Thermodynamic Properties of q-deformed massless Dirac fermions in graphene with Rashba coupling

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Abstract

We study the thermodynamic properties of massless Dirac fermions in graphene under a uniform magnetic field and Rashba spin-orbit coupling with a \(q\)–deformed Heisenberg algebra calculus. The thermodynamic functions such as the Helmholtz free energy, total energy, entropy and heat capacity are obtained by using an approach based on the zeta function and Euler-Maclaurin formula. These functions will be numerically examined for different values of \(\eta = \frac{1}{\ln(q)}\). In particular, the heat capacity in the presence of deformation, all curves coincide and reach the fixed value \(C = 6K_B\) three times greater compared to the case of undeformed massless Dirac fermions in graphene.

PACS numbers: 65.80.Ck, 03.65.-w

Keywords: Graphene, Rashba coupling, zeta function, Euler-Maclaurin formula, partition function, thermodynamic functions, \(q\)-deformed algebra.

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1 Introduction

Graphene, which is an elemental sheet of graphite, consists of a periodic, two-dimensional arrangement of carbon atoms of monoatomic thickness with a honeycomb structure. It is the latest member of the carbon allotropic family: diamond, graphite, C60 fullerenes [1] and nanotubes [2]. For the first time in 2004, a graphene sheet stable at room temperature was obtained physically by A. Geim and K. Novoselov [3]. This experiment contradicted the theory that a graphene sheet was thermodynamically unstable. As this new material developed by mechanical exfoliation has remarkable and unique properties, they were awarded the Nobel Prize in Physics in 2010. Since this discovery, graphene has been the material most studied by the scientific community for its new and unique physical properties. Indeed, it has a high superior electrical mobility [4, 5], an anomalous quantum Hall effect [6], a modulable band gap [7] and it is a transparent conductor [8] since, in the optical region, it absorbs only 2.3% of light. It also has good flexibility [9] and excellent mechanical strength, and its thermal conductivity is ten times higher than that of copper [10].

The more general framework of the $q$-deformation theory for a real parameter $q$ has found great success and has attracted considerable attention from physicists and mathematicians. The interesting physical application was started by the introduction of the $q$-deformed harmonic oscillator by Biedenharn [11] and Macfarlane [12] in 1989. Quantum mechanics can be considered as a deformation (the deformation parameter is $\hbar$) of classical mechanics and relativistic mechanics is another deformation (with $c^{-1}$ as the deformation parameter) of classical mechanics. In the same sense, quantum mechanics can be seen as the limit of a more general theory depending on one or more deformation parameters.

The study of the dynamic behavior of systems is a central question in physics and mathematics. These systems provide fundamental and general results which have found major applications not only in physics, but also in all other branches of science, as well as in technology; however, the harmonic oscillator is the simplest and most fundamental theoretical model of mechanical and electrical oscillatory phenomena. The definitions and main properties of independent and time dependent harmonic oscillators and damped harmonic oscillators have been studied by several authors [13, 14].

It was lately shown that the regular standard thermodynamics of Boltzmann-Gibb’s statistics are no longer suitable for studying all physical systems, including the attitude of complex systems controlled by the Tsallis non-extensive statistics [15] and non-equilibrium statistics of the $q$-deformed superstatistics [16, 17]. The concept of superstatistics was first developed by Wilk and Wlodarczyk [18] before Beck and Cohen [19] latter reworded the theory.

Motivated by the work done on thermodynamic proprieties under magnetic field and Rashba coupling [23] we will generalize this last work by introducing the notion of the $q$-deformed harmonic oscillator and see the influence of the parameter $q$ on the various thermodynamic quantities. For this, we consider a massless Dirac fermions in monolayer graphene with the magnetic field applied perpendicular to the graphene layer. Through investment of The $q$-deformed algebra of the quantum oscillator defined by $q$-deformed Heisenberg algebra we express our Hamiltonian in terms of creation and annihilation operators to obtain the solutions of the energy spectrum, this last will be used to determine the partition function which will help us to calculate and plot numerically the different thermodynamic functions in order to make conclusions. The present paper is organized as follows. In section 2, we give an overview on $q$-deformed Heisenberg algebra which serves to determine, explicitly,
the exact eigenvalues in terms of $q$-deformed parameter. In section 3, we will look for the partition function which will be the key to determine the different thermodynamic functions such as the free energy of Helmholtz, internal energy, entropy and heat capacity. section 4, will be devoted to the numerical results and discussions as well as comparison with literature. We conclude our results in the final section.

2 Theoretical model

2.1 $q$-deformed quantum theory

The $q$-deformed algebra of the quantum oscillator is defined by $q$-deformed Heisenberg algebra in terms of creation and annihilation operators $a^\dagger$ and $a$, respectively, and number operator $N$ by [20–22]

\[ [a, a] = [a^\dagger, a^\dagger] = 0, \quad [a, a^\dagger]_q = aa^\dagger - q^{-1}a^\dagger a = q^N, \quad [N, a^\dagger] = a^\dagger, \quad [N, a] = -a \] (1)

where deformation parameter $q$ is real and the observed value of $q$ has to satisfy the non-additivity property

\[ [x + y] \neq [x] + [y] \] (2)

In addition, the operators obey the relations

\[ [N] = a^\dagger a, \quad [N + 1] = aa^\dagger \] (3)

The $q$–Fock space spanned by orthonormalized eigenstates $|n\rangle$ is constructed according to

\[ |n\rangle = \frac{(a^\dagger)^n}{\sqrt{[n]!}} |0\rangle, \quad a|0\rangle = 0 \] (4)

Both $q$–factorial and $q$–numbers are defined, respectively, by

\[ [n]! = [n][n-1][n-2] \cdots [1], \quad [n] = \frac{q^n - q^{-n}}{q - q^{-1}} \] (5)

For $n \in \mathbb{N}$ with $[0]! = 1$. The eigenvalues of the $q$–deformed one-dimensional harmonic oscillator are

\[ E_n = \frac{\hbar \omega}{2} ([n] + [n + 1]) \] (6)

Considering the definition of basic number given in (5), and making $q = e^{i\eta}$, the eigenvalues become

\[ E_n = \frac{\hbar \omega \sin[\eta(n + \frac{1}{2})]}{2 \sin[\frac{\eta}{2}]} \] (7)

2.2 Eigenvalue problem

We consider a massless Dirac fermions in monolayer graphene with the magnetic field applied perpendicular to the graphene layer. Low energy quasiparticles in graphene with Rashba spin orbit coupling (RSOC) interaction can be well described by the Dirac-type Hamiltonian

\[ H = v_F (\eta \sigma_x \pi_x + \sigma_y \pi_y) + \lambda_R (\eta \sigma_x s_y - \sigma_y s_x) \] (8)
where the conjugate momentum $\pi_x$ and $\pi_y$ can be written in symmetric gauge $\vec{A} = \frac{B}{2}(-y, x)$ as

$$
\pi_x = p_x - \frac{eB}{2}y, \quad \pi_y = p_y + \frac{eB}{2}x.
$$

Where $B$ and $v_F = 10^6 \text{m/s}$ are respectively the uniform magnetic field and the Fermi velocity, the parameter $\eta = \pm 1$ labels the valley degrees of freedom, $\sigma = (\sigma_x, \sigma_y)$ are the Pauli matrices of pseudospin operator on $A(B)$ lattice cites. The present system presents the intrinsic spin orbit coupling (SOC), but its value is very weak compared to the RSOC \cite{23}, for this we have neglected it because it will not influence on the physical properties of the studied system.

Fixing a certain intra-Landau-level quantum number, we denote by $|r_{A,B}, n, \sigma\rangle = (a|^{n}_{\eta}\rangle r_{A,B}, n, \sigma\rangle$ a state in the $n$th Landau level with spin direction $\sigma \in \{\uparrow, \downarrow\}$, and all other eigenstates are of the form $|\Psi\rangle = (|r_A, n, \uparrow\rangle, |r_B, n - 1, \downarrow\rangle, |r_B, n, \uparrow\rangle, |r_A, n - 1, \downarrow\rangle)^T$. The Hamiltonian (8) around a single Dirac point ($\eta = +1$) with these considerations is given by

$$
H = \begin{pmatrix}
0 & 0 & v_F (\pi_x - i\pi_y) & 0 \\
0 & 0 & 0 & v_F (\pi_x + i\pi_y) \\
v_F (\pi_x + i\pi_y) & 0 & 0 & -2i\lambda_R \\
0 & v_F (\pi_x - i\pi_y) & 2i\lambda_R & 0
\end{pmatrix}.
$$

To diagonalize the Hamiltonian (10), it is convenient to introduce the usual bosonic operators in terms of the conjugate momentum

$$
a = \frac{\ell_B}{\sqrt{2\hbar}} (\pi_x - i\pi_y), \quad a^\dagger = \frac{\ell_B}{\sqrt{2\hbar}} (\pi_x + i\pi_y)
$$

which verify the commutation relation $[a, a^\dagger] = q^N$, $\ell_B = \sqrt{\frac{\hbar}{eB}}$ is the magnetic length. Express (10) in terms of $a$ and $a^\dagger$ to obtain

$$
H = \begin{pmatrix}
0 & \frac{\sqrt{2\hbar v_F}}{\ell_B} a & \frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger & 0 \\
\frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger & 0 & 0 & \frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger \\
\frac{\sqrt{2\hbar v_F}}{\ell_B} a & 0 & -2i\lambda_R & 0 \\
0 & \frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger & 2i\lambda_R & -E
\end{pmatrix}.
$$

To find the solution of the energy spectrum we act the Hamiltonian on the state $|\Psi\rangle$ leading to the eigenvalue equation

$$
\begin{pmatrix}
-E & 0 & \frac{\sqrt{2\hbar v_F}}{\ell_B} a & \frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger \\
0 & -E & 0 & \frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger \\
\frac{\sqrt{2\hbar v_F}}{\ell_B} a & 0 & -2i\lambda_R & 0 \\
\frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger & 0 & 2i\lambda_R & -E
\end{pmatrix}
\begin{pmatrix}
|r_A, n, \uparrow\rangle \\
|r_B, n - 1, \downarrow\rangle \\
|r_B, n, \uparrow\rangle \\
|r_A, n - 1, \downarrow\rangle
\end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}
$$

giving the following system of equations

$$
-E|r_A, n, \uparrow\rangle + \frac{\sqrt{2\hbar v_F}}{\ell_B} a|r_B, n, \uparrow\rangle = 0
$$

$$
-E|r_B, n - 1, \downarrow\rangle + \frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger|r_A, n - 1, \downarrow\rangle = 0
$$

$$
\frac{\sqrt{2\hbar v_F}}{\ell_B} a^\dagger|r_A, n, \uparrow\rangle - E|r_B, n, \uparrow\rangle - 2i\lambda_R|r_A, n - 1, \downarrow\rangle = 0
$$

$$
\frac{\sqrt{2\hbar v_F}}{\ell_B} a|r_B, n - 1, \downarrow\rangle + 2i\lambda_R|r_B, n, \uparrow\rangle - E|r_A, n - 1, \downarrow\rangle = 0.
$$
These can be solved to obtain a second order equation for the eigenvalues

$$E^2 \pm 2\lambda_R E - (\hbar \omega_D)^2 [n] = 0, \quad n = 0, 1, 2 \cdots$$

(18)

where $\omega_D = v_F \sqrt{2eB/\hbar}$ is the Dirac constant. The following solutions of the last equations are the form

$$E_{1,n}^\pm = -\lambda_R \pm \sqrt{(\hbar \omega_D)^2 [n] + \lambda_R^2}$$

$$E_{2,n}^\pm = \lambda_R \pm \sqrt{(\hbar \omega_D)^2 [n] + \lambda_R^2}$$

(19)

(20)

We note that the preceding energies depend to the Rashba coupling parameter $\lambda_R$ and the $q$–deformation parameter, now using the equation (5) to find

$$E_{1,n}^\pm = \lambda_R \left( -1 \pm \sqrt{1 + \left( \frac{\hbar \omega_D}{\lambda_R} \right)^2 \frac{\sin(n\eta)}{\sin(\eta)}} \right)$$

$$E_{2,n}^\pm = \lambda_R \left( 1 \pm \sqrt{1 + \left( \frac{\hbar \omega_D}{\lambda_R} \right)^2 \frac{\sin(n\eta)}{\sin(\eta)}} \right)$$

(21)

(22)

In Figure (1), we present the eigenvalues of the $q$–deformed massless Dirac fermions in graphene,

![Figure 1](image)

Figure 1 – (Color online) Eigenvalue $E$ versus $n$ for different values of $q$–deformed parameters, $\eta = 0, 0.2, 0.4, 0.6$, respectively for the values of the magnetic field and Rashba coupling parameter $B \sim 10^{-3}$ and $\lambda_R = 0.014meV$ [23].

thus, the energy levels shows that when there is no deformation the energy is quantified and has a parabolic form and symmetrical compared to the quantization axis $n$, but for a given deformation we notice that the parabolic form tends towards an ellipse, on the other hand there is an appearance of a second quantification via the periodicity of ellipses.

Now if we consider very small deformation and neglect all terms proportional to $\eta^4$, we have

$$E_{1,n}^\pm = \epsilon_{1,n}^\pm \pm \Delta \epsilon(n)$$

$$E_{2,n}^\pm = \epsilon_{2,n}^\pm \pm \Delta \epsilon(n)$$

(23)

where $\varrho$, $\epsilon_{1,n}^\pm$, $\epsilon_{2,n}^\pm$ and $\Delta \epsilon(n)$ are defined by
\[
\begin{align*}
\epsilon_1^{\pm} &= \lambda_R \left[ -1 \pm \sqrt{1 + \varrho^2 n} \right] \quad (24) \\
\epsilon_2^{\pm} &= \lambda_R \left[ 1 \pm \sqrt{1 + \varrho^2 n} \right] \quad (25) \\
\Delta \epsilon_n &= -\frac{\lambda_R q^2}{12} \frac{n^3}{\sqrt{1 + \varrho^2 n}} \quad (26) \\
\varrho &= \frac{\hbar \omega_D}{\lambda_R} \quad (27)
\end{align*}
\]

The term \( \Delta \epsilon_n \) is the correction on the energy when the deformation exists, without deformation i.e. \( q \to 1 \ (\eta \to 0) \) the last energies are reduced to the expressions already found in [23].

### 3 Thermodynamic quantities

We will study the thermodynamic properties of massless Dirac fermions in graphene with Rashba coupling in contact with a thermal reservoir at finite temperature. For simplicity, we assume that only fermions with positive energy \( (E > 0) \) are regarded to constitute the thermodynamic ensemble [23].

We start by evaluating

\[
Z = \text{Tr} e^{-\beta H} = \sum_{n=0}^{+\infty} \left( e^{-\beta \epsilon_1^{\pm}} + e^{-\beta \epsilon_2^{\pm}} \right)
\]

where \( \beta = \frac{1}{k_B T} \), \( k_B \) is the Boltzmann constant and \( T \) is the equilibrium temperature. Using (23-28), we show that \( Z \) takes the form

\[
Z = \sum_{n=0}^{+\infty} e^{-\beta (\epsilon_1^{\mp} + \Delta \epsilon_n)} + e^{-\beta (\epsilon_2^{\mp} + \Delta \epsilon_n)}
\]

\[
= \sum_{n=0}^{+\infty} e^{\beta \Delta \epsilon_n} e^{-\beta (\epsilon_1^{\mp} + \epsilon_2^{\mp})}
\]

noting here that the term \( e^{-\beta \Delta \epsilon_n} \) is very small than 1 then the development limit around 0 give

\[
Z \approx \sum_{n=0}^{+\infty} (1 + \beta \Delta \epsilon_n) e^{-\beta (\epsilon_1^{\mp} + \epsilon_2^{\mp})}
\]

\[
Z \approx \frac{Z_0 + Z_1}{Z_0}
\]

with the partitions functions of no deformed system \( Z_0 \) and the correction partition function \( Z_1 \) have as expressions

\[
Z_0 = \sum_{n=0}^{+\infty} e^{-\beta (\epsilon_1^{\mp} + \epsilon_2^{\mp})}
\]

\[
Z_1 = \sum_{n=0}^{+\infty} \beta \Delta \epsilon_n e^{-\beta (\epsilon_1^{\mp} + \epsilon_2^{\mp})}
\]

the partition function \( Z_0 \) for no deformed system is already calculated in [23] and it has the following expression

\[
Z_0 = \left[ \frac{2}{\varrho^2} (\tau^2 - 1) + 1 \right] \cosh \frac{1}{\tau}.
\]

5
Where $\tau = \frac{k_B T}{\lambda_R}$ is the reduced temperature. Indeed, the second term can be evaluated by using the Euler-Maclaurin formula; starting by the equation

$$Z_1 = \frac{\phi^2 \eta^2}{6 \tau} \cosh \frac{1}{\tau} \sum_{n=0}^{+\infty} \frac{\eta^3}{\sqrt{1 + \phi^2 n}} e^{-\frac{1}{\tau} \sqrt{1 + \phi^2 n}}$$

(33)

to solve the last sum it’s convenient to approximate integrals by finite sums, or conversely to evaluate finite sums and infinite series using integrals, indeed we put

$$f(x) = \frac{x^3}{\sqrt{1 + \phi^2 x}} e^{-\frac{1}{\tau} \sqrt{1 + \phi^2 x}}$$

(34)

using the Euler–Maclaurin formula

$$\sum_{x=0}^{+\infty} f(x) = \frac{1}{2} f(0) + \int_0^{+\infty} f(x) - \sum_{p=1}^{+\infty} \frac{B_{2p}}{2p!} f^{(2p-1)}(0)$$

(35)

$B_{2p}$ are the Bernoulli numbers, and $f^{(2p-1)}$ is the derivative of order $(2p - 1)$. Up to $p = 1$, the values $f(0)$ and $f^{(1)}(0)$ are nulls, then with the straightforward calculation the final form of $Z_1$ have the form

$$Z_1 = \frac{16 \eta^2}{\phi^6} (15 \tau^6 + 15 \tau^5 + 6 \tau^4 + \tau^3) e^{-\frac{1}{\tau}} \cosh \frac{1}{\tau}$$

(36)

Finally, the compact final form of the q-deformed partition function of the system

$$Z = \left( \frac{2}{\phi^2} (\tau^2 - 1) + 1 + \frac{16 \eta^2}{\phi^6} (15 \tau^6 + 15 \tau^5 + 6 \tau^4 + \tau^3) e^{-\frac{1}{\tau}} \right) \cosh \frac{1}{\tau}$$

(37)

Since we have inferred the partition function of our framework, we would now be able to determine all related thermodynamic quantities. The determination of all thermal properties, such as the Helmholtz free energy $F$, internal energy $U$, heat capacity $C$ and entropy $S$, can be obtained through the expression of the partition function $Z$ by using the following relations [23]:

$$F = -\lambda_R \tau \ln Z$$

(38)

$$U = \lambda_R \tau^2 \frac{\partial \ln Z}{\partial \tau}$$

$$S = \frac{1}{k_B} \frac{\partial F}{\partial \tau}$$

$$C = \frac{1}{k_B} \frac{\partial U}{\partial \tau}.$$ 

Then, we will numerically investigate the above thermodynamic functions to underline the conduct of our framework. This will be finished by giving a few plots under reasonable conditions and making various discussions.

4 Numerical Results and discussions

To make a reference to reality of graphene, we restrict our study to the low-energy regime, which may be reached by fixing an appropriate values of the Rashba coupling parameter $\lambda_R$ and the external
magnetic field $B$. Indeed, for $B \simeq 10^{-3}T$ and $\lambda_R = 0.014meV$. The thermodynamic functions versus the reduced temperature $\tau$ for the fixed values of $\eta = 0, 0.2, 0.4, 0.6, 0.8, 0.9$, respectively for the values of the magnetic field and Rashba coupling parameter $B \sim 10^{-3}T$ and $\lambda_R = 0.014meV$ [23].

It is clearly seen that the common remark between the four curves is the $\eta$-deformed parameter does not influence on the thermodynamic properties of the system in the low temperature regime. In figure (2.a) The free energy $F$ decreases gradually with increasing of temperature at a given $\eta$-deformed parameter and decreases with $\eta$ at a given temperature. In figure (2.b) we observe that at high temperature our system follows Joule’s first law in both cases, with and without deformation, thus in the case where the $\eta$—deformed parameter is not zero the internal energy in this regime is asymptotic to $U = 6\lambda_R\tau$, but when $\eta = 0$ the internal energy become asymptotic to $U = 2\lambda_R\tau$, then we observe that for two cases the internal energy in high temperature regime depends only on the reduced temperature $\tau$, then we conclude for two cases the kinetic energy of translation of molecules is the unique form of energy of $N$ atoms contained in a volume $V$ of the system. In figure (2.c) there are two remarks to report in low temperature in particular for $0 < \frac{S}{k_B} < 1.7$ the entropy is negative which can be explained by the less disorder of the system [23], in the case where $\frac{S}{k_B} > 1.7$ the entropy increases when $\eta$-parameter increases. For the three curves at the top (a,b,c) we deduce that the parameter $\eta$-parameter plays the same role of the doping of the graphene, however when $\eta$ increase the thermodynamic properties such as entropy, internal energy increases with $\eta$-parameter in the same way when we dope pure graphene with boron atoms $B$ or nitrogen $N$ and vice versa [24], and for the free
energy of Helmholtz, it decrease when \( \eta \) decrease similarly when the concentration of the doped atoms in graphene decrease. What is remarkable is in figure (2.d) we observe that without q-deformation our system at high temperature obeys to the Dulong-Petit law, but when the q-deformation is introduced, the heat capacity passes through a maximum in low temperature regime, that is, the point where the temperature changes very little as energy is supplied to the system, most of the energy is used to excite the carbon atoms of the ground state in the excited state, rather than increasing the kinetic energy of the system, that on the one hand, on the other hand at high temperature the heat capacity coincide and reach the fixed value \( C = 6k_B \) three times greater compared to the case of no deformed massless Dirac fermions in graphene which can be explained by the increasing of degree of freedom of the system due to the introduction of the \( \eta \)-deformed parameter.

5 Conclusion

In this paper, after a brief insight on the notion of the q-deformed harmonic oscillator, we have studied the thermodynamic properties of Dirac fermions in graphene in this deformation formalism, we have found the eigenvalues of the considered system via q-deformed annihilations and creations operators. It was shown that the eigenvalues of our system are more general than in the case where there is no deformation, and especially we tested them in the limiting case \( \eta = 0 \) where the ordinary results were well recovered. The eigenvalues are used together with a method based on the zeta function and Euler-Maclaurain formula to determine the partition function according to the q-deformed parameter. Therefore the thermodynamic functions, such as the Helmholtz free energy, total energy, entropy and heat capacity, were obtained in terms of the q-deformed parameter.

Subsequently, some cases were studied related to the \( q \)-deformed parameter. Indeed, we numerically analyzed the plotted curves which allowed us to make important remarks on the influence of deformation on the thermodynamic properties of our system. We also found a similarity between the doping concentration and the q-deformed parameter for the graphene system [24]. Finally, it was shown that the Dulong-Petit law is no longer verified when the q-deformed harmonic oscillator notion is introduced where the heat capacity at high temperature tends to a constant value \( C = 6k_B \) three times greater in comparison with the Dirac fermions in graphene [23].

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