Thermodynamic Properties of Polar Quantum Disc with Conical Disclination

Ritik Saklani [a)], Bhavya Kaushik[b)], and Surender Pratap*

Department of Physics & Astronomical Science, Central University of Himachal Pradesh-176206 (H.P), India.

[a)]ritiksaklani7@gmail.com
[b)]bhavayakaushik2001@gmail.com

Abstract

In this study, we have investigated the thermodynamic properties of the polar quantum disc having conical disclination. The spectrum of the non-interacting charged particle system was obtained with the aid of the Schrödinger equation with the effective mass approximation. The charged particle under investigation is confined by parabolic potential and a homogeneous magnetic field perpendicular to the quantum disc. We have shown the variation of internal energy (U) and specific heat C_v with the kink parameter α. Both U and C_v increase with the increase in α.

Keywords: Specific heat, Polar Quantum Disc, Internal energy, Thermodynamic Properties.

*** Address of correspondence**
Dr. Surender Pratap
Department of Physics & Astronomical Science, Central University of Himachal Pradesh-176206 (H.P), India

Email: suren1986dhalaria@hpcu.ac.in

How to cite this article
Ritik Saklani, Bhavya Kaushik, and Surender Pratap, Thermodynamic Properties of Polar Quantum Disc with Conical Disclination, J. Cond. Matt. 2023; 01 (02): 61-64

Available from:
https://doi.org/10.61343/jcm.v1i02.24

Introduction

The quest for low-dimensional materials rapidly increasing day by day after the successful synthesis of two-dimensional (2D) graphene [1]. The discovery of 2D graphene has opened up new avenues in the fundamental science and technology of low-dimensional materials [2,3]. Many of graphene's extraordinary features stem from its dimensionality and exceedingly unusual electronic dispersion relation, in which electrons imitate relativistic particles. The electrons in graphene are usually referred to as massless Dirac fermions, which may be thought of as electrons with zero rest mass (despite the fact that electrons are fundamental particles with characteristic mass) [4]. As a result, the unusual behavior of electrons makes graphene an ideal material to explore relativistic effects in condensed matter physics. The most remarkable consequences of the unusual behavior of electrons in graphene are the quantum Hall effect, anomalous quantum Hall effect, Klein paradox, ballistic electron propagation, metal-free magnetism, breakdown of the adiabatic Born-Oppenheimer approximation, possibility of high T_C superconductivity, and observation of relativistic phenomena such as zitterbewegung or jittery motion of a wave function under the influence of confining potentials [1].

In graphene, the inherent binary degrees of freedom, such as valleys, sublattices, and top/bottom layers in multilayers, result in a 2D electron gas with valley selective chirality of the electrons at the Fermi energy. As a result, breaking the spatial inversion symmetry through staggered AB sublattice potentials in graphene or applying a vertical electric field in rhombohedral multilayers opens up a band gap [4]. Moreover, 2D graphene is naturally anticipated to include 1D zero-line modes caused by kinks in the Dirac mass [5]. Recently, Bi *et al.* investigated the role of topological defects on the electronic and transport properties of zero-line modes in single and bilayer graphene systems. The band evolution of the quantum valley Hall edge modes and the zero-line modes in bilayer graphene ribbons reveals that the edge modes of the quantum valley Hall effect develop changing gaps as the ribbon orientation deviates from the zigzag direction, whereas the corresponding zero-line modes remain gapless all the way except in the armchair direction [6].

The study of edge states in graphene structures is currently gaining popularity. It has been discovered that zigzag graphene nanoribbons (ZGNRs) have a localized edge state near the Fermi energy, which has a significant impact on their electronic behavior [7]. In ZGNRs, the existence of edge states results in zero energy band gap, and hence these nanoribbons are always metallic [7,8]. Because the presence of an energy gap is required for many applications in nanoelectronics, controlling and manipulating the edge states in ZGNRs is a significant problem [8]. The effect of external electric potentials applied along the edges of ZGNR can produce a spectral gap, transforming the metallic behavior of ZGNR to a semiconducting one. Therefore, it has been observed that edge states are sensitive to external electric potentials and are topological in nature [9,10]. The topological defects present in the system have crucial effects on the physical properties of the system under investigation. The presence of topological defects can modify the electronic, thermal, and thermodynamic properties of the material [11]. In this study, we theoretically investigated the thermodynamic properties of the polar quantum disc with conical disclination within the presence of a uniform magnetic field $\vec{B}$. We have considered the parabolic electric potential for confinement in the polar disc. The Volterra process is used to introduce the disclination defect [12]. The partition function (Z) of the system is obtained after solving the Schrödinger equation with the effective mass approximation. The conical disclination described by the Volterra process is depicted in figure 1.

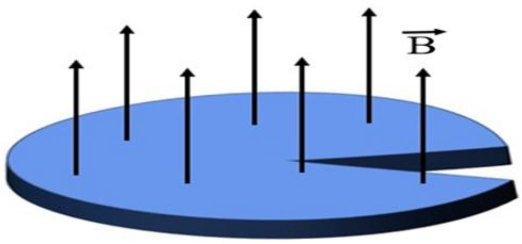

Figure 1: Volterra Construction for the polar quantum disc in which a sector is removed from the disc. The vertical arrow represents homogeneous magnetic field.

Theoretical Formulation

We have considered a polar quantum disc of radius R and height h with a topological defect in the form of conical disclination in the presence of a uniform magnetic field. The disclinated disc follows the metric given below:

$$ds^2 = dr^2 + r^2 d\varphi^2 + dz^2 \qquad \varphi \in [0, 2\pi, \alpha] \qquad \ldots(1)$$

where α is the kink parameter which is related to the deficit angle (for 0 < α <1) or surplus angle (for α >1). Disc having no conical disclination is associated with kink parameter value α equal to one. We simplify the metric using the following transformation of coordinate system [12].

$$\rho = \alpha r, \ \phi = \varphi/\alpha, \phi \in [0, 2\pi] \qquad \ldots(2)$$

the simplified metric has the form

$$ds^2 = \alpha^{-2} d\rho^2 + \rho^2 d\phi^2 + dz^2, \qquad \phi \in [0, 2\pi] \qquad \ldots(3)$$

The parabolic potential for the polar disc is defined as:

$$V(\rho, \alpha) = \begin{cases} \frac{1}{2\alpha^2}\mu\omega_{0p}\rho^2 & ; \ \rho < \alpha R \\ \infty & ; \ \rho > \alpha R \end{cases} \qquad \ldots(4)$$

The potential in the axial direction is

$$V(z) = \begin{cases} 0 & ; \ \rho < h \\ \infty & ; \ \rho > h \end{cases} \qquad \ldots(5)$$

where, μ represents the electron's effective mass, while ω_{0p} corresponds to the angular frequencies linked with the classical harmonic oscillator for the parabolic potential. The Schrödinger equation in effective mass approximation is written as [13]-

$$\frac{1}{2\mu}\left(\vec{p} + e\vec{A}\right)^2 \psi(\rho, z, \phi) + V(\rho)\,\psi(\rho, z, \phi) = E_T\,\psi(\rho, z, \phi) \qquad \ldots(6)$$

where $\vec{p} = -i\hbar\vec{\nabla}$ is the quantum mechanical momentum operator and $\vec{A} = \left(\frac{B\rho}{2\alpha}\right)\hat{\phi}$ is the vector potential with the magnetic field. Total wavefunction for electron in polar quantum disc can be written in the form:

$$\psi(\rho, z, \phi) = C_{ml}\chi_{ml}(\rho)\sin\left(\frac{n\pi z}{h}\right)e^{im\phi} \qquad \ldots(7)$$

where C_{ml} is the normalization factor, which depends on the values of the azimuthal m and radial l quantum numbers. The radial part of the electron's wavefunction satisfies a second order differential equation:

$$\frac{\alpha^2}{\rho}\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\chi(\rho)\right) + \left\{\frac{2\mu}{\hbar^2}\left[E_{ml} - \frac{m\hbar\omega_c}{2\alpha} - V(\rho)\right] - \frac{m^2}{\rho^2} - \frac{\mu^2\omega_c^2}{4\hbar^2\alpha^2}\right\}\chi(\rho) = 0 \qquad \ldots(8)$$

The solution of the radial Schrödinger equation is a linear combination of the Whittaker M and W functions

$$\chi(\rho) = \frac{C_1}{\rho}M_{\rho,v}(\xi) + \frac{C_2}{\rho}W_{\sigma,v}(\zeta) \qquad \ldots(9)$$

where $\sigma = \frac{2\alpha^2 E_{ml} - m\alpha\hbar\omega_c}{2\hbar\alpha^2\sqrt{\omega_c^2 + \omega_{0p}^2}}$, $\qquad \ldots(10)$

$$v = \frac{|m|}{2\alpha} \qquad \ldots(11)$$

$$\xi = \frac{\mu\sqrt{\omega_c^2 + 4\omega_{0p}^2}}{2\hbar\alpha^2}\rho^2 \qquad \ldots(12)$$

C_1 and C_2 are constants. In Eqn. (9), the Whittaker W function has divergent nature at origin, so $C_2 = 0$, leaving the radial component of the wave function as

$$\chi(\rho) = \frac{C_1}{\rho}M_{\rho,v}(\xi) \qquad \ldots(13)$$

Also, the electron's wave function must vanish at boundary of the wall (ρ = αR) and we obtained the following expression for the energy eigen values

$$E_T = E_{ml} + E_z = \hbar\sqrt{\omega_c^2 + 4\omega_{0p}^2}\,\sigma_R + \frac{n^2\hbar^2\pi^2}{2\mu h^2} + \frac{m\hbar\omega_c}{2\alpha} \qquad \ldots(14)$$

in which σ_R is the value of σ that satisfies the boundary condition $M_{\sigma,v}(\zeta_R) = 0$, with $\zeta_R = \zeta\,(\rho = \alpha R)$.

The partition function is given by-

$$Z = \sum_n e^{\frac{n^2 \hbar^2 \pi^2}{2\mu h^2}} \sum_m e^{\frac{m\hbar\omega_c}{2\alpha}} e^{\hbar\sqrt{\omega_c^2 + 4\omega_{0p}^2 \sigma R}} \quad \ldots(15)$$

$$Z \approx Z_1 Z_2 \quad \ldots(16)$$

$$Z_1 = \sum_n e^{\frac{n^2 \hbar^2 \pi^2}{2\mu h^2}} \to \int_0^\infty e^{-\gamma n^2}\, dn = \frac{1}{2}\sqrt{\frac{\pi}{\gamma}} \quad \ldots(17)$$

where $\gamma = e^{\frac{\hbar^2 \pi^2}{2\mu h^2}}$, and we have used the classical approximation because the order of spacing between the energy level is very less than the thermal energy that is $\Delta E \approx 10^{-42}$ J << $k_B T \approx 10^{-21}$ J, so we have replaced summation with the integration.

$$Z_1 \approx \frac{h}{\hbar}\sqrt{\frac{\mu}{2\pi\beta}} \quad \ldots(18)$$

where h is the height of disc.

Now,

$$Z_2 = 1 + e^{\chi\beta} + e^{2\chi\beta} + \cdots + e^{-\chi\beta} + e^{-2\chi\beta} \quad \ldots(19)$$

We define $\chi = \frac{\hbar\omega_c}{2\alpha}$; these are actually geometric series.

$$Z_2 \approx \frac{1}{1 - e^{-\beta\chi}}$$

$$Z = \frac{1}{1 - e^{-\beta\chi}} \frac{h}{\hbar^2}\sqrt{\frac{\mu}{2\pi\beta}} \quad \ldots(20)$$

Internal energy U is given by:

$$U = -\frac{\partial \ln Z}{\partial \beta}$$

$$U = \frac{1}{2\beta} + \frac{\chi}{e^{\beta\chi} - 1} \quad \ldots(21)$$

Specific heat is given by

$$C_v = -k_B \beta^2 \frac{\partial U}{\partial \beta}$$

$$C_v = \frac{k_B \beta^2 \chi^2 e^{\beta\chi}}{\left(e^{\beta\chi} - 1\right)^2} + \frac{k_B}{2} \quad \ldots(22)$$

Results and Discussion

In our calculations, we have taken the effective mass of electron $\mu = 0.067\ m_e$, magnetic energy $\hbar\omega_c = 5.0$ meV, thermal energy ($k_B T$) = 26 meV, and temperature (T) = 300 K. Figures 2 and 3 show the variation of internal energy and specific heat capacity with the kink parameter (α) of a polar quantum disc with conical disclination. It is clear from figure 2 that for α < 1, the increase in internal energy is very sharp, whereas, for α > 1, the internal energy slowly increases and approaches a constant value. Hence, in the presence of a uniform magnetic field, the internal energy of the system is enhanced due to the distortion produced by disclination.

For α < 1, and T = 300 K, the C_v sharply increases with a small increase in α (see figure 3). For α > 1 with the same temperature, C_v increases with α and becomes constant at higher values of α > 1.5.

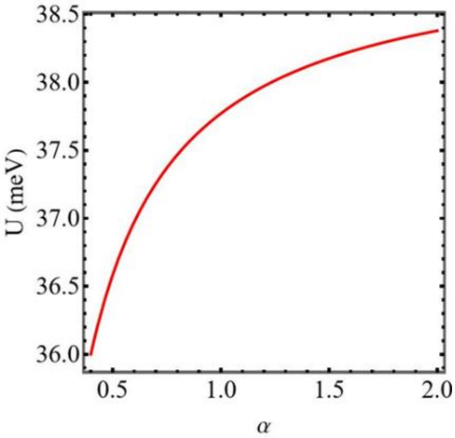

Figure 2: Variation of internal energy U with the kink parameter α for polar quantum disc with disclination.

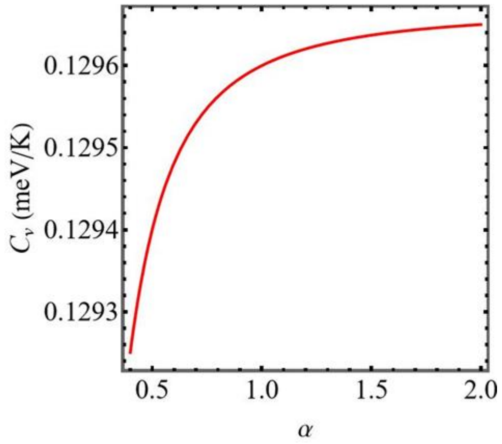

Figure 3: Variation of specific heat C_v with kink parameter α for polar quantum disc having disclination.

Conclusion

We investigated a theoretical study to calculate the internal energy & specific heat for a polar quantum disc with conical disclination. The charge particle in quantum disc is confined by parabolic electric potential in the presence of the homogeneous magnetic field perpendicular to plan of polar quantum disc. Results show that internal energy and specific heat can be modulated with the kink parameter. These findings are crucial for the design of nanodevices.

Acknowledgement

Authors wish to acknowledge the Central University of Himachal Pradesh for providing the facility during the course of this work.

References

1. A. C. Neto, F. Guinea, N. M. Peres, K. S. Novoselov, and A. K. Geim, "*The electronic properties of graphene*," Reviews of modern physics 81, 109 (2009).
2. S. Kumar, S. Pratap, V. Kumar, R. K. Mishra, J. S. Gwag, and B. Chakraborty, "*Electronic, transport, magnetic, and optical properties of graphene*

nanoribbons and their optical sensing applications: A comprehensive review," Luminescence 38, 909–953 (2023).
3. S. Pratap, N. Joshi, R. Trivedi, C. S. Rout, B. Chakraborty, et al., "*Recent development of two-dimensional tantalum dichalcogenides and their applications*," Micro and Nanostructures, 207627 (2023).
4. H. Min, B. Sahu, S. K. Banerjee, and A. MacDonald, "*Ab initio theory of gate induced gaps in graphene bilayers*," Physical Review B 75,155115 (2007).
5. W. Yao, S. A. Yang, and Q. Niu, "*Edge states in graphene: From gapped flat-band to gapless chiral modes,*" Physical review letters 102, 096801 (2009).
6. X. Bi, J. Jung, and Z. Qiao, "*Role of geometry and topological defects in the one-dimensional zero-line modes of graphene*," Physical Review B 92, 235421 (2015).
7. S. Pratap, "*Transport properties of zigzag graphene nanoribbons in the confined region of potential well*," Superlattices and Microstructures 100, 673–682 (2016).
8. S. Pratap, S. Kumar, and R. P. Singh, "*Certain aspects of quantum transport in zigzag graphene nanoribbons*," Frontiers in Physics 10, 940586 (2022).
9. P. Delplace, D. Ullmo, and G. Montambaux, "*Zak phase and the existence of edge states in graphene,*" Physical Review B 84, 195452 (2011).
10. C. K. Chiu, J. C. Teo, A. P. Schnyder, and S. Ryu, "*Classification of topological quantum matter with symmetries*," Reviews of Modern Physics 88, 035005 (2016).
11. S. Fumeron, B. Berche, F. Moraes, F. A. Santos, and E. Pereira, "*Geometrical optics limit of phonon transport in a channel of disclinations*," The European Physical Journal B 90, 1–8 (2017).
12. J. D. Castano-Yepes, D. Amor-Quiroz, C. Ramirez-Gutierrez, and E. A. Gómez, "*Impact of a topological defect and rashba spin-orbit interaction on the thermo-magnetic and optical properties of a 2d semiconductor quantum dot with gaussian confinement*," Physica E: Low-dimensional Systems and Nanostructures 109, 59–66 (2019).
13. C. Furtado, B. G. da Cunha, F. Moraes, E. B. de Mello, and V. Bezzerra, "*Landau levels in the presence of disclinations*," Physics Letters A 195, 90–94 (1994).