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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:

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

where

$$\begin{aligned}\eta^2 &= \frac{eB_0q^2}{4c\hbar 4q^2\delta^2},\qquad \beta^2 = -\frac{eB_0}{4c\hbar q\delta}\left(1+\frac{1}{\delta}+\frac{1}{4\delta}\right)\\ \varepsilon^2 &= -\frac{1}{4q^2\delta^2}\left(\left(\frac{(E-U_0)^2}{\hbar^2\upsilon_F^2}\right)^2-k^2-\frac{3eB_0}{4c\hbar}\right)\end{aligned} \tag{3}$$

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,

$$\begin{aligned}E(k) &= \mathrm{sgn}(n)\sqrt{\hbar^2\upsilon_F^2\big(-[a_1n+a_2]^2+a_3eB_0+k^2\big)^{1/2}}+U_0\\ a_1 &= 4\delta q,\quad a_2 = 2q\delta\left(\delta+\frac{5}{4}\right),\quad a_3=\frac{3}{4c\hbar}\end{aligned} \tag{5}$$

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: $\int_0^\infty|\psi_B(r)|^2dr = 1$. Therefore, we have:

$$C_{n,m}^{-2}=\left[\frac{n!\Gamma(2|\varepsilon|+\frac{1}{2})}{\Gamma(n+2|\varepsilon|+\frac{1}{2})}\right]^2\times\int_0^\infty x^{4|\varepsilon|}\mathrm{e}^{-\eta x^2}\left[L_n^{|\varepsilon|}(\eta x^2)\right]^2\mathrm{d}(\eta x^2) \tag{9}$$

Now, we use the integral formula $\int_0^\infty x^{\alpha-1}\exp(-\lambda x)L_m^\beta(\lambda x)L_n^\gamma(\lambda x)\mathrm{d}x$ for the calculation of the normalization constant of the radial wave function. Thus, we obtain the normalization constant as follows:

$$C_{n,m}=\left(\frac{-2^{4|\varepsilon|+1}\Gamma(n+2|\varepsilon|+1/2)\eta^{2|\varepsilon|+1}}{\Gamma(n+4|\varepsilon|+1)\Gamma(n-1/2)_3F_2(-n,2|\varepsilon|+1,3/2;-n+3/2,2|\varepsilon|+1/2;1)}\right)^{\frac{1}{2}} \tag{10}$$

where $F_2(a,b,c;d,e;1)$ is defined as the Barnes extended hypergeometric function [21]. Finally, we obtain the normalized radial wave function as:

$$\begin{aligned}\psi_{\mathrm{B}}(x)=&\sqrt{\frac{\eta}{{}_3F_2(-n,2|\varepsilon|+1,3/2;-n+3/2,2|\varepsilon|+1/2;1)}}\\&\times\left[\frac{-1}{((-n+3/2)_\delta(n+2|\varepsilon|-1/2)(-n-2|\varepsilon|-3/2)_{\delta-1}(2|\varepsilon|+1))}\right]^{\frac{1}{2}}\\&\times n!\left(-\eta x^2\right)^{|\varepsilon|}\exp\left(-\frac{\eta x^2}{2}\right)L_n^{2|\varepsilon|-1/2}\left(-\eta x^2\right)\end{aligned} \tag{11}$$

and $(a)_\delta$ is the Pochhammer symbol in the theory of the special function, defined as $(a)_\delta=\Gamma(a+\delta)/\Gamma(a)$.

2.2. Second magnetic potential

Secondly, by choosing the vector potential as $\vec{A}=(0,\{B_0\exp(-2\delta x)/[1+q\exp(-2\delta x)]\},0)$, where δ and $q>0$ are the screening and real parameters, respectively, B_0 corresponds to a constant magnetic field along the z direction, which is perpendicular to the graphene plane, and the electric potential as $U(x)=U_0$, splitting the 2-spinor into its sublattice parts $\psi(x,y)=\mathrm{e}^{\mathrm{i}ky}(\psi_{\mathrm{A}},\mathrm{i}\psi_{\mathrm{B}})^{\mathrm{T}}$ and using a new variable $s=\exp(-2\delta x)$ that maps $x\in(0,\infty)$ to $s\in(0,\infty)$, we obtain the second-order differential equation satisfying the radial wave function $\psi_{\mathrm{B}}(s)$ of the same Eq. (2) with

$$\begin{aligned}\eta^2&=-\left[\left(\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right)^2-k^2\right]q^2+\frac{2keB_0}{c\hbar}q+\left(\frac{eB_0}{c\hbar}\right)^2\\\beta^2&=\frac{-2\delta B_0e}{c\hbar}+2\left[\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right]^2-2k^2-\frac{2keB_0}{c\hbar},\qquad\varepsilon^2=-\left[\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right]^2+k^2\end{aligned} \tag{12}$$

Now, to avoid repetitions in our solution, we finally arrive at the following transcendental energy formula for this state,

$$\begin{aligned}&-D(\delta+k)-\xi=[2n+1+\xi]\sqrt{\xi q^2+2kDq+D^2}\\&D=\frac{eB_0}{c\hbar},\quad\xi=\left[-\left(\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right)^2+k^2\right]\end{aligned} \tag{13}$$

and obtain the corresponding radial wave function (Eq. (11)) by substituting the parameters of Eq. (12).

2.3. Third magnetic potential

Thirdly, by choosing the vector potential as $\vec{A}=(0,[B_0\exp(-\delta x)/x],0)$, the electric potential as $U(x)=U_0$, splitting the 2-spinor into its sublattice parts $\psi(x,y)=\mathrm{e}^{\mathrm{i}ky}(\psi_{\mathrm{A}},\mathrm{i}\psi_{\mathrm{B}})^{\mathrm{T}}$ and using a new variable $s=\exp(-2\delta x)$ that maps $x\in(0,\infty)$ to $s\in(0,\infty)$, we obtain the second-order differential equation satisfying the radial wave function $\psi_{\mathrm{B}}(s)$ of the same Eq. (2) by substituting the following parameters:

$$\begin{aligned}-\eta^2&=\left[\left(\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right)^2-k^2\right]q^2+\frac{2keB_0}{c\hbar}q+\left(\frac{eB_0}{c\hbar}\right)^2\\\beta^2&=\frac{-2\delta B_0e}{c\hbar}+2\left[\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right]^2-2k^2-\frac{2keB_0}{c\hbar}\\\varepsilon^2&=-\left[\frac{(E-U_0)^2}{\hbar^2\upsilon_{\mathrm{F}}^2}\right]^2+k^2\end{aligned} \tag{14}$$

In here, we used the following approximation as [22]:

$$\frac{1}{r^2} \approx \frac{4\delta^2 e^{-2\delta r}}{(1-qe^{-2\delta r})^2} \to \frac{1}{r} \approx \frac{2\delta e^{-\delta r}}{1-qe^{-2\delta r}} \tag{15}$$

Now, to avoid repetition, we obtain the energy formula corresponding to this stage,

$$\begin{aligned} &-D(\delta+k)-\xi = [2n+1+\xi]\sqrt{\xi q^2+2kDq+D^2}, \\ &D=\frac{eB_0}{c\hbar}, \quad \xi=\left[k^2-\left(\frac{(E-U_0)^2}{\hbar^2\upsilon_F^2}\right)^2\right] \end{aligned} \tag{16}$$

and the corresponding radial wave function is obtained by substituting the parameters of Eq. (14) in Eq. (11).

2.4. Fourth magnetic potential

At the end, by choosing the vector potential as $\vec{A}=(0,[B_0x-\lambda/x],0)$, where λ is a constant and B_0 corresponds to a constant magnetic field along the z direction, which is perpendicular to the plane of graphene, and choosing the electrostatic potential as $U(x)=U_0$ and using a new variable $\chi=\sqrt{e|B_0|/c\hbar}x$, then after simple calculations, we have

$$\begin{aligned} &\frac{d^2\psi_B(\chi)}{d\chi^2}+\left\{\frac{\varepsilon_{k,\lambda}c\hbar}{e|B_0|}+\frac{e\lambda}{c\hbar}\left(\frac{e\lambda}{c\hbar}-1\right)\frac{1}{\chi^2}\right. \\ &\left.+\frac{2ek\lambda}{\sqrt{c\hbar e|B_0|}}\frac{1}{\chi}+\frac{2keB_0}{\sqrt{c\hbar e|B_0|}}\chi-\chi^2\right\}\psi_B(\chi)=0 \end{aligned} \tag{17}$$

where $\varepsilon_{k,\lambda}=\frac{(E-U_0)^2}{\hbar^2\upsilon_F^2}-k^2+\frac{eB_0}{c\hbar}+\frac{2e^2B_0\lambda}{c^2\hbar^2}$. Now, we choose the radial component of $\psi_B(\chi)$ as:

$$\psi_B(\chi)=\chi^{e\lambda/c\hbar}\exp\left[-\frac{1}{2}\chi\left(\chi-\frac{2kB_0}{|B_0|}\sqrt{\frac{c\hbar}{e|B_0|}}\right)\right]F(\chi)$$

Inserting this ansatz into Eq. (17), we will have:

$$\begin{aligned} &\chi\frac{d^2F(\chi)}{d\chi^2}+\left[2\frac{e\lambda}{c\hbar}+\frac{2keB_0}{\sqrt{c\hbar e|B_0|}}\chi-2\chi^2\right]\frac{dF(\chi)}{d\chi} \\ &+\left[\left(1+\frac{B_0}{|B_0|}\right)\frac{2ek\lambda}{\sqrt{c\hbar e|B_0|}}+\left(\frac{\varepsilon_{k,\lambda}c\hbar}{e|B_0|}+\frac{keB_0}{2\sqrt{c\hbar e|B_0|}}-2\left(\frac{e\lambda}{c\hbar}+1\right)-\frac{B_0}{|B_0|}\right)\chi\right]F(\chi)=0 \end{aligned} \tag{18}$$

Equation (18) is the biconfluent Heun's differential equation [23], whose solution is the so-called biconfluent Heun (BCH) function, H_B:

$$F(\chi)=H_B\left(2\frac{e\lambda}{c\hbar}-1,\frac{2keB_0}{\sqrt{c\hbar e|B_0|}},\frac{\varepsilon_{k,\lambda}c\hbar}{e|B_0|}+\frac{ek^2B_0^2}{c\hbar|B_0|}-\frac{B_0}{|B_0|},\frac{4ek\lambda}{\sqrt{c\hbar e|B_0|}},-\chi\right) \tag{19}$$

Also, after substituting $\psi_A(\chi)$ with $\psi_A(\chi)=\chi^{(e\lambda/c\hbar)+1}\exp\{-\chi[\chi-(2kB_0/|B_0|)\sqrt{c\hbar/e|B_0|}]/2\}H(\chi)$, we obtain:

$$H(\chi)=H_B\left(2\frac{e\lambda}{c\hbar}+1,\frac{2keB_0}{\sqrt{c\hbar e|B_0|}},\frac{\varepsilon_{k,\lambda}c\hbar}{e|B_0|}+\frac{ek^2B_0^2}{c\hbar|B_0|}+\frac{B_0}{|B_0|},\frac{4ek\lambda}{\sqrt{c\hbar e|B_0|}},-\chi\right) \tag{20}$$

We can calculate the probability density for an eigenfunction $\rho_n(x)=\psi_n^+(x,y)\psi_n(x,y)=\psi_A^2(x)+\psi_B^2(x)$, and the current density in the y direction for this eigenfunction $j_n(x)=e\upsilon_F\psi_n^+(x,y)\sigma_y\psi_n(x,y)=2e\upsilon_F\psi_A(x)\psi_B(x)$ [24]. Also, we can calculate the local density of state using the representation $N=\sum_{n,m}|\psi_{n,m}(r)|^2\delta(E-E_{n,m})$ [25].

But we would like that to follow the analyses drawn from Eq. (19). To accomplish this, we define the constants A, B, D, and the function G representing F as follows:

$$\begin{cases} A=\dfrac{e\lambda}{c\hbar}, \quad B=1+\dfrac{B_0}{|B_0|}, & \text{if } G=F \\ D=\dfrac{\varepsilon_{k,\lambda}c\hbar}{e|B_0|}+\dfrac{keB_0}{2\sqrt{c\hbar e|B_0|}}-2\left(\dfrac{e\lambda}{c\hbar}+1\right)-\dfrac{B_0}{|B_0|}, & \text{if } G=F \end{cases} \tag{21}$$

Now, by making use of these definitions, Eq. (18) be as

$$\chi\frac{\mathrm{d}^2G(\chi)}{\mathrm{d}\chi^2}+\left[2A+\frac{2keB_0}{c\hbar}\sqrt{\frac{c\hbar}{e|B_0|}}\chi-2\chi^2\right]\frac{\mathrm{d}G(\chi)}{\mathrm{d}\chi}+\left[B\frac{2ek\lambda}{c\hbar}\sqrt{\frac{c\hbar}{e|B_0|}}+D\chi\right]G(\chi)=0 \tag{22}$$

Now, we substitute $G(\chi)=\sum_n C_n\chi^n$ in Eq. (22) and use the Frobenius method; then we can simply obtain the recurrence relation as follows:

$$C_{n+2}=\frac{-1}{(n+2)(n+2A+1)}\left\{\left[\frac{2k[e\lambda B+B_0(n+1)]}{\sqrt{c\hbar e|B_0|}}\right]C_{n+1}+(D-2n)C_n\right\}$$
$$C_1=-\frac{ek\lambda B}{A\sqrt{c\hbar e|B_0|}}C_0 \tag{23}$$

By using Eq. (23), and assuming that $C_0=1$, the first three coefficients of the expansion are as follows:

$$C_2=\frac{1}{2(2A+1)}\left[\frac{2k^2B\lambda}{A}\left(\frac{(e\lambda B+B_0)}{c\hbar|B_0|}\right)-D\right]$$
$$C_3=\frac{-1}{6(A+1)}\left\{\frac{k(Be\lambda+2B_0)}{(2A+1)\sqrt{c\hbar e|B_0|}}\times\left[D-\frac{2k^2B\lambda}{A}\left(\frac{(e\lambda B+B_0)}{c\hbar|B_0|}\right)\right]+\frac{Bek\lambda}{A\sqrt{c\hbar e|B_0|}}(D-2)\right\} \tag{24}$$

At this point, we can obtain an analytical solution to the radial equation by breaking the series expansion of the biconfluent Heun function into a Heun polynomial of degree n. By imposing the two conditions $C_{n+1}=0$ and $D=2n$ with $(n=1,2,3,\ldots)$ on the coefficients, this can be achieved. From the condition $D=2n$, it is possible we obtain a formal expression for the energy. However, the biconfluent Heun series becomes a polynomial of degree n when [26,27]

$$\frac{\varepsilon_{k,\lambda}c\hbar}{e|B_0|}+\frac{1}{4}\left(\frac{2kB_0}{|B_0|}\right)^2\frac{c\hbar}{e|B_0|}=2n+2-\left(1+4\frac{e\lambda}{c\hbar}\left(\frac{e\lambda}{c\hbar}-1\right)\right)^{1/2} \tag{25}$$

with $(n=1,2,3\ldots)$. Finally, we can obtain the energy spectrum from Eq. (25) as follows:

$$E_n=\mathrm{sgn}(n)\sqrt{\frac{2\upsilon_F^2\hbar e|B_0|}{c}\left[n+\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}\left(\frac{e\lambda}{c\hbar}-1\right)}\Big/2-\frac{e\lambda}{c\hbar}\right]}+U_0 \tag{26}$$

where $n>0$ corresponds to electron-like Landau level energy and $n<0$ corresponds to hole-like Landau level energy. There is a single Landau level exactly at $E=0$, corresponding to $n=0$, as a result of chiral symmetry and particle–hole symmetry. Now, for $U_0=0$, $\lambda=0$ and $\hbar=c=1$, we have $E_n=\pm\upsilon_F\sqrt{2e|B_0|n}$, which is the known expression giving the relativistic Landau levels for massless fermions in the presence of a constant orthogonal magnetic field.

Let us study only the thermodynamical properties for the above case. In fact, we can use the energetic spectrum formula (26) to study the thermodynamics properties of such a system in the presence and the absence of a magnetic field. Here, we assume that the electrostatic potential is zero. Having calculated the energy, we can immediately obtain the thermodynamical quantities of the system in a systematic manner. The thermodynamics properties of graphene and graphene nanoribbons have been studied under electric and magnetic modulations from the theoretical and experimental viewpoints (see [28–32]). In order to obtain all thermodynamic quantities of the pseudo-relativistic electrons system, we should concentrate, at first, on the calculation of the partition function Z. The partition function Z at temperature T is obtained through the Boltzmann factor as $Z=\sum_{n=0}^{\infty}\mathrm{e}^{-(E_n-E_0)\beta}$, where $\beta=1/k_BT$, k_B is the Boltzmann constant [33], and E_0 is the ground state energy correspondent to $n=0$. The partition function Z of this problem at temperature T is obtained as [34]:

$$Z=\exp\left(\beta\upsilon_F\sqrt{\frac{2\hbar e|B_0|}{c}\left[\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}\left(\frac{e\lambda}{c\hbar}-1\right)}\Big/2-\frac{e\lambda}{c\hbar}\right]}\right)$$
$$\times\sum_{n=0}^{n}\exp\left(-\beta\upsilon_F\sqrt{\frac{2\hbar e|B_0|}{c}\left[n+\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}\left(\frac{e\lambda}{c\hbar}-1\right)}\Big/2-\frac{e\lambda}{c\hbar}\right]}\right) \tag{27}$$

Since $\exp(\beta\upsilon_F\sqrt{\frac{2\hbar e|B_0|}{c}[\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}(\frac{e\lambda}{c\hbar}-1)/2-\frac{e\lambda}{c\hbar}}])\approx 1$, the partition function Z can therefore be written as:

$$Z=\sum_{n=0}^{n}\exp\left(-\beta\upsilon_F\sqrt{\frac{2\hbar e|B_0|}{c}\left[n+\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}\left(\frac{e\lambda}{c\hbar}-1\right)}\Big/2-\frac{e\lambda}{c\hbar}\right]}\right) \tag{28}$$

We assumed that the electrostatic potential is zero in this case. In order to cover all the temperature range, we use the Hurwitz zeta function method. Now, by using the formula [35,36]

$$\mathrm{e}^{-x} = \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{d}s x^{-s} \Gamma(s), \tag{29}$$

Eq. (28) is transformed into

$$\begin{aligned}
&\sum_n \mathrm{e}^{(-\beta \upsilon_\mathrm{F} \sqrt{\frac{2\hbar e|B_0|}{c}[n+\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}(\frac{e\lambda}{c\hbar}-1)}/2-\frac{e\lambda}{c\hbar}]})} \\
&= \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{d}s \left(\beta \upsilon_\mathrm{F} \sqrt{\frac{2\hbar e|B_0|}{c}}\right)^{-s} \\
&\quad \times \sum_n \left[n + \frac{c(1-\sqrt{1+4(e\lambda/c\hbar)[(e\lambda/c\hbar)-1]}-(e\lambda/c\hbar))}{4\hbar e|B_0|}\right]^{-s/2} \Gamma(s) \\
&= \frac{1}{2\pi \mathrm{i}} \int_C \mathrm{d}s \left(\beta \upsilon_\mathrm{F} \sqrt{\frac{2\hbar e|B_0|}{c}}\right)^{-s} \\
&\quad \times \zeta_\mathrm{H}\left(\frac{s}{2}, \frac{c(1-\sqrt{1+4(e\lambda/c\hbar)[(e\lambda/c\hbar)-1]}-(e\lambda/c\hbar))}{4\hbar e|B_0|}\right) \Gamma(s)
\end{aligned} \tag{30}$$

where $x = \beta \upsilon_\mathrm{F} \sqrt{\frac{2\hbar e|B_0|}{c}[n+\frac{1}{2}-\sqrt{1+4\frac{e\lambda}{c\hbar}(\frac{e\lambda}{c\hbar}-1)}/2-\frac{e\lambda}{c\hbar}]}$, $\Gamma(s)$ is the Euler function and $\zeta_\mathrm{H}(\frac{s}{2}, \frac{c(1-\sqrt{1+4(e\lambda/c\hbar)[(e\lambda/c\hbar)-1]}-(e\lambda/c\hbar))}{4\hbar e|B_0|})$ is the Hurwitz zeta function. The Hurwitz zeta function ζ_H [37] is as follows:

$$\zeta_H(s,\alpha) = \sum_{n=0}^{\infty} \frac{1}{(n+\alpha)^s} \tag{31}$$

where $0 < \alpha \leq 1$ is a well-defined series when $\Re e(s) > 1$, and can be analytically continued to the whole complex plane with one singularity, a simple pole with residue 1 at $s = 1$. An integral representation of the Hurwitz zeta function is:

$$\zeta_\mathrm{H}(s,\alpha) = \frac{1}{\Gamma(s)} \int_0^{\infty} t^{s-1} \frac{\mathrm{e}^{-t\alpha}}{1-\mathrm{e}^{-t}} \mathrm{d}t, \quad \Re(s) > 1,\ \Re(\alpha) > 0 \tag{32}$$

The properties of the Hurwitz zeta function $\zeta_\mathrm{H}(s,\alpha)$ are as follows [37,38]:

$$\zeta_\mathrm{H}(0,\alpha) = \frac{1}{2} - \alpha \tag{33}$$

$$\zeta_\mathrm{H}(-p,\alpha) = \frac{B_{p+1}(\alpha)}{p+1}, \quad p \in \mathrm{N} \tag{34}$$

where $B_r(\alpha)$ being the Bernoulli polynomials. The asymptotic series corresponding to the Hurwitz zeta function is as:

$$\zeta_\mathrm{H}(1+z,\alpha) = \frac{1}{2}\alpha^{-z} + \frac{1}{2}\alpha^{-1-z} + \frac{1}{z}\sum_{i=2}^{\infty} \frac{B_i \Gamma(z+i)}{\Gamma(z)} \alpha^{-z-i} \tag{35}$$

with B_i are Bernoulli's numbers.

The Hurwitz zeta function $\zeta_\mathrm{H}(s,\alpha)$ has only singularity—namely a simple pole at $s = 1$ with residue 1. It can be analytically continued to the rest of the complex s-plane. Now, for the two poles $s = 0$ and $s = 2$, we apply the residues theorem. Therefore, the desired partition function is written as:

$$Z = \vartheta/\beta^2 \upsilon_\mathrm{F}^4 + \zeta_H(0,\vartheta), \qquad \vartheta = \left[\frac{c(1-\sqrt{1+4(e\lambda/c\hbar)[(e\lambda/c\hbar)-1]}-(e\lambda/c\hbar))}{4\hbar e|B_0|}\right] \tag{36}$$

Finally, the final partition function can be written by using Eq. (33) as:

$$Z = \vartheta\left(\frac{1}{\beta^2 \upsilon_\mathrm{F}^4} - 1\right) + \frac{1}{2} \tag{37}$$

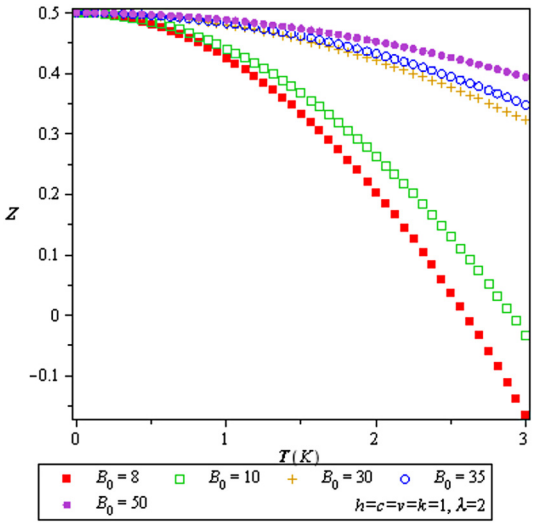

Fig. 1. Partition function as a function of T for various values of B_0.

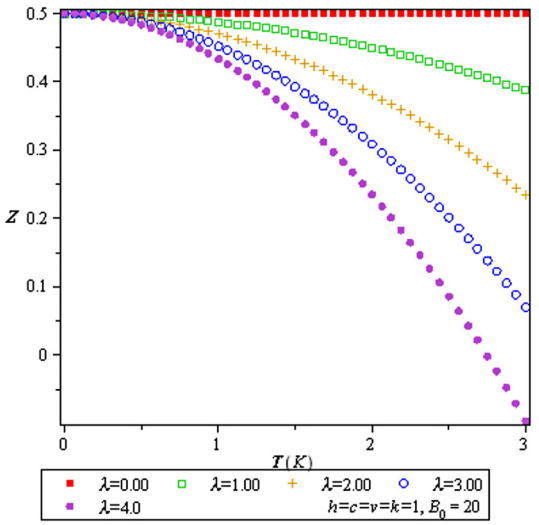

Fig. 2. Partition function as a function of B for various values of λ.

In Figs. 1 and 2, we show the dependence of the partition function Z of the graphene as a function of T with various values of B_0 and λ. In fact, this clearly illustrates that the results calculated by the analytical expression for the partition function decrease with increasing temperature. Extending the calculated partition function to an interaction-free N-body system can be done via $Z = Z^N$. The dependence on N and on volume comes via the dependence on the energy eigenvalues E_n.

The thermodynamical properties of the system can be obtained from the partition function [34]. In fact, any other parameter that might contribute to the energy should also appear in the argument of Z [34], as in the Helmholtz free energy F, which is alternatively defined as $F = -\ln(Z)/\beta$:

$$F = -\ln\left\{\vartheta\left(\frac{1}{\beta^2\upsilon_{\mathrm{F}}^4} - 1\right) + \frac{1}{2}\right\}\Big/\beta \tag{38}$$

In Fig. 3, we show the dependence of the Helmholtz free energy F function as a function of the T with $\lambda = (0.00, 1.00, 2.00, 3.00, 4.00)$. In fact, this clearly illustrates that the results calculated by the analytical expression for the Helmholtz free energy function increase with increasing temperature. And the mean energy is:

$$U = 2\vartheta/\beta^3\upsilon_{\mathrm{F}}^4\left\{\vartheta\left(\frac{1}{\beta^2\upsilon_{\mathrm{F}}^4} - 1\right) + \frac{1}{2}\right\} \tag{39}$$

Here, the vibrational entropy S that is as $S = -\partial F/\partial T$ or

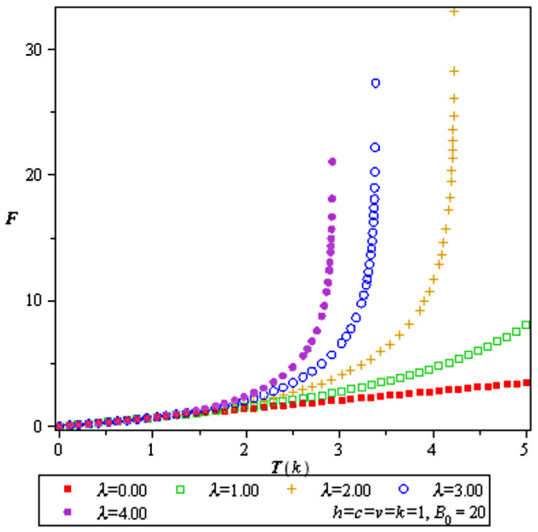

Fig. 3. Helmholtz free-energy function as a function of T for various values of λ.

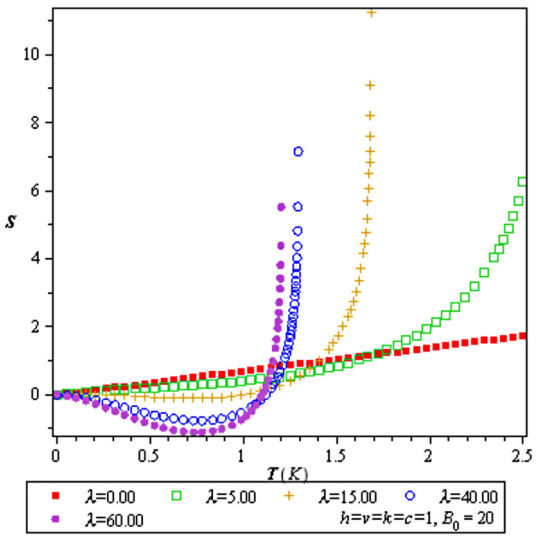

Fig. 4. Mean energy function as a function of T for various values of λ.

$$\begin{aligned} S &= k_B \ln(Z) - k_B\beta\frac{\partial}{\partial\beta}\ln(Z) \\ &= k_B \ln\left\{\vartheta\left(\frac{1}{\beta^2\upsilon_F^4}-1\right)+\frac{1}{2}\right\} - 2\vartheta\Big/\beta^3\upsilon_F^4\left\{\vartheta\left(\frac{1}{\beta^2\upsilon_F^4}-1\right)+\frac{1}{2}\right\} \end{aligned} \tag{40}$$

In Figs. 4, we show the dependence of the Helmholtz free energy F function as a function of T with λ. In fact, this clearly illustrates that the results calculated by the analytical expression for the entropy increase with increasing temperature. And the specific heat can be found as $C = \partial U/\partial T$ or

$$C = -k_B\beta^2\frac{\partial U}{\partial\beta} = -4k_B\vartheta\left(\vartheta\left[1-3\beta^2\upsilon_F^4\right]+\frac{3\beta^2\upsilon_F^4}{2}\right)\Big/\left(\vartheta\left[1-\beta^2\upsilon_F^4\right]+\frac{\beta^2\upsilon_F^4}{2}\right)^2 \tag{41}$$

Also, with the energy spectrum specified or the partition function, and using the Gibbs statistics, the thermodynamic potential for the electrons, Ω_e, and the holes, Ω_h, as

$$\Omega_e = -\frac{k_B T}{\pi\ell_B^2}\left[2\sum^{\infty}\ln\left\{1+\left(\vartheta\left(\frac{1}{\beta^2\upsilon_F^2}-1\right)+\frac{1}{2}\right).e^{\mu}\right\}+\ln\left(1+\exp(\mu/k_B T)\right)\right] \tag{42}$$

and $\Omega_{\rm h} = (-\mu, T)$, we can calculate the quantum capacitance of the graphene quantum dot placed in the magnetic field by using Eqs. (2) and (4) and the method given in Ref. [39] with Eq. (42), and the total charge density $Q = e(N - P)$. Finally, using the above equations, we can easily find other thermodynamic quantities.

3. Conclusion

Exact solutions of the Dirac–Weyl equation in the presence of both electric and magnetic fields with various q-parameters were obtained by using the Nikoforov–Uvarov and Frobenius methods analytically. In addition, we calculated some of the thermodynamic physical quantities for the final state. We also used from the Hurwitz zeta function method for the calculation of the partition function.

Appendix A. Nikoforov–Uvarov method

We give a brief description of the conventional NU method [18]. This method is based on solving the second-order differential equation of hypergeometric type by means of special orthogonal functions

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0 \tag{A.1}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of degree at most 2, and $\tilde{\tau}(s)$ is a polynomials of degree at most 1. If we take the following factorization $\psi_n(s) = \phi(s)y_n(s)$, (A.1) becomes:

$$\sigma(s)y_n''(s) + \tau(s)y_n'(s) + \lambda y_n(s) = 0 \tag{A.2}$$

where

$$\pi(s) = \sigma(s)\frac{\mathrm{d}}{\mathrm{d}s}\big(\ln\varphi(s)\big) \tag{A.3}$$

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \qquad \tau'(s) < 0 \tag{A.4}$$

where $\pi(r)$ is a polynomial of order at most one.

The $y_n(s)$ can be expressed in terms of the Rodrigues relation:

$$y_n(s) = \frac{a_n}{\rho(s)}\frac{\mathrm{d}^n}{\mathrm{d}s^n}\big[\sigma^n(s)\rho(s)\big] \tag{A.5}$$

where a_n is a normalization constant and the weight function $\rho(s)$ must satisfy the differential equation:

$$\omega'(s) - \left(\frac{\tau(s)}{\sigma(s)}\right)\omega(s) = 0, \qquad \omega(s) = \sigma(s)\rho(s) \tag{A.6}$$

The function $\pi(s)$ and the parameter λ in the above equation are defined as follows:

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \tag{A.7}$$

$$\lambda = k + \pi'(s) \tag{A.8}$$

The determination of k is the essential point in the calculation of $\pi(s)$. It is simply defined by setting the discriminate of the square root to zero. Thus, a new eigenvalues equation is:

$$\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s) \quad n = 0, 1, 2, \ldots \tag{A.9}$$

For a more simple application of the method, we develop a parametric generalization of the NU method, which is valid for any potential under consideration by an appropriate coordinate transformation $s = s(r)$.

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