

ANALYTIC STUDY OF FERMIONS IN GRAPHENE; HEUN FUNCTIONS AND BEYOND

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Received October 9, 2012

Starting with the wave function characterizing massless fermions evolving in orthogonal electric and magnetic fields, written in terms of Heun Biconfluent functions, we analyse some physically interesting cases. When the *HeunB* function truncates to a polynomial form, one may easily compute the essential components of the conserved current density. For a vanishing electric field, we get the familiar Hermite associated functions and discuss the current dependence on the sample width. In the opposite case, corresponding to an electric static field alone, one has to deal with *HeunB* functions of complex variable and parameters.

Key words: Quantum Hall Effect, relativistic Dirac equation, Heun’s Functions graphene.

PACS: 03.65.-w, 11.10.-z, 11.15.-q..

1. INTRODUCTION

By “graphene”, one generally denotes one planar layer of carbon atoms, arranged on a honeycomb structure made out of hexagons. Its low-energy excitations are massless, chiral, pseudo-particles, moving with a speed 300 times smaller than the speed of light [1].

As a special feature and also a trademark of Dirac fermion behaviour, which makes graphene a very attractive material from a theoretical point of view, is the anomalous integer quantum Hall effect measured experimentally [2], at room temperature [3].

Because the energetic states of the positrons within the barrier are aligned to the continuous energetic states of the electrons outside the barrier, these carriers are transmitted with unit probability [4]. As a result to the insensitivity to external electrostatic potentials, they evolve in an unusual way in the presence of confining potentials that can be easily produced by disorder [5].

The properties of chiral massless particles, belonging to the distinct sub-lattices in graphene and described by the Dirac equation near the two points K and K' , being an active field of research, in a previous paper [6], we have considered a strong magnetic induction orthogonal to a weak electrostatic intensity. By employing the

perturbation theory, we have derived the first-order transition amplitudes and the corresponding current. Then, we have generalized this analysis for arbitrary static magnetic and electric fields, and concluded that the Dirac-type equation of massless fermions is satisfied by the *Heun* biconfluent functions [7]. Even though these functions have been intensively worked out in the last years, in situations relevant to physics, chemistry and engineering [8], there are problems when dealing with the general expressions. That is why, for having a better understanding of the physical phenomena, in the present paper, we focus on particularly interesting cases which can be investigated by using the corresponding series expansions, for some ranges of the parameters.

2. DIRAC-TYPE EQUATION AND FERMIONS' WAVE FUNCTION

In natural units, *i.e.* $\hbar = c = 1$, the four-dimensional Dirac equation describing a massless fermion evolving in an electric field orthogonal to a magnetic field, oriented along Ox and Oz respectively, is

$$\gamma^i D_i \Psi = 0, \quad D_i = \partial_i - iqA_i, \quad (1)$$

where the covariant derivatives D_i contains the components of the 4-potential

$$A_2 = B_0 x, \quad A_4 = E_0 x.$$

Using the Dirac representation for γ matrices,

$$\gamma^\mu = -i\beta\alpha^\mu, \quad \gamma^4 = -i\beta, \quad (2)$$

with

$$\beta = \begin{pmatrix} \mathcal{I} & 0 \\ 0 & -\mathcal{I} \end{pmatrix}, \quad \alpha^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \sigma^\mu & 0 \end{pmatrix},$$

where σ^μ are the usual Pauli matrices, we are looking for the positive-energy solution

$$\Psi(x, y, z, t) = e^{i(p_y y + p_z z - \omega t)} \begin{pmatrix} \xi(x) \\ \varphi(x) \end{pmatrix}, \quad (3)$$

where ξ and φ are the two-component spinors

$$\xi(x) = \begin{pmatrix} \xi_1(x) \\ \xi_2(x) \end{pmatrix}, \quad \varphi(x) = \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix}. \quad (4)$$

Thus, the Dirac equation (1) leads to the system of coupled equations

$$\begin{aligned} \text{(a)} \quad & \sigma^1 \xi' + i\sigma^2 (p_y - qB_0 x) \xi + i\sigma^3 p_z \xi = i[\omega + qE_0 x] \varphi; \\ \text{(b)} \quad & \sigma^1 \varphi' + i\sigma^2 (p_y - qB_0 x) \varphi + i\sigma^3 p_z \varphi = i[\omega + qE_0 x] \xi, \end{aligned} \quad (5)$$

where ' stands for the derivative with respect to x .

Following the usual procedure, we express $\varphi(x)$, from (5.a) and, by replacing it into (5.b), we come to the following second-order differential equation for the spinor ξ :

$$\xi'' - \frac{qE_0}{\omega + qE_0x} \xi' - \frac{iq}{\omega + qE_0x} \{[\omega B_0 + p_y E_0] \sigma^1 \sigma^2 + E_0 p_z \sigma^1 \sigma^3\} \xi = \left[-(\omega + qE_0x)^2 + (p_y - qB_0x)^2 + p_z^2 \right] \xi. \quad (6)$$

As in [7], because the complicated form of the above equation, in the followings, we are working out the case $p_z = 0$. This assumption which appears in most of the works devoted to the (2+1)-quantum-relativistic study of graphene [9], is motivated by the fact that the characteristic magnitude of p_z is actually \hbar/a_z , where a_z is a length scale measuring the extent of the P_z orbitals.

Thus, we come to the following decoupled equations for the two components of the spinor ξ

$$\frac{d^2 \xi_{1,2}}{dx_*^2} - \frac{1}{x_*} \frac{d\xi_{1,2}}{dx_*} + \frac{\varepsilon p}{x_*} \xi_{1,2} + \left[d^2 x_*^2 - b^2 \left(x_* - \frac{p}{b} \right)^2 \right] \xi_{1,2} = 0, \quad (7)$$

where $\varepsilon = \pm 1$, for ξ_1, ξ_2 respectively, and we have introduced the notations

$$x_* \equiv x + \frac{\omega}{qE_0}, \quad b \equiv qB_0, \quad d \equiv qE_0, \quad p \equiv p_y + \omega \frac{B_0}{E_0}. \quad (8)$$

For $p = 0$ and $E_H = -E_0$, the last relation in (8) is the quantum analog of the well-known classical Hall relation, $E_H = B_0 v$ and the solutions of (5) are expressed in terms of the trigonometric *sine* and *cosine* functions, for $d > b$, and hyperbolic *Sinh* and *Cosh* functions, for $b > d$.

For $p \neq 0$ and arbitrary external static fields, whose intensities are related to each other as $b > d$, the perturbative approach developed in [6] is no longer valid. Thus, in order to solve the equation (7), we have introduced, in [7], the new function, $u(x_*)$, by

$$\xi(x_*) = x_*^2 \exp [C_1 x_*^2 + C_2 x_*] u(x_*), \quad (9)$$

where the parameters C_1 and C_2 are

$$C_1 = -\frac{1}{2\lambda^2}, \quad C_2 = bp\lambda^2, \quad (10)$$

with

$$\lambda^2 = \frac{1}{\sqrt{b^2 - d^2}} = \ell_B^2 \left[1 - \frac{d^2}{b^2} \right]^{-1/2}, \quad (11)$$

$\ell_B = \sqrt{\hbar/qB_0}$ being the magnetic length.

With the dimensionless variable $\zeta = x_*/\lambda$, the function u satisfies the second

order differential equation

$$\frac{d^2u}{d\zeta^2} + \frac{1}{\zeta} [-2\zeta^2 + 2bp\lambda^3\zeta + 3] \frac{du}{d\zeta} + [(p^2d^2\lambda^6 - 4)\zeta + p\lambda(3b\lambda^2 + \varepsilon)] \frac{u}{\zeta} = 0, \quad (12)$$

which can be compared with the so-called *Heun Biconfluent Equation* [10]

$$\frac{d^2u}{d\zeta^2} + \frac{1}{\zeta} [-2\zeta^2 - \beta\zeta + \alpha + 1] \frac{du}{d\zeta} + \left[(\gamma - \alpha - 2)\zeta - \frac{\delta + \beta + \alpha\beta}{2} \right] \frac{u}{\zeta} = 0, \quad (13)$$

so that u is the function $\text{HeunB}[\alpha, \beta, \gamma, \delta; \zeta]$, with the parameters

$$\alpha = 2, \quad \beta = -2bp\lambda^3, \quad \gamma = p^2d^2\lambda^6, \quad \delta = -2\varepsilon p\lambda. \quad (14)$$

Generally, for a differential equation which can be cast in the form

$$[F(D) + P(x, d/dx)]u(x) = 0,$$

where $D \equiv x \frac{d}{dx}$, $F(D) = \sum_n a_n D^n$ is a diagonal operator in the space of monomials and $P(x, d/dx)$ is an arbitrary polynomial function of x and d/dx , the necessary condition for a polynomial form of u is [11]

$$F(D)x^n = 0. \quad (15)$$

By inspecting the equation (12), one can identify $F(D) = -2D + p^2d^2\lambda^6 - 4$, so that the condition (15) concretely becomes

$$p^2d^2\lambda^6 - 4 = 2n, \quad (16)$$

leading to the following energy quantization law

$$\omega_n = c\sqrt{2(n+2)qB_0\hbar} \left[1 - \left(\frac{E_0}{cB_0} \right)^2 \right]^{3/4} - p_y \frac{E_0}{B_0}, \quad (17)$$

where we have restored c and \hbar for a better comparison with data.

Besides the Hall term $p_y E_0 / B_0$, the first term in the right hand side is typical for the energy levels of graphene's carriers evolving in static magnetic inductions [2].

Putting everything together, we are able to write down the full expression of the wave function (3), up to a normalization factor \mathcal{N} , as

$$\Psi = \mathcal{N} e^{i(p_y y - \omega t)} \exp \left[-\frac{\zeta^2}{2} + a\zeta \right] \times \begin{pmatrix} \zeta^2 \text{HB}_1 \\ \zeta^2 \text{HB}_2 \\ -\frac{i}{d\lambda^2} \left[2 - (b\lambda^2 + 1)(\zeta^2 - p\lambda\zeta) + \zeta \frac{d}{d\zeta} \right] \text{HB}_2 \\ -\frac{i}{d\lambda^2} \left[2 + (b\lambda^2 - 1)(\zeta^2 + p\lambda\zeta) + \zeta \frac{d}{d\zeta} \right] \text{HB}_1 \end{pmatrix}, \quad (18)$$

where

$$a \equiv (p\lambda)(b\lambda^2) = \sqrt{2(n+2)} \frac{b}{d} \quad (19)$$

and $\text{HB}_{1,2} \equiv \text{HeunB} [2, -2a, p^2 d^2 \lambda^6, \mp 2p\lambda; \zeta]$.

3. THE HALL-TYPE CURRENT

Even though we got an analytical solution to the equation (1), it is not easy to deal with the HeunB functions in (18) since they are very sensitive to the parameters values and, up to know, their normalization procedure is not well understood.

According to the exponential argument, for $\zeta \in [0, 2a]$, we experience the most interesting behaviour. Thus, for $\zeta \in [0, 1]$ and $a > 1$, we are in the region of amplification whose amplitude increases as a gets larger.

The physically interesting case corresponding to $\zeta \ll 1$, is leading, in view of (8, 11, 17), to the following conditions which should be satisfied by the model parameters:

$$x \ll \lambda = \ell_B \left[1 - \frac{d^2}{b^2} \right]^{-1/4}$$

and

$$\omega \ll d\lambda \Rightarrow n+2 \ll \frac{b^2 d^2}{2(b^2 - d^2)^2}.$$

Besides the sample's width, the above relation is imposing d close enough to b and a maximum value of the quantum number n . However, in many theoretical studies, the energy separation between the Landau levels is considered to be large enough to justify the use of the lowest Landau level (LLL) approximation.

For $\zeta \ll 1$, one may use the following series expansions for u and its derivatives

$$\begin{aligned} u &= 1 + c_1 \zeta + c_2 \zeta^2 + \dots = \sum_{n=0}^{\infty} c_n \zeta^n, \\ u' &= c_1 + 2c_2 \zeta + 3c_3 \zeta^2 + \dots = \sum_{n=1}^{\infty} n c_n \zeta^{n-1}, \\ u'' &= 2c_2 + 6c_3 \zeta + 12c_4 \zeta^2 + \dots = \sum_{n=2}^{\infty} n(n-1) c_n \zeta^{n-2}, \end{aligned} \quad (20)$$

and, by setting to zero the coefficients of ζ^{-1} , ζ^0 and ζ , we get

$$\begin{aligned} c_1 &= -p\lambda \left(b\lambda^2 + \frac{\varepsilon}{3} \right) < 0; \\ c_2 &= \frac{(p\lambda)^2}{2} \left[b\lambda^2 \left(b\lambda^2 + \frac{5}{12} \varepsilon \right) + \frac{1}{4} \right] + \frac{1}{2} > 0; \\ c_3 &= -\frac{(p\lambda)^3}{6} \left[(b\lambda^2)^2 \left(b\lambda^2 + \frac{13}{20} \varepsilon \right) + \frac{5}{6} \left(b\lambda^2 + \frac{11}{50} \varepsilon \right) \right] - \frac{p\lambda}{6} \left[\frac{19}{5} b\lambda^2 + \varepsilon \right]. \end{aligned} \quad (21)$$

Since the quantity $a\zeta$ is also much less than 1, one can approximate the function u in (20), with the coefficients (21), with $\exp[-a\zeta]$. This allows us to write down the following easily handling expression for the wave function (18),

$$\Psi = \mathcal{N} e^{i(p_y y - \omega t)} \exp \left[-\frac{\zeta^2}{2} \right] \begin{pmatrix} \zeta^2 \\ \zeta^2 \\ -\frac{i}{d\lambda^2} [2 + p\lambda\zeta - (b\lambda^2 + 1)\zeta^2] \\ -\frac{i}{d\lambda^2} [2 - p\lambda\zeta + (b\lambda^2 - 1)\zeta^2] \end{pmatrix}, \quad (22)$$

which obviously is the superposition of two orthogonal modes, associated to the pseudo-spin states belonging to the two sub-lattices that exist in graphene [1],

$$\begin{aligned} \Psi^{up} &= \mathcal{N} e^{i(p_y y - \omega t)} \exp \left[-\frac{\zeta^2}{2} \right] \begin{pmatrix} \zeta^2 \\ 0 \\ -\frac{i}{d\lambda^2} [2 - \zeta^2] \\ \frac{i}{d\lambda^2} [p\lambda\zeta - b\lambda^2\zeta^2] \end{pmatrix}; \\ \Psi^{down} &= \mathcal{N} e^{i(p_y y - \omega t)} \exp \left[-\frac{\zeta^2}{2} \right] \begin{pmatrix} 0 \\ \zeta^2 \\ -\frac{i}{d\lambda^2} [p\lambda\zeta - b\lambda^2\zeta^2] \\ -\frac{i}{d\lambda^2} [2 - \zeta^2] \end{pmatrix}. \end{aligned} \quad (23)$$

The non-vanishing components of the current density defined as

$$j^i = iq \bar{\Psi} \gamma^i \Psi, \quad \bar{\Psi} = \Psi^\dagger \beta, \quad (24)$$

are the electric charge density

$$\rho_e = q \Psi^\dagger \Psi,$$

which is generating an electric potential through the Poisson equation and the spatial component, j_y , whose dependence on the external fields intensities is

$$\begin{aligned} j_y &= q \Psi^\dagger \alpha^2 \Psi = \frac{4q}{d} |\mathcal{N}|^2 \frac{\zeta^2}{\lambda^2} [p\lambda\zeta - b\lambda^2\zeta^2] \exp[-\zeta^2] \\ &= \frac{4}{E_0} |\mathcal{N}|^2 \frac{x_*^2}{\lambda^4} \left[\left(p_y + \omega \frac{b}{d} \right) x_* - b x_*^2 \right] \exp \left[-\frac{x_*^2}{\lambda^2} \right] \\ &\approx \frac{4q^2}{E_0} |\mathcal{N}|^2 \left(x + \frac{\omega}{qE_0} \right)^3 (B_0^2 - E_0^2) (p_y - qB_0 x), \end{aligned} \quad (25)$$

ω being quantized as in (17).

4. THE MAGNETIC FIELD ALONE

The case corresponding to a zero electric field deserve a closer look. Now, for $\omega \neq 0$ and $p_z = 0 = E_0$, the equation (6) gets a simpler form,

$$\frac{d^2 \xi_{1,2}}{dx^2} + \left[\omega^2 - (p_y - qB_0x)^2 \pm qB_0 \right] \xi_{1,2} = 0, \quad (26)$$

which is, for each component of ξ , an oscillator-type equation. The solution

$$\xi = (qB_0)^{1/4} \begin{pmatrix} \psi_n(\tau) \\ \psi_{n-1}(\tau) \end{pmatrix},$$

is leading, using (5.a) written as

$$\sigma^1 \frac{d\xi}{dx} + i\sigma^2 (p_y - qB_0x)\xi = i\omega\varphi,$$

to

$$\varphi = i(qB_0)^{1/4} \begin{pmatrix} \psi_n(\tau) \\ -\psi_{n-1}(\tau) \end{pmatrix},$$

with

$$\psi_n(\tau) = C_n e^{-\tau^2/2} H_n(\tau),$$

where C_n is the normalization constant of the Hermite associated functions of dimensionless variable

$$\tau \equiv \frac{1}{\sqrt{qB_0}} (qB_0x - p_y) = \frac{x}{\ell_B} - p_y \ell_B. \quad (27)$$

The full wave function corresponding to the spectrum $\omega_n = \sqrt{2nqB_0}$, with $n \geq 1$, being

$$\Psi_0 = \frac{\sqrt{\omega_n}}{2\pi} (qB_0)^{1/4} \begin{pmatrix} \psi_n \\ \psi_{n-1} \\ i\psi_n \\ -i\psi_{n-1} \end{pmatrix} e^{i(p_y y - \omega t)}, \quad (28)$$

the observed current along Oy , in a given quantum state, for $-D/2 \leq x \leq D/2$, where D is the sample width, can be computed as

$$\begin{aligned} \mathcal{J}_n &= \frac{q}{\pi^2} \omega_n \sqrt{qB_0} \int_{-D/2}^{D/2} \psi_n(\tau) \psi_{n-1}(\tau) dx \\ &= \frac{q}{\pi^2} \omega_n \int_{-\frac{D}{2\ell_B} - p_y \ell_B}^{\frac{D}{2\ell_B} - p_y \ell_B} \psi_n(\tau) \psi_{n-1}(\tau) d\tau, \end{aligned} \quad (29)$$

obviously vanishing for $D \gg \ell_B$.

For a semi-infinite graphene plane perpendicular to the magnetic field B_0 , without any boundary condition, the current along Oy , has the following expressions for even respectively odd n -values,

$$\mathcal{J}_n^{even} = \frac{q}{\pi^2} \omega_n \frac{2^{n-1} \sqrt{2\pi}}{\sqrt{(n-1)! n!}} \frac{1}{[\Gamma(\frac{1-n}{2})]^2} \left(1 + \frac{p_y^2}{qB_0}\right),$$

$$\mathcal{J}_n^{odd} = \frac{q}{\pi^2} \omega_n \frac{2^{n-1} \sqrt{2\pi}}{\sqrt{(n-1)! n!}} \frac{2}{n [\Gamma(-\frac{n}{2})]^2} \left(1 - \frac{p_y^2}{qB_0}\right),$$

where

$$\frac{\mathcal{J}_{n=2k}}{\mathcal{J}_{n=2k+1}} = \frac{2k}{2k+1},$$

for $p_y^2 \ll qB_0$.

In the opposite case, meaning $D \ll \ell_B = 25/\sqrt{B_0}$ (nm), to first order in D/ℓ_B and $p_y \ell_B \ll 1$, the current (29) is linearly depending on D

$$\mathcal{J}_n \sim \frac{q}{\pi^2} \omega_n p_y D.$$

For $\omega = 0$, the equations in the system (5) (with $E_0 = 0$ and $p_z = 0$) decouple and the wave function corresponding to this dispersionless energy band is

$$\Psi^0 \sim \exp\left(-\frac{1}{2}\tau^2\right) \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix},$$

with τ given by (27). One may notice that the above expression exists also for zero-magnetic field, when it behaves like e^{xp_y} , being an edge state, for $p_y < 0$.

5. CONCLUSIONS

For massless fermions evolving in orthogonal electric and magnetic fields, the solution to the Dirac equation is expressed in terms of the biconfluent Heun functions. The exponential in (18) gets a maximum value for $\zeta = a$, meaning in view of (8),

$$x \sim \frac{\omega}{qE_0} \frac{E_0^2/c^2}{B_0^2}$$

and is exponentially dumping, for $a \gg 1$, once $\zeta > a$. However, one should be careful about the size, especially in strong magnetic fields since, once the samples get narrower (than about 40 nm), the electrical characteristics of the devices are more sensitive to temperature and to current fluctuations (current noise). These are significantly increasing as the device dimension shrinks [12] as an impact of the edge states.

If the electric field vanishes, the situation gets significantly simpler because the chiral wave function gets a familiar form expressed in terms of the Hermite associated functions, for unconfined harmonic oscillators, exhibiting n zeros.

For the physically relevant case of a semi-infinite graphene sheet with zigzag edges [13], the condition of an additional zero for the functions ψ_n in the origin of axes, provides a transcendental equation for the allowed values of the particle momentum along Oy ,

$$\psi_n \left(-\frac{p_y}{\sqrt{qB_0}} \right) \equiv 0.$$

Once an weak electric field along Ox is applied, one may employ the perturbation theory, [6], to evaluate the first-order transition amplitude between initial and final states characterized by the wave functions (28).

As a final remark, we would like to say that even though today it is no doubt that Heun's functions are successfully succeeding the hypergeometric ones in studying a whole range of phenomena, starting with the theory of quantum systems [14] to astrophysics [15], to the best of our knowledge, there are problems with their normalization and in evaluating the power-series representations, for some domains of the variable [16].

For example, in the physically interesting case corresponding to $B_0 = 0$, the equation (7) will be replaced by

$$\frac{d^2 \xi_{1,2}}{dx_*^2} - \frac{1}{x_*} \frac{d\xi_{1,2}}{dx_*} + \varepsilon \frac{p_y}{x_*} \xi_{1,2} + [d^2 x_*^2 - p_y^2] \xi_{1,2} = 0, \quad (30)$$

where d and x_* are defined in (8). Following the same procedure as in section 2, the function $u(x_*)$, introduced by

$$\xi(x_*) = x_*^2 \exp \left[i \frac{dx_*^2}{2} \right] u(x_*), \quad (31)$$

is the HeunB function of complex variable

$$\zeta = \sqrt{-id} x_* = -\frac{1}{\sqrt{2}} (1-i) \sqrt{d} x_*,$$

and complex γ and δ parameters. This can be understood as a sort of complex duality, which operates in between the Hermite and the parabolic cylinder functions (of variable $(1 \pm i)\tau$), respectively.

In terms of available soft, the treatment of Heun's equations can be done only with MAPLE routines which are working well in particular cases, but are breaking down for values of the parameters which might be of interest. That is why, as the aim of a coming paper, we plan to compare the analytical results derived in this work to

the ones obtained within a numerical analysis of the original system (5).

Acknowledgments. Ovidiu Buhucianu acknowledges the support of the European Social Fund in Romania, under the responsibility of the Managing Authority for the Sectorial Operational Programme for Human Resources Development 2007-2013, Grant POSDRU/88/1.5/S/47646.

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