $\Omega_\pm$ are solutions by themselves. However, there are no physical solutions among the solutions of the free motion equation because it is impossible to satisfy physical boundary conditions (8).

If $U(x) \to 0$ as $x \to \infty$, then the asymptotic form of solutions at infinity resembles those of the free motion equation. Thus, **a** is proven.

b. Two families of stationary points of the free motion equation (which represent the whole set of attractors and repellors of Eq. (7)) obviously arise from the equation $\sin\Omega_\pm = -E/p_y$.

c. We demonstrate that Ω_+ are repellors as $x \to \to +\infty$ and attractors as $x \to -\infty$. We consider the solution that comes close to Ω_+ at some point x^* and represent it in the form $\Omega(x) = \Omega_+ - \epsilon + \delta\Omega(x)$, $\delta\Omega(x^*) = 0$, where ϵ is a small deviation from Ω_+ at $x = x^*$. Substituting it in Eq. (7) and expanding in view of the smallness of $\delta\Omega(x)$ in the vicinity of x^* yields

$$\delta\Omega'(x) \approx 2U(x) + 2k(\delta\Omega(x) - \epsilon), \tag{34}$$

where we used the relation $p_y\cos\Omega_+ = -k$, $k = = \sqrt{p_y^2 - E^2} > 0$. The solution with an appropriate boundary condition is

$$\delta\Omega(x) = 2\int\limits_{x^*}^{x} U(x')e^{2k(x-x')}\,dx' + \\ + \epsilon\left(1 - e^{2k(x-x^*)}\right). \tag{35}$$

In the region $x > x^*$, both terms in (35) diverge exponentially as $x \to +\infty$ ($x - x' \ge 0$ in the integrand). Hence, the solution that comes close to Ω_+ (up to some arbitrarily small value ϵ) runs away exponentially. This proves the statement that Ω_+ are repellors as $x \to +\infty$.

In the region $x < x^*$, $\delta\Omega(x) \to \epsilon$ exponentially fast ($x - x' \le 0$ in the integrand) as $x \to -\infty$, and hence $\Omega(x) \to \Omega_+$. This proves that Ω_+ are attractors as $x \to -\infty$.

We can prove the statement for Ω_- in **c** similarly. For this, we just note the change of sign in exponents because $p_y\cos\Omega_- = k$.

We have to remark, however, that we can fine-tune the constant ϵ to cancel the exponential divergence in the integral part of (35) as $x \to +\infty$. As we see below, such solutions indeed exist!

d. As follows from **c**, the asymptotes Ω_+ (Ω_-) are unstable as $x \to +\infty$ ($x \to -\infty$). However, we can require the solutions to satisfy one of the initial conditions (32). We call such solutions left and right separatrices because they separate all solutions by regions. For example, the separatrix Ω_r separates solutions that are above or below its value Ω_+ at $+\infty$ just according the fact that Ω_+ is a repellor at $+\infty$.

We demonstrate that once we fixed one of conditions (32), it defines a single solution. To be more specific, we consider $\Omega_r(x)$. To demonstrate the existence of such a solution, we need to set $x^* = +\infty$ and $\epsilon = 0$ in the preceding item. Then $\Omega_r(x) = \Omega_+ + \delta\Omega_r(x)$, where, as $x \to +\infty$, by analogy with (35) we can write

$$\delta\Omega_r(x) = 2\int\limits_{+\infty}^{x} U(x')e^{2k(x-x')}\,dx',$$

where $\delta\Omega_r(x) \to 0$ as $x \to +\infty$, which proves the existence of a solution. To show its uniqueness, we suppose that there are two solutions with the same condition $\Omega_{1,2}(x) \to \Omega_+$ as $x \to +\infty$ and consider its difference $\delta\Omega = \Omega_2 - \Omega_1$, which continuously tends to zero as $x \to +\infty$. While $\delta\Omega$ is small, it satisfies the equation

$$\delta\Omega' = -2p_y \cos\Omega_1(x)\delta\Omega$$

with the solution

$$\delta\Omega(x) = \delta\Omega(x_0)\exp\left\{-2p_y\int\limits_{x_0}^{x}\cos\Omega_1(x')\,dx'\right\},$$

$x \le x_0 \to +\infty$. While x_0 is fixed, we use the limit relation $p_y\cos\Omega_1(x) \to -k$ as $x \to +\infty$, which exposes the exponential divergence at any nonzero $\delta\Omega(x_0)$, whence $\delta\Omega(x) \equiv 0$.

We emphasize that the uniqueness of solutions with conditions (32) does not hold if $E = \pm p_y$!

e. We next compare boundary conditions (8) for solutions that correspond to physical states with initial conditions (32) for two families of separatrices. The physical solution must satisfy both conditions, which is possible only when two separatrix families merge! Hence, the bound-state problem is equivalent to the degeneracy of separatrices of Eq. (7).

□

We note that the physical solutions are stated by degenerated separatrices, and when the degeneracy occurs, the corresponding parameter E is a discrete energy level in a given potential $U(x)$.

We let Ω_l and Ω_r denote the whole families of separatrices. If we need some particular function from the family, we indicate the dependence on x: $\Omega_l(x)$ and $\Omega_r(x)$. And again, we use the notation Ω_+ and Ω_- to describe the whole families of attractors and repellors if we do not specify some particular point of these families.

Lemma 3 (of boundedness). Let $U(x) \to 0$ as $x \to \pm\infty$. Let the primitive integral $f_{x_0}(x) = \int_{x_0}^{x} U(x')\,dx'$ of the potential $U(x)$ be a continuous function and the limit $\lim\limits_{x\to\pm\infty} f_{x_0}(x)$ exist (which may be infinite). Then

a. Any solution of Eq. (7) is a bounded function for any parameter $E \in (-p_y, p_y)$.

b. If $|\lim\limits_{x\to\pm\infty} f_{x_0}(x)| < \infty$, then all solutions of Eq. (7) are bounded functions for any parameter $E \in [-p_y, p_y]$.

Proof. a. We first consider the situation when $k \neq 0$ or $E \in (-p_y, p_y)$.

The continuity of $f_{x_0}(x)$ results in that $\Omega(x)$ is continuous function by Lemma 1. We suppose that $\Omega(x)$ diverges as $+\infty$. From the continuity, we can then always find an arbitrarily large positive x_0 such that $p_y\cos\Omega(x_0) = k > 0$. We expand $\Omega(x)$ in the vicinity of x_0: $\Omega(x) = \Omega(x_0) + \delta\Omega(x)$. Through the first order in $\delta\Omega$, we then have

$$\delta\Omega'(x) = 2U(x) - 2k\delta\Omega(x), \qquad (36)$$

which yields the solution

$$\delta\Omega(x) = 2\int\limits_{x_0}^{x} U(x')e^{-2k(x-x')}\,dx'. \qquad (37)$$

We clearly see that $\delta\Omega(x)$ converges as $x \to +\infty$ even at arbitrarily small $k > 0$. Hence, we arrived at a contradiction with our initial assumption of the unboundedness of $\Omega(x)$ at $+\infty$.

We can similarly prove the boundedness of any solution of Eq. (7) as $x \to -\infty$. We choose arbitrarily large negative x_0 such that $p_y\cos\Omega(x_0) = -k$.

We note that $\delta\Omega(+\infty) = 0$. Indeed, we integrate Eq. (36) and substitute (37) in the right-hand side. On the one hand, we have

$$\int\limits_{x_0}^{\infty}\delta\Omega(x)\,dx = 2\int\limits_{x_0}^{\infty}\int\limits_{x_0}^{x} U(x')e^{-2k(x-x')}\,dx\,dx' = \frac{f_{x_0}(+\infty)}{k}.$$

On the other hand, direct integration of Eq. (36) yields

$$\delta\Omega(+\infty) = 2f_{x_0}(+\infty) - 2k\int_{x_0}^{\infty}\delta\Omega(x)\,dx.$$

Hence, $\delta\Omega(+\infty) = 0$ or $\Omega(+\infty) = \Omega(x_0)$. This result is not surprising because we intentionally chose x_0 such that $\Omega(x_0) = \Omega_-$, which is attractor at $x \to +\infty$.

b. If $f_{x_0}(x)$ has finite limits at $x \to \pm\infty$, it can be shown that solutions of Eq. (7) are bounded on the closed interval $E \in [-p_y, p_y]$. To show this, we need to see what happens on the boundaries of the continuum when $E = \mu p_y$, $\mu = \pm 1$, and $k = 0$.

As in item **a**, we assume that $\Omega(x)$ diverges as $x \to +\infty$, and we can therefore write $\Omega(x) = \Omega(x_0) + \delta\Omega(x)$ and $\sin\Omega(x_0) = \mu$, where x_0 can be an arbitrarily large positive number. In Eq. (36), we omitted summands of the order $\delta\Omega^2$ and higher because $k \neq 0$ there. In this case, we have to account for the first nonzero term, which is quadratic in $\delta\Omega$:

$$\delta\Omega'(x) = 2U(x) - \mu p_y \delta\Omega^2(x).$$

This equation resembles that in the nonrelativistic limit with zero nonrelativistic energy. There are three possible scenarios of the behavior at $+\infty$. The first, where $\delta\Omega^2(x) \sim U(x)$, $x \to +\infty$, gives explicit convergence of $\delta\Omega$ because $U(x) \to 0$ as $x \to +\infty$. The second corresponds to $\delta\Omega^2(x) \sim \delta\Omega'(x)$, which yields the convergence $\delta\Omega \sim 1/x$. And the last situation is $\delta\Omega'(x) \sim U(x)$, which gives the convergence if and only if $f_{x_0}(x)$ converges at infinity.

Hence, any solution of Eq. (7) is bounded at any parameter $E \in [-p_y, p_y]$ as long as $f_{x_0}(x)$ is continuous and converges at infinity.

□

As can be seen from Lemma 2, we are interested in separatrix solutions because only those solutions are related to physical ones. For all discussions in what follows, we choose the family of left separatrices Ω_l. We want to show that the total variance

$$\Delta\Omega_l(E) = \Omega_l(+\infty) - \Omega_l(-\infty)$$

as a function of energy contains the full information of the discrete spectrum. This is stated in the following theorem.

Theorem (Levinson). Let $f_{x_0}(x)$ be a continuous function that converges at infinity, and $E \in [-p_y, p_y]$. Then

a. $\Delta\Omega_l(E)$ is a bounded function on the interval $E \in [-p_y, p_y]$.

b. $\Delta\Omega_l(E)$ is an integer multiple of 2π if $E \notin \mathrm{Spec}(U, p_y)$, and $\mathrm{Spec}(U, p_y)$ is the discrete spectrum of $U(x)$ at a given p_y.

c. Any $E \notin \mathrm{Spec}(U, p_y)$ is a point of continuity of $\Delta\Omega_l(E)$.

d. $\Delta\Omega_l(E)$ has finite jumps of -2π at each point $E_d \in \mathrm{Spec}(U, p_y)$:

$$\Delta\Omega_l(E_d + 0) - \Delta\Omega_l(E_d - 0) = -2\pi. \tag{38}$$

e. The total number $N_d(p_y)$ of discrete levels of $U(x)$ at a given $p_y > 0$ is given by

$$N_d(p_y) = \frac{\Delta\Omega_l(-p_y) - \Delta\Omega_l(p_y)}{2\pi}. \tag{39}$$

Proof. a. We know from Lemma 3 that under conditions of the theorem, $\Omega_l(x)$ is a bounded function of $x \in (-\infty, \infty)$ at any parameter $E \in [-p_y, p_y]$. In other words, $\Delta\Omega_l(E)$ is finite for any $E \in [-p_y, p_y]$ or $\Delta\Omega_l(E)$ is a bounded function of E.

b. According to Lemma 2, **e**, two families Ω_l and Ω_r of separatrices merges if and only if the parameter E corresponds to some discrete energy level. Let $E \notin \mathrm{Spec}(U, p_y)$. Then Ω_l and Ω_r are disjoint families; $\Omega_l(x)$ starts from some Ω_- at $x = -\infty$ and maybe comes to some other Ω_- from the family at $x = +\infty$. Indeed, otherwise $\Omega_l(x)$ must tend to Ω_+ at $+\infty$, whence $\Omega_l(x) = \Omega_r(x)$, which violates our assumption that $E \notin \mathrm{Spec}(U, p_y)$. Hence, $\Delta\Omega_l(E)$ is a multiple of 2π.

c. Let $E \notin \mathrm{Spec}(U, p_y)$, where it is natural to assume that $\mathrm{Spec}(U, p_y)$ is a discrete set. Then some δ-vicinity of E is disjoint with $\mathrm{Spec}(U, p_y)$, $\delta > 0$. We consider how $\Omega_l(x, E)$ changes with a small variation in the parameter E:

$$\delta\Omega_l(x, E, \epsilon) = \Omega_l(x, E + \epsilon) - \Omega_l(x, E),$$

where $0 < |\epsilon| < \delta$. In contrast to the foregoing, where E was fixed, we here indicate E as an argument. Subtracting Eqs. (7) for $\Omega_l(x, E+\epsilon)$ and $\Omega_l(x, E)$, we arrive at an equation for the variation function:

$$\delta\Omega_l' \approx -2\epsilon - 2p_y \cos\Omega_l(x, E)\,\delta\Omega_l. \tag{40}$$

We note that the initial condition depends on ϵ because

$$\delta\Omega_l(-\infty, E, \epsilon) = \Omega_-(E + \epsilon) - \Omega_-(E) \approx -\frac{\epsilon}{k}. \tag{41}$$

The solution is

$$\delta\Omega_l(x, E, \epsilon) = = -2\epsilon\int_{-\infty}^{x} \exp\left\{2p_y\int_{x}^{y}\cos\Omega_l(y', E)\,dy'\right\} dy. \tag{42}$$

We first demonstrate that (42) satisfies initial condition (41). According to (32), we can approximate $p_y \cos\Omega_l(y', E) \to p_y \cos\Omega_- = k$ as $x \to -\infty$ because $y \le y' \le x$. Hence, we see that

$$\delta\Omega_l(-\infty, E, \epsilon) \to -2\epsilon \int\limits_{-\infty}^{x} e^{2k(y-x)}\, dy = -\frac{\epsilon}{k}$$

as $x \to -\infty$. Now we are ready to show the convergence of (42) at $+\infty$ and, moreover, that $\delta\Omega_l(+\infty, E, \epsilon) = -\epsilon/k$. We first, divide (42) into two parts: the first part is the y-integral where $-\infty < y < x_0$, and the second part is the y-integral where $x_0 < y < x$, with $x_0 < x$ being a large positive number such that we can use the approximation $p_y \cos\Omega_l(y', E) \approx p_y \cos\Omega_- = k$ for $y' > x_0$. The first part can be estimated as $x \to +\infty$ as follows:

$$-2\epsilon \int\limits_{-\infty}^{x_0} \exp\left\{ 2p_y \left(\int\limits_{x}^{x_0} + \int\limits_{x_0}^{y} \right) \cos\Omega_l(y', E)\, dy' \right\} dy \approx$$

$$\approx -2\epsilon \int\limits_{-\infty}^{x_0} \exp\left\{ 2p_y \int\limits_{x_0}^{y} \cos\Omega_l(y', E)\, dy' \right\} dy \times$$

$$\times e^{-2k(x-x_0)} = \delta\Omega_l(x_0, E, \epsilon) e^{-2k(x-x_0)} \to 0.$$

The second part gives the desired limit $\delta\Omega_l(+\infty, E, \epsilon)$:

$$-2\epsilon \int\limits_{x_0}^{x} \exp\left\{ 2p_y \int\limits_{x}^{y} \cos\Omega_l(y', E)\, dy' \right\} dy \approx$$

$$\approx -2\epsilon \int\limits_{x_0}^{x} e^{2k(y-x)}\, dy \to -\frac{\epsilon}{k}.$$

Hence,

$$\delta\Omega_l(+\infty, E, \epsilon) = \delta\Omega_l(-\infty, E, \epsilon) = -\epsilon/k + O(\epsilon^2).$$

We note the equality of the values of $\delta\Omega_l$ at $\pm\infty$ not just up to the order ϵ^2 because we proved here that the difference tends to zero with ϵ, but according to item **b** of this theorem, the difference must be a multiple of 2π, whence only one opportunity is possible. Finally, we conclude that

$$\Delta\Omega_l(E+\epsilon) - \Delta\Omega_l(E) = \\ = \delta\Omega_l(+\infty, E, \epsilon) - \delta\Omega_l(-\infty, E, \epsilon) = 0.$$

Hence, we proved that any $E \notin \mathrm{Spec}(U, p_y)$ is a point of continuity of the function $\Delta\Omega_l(E)$. We also proved that $\Delta\Omega_l(E)$ is a piecewise-constant function with only possible discontinuity points from $\mathrm{Spec}(U, p_y)$.

We emphasize that the statement of this item is true even for the boundaries of the continuum where $E = \pm p_y$ because $E = \pm p_y$ are not limit points of $\mathrm{Spec}(U, p_y)$ (see Remark 1). For example, for $E = p_y$, we take

$$\delta\Omega_l(x, E = p_y, \epsilon) = \Omega_l(x, p_y - \epsilon) - \Omega_l(x, p_y),$$

where $\epsilon \approx k^2/(2p_y) \to +0$. Then condition (41) holds because $\epsilon/k \approx k/(2p_y) \to 0$.

d. Now we understand the behavior of $\Delta\Omega_l(E)$ with $E \notin \mathrm{Spec}(U, p_y)$. In this item, we consider the situation when $E = E_d \in \mathrm{Spec}(U, p_y)$, where we assume that $\mathrm{Spec}(U, p_y)$ is a discrete set or each element is an isolated point. As follows from Lemma 2, **e**, two separatrix families merge when $E = E_d$. We call this merged separatrices the Ω_d family.

Because E_d is isolated point of $\mathrm{Spec}(U, p_y)$, there exists a $\delta > 0$ such that the δ-vicinity of E_d does not contain any other points from $\mathrm{Spec}(U, p_y)$ except E_d. We consider the variation function

$$\delta\Omega_l(x, E_d, \epsilon) = \Omega_l(x, E_d + \epsilon) - \Omega_d(x, E_d),$$

where ϵ can be arbitrarily small, $0 < |\epsilon| < \delta$. We then repeat the procedure in item **c** of the theorem, which gives exactly the same initial condition (41), and we need to substitute $\Omega_l(y', E) \to \Omega_d(y', E_d)$ in Eq. (40). Hence, the approximate solution for $\delta\Omega_l(x, E_d, \epsilon)$ is given by

$$\delta\Omega_l(x, E_d, \epsilon) = \\ = -2\epsilon \int\limits_{-\infty}^{x} \exp\left\{ 2p_y \int\limits_{x}^{y} \cos\Omega_d(y', E_d)\, dy' \right\} dy. \quad (43)$$

But the analysis of Eq. (43) at $x \to +\infty$ gives different result from those in Eq. (42). The reason is that $\Omega_d(x, E_d)$ tends to Ω_+ as $x \to +\infty$ in accordance with conditions (8). This gives $p_y \cos\Omega_d(+\infty, E_d) = p_y \cos\Omega_+ = -k$, which yields the exponential divergence of $\delta\Omega_l(x, E_d, \epsilon)$ as $x \to +\infty$ for any $|\epsilon| > 0$. Formally, this divergence indicates the instability of the solution $\Omega_d(x, E_d)$ under infinitely small variations from the parameter E_d. But this conclusion is already obvious because we know that at $E = E_d + \epsilon$, we have two disjoint families of separatrices and our separatrix Ω_l tends to Ω_- as $x \to +\infty$.

A nontrivial conclusion that can be drawn from (43) is that

$$\mathrm{sign}\,(\delta\Omega_l) = -\,\mathrm{sign}(\varepsilon). \quad (44)$$

We next show that it leads to (38).

We can use approximate solution (43) in the region $x < R$ if the condition $\delta\Omega_l(x < R, E_d, \epsilon) \ll 1$ holds. Fix some small value of $\delta\Omega_l$,

$$\delta\Omega_l(R, E_d, \epsilon) \equiv \alpha.$$

This means that R is a function of two parameters α and ϵ and $R(\alpha, \epsilon) \to +\infty$ at a fixed α and $\epsilon \to 0$. We introduce the variance

$$\delta\Omega_d = \Omega_d(R(\alpha, \epsilon), E_d) - \Omega_+,$$

where $\delta\Omega_d \to 0$ as $R \to +\infty$. Finally, for the left separatrix, we have

$$\Omega_l(R(\alpha, \epsilon), E_d + \epsilon) = \Omega_+ + \delta\Omega_d + \alpha,$$

where α is fixed and $\delta\Omega_d \to 0$ as $\epsilon \to 0$ or, equivalently,

$$\Omega_l(R(\alpha, \epsilon), E_d + \epsilon) \to \Omega_+ + \alpha$$

at $\epsilon \to 0$ and an arbitrarily small but fixed α. In accordance with the definition of α and Eq. (44), we obtain

$$\operatorname{sign}(\alpha) = -\operatorname{sign}(\epsilon).$$

This means that at $\epsilon > 0$ ($\epsilon < 0$), the left separatrix $\Omega_l(R, E_d + \epsilon) < \Omega_+$ ($\Omega_l(R, E_d + \epsilon) > \Omega_+$) at $R \to +\infty$ and hence $\Omega_l(x, E_d + \epsilon)$ falls onto the asymptote Ω_-, which is right under (above) the asymptote $\Omega_+ = \Omega_d(+\infty, E_d)$. Hence,

$$\Omega_l(+\infty, E_d + 0) - \Omega_l(+\infty, E_d - 0) = -2\pi$$

or equivalently,

$$\Delta\Omega_l(E_d + 0) - \Delta\Omega_l(E_d - 0) = -2\pi.$$

We used the fact that $\Omega_l(-\infty, E_d + 0) = \Omega_l(-\infty, E_d - 0)$ here.

It can be shown similarly that the right separatrix experiences jumps with the same sign:

$$\Delta\Omega_r(E_d + 0) - \Delta\Omega_r(E_d - 0) = -2\pi.$$

In this sense, the right separatrix does not give any additional information about the discrete spectrum.

e. We proved that $\Delta\Omega_l(E)$ is a bounded piecewise-constant function that experiences final jumps of -2π at every point E_d of the discrete spectrum of the confinement potential $U(x)$ and $\Delta\Omega_l(E)$ is continuous at any other points where $E \notin \operatorname{Spec}(U, p_y)$. This allows us to calculate the total number of discrete levels as the difference of $\Delta\Omega_l(E)$ on the ends of the interval $[-p_y, p_y]$, which immediately gives Eq. (39).

We remark, however, that we understand $\Delta\Omega_l(\pm p_y)$ only in the sense of the limit relation

$$\Delta\Omega_l(\pm p_y) = \lim_{\epsilon \to +0} \Delta\Omega_l(\pm(p_y - \epsilon))$$

because separatrices are not well defined at the boundaries of the continuum, as we saw in Lemma 2.

□

Remark 1 (for the Levinson theorem). We note that the assumptions made in the statement of the Levinson theorem ensure that $\operatorname{Spec}(U, p_y)$ is a discrete set. Indeed, we suppose that $\operatorname{Spec}(U, p_y)$ has one limit point $E_0 \in [-p_y, p_y]$. This means that the infinitesimal vicinity of this point contains an infinite number of isolated points from $\operatorname{Spec}(U, p_y)$. But for any isolated point, item **d** of the theorem applies, whence $\Delta\Omega_l(E \to E_0) \to \infty$, which contradicts item **a** of the theorem, the boundedness of this function for any $E \in [-p_y, p_y]$. Hence, $\operatorname{Spec}(U, p_y)$ does not contain limit points.

Remark 2 (for the Levinson theorem). Even if $|\lim_{x \to \pm\infty} f_{x_0}(x)| = \infty$, all proofs and statements of the theorem are valid for the open interval $E \in (-p_y, p_y)$ because $k = \sqrt{p_y^2 - E^2} > 0$. However, at least one of the points $E = \pm p_y$ is a limit point of $\operatorname{Spec}(U, p_y)$, which makes $\Delta\Omega_l(E)$ unbounded on the closed interval $E \in [-p_y, p_y]$.

Remark 3 (for the Levinson theorem). We can find the number of discrete levels between any two given energies $|E_{1,2}| \le p_y$, $E_{1,2} \notin \operatorname{Spec}(U, p_y)$:

$$N_d(p_y, E_1, E_2) = \left| \frac{\Delta\Omega_l(E_2) - \Delta\Omega_l(E_1)}{2\pi} \right|. \qquad (45)$$

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

Example with a δ-potential

Finally, we give an example in the simple case of the δ-potential $U(x) = G\delta(x)$. We demonstrate that the total number of discrete levels $N_d(p_y) = 1$ at any $p_y \ne 0$ and $G \ne \pi n$, where n is an integer and N_d is defined by Eq. (39). We need to consider Eq. (7) only at $E = \pm p_y$.

All solutions of Eq. (7) are constructed from solutions of the free motion equation (33) separately at $x < 0$ and $x > 0$ with the matching condition

$$\Omega(+0) = \Omega(-0) + 2G. \qquad (46)$$

We first analyze the solutions of Eq. (33). If $E = p_y$, then we have $\Omega'(x) = -2p_y(1 + \sin\Omega) \le 0$ and

$\Omega'(x) = 0$ only in the case of stationary points $\Omega_0 \equiv \Omega_\pm = -\pi/2 + 2\pi n$. Hence, all nonstationary solutions of Eq. (33) decrease strictly monotonically from some stationary point $\Omega_0 + 2\pi$ at $x = -\infty$ to Ω_0 at $x = +\infty$. We note that two families of stationary points merge at $E = \pm p_y$.

In the case where $E = -p_y$, all nonstationary solutions of Eq. (33) increase strictly monotonically from some stationary point $\Omega_0 - 2\pi$ at $x = -\infty$ to Ω_0 at $x = +\infty$.

We represent the confinement strength in the form

$$G = \pi(n_G + \delta n_G),$$

where n_G is an integer and $\delta n_G \in (0, 1)$. Then

$$\Omega_l(x < 0, \pm p_y) = \Omega_-(\pm p_y)$$

and

$$\Omega_l(+0, \pm p_y) = \Omega_-(\pm p_y) + 2\pi n_G + 2\pi\delta n_G,$$

where $\Omega_0 = \Omega_- + 2\pi n_G$ is a stationary point and $2\pi\delta n_G \in (0, 2\pi)$, which means that $\Omega_l(x, \pm p_y)$ at $x > 0$ comes along some nonstationary solution that decreases (increases) at $E = p_y$ ($E = -p_y$), whence $\Omega_l(+\infty, p_y) = \Omega_0$ ($\Omega_l(+\infty, -p_y) = \Omega_0 + 2\pi$) at $E = p_y$ ($E = -p_y$). Equivalently, $\Delta\Omega_l(p_y) = 2\pi n_G$ and $\Delta\Omega_l(-p_y) = 2\pi n_G + 2\pi$. Hence, $N_d(p_y) = 1$.

7. GEOMETRICAL INTERPRETATION OF THE RELATIVISTIC LEVINSON THEOREM

The problem of bound states in graphene stripes can be analyzed similarly to what happens in mechanical autonomous systems. We consider the system of equations

$$\begin{aligned} &U'(x) = G(U), \\ &\Omega'(x) = 2\,(U(x) - E) - 2p_y \sin\Omega(x), \end{aligned} \tag{47}$$

where the second equation is just Eq. (7). We can assume that Eq. (47) represents integral curves of some vector field

$$\mathbf{F}(U, \Omega) = \begin{pmatrix} G(U) \\ 2\,(U - E) - 2p_y \sin\Omega \end{pmatrix},$$

and the coordinate x is just some parameterization of these curves. Although our system (47) is not Hamiltonian as in usual mechanics, it is still an autonomous system of differential equations, and it can therefore be analyzed in terms of phase trajectories in the so-called phase space $\mathfrak{D}$. In our case, the phase space $\mathfrak{D}$ is the (U, Ω)-stripe:

$$\mathfrak{D} = \{(U, \Omega) | U \in [\inf_{x\in\mathbb{R}} U(x), \sup_{x\in\mathbb{R}} U(x)], \Omega \in \mathbb{R}\},$$

where $\mathbb{R} = (-\infty, +\infty)$.

However, our system (47) is more complicated than the usual autonomous systems. To see this, we note that the function $G(U)$ is different for each monotonicity interval $I_j = [x_{j-1}, x_j]$ of $U(x)$. This means that we have different maps for each I_j and we need to match these maps continuously. In other words, instead of one autonomous system, we have a chain of systems:

$$\mathbf{F}_j(U, \Omega) = \begin{pmatrix} U'(x) \\ \Omega'(x) \end{pmatrix} = \begin{pmatrix} G_j(U) \\ 2\,(U - E) - 2p_y \sin\Omega \end{pmatrix}, \tag{48}$$

which are autonomous on the corresponding intervals I_j, $x \in I_j$ is some parameterization, and $\mathbf{F}_j(x_j) = \mathbf{F}_{j+1}(x_j)$. All trajectories of the field $\mathbf{F}_j$ fill the whole stripe:

$$\mathfrak{D}_j = \{(\Omega, U) | U \in [\inf_{x\in I_j} U(x), \sup_{x\in I_j} U(x)], \Omega \in \mathbb{R}\}.$$

We formulate the following Lemma.

Lemma 4 (of stationary points). Let $U(x) \in C^1$ have a finite number N of monotonicity intervals $I_j = [x_{j-1}, x_j]$, $x_0 = -\infty < x_1 < \ldots < x_{N-1} < x_N = +\infty$. Let $U(x)$ be a strictly monotonic function on each I_j. Let $U(x) \to 0$ as $x \to \pm\infty$. Then

a. $U'(x) \to 0$ as $x \to \pm\infty$.

b. The functions $G_j(U)$ are definite on the corresponding intervals I_j, $j = 1, \ldots, N$, and $G_1(0) = G_N(0) = 0$.

c. The number of stationary points of the jth equation (48) is exhausted by the series

$$\left(U_\sigma, \arcsin\left(\frac{U_\sigma - E}{p_y}\right) + 2\pi n\right)$$

or

$$\left(U_\sigma, \pi - \arcsin\left(\frac{U_\sigma - E}{p_y}\right) + 2\pi n\right),$$

where n is an integer, $|U_\sigma - E| \le p_y$, and $G_j(U_\sigma) = 0$.

Proof. a. It is straightforward from the monotonic behavior of $U(x)$ at infinity and the fact that $U(x) \to 0$ as $x \to \infty$.

b. Because $U(x)$ is strictly monotonic on each I_j, the inverse function $x_j(U)$ exists. Then $G_j(U) = U'(x_j(U))$.

We know that $I_1 = (-\infty, x_1]$, $I_N = [x_{N-1}, +\infty)$, and $U'(x) \to 0$ as $x \to \pm\infty$, where $U(x) \to 0$. This immediately yields $G_1(0) = \lim_{x\to-\infty} U'(x) = 0$ and $G_N(0) = \lim_{x\to+\infty} U'(x) = 0$.

c. To prove this statement, if suffices to solve the simple equation

$$\mathbf{F}_j(U,\Omega) = 0.$$

□

In what follows, we let $\mathbf{F}(U,\Omega)$ denote the entire chain of connected maps for $\mathbf{F}_j(U,\Omega)$, where each trajectory from $\mathfrak{D}$ corresponds to some solution of Eq. (47). The properties of these trajectories are formulated in the following theorem.

Theorem (of Poincaré indices). Let all restrictions of Lemma 4 be valid. We consider the map $\mathfrak{D} \to \mathfrak{R}$ defined by the rule

$$X(U,\Omega) = (U + ap_y)\cos\Omega, \quad Y(U,\Omega) = (U + ap_y)\sin\Omega, \tag{49}$$

where $+\infty > ap_y > -\inf_{x\in\mathbb{R}} U(x)$ is some parameter, and $E \in (-p_y, p_y)$, $E \notin \mathrm{Spec}(U,p_y)$. Then

a. All stable trajectories of the vector field

$$\mathbf{P}(X,Y) = \mathbf{F}(U(X,Y),\Omega(X,Y)),$$

$(X,Y) \in \mathfrak{R}$ are open. All unstable trajectories (separatrices) are closed.

b. In the preceding section, we introduced the total variance $\Delta\Omega_s(E)$, where s indicates the left or right separatrix. The fraction $\Delta\Omega_s(E)/(2\pi)$ equals the integer number $\mathfrak{p}$ of full rotations of the corresponding closed trajectory in the phase space $\mathfrak{R}$:

$$\Delta\Omega_s(E) = 2\pi\mathfrak{p}_s;$$

$\mathfrak{p}_s$ is the Poincaré index of a closed trajectory.

Proof. a. Map (49) is a map of the stripe $\mathfrak{D}$ to the annulus $\mathfrak{R}$ where all points $(U, \Omega + 2\pi n)$, where n is an integer, are identified.

The asymptotic behavior of stable trajectories of the field $\mathbf{P}(X,Y)$ is related to stable solutions of Eq. (7) that start from the attractor Ω_+ at $x \to -\infty$ and finish at the attractor Ω_- at $x \to +\infty$ in accordance with Lemma 2. Because $U(x) \to 0$ as $x \to \pm\infty$, we conclude that stable trajectories in $\mathfrak{R}$ start from the point

$$P_i = (-ak, -aE)$$

because $X_i = ap_y \cos\Omega_+$ and $Y_i = ap_y \sin\Omega_+$, and finish at another point

$$P_f = (ak, -aE)$$

because $X_f = ap_y\cos\Omega_-$, $Y_f = ap_y \sin\Omega_-$. If $E \in (-p_y, p_y)$, then $k > 0$ and $P_f \neq P_i$. This means that stable trajectories are open.

According to (32), if $E \notin \mathrm{Spec}(U,p_y)$, then Ω_l (Ω_r) starts and finishes on the asymptotes from the same family: Ω_- for Ω_l and Ω_+ for Ω_r. Then, P_i and P_f are identical for them or, equivalently, their trajectories in the space $\mathfrak{R}$ are closed.

b. As follows from the Levinson theorem, $\Delta\Omega_l(E) = 2\pi\mathfrak{p}_l$, where $\mathfrak{p}_l$ is an integer. But from the continuity of $\Omega_l(x)$ we conclude that $\mathfrak{p}_l$ is the number of full rotations of the closed trajectory corresponding to the separatrix Ω_l in $\mathfrak{R}$. In other words, $\mathfrak{p}_l$ is the Poincaré index of this closed trajectory [34].

□

We present a simple example of the spectral analysis for the Lorentzian-shaped confinement potential

$$U(x) = -U_0/(x^2+1).$$

We plot the vector field $\mathbf{F}(U,\Omega)$ and calculate the number of bound states at some particular p_y and U_0.

First, we need to find $G_j(U)$ for each interval of monotonicity $I_1 = (-\infty, 0)$ and $I_2 = (0, +\infty)$:

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

for the interval I_n, $n = \{1,2\}$, $U \in [-U_0, 0]$.

Then we set the parameters $p_y = 0.1$ and $U_0 = 1$. To find the total number of confined modes, we use Eq. (39). Hence, we need to plot the phase portrait only for two energies $E = \pm p_y$. For the vector field $\mathbf{F}(E = p_y)$, Figs. 1 and 2 show the approximate trajectory $(U, \Omega_l(x(U)))$ (red line) for two intervals $I_{1,2}$. We 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 the trajectories corresponding to the intervals I_1 and I_2 (black points in Figs. 1 and 2), we finally obtain the variance $\Delta\Omega_l(p_y) = -4\pi$. Similarly, drawing such pictures for $E = -p_y$, we obtain that $\Delta\Omega_l(p_y) = 0$. Equation (39) yields $N_d(p_y) = 2$ confined energy levels for $p_y = 0.1$.

We have to remark that the initial condition for Ω_l must be perturbed from the ideal point ($U = 0$, $\Omega = \Omega_-$) because it is a stationary point of Eq. (47) according to Lemma 4. But the result is stable under small variations in the initial conditions because of the stability of the Poincaré index or the so-called topological charge.

8. CONCLUSIONS

The variable-phase method has been developed herein for electrostatically confined 2D massless Dirac–Weyl particles such as electrons in graphene devices. The desired phase function $\Omega(x)$ appears as the

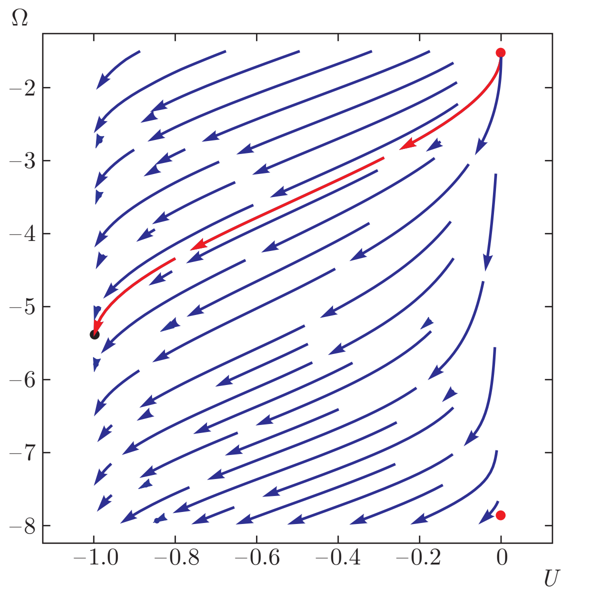

Fig. 1. (Color online.) The vector field $\mathbf{F}(E=p_y)$ with $p_y = 0.1$ and $U_0 = 1$ on the interval $I_1 = (-\infty, 0)$. The trajectory $(U, \Omega_l(x_1(U)))$ corresponding to the separatrix $\Omega_l(x)$ (red streamline) starts from the initial (red) point ($U = 0$, $\Omega = -\pi/2$) and ends where $U = -U_0 = -1$ (black point). The distance between red points is 2π

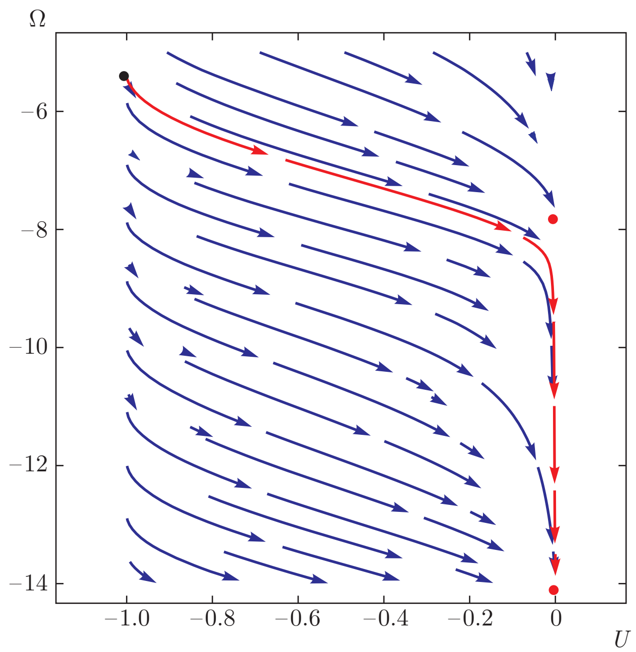

Fig. 2. (Color online.) The vector field $\mathbf{F}(E=p_y)$ with $p_y = 0.1$ and $U_0 = 1$ on the interval $I_2 = (0, +\infty)$. The trajectory $(U, \Omega_l(x_2(U)))$ corresponding to the separatrix $\Omega_l(x)$ (red streamline) starts from the black point, which provides the continuity of $\Omega_l(x)$ at $x = 0$, and ends at the red point ($U = 0$, $\Omega = -9\pi/2$). The distance between red points is 2π

phase between two chiral states whose superposition yields the wave function of the confined state. In addition to the well-known nonrelativistic and semiclassical limits, it has been shown that confined states with small p_y (see condition (18)) are successfully described in the so-called δ-potential limit that is valid for each integrable potential $U(x)$. 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 a given p_y has been derived. Finally, a geometrical approach to finding the function $\Delta\Omega_l(E)$ has been proposed.

We note that this paper is dedicated exclusively to the discrete part of the spectrum. The developed approach can be extended to the analysis of half-bound and quasi-bound states, the last ones being important for better understanding the supercriticality.

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APPENDIX

Unique solution of the δ-potential

One can find in the literature that $U(x) = G\delta(x)$ does not have definite solutions of the Dirac–Weyl equation [35, 36]. This problem arises from the fact that the wave function is discontinuous at $x = 0$, and it results in an ambiguous integral of the type

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

which takes an arbitrary value from the segment $[0, 1]$, where $\theta(x)$ is the Heaviside step function and $\epsilon \to +0$. This problem was circumvented in [5], where the wave function $\Psi(x)$ was represented as the x-ordered exponential (an analogue of the evolution operator) acting on the wave function at the initial point x_0. We here quote the exact solution of Eq. (3) in order to explicitly demonstrate the absence of any ambiguities.

We start from Eq. (3):

$$g''(x) + 2i\,(E - G\delta(x))\, g'(x) - p_y^2 g(x) = 0. \quad (50)$$

The function $g(x)$ appears to be continuous, and $g'(x)$ is discontinuous at $x = 0$. We assume that $g'(\pm 0) \neq \neq 0$ and divide this equation by the function $g'(x)$,

$x \in I_\epsilon = (-\epsilon, \epsilon)$. Integrating this equation over the interval I_ϵ and taking the limit $\epsilon \to +0$, we then arrive at the correct matching condition

$$\frac{g'(+0)}{g'(-0)} = e^{2iG}. \tag{51}$$

If we are interested in the discrete spectrum of this problem, we have to apply condition (51) to the function $g(x) = g_0 \exp(-iEx)\exp(-k|x|)$, which represents the common form of a bounded solution of Eq. (50) continuous at $x = 0$, $k = \sqrt{p_y^2 - E^2}$. This manifestly yields the spectrum in Eq. (19). The initial assumption that $g'(\pm 0) \neq 0$ is obviously valid for such functions $g(x)$.

If we consider the scattering problem with a fixed $|E| > p_y$, then the continuous function $g(x)$ has the form

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

$k = \sqrt{E^2 - p_y^2}$. Applying condition (51), we can obtain the transmission coefficient:

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

Finally, we have to verify that the initial assumption $g'(\pm 0) \neq 0$ is not violated. $g'(+0) \neq 0$ as long as $E \neq k$ for $p_y \neq 0$. We then suppose 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 does not depend on the parameter G in this case. Hence, the unique solution in the case of a δ-potential is provided.

We can suggest an easier way to obtain the discrete spectrum for this potential. For this, integrating Eq. (7) and applying boundary conditions (8), we finally obtain

$$\Delta\Omega = \Omega_+ - \Omega_- = 2G \tag{52}$$

which explicitly gives spectrum (19).

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