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Original article

Exact solution of the Dirac–Weyl equation in graphene under electric and magnetic fields

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ABSTRACT

In this paper, we have obtained exact analytical solutions for the bound states of a graphene Dirac electron in magnetic fields with various q-parameters under an electrostatic potential. In order to solve the time-independent Dirac–Weyl equation, the Nikoforov–Uvarov (NU) and Frobenius methods have been used. We have also investigated the thermodynamic properties by using the Hurwitz zeta function method for one of the states. Finally, some of the numerical results are also shown.

1. Introduction

Graphene is a two-dimensional layer of graphite, which has received an enormous attention as it is expected to be an appropriate material for developing electronic devices [1–3]. In fact, there is a great challenge in the design of electronic devices. This challenge is in confining electrons in graphene. Since Dirac electrons cannot be confined in graphene by electrostatic potentials due to the Klein paradox, it was suggested that magnetic confinement should be considered [4–10].

Recently, a series of studies concerning the interaction of graphene electrons moving in magnetic fields perpendicular to the graphene surface [11–13] and/or including electrostatic fields parallel to the surface [14] have been carried out in order to find a way for confining the charges. In all these works, the Dirac–Weyl equation is considered for studying the electrons in graphene. These studies concluded that the charged massless carriers can be confined by appropriate electric and magnetic barriers, but only a limited number of examples have been considered. On the other hand, no experiments have been reported as yet, and we believe that it is because such field configurations are not easy to implement in the laboratory. However, different configurations of electric and magnetic fields have different effects. Further, under the combined effects of electric and magnetic fields, they may be used as near-linearly-controlled frequency filters or switches through appropriate designs [15]. For example, the graphene samples are mechanically cut into suitable shapes [16], and suitable magnetic fields and electric fields are employed through gates with suitable size to overcome the Klein effect, making them possible building blocks of nanoelectronic devices.

In this paper, we are going to obtain the exact analytical solutions of the Dirac–Weyl equation in the presence of both electric and magnetic fields with various q-parameters. We will use the Nikoforov–Uvarov and the Frobenius methods. Thus, we calculate some of the thermodynamic physical quantities for the final state. We also use the Hurwitz zeta function method for the calculation of the partition function.

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2. Theory

The effective Hamiltonian around Dirac points have the form $H = \pm\hbar\upsilon_F \sigma \cdot (-i\hbar\nabla)$, where $\sigma = (\sigma_x, \sigma_y)$ are the Pauli matrices and $\upsilon_F \approx 0.86 \times 10^6$ m/s is the Fermi velocity in graphene, and the $+(-)$ sign corresponds to the approximation that the wave vector k is near the Dirac points which are labeled as $K(K')$. Now, we are going to consider a Dirac electron moving in graphene under electric and magnetic fields acting toward the x–y plane of graphene. Under these circumstances, the low-energy spectrum is correctly described by the Dirac–Weyle equation for massless particle around the K-Dirac point in the Brillouin zone, which is given by:

$$\hbar\upsilon_F\left[\sigma \cdot \left(p + \frac{e}{c}A\right)\right]\psi(x, y) = \big(E - U(x)\big)\psi(x, y) \tag{1}$$

2.1. First magnetic potential

Firstly, by choosing the vector potential as $A(x) = (0, B_0 \cosh_q(\delta x)\exp(-\delta x), 0)$, the electric potential as $U(x) = U_0$, splitting the 2-spinor into its sublattice parts $\psi(x, y) = e^{iky}(\psi_A, i\psi_B)^T$ and using a new variable $s = \exp(-\delta x)$ that maps $x \in (0, \infty)$ to $s \in (0, \infty)$, we obtain the second-order differential equation satisfying the radial wave function $\psi_B(s)$ as:

$$\begin{aligned}&\left[\frac{d^2}{ds^2} + \frac{1}{s}\frac{d}{ds} + \frac{1}{s^2}\left(-\eta^2 s^2 + \beta^2 s - \varepsilon^2\right)\right]\psi_B(s) = 0\\ &\big(\psi_B(0) = 0, \psi_B(\infty) = 0\big)\end{aligned} \tag{2}$$

where

$$\begin{aligned}&\eta^2 = \frac{eB_0 q^2}{4c\hbar 4q^2\delta^2}, \qquad \beta^2 = -\frac{eB_0}{4c\hbar q\delta}\left(1 + \frac{1}{\delta} + \frac{1}{4\delta}\right)\\ &\varepsilon^2 = -\frac{1}{4q^2\delta^2}\left(\left(\frac{(E - U_0)^2}{\hbar^2\upsilon_F^2}\right)^2 - k^2 - \frac{3eB_0}{4c\hbar}\right)\end{aligned} \tag{3}$$

where δ and $q > 0$ are the screening and real parameters, respectively, and B_0 corresponds to a constant magnetic field along the z direction, which is perpendicular to the graphene plane. In this calculation, we applied the deformed hyperbolic functions introduced for the first time by Arai [17]. Now, we use the NU method [18] and the parametric NU derived in [19] to obtain the following energy-spectrum equation:

$$\beta^2 = 2(2n + 1 + \varepsilon)\eta \tag{4}$$

where the constant parameters used in our calculations have been displayed in Table 1 [20]. As a reminder, the NU method has been shown in Appendix A. Using Eqs. (3) and (4), we finally arrive at the following transcendental energy formula,

$$\begin{aligned}&E(k) = \operatorname{sgn}(n)\sqrt{\hbar^2\upsilon_F^2\left(-[a_1 n + a_2]^2 + a_3 eB_0 + k^2\right)^{1/2}} + U_0\\ &a_1 = 4\delta q, \quad a_2 = 2q\delta\left(\delta + \frac{5}{4}\right), \quad a_3 = \frac{3}{4c\hbar}\end{aligned} \tag{5}$$

where $n > 0$ is for the positive energy band and $n < 0$ is for the negative energy band. Using Eq. (38) in [19] and Table 1 [20], we obtain the corresponding radial wave function $\psi_B(x)$ as

$$\psi_B(x) = C_{n,m} x^{|\varepsilon|} e^{-\eta x^2/2} F\big(-n, |\varepsilon| + 1; \eta x^2\big) \tag{6}$$

where $C_{n,m}$ is a constant and

$$F(-n, \gamma, z) = \sum_{j=0}^{n} \frac{(-1)^j n! \Gamma(\gamma)}{(n - j)! j! \Gamma(\gamma + j)} z^j \tag{7}$$

is the Kummer confluent hypergeometric function [21]. Now, we write Eq. (7) in terms of Laguerre polynomials as follows: $L_n^n(x) = \frac{\Gamma(n+\varsigma+1)}{n!\Gamma(\varsigma+1)} F(-n, \varsigma + 1, x)$, and considering Eqs. (6) and (3) to obtain the radial wave functions. Thus, we have:

$$\psi_B(x) = C_{n,m} x^{|\varepsilon|} e^{-\eta x^2/2} \frac{n! \Gamma(2|\varepsilon| + \frac{1}{2})}{\Gamma(n + 2|\varepsilon| + \frac{1}{2})} L_n^{2|\varepsilon| - \frac{1}{2}}\big(\eta x^2\big) \tag{8}$$

To calculate the normalization constant $C_{n,m}$ in closed form, we use the normalization condition: $\int_0^\infty |\psi_B(r)|^2 dr = 1$. Therefore, we have: