Fractional edge charge of $e/2$ in interacting disordered graphene zigzag nanoribbon

S.-R. Eric Yang$^1$*, Min-Chul Cha$^2$, and Hye Jeong Lee$^1$

$^1$Department of Physics, Korea University, Seoul, Korea
$^2$Department of Photonics and Nanoelectronics, Hanyang University, Ansan, Korea

We numerically compute the density of states (DOS) of interacting disordered zigzag graphene nanoribbon (ZGNR) having midgap states showing $e/2$ fractional edge charges. The computed Hartree–Fock DOS is linear at the critical disorder strength where the gap vanishes. This implies an $I$-$V$ curve of $I \propto V^2$. Thus, $I$-$V$ curve measurement may yield evidence of fractional charges in interacting disordered ZGNR. We show that even a weak disorder potential acts as a singular perturbation on zigzag edge electronic states, producing drastic changes in the energy spectrum. Spin–charge separation and fractional charges play a key role in the reconstruction of edge antiferromagnetism. Our results show that an interacting disordered ZGNR is a topologically ordered Mott–Anderson insulator.

PACS numbers:

Graphene has numerous remarkable properties \cite{1}. One prominent feature is that, in the absence of disorder, zigzag graphene nanoribbons (ZGNRs) can support chiral symmetry protected topological (SPT) \cite{4,7} edge states displaying an integer charge \cite{2}. Disorder has profound effects on ZGNRs. In particular, an interacting disordered ZGNR becomes a Mott–Anderson insulator \cite{10} with spin-split energy levels \cite{11}. Furthermore, localized gap-edge states reduce the size of the gap between the occupied and unoccupied midgap states with energies $-\Delta_s/2$ and $\Delta_s/2$, respectively, to $\Delta_s$ (see Fig. 1). In the weak disorder regime, solitonic midgap states \cite{12,13} may have an $e/2$ fractional charge on each of the opposite zigzag edges, i.e., \textit{there is one for each edge}, where $e$ is the electron charge. These fractional charges have small disorder-induced charge variances. In addition, the charge fractionalization is protected against quantum charge fluctuations by the non-zero $\Delta_s$ \cite{11}. Here, $\Delta_s \lesssim 10^{-2} \Delta \sim 1$ THz, where $\Delta$ is the gap value; this is sufficiently large that quantum charge fluctuations can be ignored (see Girvin \cite{14}). In the absence of disorder, typically, $\Delta \sim 0.2t$ \cite{15}, where $t \sim 3$ eV is the hopping constant.

An excellent opportunity to observe these boundary charges has recently arisen, as rapid progress has been made in the fabrication of atomically precise GNRs \cite{16}. The chiral Luttinger liquid theory of fractional quantum Hall edges \cite{17,18} predicts an $I$-$V$ curve of $I \propto V^{1/\nu}$. The corresponding DOS is given by $\rho(E) \propto E^{1/\nu-1}$, where $\nu$ is the filling factor, and the energy $E$ is determined from the Fermi energy (these edges support gapless excitations). This predicted $I$-$V$ curve has been experimentally confirmed \cite{19}. It should be noted that Laughlin quasi-particles have an odd denominator fractional charge $e\nu$, and an even denominator fractional charge $e/2$ is not found in fractional quantum Hall systems. The aforementioned $I$-$V$ curve may be derived heuristically by assuming that a tunneling electron fractionalizes into $m = 1/\nu$ fractionally charged quasi-particles \cite{20}, where $e \rightarrow e/m + \cdots + e/m$. However, the chiral Luttinger liquid theory does not apply to ZGNRs. Furthermore, the gap-edge states are all localized along the ribbon direction, in contrast to the fractional quantum Hall edge states. Moreover, the average edge charge of the gap-edge states with energies within a small interval $\delta E$ is $e/2$; however, significant disorder-induced charge fluctuations may occur. Some of these states are more localized on the left or right zigzag edges. This tendency increases as the electron energy deviates from

\*corresponding author, eyang812@gmail.com
\[ \pm \Delta_s / 2. \] Despite this, if we apply the above heuristic argument to a ZGNR with \( m = 2 \), we find that the I-V curve is given by \( I \propto \int dx \int \frac{\pi}{\epsilon_1 - \epsilon_2} \propto V^2 \), where \( \theta \) and \( \epsilon_{1,2} \) are the step function and quasi-particle energies, respectively. This I-V curve is equivalent to a linear tunneling DOS. In contrast to what is usually expected of a topological insulator, a disorder potential profoundly affects an interacting ZGNR. However, the physical processes involved in this effect and the properties of the interacting disordered state are not well understood.

In this study, we propose an experiment that may provide evidence of the presence of \( e^2 / 2 \) fractional charges in interacting disordered ZGNRs. We compute the DOS of an interacting disordered ZGNR and find that, for the critical disorder strength where the ZGNR supports gapless excitations (i.e., where \( \Delta_s \) vanishes), our computed Hartree–Fock (HF) DOS is linear near the Fermi energy. This finding is in agreement with the heuristic argument given above. In addition, our results show that even a weak disorder potential behaves similar to a singular perturbation on zigzag edge electronic states, generating drastic changes in the energy spectrum. It also induces a magnetic zigzag edge reconstruction in which fractional edge charges and spin-charge separation play a significant role. Moreover, disorder also changes an SPT phase to a topologically ordered phase [3].

We applied a Hubbard model to the interacting disordered ZGNRs and used a self-consistent HF approximation; this is because the self-consistency provides an excellent approximation when both disorder and interactions are present [21][22]. In this model, the range of each impurity potential is shorter than or comparable to the carbon–carbon distance. For a short-range potential, a significant wave vector transfer occurs upon backscattering for \( |k - k'| \sim 1 / a_0 \). This transfer couples the chiral zigzag edge state \( R \uparrow \) near \( k = -\pi / a_0 \) to another chiral zigzag edge state \( L \uparrow \) on the opposite zigzag edge near \( k = \pi / a_0 \) [23] (see Fig. 1). In this study, the disorder potential strength was chosen randomly from the energy interval \( [-\Gamma, \Gamma] \). The ratio between impurities/defects and the number of carbon atoms was denoted by \( n_{\text{imp}} \), and the on-site electron repulsion and hopping parameter were indicated by \( U \) and \( t \), respectively. The ratio between the disorder strength and interaction strength is \( \kappa = \Gamma \sqrt{n_{\text{imp}}} / U \ll 1 \) in the weak disorder regime. Varying the strength \( \Gamma \) is approximately equivalent to changing \( \sqrt{n_{\text{imp}}} \). In this work, the ribbon width was set to \( w = 7.1 \AA \) and the on-site repulsion was \( U = t \).

Disorder behaves similar to a singular perturbation on zigzag edge electronic states. This singular perturbation is analogous to the non-perturbative coupling between the left and right wells of a double quantum well (the non-perturbative aspect can be seen by using instantons of the inverted double well potential). Disorder potential produces drastic changes in the energy spectrum when compared to the disorder-free behavior, see Fig. 2. It shows the probability of finding an electron of a gap-edge state on \( A \) carbon sites \( i \), \( q_A = \sum_{i \in \mathcal{A}} |\psi_i|^2 \), as a function of \( E \) for \( \Gamma = 0.1t \). Note that particle-hole symmetry (chiral symmetry) is broken. In contrast to the case of \( \Gamma = 0 \), shown in Fig. 2(b), there are numerous states with \( q_A \approx 1 / 2 \) in the energy range \( |E| < \Delta / 2 \). If the disorder potential experienced by the left and right edges differ, charge fluctuations will arise. Even a weaker disorder potential with \( \Gamma = 0.03t \) produces similar drastic changes in the energy spectrum when compared to the disorder-free behavior. We have found that the localization length along the edges decreases as \( |E| \) decreases toward \( \Delta_s / 2 \).

A small localization length means that the repulsive energy between an electron in a soliton state and an added electron in another soliton state can be small. (They can avoid each other). This effect determines the magnitude of \( \Delta_s \).

The midgap states with \( |E| \approx \Delta_s / 2 \ll \Delta / 2 \) and \( q_A \approx 1 \) represent soliton states. For the sake of conceptual clarity we briefly summarize the properties of soliton midgap states obtained in Ref. [11]. They consist of almost equal contributions from the valence \( R \) and conduction band \( L \) states with energies near \( -\Delta / 2 \) and \( \Delta / 2 \), respectively, as shown in Fig. 1. A soliton state has small disorder induced charge fluctuations. For a given disorder realization, greater spin-splitting occurs for states with \( |E| \approx \Delta_s / 2 \) than for those with \( |E| \approx \Delta / 2 \). In the limit \( \Gamma \to 0 \) and \( \ell \to \infty \) the energy of a soliton decreases with very small fluctuations of \( q_A \).

The \( e^2 / 2 \) fractional charge fluctuations decrease as \( |E| \to \Delta_s / 2 \). Thus, we investigated the effect of this behavior on the DOS near the Fermi energy. Note that the tunneling DOS measures the number of quasiparticle excitations of the interacting disordered ZGNR. We performed finite-size calculations and computed the DOS given by \( \rho(E) = \frac{D_{\text{eff}}(E)}{N_{\text{site}} \delta E} \), where \( D_{\text{eff}}(E) \) is the total number of states in the energy histogram interval \( \delta E \). We
defined the critical point \( \Gamma_c \) as the value where \( \Delta_s \) is zero, i.e., where the gap closes. The heuristic argument given above suggests that the DOS at \( \Gamma_c \) is linear near the Fermi energy. The DOS result for \( \Gamma = 0.18t \geq \Gamma_c \) is plotted in Fig. 3. Our numerical results show that the energy range where the DOS is linear increases as \( \ell \) grows and that fluctuations in the DOS also decreases. Below \( \Gamma < \Gamma_c \), a gap develops in the DOS, and even a weak potential can form a soft gap in the limit \( \ell \to \infty \). Note that \( \Gamma_c \) does not represent a metal–insulator transition point, and the gap–edge states are all localized in the interacting disordered ZGNR. Note also that \( \Gamma_c \) decreases as \( \ell \) increases (this is a finite-size effect).

Let us try to understand how the singular disorder potential disrupts the SPT phase. Suppose that the site occupation numbers of the disorder-free left edge are \( n_{i\uparrow} = 0.7 \) and \( n_{i\downarrow} = 0.3 \). Then, those of the right edge are \( n_{i\uparrow} = 0.3 \) and \( n_{i\downarrow} = 0.7 \), respectively. Assume that disorder generates one spin-up and one spin-down occupied soliton state near the gap edge displaying charge fractionalization. In other words, a spin-up electron on the left zigzag edge of the interacting ZGNR is replaced by two \( e/2 \) fractional charges, one of which resides on the left zigzag edge while the other resides on the right zigzag edge (Fig. 4(a)). Similarly, a spin-down electron on the right zigzag edge is also replaced by two \( e/2 \) fractional charges, with one each residing on the left and right zigzag edges (Fig. 4(a)). Hence, the total \( z \)-component of the site spin on the zigzag edges changes sign along the edge direction, as shown in Fig. 4(b). The total occupation number of each site is now close to one (i.e., the ZGNR is half-filled). Note that the disorder potential creates an even number of solitons to minimize the energy cost of double occupancy of a site (a soliton consists a pair of fractional charges). Thus, even if the disorder potential is weak it can still disrupt the SPT phase. In addition, the magnetic zigzag edge reconstruction can also lead to a spin–charge separation [12, 20]. Figures 4 (c) and 4 (d) show how a charge fractionalization process results in an object \( (e_L, 0) \) that display spin–charge separation. Here \( e_L \) denotes an electron charge located on the left edge and number 0 means no spin. When such an object moves along the zigzag edge it will carry charge but no spin.

We now explain the essential physics of charge fractionalization and the physical nature of interacting disordered ZGNRs. In each disorder realization particle–hole symmetry (chiral symmetry) is broken, but after disorder averaging the symmetry is restored. This implies that the average edge charge is \( e/2 \) at each energy \(|E| < \Delta/2\), but with a significant charge variance. However, if the tunneling DOS develops a soft gap [21, 24] then the charge variance near zero energy will be negligible in the weak disorder regime, see Fig. 2 (a). What is the physical origin of a soft gap? The essential physics is that it is difficult for the tunneling electron to avoid other electrons since it takes long time for interacting electrons to diffuse away from each other (see Girvin and Yang, Ref. [20], pages 290 and 645). Our numerical simulation shows that an interacting disordered ZGNR cannot be reached iteratively from a disorder–free chiral SPT state. Moreover, an interacting disordered ZGNR has a doubly degenerate ground state, \( e/2 \) fractional charges, and broken chiral symmetry. Thus we expect that it is in a topological ordered phase rather than in an SPT phase (see Wen [2] for the distinction between them). An interacting disordered ZGNR is somewhat analogous to topologically ordered Laughlin states. In both systems fractional charge and ground state degeneracy are intimately related [2, 20].

In conclusion, an interacting disordered ZGNR is a one-dimensional topologically ordered insulator with \( e/2 \) solitonic fractional charges and with two-fold ground state degeneracy. Even a weak disorder potential behaves similar to a singular perturbation, producing spin-splitting and drastically modifying the energy spectrum.
We conducted a numerical study showing that the DOS is linear at the critical disorder strength. Measurement of the $I$-$V$ curve may thus provide evidence for the presence of fractional charges in an interacting disordered ZGNR. We also found that spin–charge separation and fractional edge charges play a significant role in the reduction of edge antiferromagnetism. We hope that our work will stimulate experimental tests investigating the fractional edge charges in interacting disordered ZGNRs. However, several experimental possibilities and challenges exist. In particular, investigation of tunneling between zigzag edges, as in fractional quantum Hall bar systems [25], may be fruitful. Quantum shot noise may directly measure [26] the tunneling fractional charge of a ZGNR. Resonant tunneling measurement through a quantum dot structure made of a rectangular ZGNR may also be explored [27]. Finally, it would be interesting to investigate other zigzag nanoribbon systems that exhibit antiferromagnetism, e.g., silicene and boron nitride nanoribbons [28, 29]. Disorder can couple the left and right zigzag edges and lead to charge fractionalization.

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-2018R1A1A09082332 (S.R.E.Y.) and NRF-2019R1F1A1062704 (M.C.C.)).

[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] X.-G. Wen, Rev. Mod. Phys. 89, 041004 (2017); X.-G. Wen, ISRN Condensed Matter Physics 2013, 1 (2013).
[5] J. Wang, L. H. Santos, X.-G. Wen, Phys. Rev. B 91, 195134 (2015).
[6] S. Ryu and Y. Hatsugai, Phys. Rev. Lett. 89, 077002 (2002).
[7] Y. H. Jeong and S.-R. Eric Yang, Ann. Phys. 385, 688 (2017).
[8] Y. H. Jeong, S. C. Kim, and S.-R. Eric Yang, Phys. Rev. B 91, 205441 (2015).
[9] K. Wbakayashi, M. Sigrist and M. Fujita, J. Phys. Soc. Jap. 67, 2089 (1998).
[10] V. Dobrosavljevic, N. Trivedi, and J. M. Valles, Jr., eds., Condenser Insulator Quantum Phase Transitions, (Oxford University Press, Oxford, 2012); D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. 66, 261 (1994).
[11] Y. H. Jeong, S.-R. Eric Yang, and M.-C. Cha, J. Phys.: Condens. Matter 31, 265601 (2019).
[12] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979); A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W. P. Su, Rev. Mod. Phys. 60, 781 (1988).
[13] S.-R. Eric Yang, Nanomaterials 9, 885 (2019).
[14] S. M. Girvin, in Topological Aspects of Low Dimensional Systems, edited by A. Comtet, T. Jolicoeur, S. Ouvry, and F. David (Springer Verlag, Berlin and Les Editions de Physique, Les Ulis, 2000).
[15] L. Yang, C. H. Park, Y. W. Son, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. 99, 186801 (2007).
[16] P. Ruffieux, S. Wang, B. Yang, C. Sanchez-Sanchez, J. Liu, T. Dienel, L. Talirz, P. Shinde, C. A. Pinedolodi, and D. Passeurone, Nature 531, 489 (2017).
[17] X.-G. Wen, Int. J. Mod. Phys. B6, 1711 (1992).
[18] C. de Chamon and E. Fradkin, Phys. Rev. B 56, 2012 (1997).
[19] M. Grayson, D. C. Tsui, L. N. Pfeiffer, K. W. West, and A. M. Chang, Phys. Rev. Lett. 80, 1062 (1998).
[20] S. M. Girvin and K. Yang, Modern Condensed Matter Physics, (Cambridge University Press, Cambridge, 2019).
[21] S.-R. Eric Yang and A. H. MacDonald, Phys. Rev. Lett. 70, 4110 (1993).
[22] S.-R. Eric Yang, A. H. MacDonald, and B. Huckestein, Phys. Rev. Lett. 74, 3229 (1995).
[23] L. R. F. Lima, F. A. Pinheiro, R. B. Capaz, C. H. Lewenkopf and E. R. Mucciolo, Phys. Rev. B 86, 205111 (2012).
[24] A. L. Efros and B. I. Shklovskii , J. Phys. C 8, L49 (1975).
[25] W. Kang, H. L. Stormer, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Nature 403, 59 (2000); I. Yang, W. Kang, K. W. Baldwin, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. 92, 056802 (2004).
[26] R. de-Picciotto, M. Reznikov, M. Heiblum, V. Usmansky, G. Bunin, and D. Mahalu, Nature 389, 162 (1997); L. Saminadayar, D. C. Glattli, Y. Jin, and B. Etienne, Phys. Rev. Lett. 79, 2526 (1997).
[27] V. J. Goldman and B. Su, Science 267, 1010 (1995).
[28] Y. Yao, A. Liu, J. Bai, X. Zhang and R. Wang, Nanoscale Res. Lett., 11, 371 (2016).
[29] V. Barone and J. E. Peralta, Nano Lett., 8 (8), 2210 (2008).