Topological entanglement entropy of interacting disordered zigzag graphene ribbons

Young Heon Kim, Hye Jeong Lee, and S.-R. Eric Yang
Department of Physics, Korea University, Seoul, Korea

Interacting disordered zigzag graphene nanoribbons have fractional charges, are quasi-one-dimensional, and display an exponentially small gap. Our numerical computations showed that the topological entanglement entropy of these systems has a small finite but universal value, independent of the strength of the interaction and the disorder. The result that was obtained for the topological entanglement entropy shows that the disorder-free phase is critical and becomes unstable in the presence of disorder.

PACS numbers:

I. INTRODUCTION

Graphene structures have many fascinating physical properties, such as massless Dirac electrons and the quantum Hall effect [1–4]. Recent years have seen rapid progress in the fabrication of atomically precise graphene nanoribbons [5]. Recent studies showed [6, 7] that interacting disordered zigzag graphene nanoribbons [8] are topologically ordered [9, 10]. The ground states of these quasi-one-dimensional Mott-Anderson insulators are doubly degenerate: the two degenerate ground states are related to each other in that their electron spins are reversed (see Fig.1). They have an exponentially small gap, $\Delta_s$, in the DOS (see Fig.2) and their boundary zigzag edges can support $1/2$ fractional charges. These objects are solitonic in nature [11, 12]. Moreover, the zigzag edges induce spin-splitting in the bulk [13] and can display spin-charge separation. Disorder in interacting zigzag graphene ribbons induces a transition between symmetry-protected and topologically ordered phases.

In this study, we investigated the entanglement in many-body topological insulators [14, 15] of interacting disordered zigzag graphene nanoribbons. A region $D$ of a topologically ordered gapful system with one boundary has an entanglement entropy of [16, 18]

$$ S_D = \alpha L - \beta, \quad (1) $$

where $L$ is the length of the boundary and $\alpha$ is non-universal. The topological entanglement entropy $\beta$ is universal and

$$ \beta > 0. \quad (2) $$

In the case of non-negligible finite-size effects and disorder fluctuations, the following method can be used to compute $\beta$. Consider a loop that wraps non-trivially around a region [19, 20], see Fig.3. The topological entanglement entropy of the loop domain can be written as

$$ S_{\text{top}} = 2\beta = (S_{AB} - S_B) - (S_{ABC} - S_{BC}). \quad (3) $$

FIG. 1: (a) Zigzag edge antiferromagnetism of an interacting zigzag graphene nanoribbon without disorder showing the two degenerate ground states. (b) Schematic band structures of interacting (solid curves) and non-interacting (dashed curves) zigzag graphene nanoribbons. Unoccupied and occupied states near the wave vectors $k = \pm \pi/a_0$: $R$ and $L$ represent the states confined to the zigzag edges on the right and left, respectively (the length of the unit cell of a ribbon is $a_0$). The small arrows indicate the spins. Spin-split energy levels of the spin-up (solid lines) and spin-down (dashed lines) gap–edge states of the interacting disordered interacting zigzag graphene nanoribbons.

FIG. 2: Dashed line: the exponentially small soft gap with $\alpha \sim 1/\sqrt{\Delta}$ near the Fermi energy of the tunneling density of states of an interacting disordered zigzag graphene nanoribbon. Solid line: the hard gap, $\Delta$, of the tunneling density of states of an interacting zigzag graphene nanoribbon in the absence of disorder.

*These two authors contributed equally
†corresponding author: eyang812@gmail.com
This expression reduces the finite-size effects and is more suitable for numerical calculations. The entanglement entropy $S_{AB} - S_B$ has contributions from $A$. Similarly, $S_{ABC} - S_{BC}$ has contributions from the same region. The difference between these two contributions $(S_{AB} - S_B)$ and $(S_{ABC} - S_{BC})$ is the topological entanglement entropy. Note that other regions have only one boundary, whereas $ABC$ has two boundaries, i.e., one inner and one outer, as shown in Fig. 3. Except near a critical point, the value of the topological entanglement entropy is universal and is independent of system parameters. Moreover, when the finite-size effects are small, the entropy does not depend on the shape of the regions.

Several questions regarding the entropy of interacting disordered zigzag graphene nanoribbons remain unanswered. For example, it is unclear whether these ribbons should have non-zero topological entanglement entropy. As mentioned above, the presence of fractional charges suggests that the topological entanglement entropy is finite, although the magnitude thereof is unknown. However, the presence of an exponentially small gap may be compatible with zero topological entanglement entropy. In addition, the behavior of the topological entanglement entropy near the critical point is unclear. In this work, we numerically computed the topological entanglement entropy and showed that it is finite and universal, and independent of the strength of both the interaction and disorder. Our results also showed that the disorder-free phase is critical, and that this phase becomes unstable in the presence of disorder.

**II. MODEL**

We applied a Hubbard model to the interacting disordered zigzag graphene nanoribbons and used a self-consistent Hartree-Fock approximation [15] [21]. We included both electron–electron interactions and disorder in a tight-binding model at half-filling. When the on-site repulsion is $U = 0$, the effect of disorder can be described exactly within the Hartree-Fock approximation, whereas in the other limit, where disorder is absent, the interaction effects are well represented by the Hartree-Fock approximation, which is widely used in graphene-related systems [22]. The ground state is doubly degenerate and can be written as a product of spin-up and -down Slater determinants:

$$
\Psi_1 = \Psi_{L,\uparrow}(\vec{r}_1, \ldots, \vec{r}_{N/2})\Psi_{R,\downarrow}(\vec{r}_{N/2+1}, \ldots, \vec{r}_N), \\
\Psi_2 = \Psi_{R,\uparrow}(\vec{r}_1, \ldots, \vec{r}_{N/2})\Psi_{L,\downarrow}(\vec{r}_{N/2+1}, \ldots, \vec{r}_N),
$$

where $\Psi_{L,\sigma}$ ($\Psi_{R,\sigma}$) describes $N/2$ electrons with spin $\sigma$, containing electrons localized on the left (right) zigzag edge. In the first state the spin of the magnetization of the zigzag edge on the left (right) is dominantly upward (downward), see Fig 1(a). In the second state, the magnetization is the opposite. The total number of electrons is $N$.

The total Hamiltonian in the Hartree-Fock approximation is

$$
H = - \sum_{<ij>\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} V_i c_{i\sigma}^\dagger c_{i\sigma} \\
+ U \sum_i (n_{i\uparrow} n_{i\downarrow} - n_{i\uparrow}^2 - n_{i\downarrow}^2) \\
- \frac{U}{2} \sum_i (n_{i\uparrow} + n_{i\downarrow}),
$$

where $c_{i\sigma}^\dagger$ and $n_{i\sigma}$ are the electron creation and occupation operators at site $i$ with spin $\sigma$. Because the translational symmetry is broken, the Hamiltonian is written in the site representation. In the hopping term, the summation is over the nearest neighbor sites (the value of the hopping parameter is $t \sim 3eV$). The eigenstates and eigenenergies are computed numerically by solving the tight-binding Hamiltonian matrix self-consistently. The self-consistent occupation numbers $\langle n_{i\sigma} \rangle$ in the Hamiltonian are the sum of the probabilities of finding electrons of spin $\sigma$ at site $i$:

$$
\langle n_{i\sigma} \rangle = \sum_{E \leq E_F} \left| \psi_{i\sigma}(E) \right|^2.
$$

The summation is over the energy $E$ of the occupied eigenstates below the Fermi energy $E_F$. Note that $\psi_{i\sigma}(E)$ represents an eigenvector of the tight-binding Hamiltonian matrix with energy $E$. The on-site impurity energy $V_i$ is chosen randomly from the energy interval $[-\Gamma, \Gamma]$. 

![Image](https://via.placeholder.com/150)
The entanglement entropy of

where \( n \) depend on the size of the system. We used another data we obtained display significant disorder fluctuations entanglement entropy from Eq. (1) is not accurate: the 

of disorder, the method for computing the topological nearly zero energy exist [6, 7]. However, in the presence zero-energy zigzag edge states exist, as shown in Fig. 2. 

Let us divide the zigzag ribbon into two parts \( A \) and \( B \). We restrict the indices \( i \) and \( j \) to \( A \) and define the correlation function [23, 24]

\[
C_{ij} = \langle \Psi | \sum_k \sum_{j'} a_k^\dagger a_{j'}^\dagger \sum_{k'} B_{jj'} B_{kk'} | \Psi \rangle
\]

where \( \Psi = \Psi_1 \) is chosen (\( \Psi_2 \) is an equally good choice). This can be written as

\[
C_{ij} = \langle \Psi | \sum_k \sum_{k'} a_k^\dagger B_{kk'} a_{j'}^\dagger B_{j'j} | \Psi \rangle
\]

\[
= \sum_k B_{ki}^\dagger B_{kj} n_k.
\]

Here we have used

\[
\langle \Psi | a_k^\dagger a_{k'}^\dagger | \Psi \rangle = \delta_{kk'} n_k,
\]

where \( n_k \) is the number of occupied Hartree-Fock states. The entanglement entropy of \( A \) is given by

\[
S_A = - \sum_i [\lambda_i \ln \lambda_i + (1 - \lambda_i) \ln (1 - \lambda_i)],
\]

where \( \lambda_i \) are the eigenvalues of the matrix \( C \).

We compute \( S/L \) as a function of \( 1/L \) and extract the topological entanglement entropy from the result. For an interacting but disorder-free system, we find \( \beta \approx 0 \). Note that, in this case, a hard gap exists in the DOS and no zero-energy zigzag edge states exist, as shown in Fig. 2.

The DOS of interacting disordered zigzag nanoribbons develops a soft gap, and a few zigzag edge states with nearly zero energy exist [5, 6]. However, in the presence of disorder, the method for computing the topological entanglement entropy from Eq. (1) is not accurate: the data we obtained display significant disorder fluctuations that depend on the size of the system. We used another method based on a ring domain (the Wilson loop) to compute \( S_{top} = 2 \beta \) given in Eq. (3). Our investigation shows significant finite-size effects that depend on the shape of the ring, and a careful analysis is required to reduce these effects. Two conditions must be met to reduce these finite-size effects: [1] the lengths of the inner and outer boundaries of the ring must be nearly equal. [2] Because \( \Gamma/U = 0 \) is a critical point, the topological entanglement entropy should be \( \beta \approx 0 \) near \( \Gamma/U \approx 0 \). We investigated different types of rings (one of which is shown in Fig. 4). Our numerical investigation showed that the ring domain
shown in Fig. 3 satisfies these conditions.

The results of the topological entanglement entropy for this ring domain are displayed in Fig. 5. The topological entanglement entropy of interacting disordered zigzag graphene nanoribbons is \( \beta \approx 0.046 \) and independent of the strength of the interaction and the disorder, that is, independent of \( \Gamma/U \). We consider this small value of \( \beta \) to be related to the presence of an exponentially small soft gap of interacting disordered ribbons [7]. As expected, as the critical point is approached, \( \Gamma/U \rightarrow 0 \), the value of the topological entanglement entropy varies rather abruptly to zero in a non-universal manner [18]. (In limit of infinitely large systems the transition occurs discontinuously at \( \Gamma/U = 0 \).)

In conclusion, our numerical work showed that the topological entanglement entropy of interacting disordered zigzag graphene nanoribbons is small but finite and universal. Disorder-free interacting zigzag graphene nanoribbons are in a critical phase that becomes unstable in the presence of disorder. It would be interesting to find other systems with a pseudo gap that belongs to the same universality class. It may be worthwhile to analytically compute \( S_{\text{top}} \) of a quasi-one-dimensional system in the presence of an exponentially small gap.

Acknowledgments

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF), funded by the Ministry of Education, ICT & Future Planning (MSIP) (NRF-2018R1D1A1A09082332).

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Nature 438, 197 (2005).
[2] Y. Zhang, Y. W. Tan, H. L. Stormer, and P. Kim, Nature 438, 201 (2005).
[3] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109 (2009).
[4] A. K. Geim and A. H. MacDonald, Physics Today, 60, 8, 35 (2007).
[5] P. Ruffieux, S. Wang, B. Yang, C. Sanchez-Sanchez, J. Liu, T. Dienel, L. Talirz, P. Shinde, C. A. Pignedoli and D. Passerone, Nature 531, 489 (2016).
[6] Y. H. Jeong, S.-R. Eric Yang, and M. C. Cha, J. Phys.: Condens. Matter 31, 265601 (2019).
[7] S.-R. Eric Yang, M. C. Cha, H. J. Lee, and Y. H. Kim, Phys. Rev. Res. 2, 033109 (2020).
[8] M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, J. Phys. Soc. Jpn. 65, 1920 (1996); L. Yang, C. H. Park, Y. W. Son, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 99, 186801 (2007).
[9] X.-G. Wen, Rev. Mod. Phys. 89, 041004 (2017).
[10] X.-G. Wen, ISRN Condensed Matter Physics 2013, 198710 (2013).
[11] Y. H. Jeong, S. C. Kim, and S.-R. Eric Yang, Phys. Rev. B 91, 205441 (2015).
[12] M. P. López-Sancho and L. Brey, 2D Materials 5, 015026 (2017).
[13] Y. H. Jeong and S.-R. Eric Yang, Ann. Phys 385, 688 (2017).
[14] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
[15] S. M. Girvin and K. Yang, Modern Condensed Matter Physics, (Cambridge University Press, 2019).
[16] J. Eisert, M. Cramer, and M.B. Plenio, Rev. Mod. Phys. 82, 277 (2010).
[17] J. K. Pachos, Introduction to Topological Quantum Computation, (Cambridge University Press, Cambridge, 2012).
[18] B. Zeng, X. Chen, D.-L. Zhou, and X.-G. Wen, Quantum Information Meets Quantum Matter (Springer, 2019).
[19] A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404 (2006).
[20] M. Levin and X.-G. Wen, Phys. Rev. Lett. 96, 110405 (2006).
[21] S.-R. Eric Yang and A. H. MacDonald, Phys. Rev. Lett. 70, 4110 (1993).
[22] T. Stauber, P. Parida, M. Trushin M. V. Ulybyshev, D. L. Boyda, and J. Schliemann, Phys. Rev. Lett. 118, 266801 (2017).
[23] I. Peschel, J. Phys. A Math. Gen. 36, L205 (2003).
[24] J. I. Latorre and A. Riera, J. Phys. A: Math. Theor. 42, 504002 (2009).