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free energy, persistent current, and entanglement entropy**

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Visualization of Higher Genus Carbon Nanomaterials: Free Energy, Persistent Current, and Entanglement Entropy

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Abstract—The goal of this project is to explore computational nanoscience. We theoretically investigate the fascinating quantum structures, as well as electrical and chemical properties of carbon-based nanomaterials. We examine the toroidal topology of a tight-binding model of carbon-based nanomaterials with magnetic flux using visualization and simulation with applications of nanoelectronics and beyond Moores Law computing. Our method starts with constructing a 3D structure with molecular editing and modeling program, such as Avogadro and Visual Molecular Dynamics (VMD). Then we generate an adjacency matrix of each structure using C++ code and determine the eigenvalues from the adjacency matrix. Finally, we animate these nanomaterials properties at a finite temperature, density, and flux potential to observe how the free energy, persistent current, and entanglement entropy changes shape for each of the carbon-based nanomaterial structures such as ring, double rings, Möbius strip, nanotorus, and double nanotorus. Additionally, each illustrative calculation will be exported as a 3D animated plot video, and the geometry of each material will be 3D printed and view on virtual reality (VR) headsets using UnityMol as well as high resolution displays.

I. INTRODUCTION

Carbon is capable of forming many allotropes due to its valency. There are three well known allotropic forms of crystalline carbon: fullerene, diamond, and graphite. Fullerenes are carbon-based molecules with a hollow cage line structure. In 1985, Robert Curl, Harold Kroto, and Richard Smalley discovered the buckminsterfullerene or the buckyball consists of molecules containing 60 carbon atoms joined together forming a hollow sphere.

In 2004, Andre Geim and Konstantin Novoselov, decided to strip away just a single layer of a slab of graphite, a 2D sheet of graphene made up of a hexagonal lattice of carbon atoms in honeycomb like structure was formed. Despite being one atom thick, it is a superb conductor and a perfect barrier that helium atoms cannot pass through. Graphene is extremely strong, yet it is incredibly flexible and semi-transparent. Moore's Law, the prediction that the number of transistors can be doubled every two years, is being stretched to its limits. Packing more transistors on a microchip becomes increasingly difficult as shortening the distance between conductive channels increases the likelihood of current leakage. Because of graphene ex-

traordinary conductive properties, graphene would be a great replacement for silicon in microchips.

Joined fullerene particles or rolled-up sheets of graphene held together by van der Waals forces, can form a single-walled carbon nanotubes (CNTs). These graphene sheets are rolled at specific and discrete chiral angles, and the combination of the rolling angle and radius decides the CNTs properties. These CNTs have massive surface areas compared to their volumes, which makes them an excellent catalyst. Furthermore, CNTs are the strongest and stiffest materials ever discovered.

When a single-walled CNT is bent so that its ends meet and yield a toroidal shape, a carbon nanotorus (TCNT) is produced. Since, TCNT unique mechanical and electrical properties similar to graphene, TCNT plays a crucial role in electromagnetic oscillators. Due to TCNT's unique characteristics, we attempt to visualize various electromagnetic and thermodynamic properties of all the carbon nanostructures with induced magnetic flux listed in the abstract. Also the effect of dispersion relation of graphene sheet in carbon nanotori. The paper is structured as follows: after summarizing the background and formulas in the first two sections, we visualize the result in section III through VIII, then we discuss the conclusion and future works in the last section.

II. FREE ENERGY, PERSISTENT CURRENT, AND ENTANGLEMENT ENTROPY

In order to obtain the free energy, persistent current, and entanglement entropy, it is necessary to calculate the energy eigenvalues. Using the adjacency matrix in Fig. 4, we can calculate the energy eigenvalues of the TCNT. Equivalently, we can also calculate the energy eigenvalues of TCNT mathematically using the dispersion relation [1] expression below,

$$\epsilon_n(\mathbf{k}, \phi_1, \phi_2) = \gamma_0 \sqrt{1 + 4 \cos\left(\frac{3k_x a}{2} + \phi_1\right) \cos\left(\frac{\sqrt{3}k_y a}{2} + \phi_2\right) + 4 \cos^2\left(\frac{\sqrt{3}k_y a}{2} + \phi_2\right)} \quad (1)$$

where $N = 2(mn - pq)$

$$k_x = \frac{2\pi}{3a} \frac{l_t(m - n) + l_n(p - q)}{mp - nq}$$
$$k_y = \frac{2\pi}{\sqrt{3}a} \frac{l_t(m + n) - l_n(p + q)}{mp - nq}$$

where j and k are restricted to the interval $A : -s \leq i, j, k \leq s$ and $2s + 1 = n$. The entanglement entropy formulas apply to bosons such as phonons [4].

have magnetic flux in both x and y directions. Note: In Fig. 4 (a) we label ϕ_1 for the magnetic flux in the x direction and ϕ_2 for the magnetic flux in the y direction. Let focus on atom 6 in Fig. 4 (a) or row 7 in Fig. 3 for example. Each atom in the TCNT will have three neighbors next to them, because we rolled the graphene sheet in both x and y directions. Atom 2 is the only neighbor of atom 6 in the y direction, so we put $te^{i\phi_2}$ in column 3. Atom 5 is the left neighbor, so we put $te^{-i\phi_1}$ in column 6. Lastly, atom 7 is the right neighbor, so we put $te^{i\phi_1}$ in column 8 for the adjacency matrix.

Fig. 4: (a) Schematic illustration of a 2D lattice of graphene with $N = 16$. (b) 3D model of a $N = 144$ TCNT. (c) Dispersion relation of graphene has valance and conduction bands touch at the Fermi energy in the first Brillion zone plotted using equation (1) where ϕ_1 and $\phi_2 = 0$. (d) Dispersion relation of graphene near one of the corner of the Brillion zone, called Dirac point (K), where the energy is zero.

As indicated in Fig. 5 below, the saddle points between the local maxima progressively increases as the temperature increases. Eventually, the free energy decreases at a very slow rate and become stabilize at high temperatures, similarly to the carbon nanoring in Fig. 2.

Fig. 5: Free energy of a $N = 144$ TCNT. Plot (a) represent the free energy at 1000 Kelvins and plot (b) represents the free energy at 6000 Kelvins.

By varying the temperature as described in Fig. 6, all of the persistent current plots of a $N = 144$ TCNT behave similar to the carbon nanoring in Fig. 2. The saddle points between the local maxima and local minima of each plots gradually increase, while the persistent current decreases as the temperature increases. Note that the purpose of this paper is to simulate and visualize the electromagnetic and thermodynamic properties of carbon nanostructures, so the temperature values are not realistic.

Fig. 6: Persistent current of $N = 144$ TCNT at 1000K, 4000K, and 6000K. Plots (a), (b), and (c) represents the partial derivative with respect to ϕ_1 . Plots (d), (e), and (f) represents the partial derivative with respect to ϕ_2 .

V. DOUBLE CARBON NANORINGS

Fig. 7: (a) 3D model of a $N = 16$ double carbon nanorings. (b) Lattice model of a double closed ring with $N = 16$. The black dots represent the atoms in the ring and being number from 0 to 15. Notice there is a coupling in the middle that link the two rings.

$$\begin{bmatrix} 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & te^{-i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ te^{-i\phi_1} & 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & te^{-i\phi_1} & 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & te^{-i\phi_1} & 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & te^{-i\phi_1} & 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & te^{-i\phi_1} & 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & te^{-i\phi_1} & 0 & te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ te^{i\phi_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Fig. 8: Adjacency matrix of $N = 16$ carbon nanorings.

In Fig. 7, the vector potential goes around the ring with enclosed magnetic flux ϕ_1 and ϕ_2 coming out of the plane. Notice inside the red box in Fig. 8, atom 0 and atom 8 will have 3 neighbors because there is a coupling representing a

bridge connecting the two rings, where electrons can travel between two rings. While, all the other atoms will have 2 neighbors. The two V_0 s inside the red box represent coupling and V_0 is a positive integer. If $V_0 = 0$, then there is no coupling, therefore $V_0 \neq 0$.

Fig. 9: Free energy of a $N = 16$ double carbon nanorings. Plot (a) represent the free energy at 1000 Kelvins and plot (b) represents the free energy at 6000 Kelvins.

As illustrated in Fig. 9, both plots are symmetrical on both axis unlike the free energy of the TCNT. The local maxima decrease at a much faster rate than the local minimum. Eventually, the plot flattens out at high temperature but still maintains its symmetry similar to the single carbon nanoring in section III.

Fig. 10: Entanglement entropy of a $N = 16$ double carbon nanorings.

Fig. 10 (a) represents the entanglement entropy vs. n (a subset of atoms inside of N) at various temperatures. Since $n = 2s + 1$ we choose n to be an odd number for simplicity. Each point is calculated numerically, then we used interpolation to obtain the entanglement entropy for the even number of n . Fig. 10 (b) represents the entanglement entropy versus temperature in Kelvins with various n . In both plots, the entanglement entropy depends exponentially on both the n and temperature.

VI. MÖBIUS STRIP

Fig. 11: (a) 3D model of a $N = 48$ Möbius strip. (b) Represents the free energy of a $N = 16$ Möbius strip. (c) 16×16 adjacency matrix of a $N = 16$ Möbius strip.

In Fig. 11 (b), the local maxima decrease and gradually become the local minima as temperature increases and doubles the amount of oscillation.

VII. GENUS 2 CARBON DOUBLE NANOTORUS

Fig. 12: A 3D model of a genus 2 double torus.

In future work, we will compute the free energies numerically as there is no exact formula for the $g = 2$ TCNT. However, the work on the double ring should provide an excellent guide.

VIII. CONCLUSION

We theoretically simulated and visualized the electronic and thermodynamic properties of various types of tight-binding carbon nanostructures at finite temperatures with magnetic flux. For further development, we would like to develop a program to construct a 3D model of tight-binding carbon nanostructures in conjunction with generating the adjacency matrices. Also we would like to utilize super computers that have the capability to handle structures consisting of hundreds and thousands of atoms to calculate the electronic and thermodynamic properties of genus 2, 3, and 4 TCNTs.

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