Compressibility as a probe of quantum phase transitions in topological superconductors

David Nozadze and Nandini Trivedi
Department of Physics, The Ohio State University, 191 W. Woodruff Avenue, Columbus, OH 43210, USA
(Dated: April 2, 2015)

We investigate the behavior of the local compressibility $\kappa$ in a $p$-wave superconducting Kitaev chain. For a closed chain in the absence of any impurity, we show that the topological phase transition is signaled by the divergence of $\kappa$ at the quantum critical point tuned by the chemical potential $\mu$. We also show that a single strong impurity potential can lead to a local negative compressibility that is a diagnostic of the topological phase transition in the bulk. The origin of such anomalous behavior can be traced to the formation of bound states at the topological to trivial phase transition. Our results have implications for gate-tunable scanning compressibility that includes contributions from both single particle states and collective modes and is therefore distinct from scanning tunneling spectroscopy that is sensitive to only the single particle density of states.

PACS numbers: 71.10Pm, 03.67.Lx, 74.45.+c, 74.90.+n

Introduction
Recently, the search for Majorana fermions in condensed matter systems has attracted a lot of attention because of their non-Abelian statistics and possible application in topological quantum computation\textsuperscript{1–5}. There are several promising proposals for practical realization of Majorana fermions both in one (1D) and two-dimensional (2D) systems. Majorana fermions can emerge in systems, such as topological insulator-superconductor interfaces\textsuperscript{6,7}, quantum Hall states with filling factor $5/2$, $p$-wave superconductors\textsuperscript{8}, semiconductor heterostructures\textsuperscript{9,10}, half-metallic ferromagnets\textsuperscript{11,12} and metallic chains\textsuperscript{13}. As shown by Kitaev\textsuperscript{14}, Majorana fermions can emerge at the ends of 1D spinless $p$-wave superconducting chain when the chemical potential is in the topological regime. A realization of the Kitaev chain based on a quantum nanowire made of a semiconductor-superconductor hybrid structure has been proposed. In this hybrid, an ordinary $s$-wave superconductor is proximity coupled to a semiconducting nanowire with strong intrinsic spin-orbit coupling and an applied Zeeman spin splitting\textsuperscript{15,16}. The quantum nanowire undergoes a quantum phase transition from a topologically trivial superconducting phase to the topological one by increasing the magnetic field parallel to the wire beyond a critical value.

There have been recent reports of observations of Majorana fermions in tunneling and the fractional Josephson effect\textsuperscript{17–20}. Ref.\textsuperscript{21} has reported significant progress in creating the Majorana states where spatial location of Majoranas are detected using a scanning tunneling microscope. All these experimental observations of the existence of Majorana fermions rely on the fact that the system is in the topological phase. However, local probes and identifiers that characterize the topological phase transitions are still missing and that is what our paper proposes to investigate.

In this paper, we propose the gate-tuned compressibility as a probe of the topological phase transition in the Kitaev chain. For the clean closed chain, we find that the compressibility is finite and almost constant in the topological phase, and diverges at the transition (see Fig. 1). It rapidly decreases in the trivial phase, with increasing chemical potential. A single impurity can dramatically change the local response: a strong impurity leads to the formation of a bound state and surprisingly this results in a local negative compressibility with a dip at the topological phase transition. An extra peak associated with the bound state appears in the local compressibility in the trivial phase.

Model and Method
We consider a 1D tight-binding Hamiltonian

$$H = -\sum_i \mu_i c_i^\dagger c_i - \sum_i t_i (c_i^\dagger c_{i+1} + \text{h.c.}) - \frac{U}{2} \sum_i c_i^\dagger c_i c_{i+1}^\dagger c_{i+1}^\dagger,$$  \hspace{1cm} (1)

where $c_i^\dagger$ ($c_i$) is the creation (destruction) operator for

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{fig1.pdf}
\caption{(Color online). The particle density $n$ (dashed line) and the compressibility $\kappa$ (solid line) versus chemical potential $\mu/t$ for a clean closed chain at $T = 0$. The compressibility diverges logarithmically at the quantum critical point $\mu = \pm 2t$.}
\end{figure}
an electron on a site $i$, $t_i$ the near-neighbor hopping, $\mu_i$ and $U_i$ are the chemical potential and pairing interaction, respectively. The mean-field decomposition of the interaction term gives the $p$-wave gap function

$$\Delta_i = U (c_i^\dagger c_{i+1}^\dagger),$$

which results in the Kitaev 1D spinless tight-binding Hamiltonian with $p$-wave superconducting pairings. In addition we can add an on-site impurity potential or a weak link described by,

$$H = \sum_i \left( V_i - \mu_i \right) c_i^\dagger c_i - \sum_i t_i (c_i^\dagger c_{i+1} + \text{h.c.}) - \sum_i \Delta_i (c_i^\dagger c_{i+1}^\dagger + \text{h.c.}).$$

In the clean limit, $t_i = t$, $\Delta_i = \Delta$, $\mu_i = \mu$ and $V_i = 0$, the system reduces to the 1D Kitaev chain. We use both $T$-matrix and inhomogeneous Bogoliubov-de Gennes (BdG) equations, including self consistency as discussed below. Even though this is a one-dimensional problem we are justified in ignoring the quantum fluctuations, primarily because we envisage the system as proximity coupled to a bulk superconductor which damps out the fluctuations.

**T-matrix approach:** The Green’s function for a clean SC system is given by

$$G_0(k, \omega) = \frac{1}{D} \begin{pmatrix} \omega + \epsilon_k & 2i\Delta \sin(k) \\ -2i\Delta \sin(k) & \omega - \epsilon_k \end{pmatrix},$$

where

$$D(\omega) = \omega^2 - \epsilon_k^2 - 4\Delta^2 \sin^2(k).$$

The full Green’s function in the single-impurity problem within the $T$-matrix approximation can be written as

$$G(k, k', \omega) = G_0(k, \omega) \delta_{kk'} + G_0(k, \omega) T(k, k', \omega) G_0(k', \omega).$$

From standard perturbation theory:

$$T(\omega) = [I_2 - \tilde{V} g_0(\omega)]^{-1} \tilde{V},$$

where $g_0(\omega) = \int \frac{dk}{2\pi} G_0(k, \omega)$ and $\tilde{V} = V_i \sigma_3$ corresponds to the non-magnetic impurity potential. The impurity induced bound state can be determined from $\text{Det}(T^{-1}(\omega)) = 0$. We solve this equation numerically and show that the locations of the bound states agree with the peaks in the density of states obtained from the BdG method discussed below, in the absence of self consistency. The bound state at $\omega = 0$ occurs when $V_i = 2\mu/(1 - \text{sign}(4t^2 - \mu))$ in the trivial phase. Bound state formation by an on-site impurity in the related problem of spin-orbit coupled superconductors was also studied within non-self consistent T-matrix approach.

Bogoliubov-de Gennes (BdG) approach: We go beyond non-self consistent $T$-matrix by using the self consistent BdG method to study the effects of link defects and on-site impurities. We diagonalize Eq. (3) by defining the operator $\gamma_i = \sum_n \left( c_n u_n(i) - c_n^\dagger v_n^*(i) \right)$ that leads to BdG equations

$$\begin{pmatrix} h_0 - \Delta^\dagger & u_n(j) \\ \Delta - h_0 & v_n(j) \end{pmatrix} = E_n \begin{pmatrix} u_n(j) \\ v_n(j) \end{pmatrix},$$

where the excitation eigenvalues $E_n \geq 0$. $h_0 u_n(i) = (-\mu_i + V_i - t_i(u_n(i+1) + u_n(i-1)))$ and $\Delta u_n(i) = \Delta_i u_n(i+1) + \Delta_{i-1} u_n(i-1)$. The self-consistency cond-
The density of particles on site \( i \) is
\[
n_i = \left\langle n_i^\dagger n_i \right\rangle = \sum_n \left[ |u_n(i)|^2 f(E_n) + |v_n(i)|^2 (1 - f(E_n)) \right],
\]
where \( f(E_n) \) is the Fermi function and the local single-particle density of states (LDOS) is given by
\[
N_i(\omega) = \sum_n \left[ |u_n(i)|^2 \delta(\omega - E_n) + |v_n(i)|^2 \delta(\omega + E_n) \right].
\]

When the order parameter \( \Delta_i \) is solved for self-consistently in the presence of single impurity, we find that it becomes inhomogeneous around the impurity. This however changes our results for the local compressibility only quantitatively.

**Compressibility at the topological phase transition:** In the clean limit, the Hamiltonian can be diagonalized
\[
H = \sum_k E_k a_k^\dagger a_k
\]
using the Bogoliubov transformation
\[
a_k = u_k c_k + v_k c_k^\dagger \quad \text{with} \quad |u_k|^2 = 1/2 \left( 1 + \epsilon_k/E_k \right) \quad \text{and} \quad |v_k|^2 = 1 - |u_k|^2.
\]
The quasiparticle excitation energy is given by
\[
E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2} \quad \text{where} \quad \Delta_k = 2t \sin(k) \quad \text{and} \quad \epsilon_k = -\mu - 2t \cos(k).
\]

From the number equation
\[
N = \frac{1}{2} \sum_k \left( 1 - \frac{\epsilon_k}{E_k} \tanh \left( \frac{E_k}{2T} \right) \right),
\]
we can obtain the isothermal compressibility at finite temperature \( \kappa(T) = \frac{\partial N}{\partial T} \) to be
\[
\kappa(T) = \sum_k \frac{|\Delta_k|^2}{2E_k^3} \tanh \left( \frac{E_k}{2T} \right) + \sum_k Y_k \frac{\epsilon_k}{E_k^3},
\]
where \( Y_k = 1/4T \text{sech}^2 \left( E_k/2T \right) \) is the Yoshida function.

The low temperature compressibility diverges logarithmically at the quantum critical point \( \kappa \sim \log(1/|\mu| - 2t)/T \) as shown in Fig. 1. This divergence is caused by the gap in the topological phase \( |\mu| < 2t \) closing at the topological phase transition and reopening again in the trivial phase \( |\mu| > 2t \). At \( T=0 \) and for fixed \( \mu \), deep in the topological phase \( |\mu| \ll 2t \), \( \kappa \sim \Delta^2/t^3 \) for \( t \gg \Delta \).

It is useful to contrast the compressibility which captures the single particle density of states (DOS) as well as the pairs, from the behavior of the spectral function \( A_k(\omega) = |u_k|^2 \delta(E_k - \omega) + |v_k|^2 \delta(E_k + \omega) \) and the single particle density of states \( N(\omega) = \sum_k A_k(\omega) \). As seen in Fig. 2, the DOS shows a gap in both the topological and the trivial phases except at the transition. However, \( \kappa \) is non-zero because of the contribution from the pairs.

**Weak link:** In the presence of a weak link the system becomes inhomogeneous with the local particle number defined in Eq. \( 3 \). From that we obtain the local compressibility \( \kappa_i = \partial n_i/\partial \mu \) by differentiating it with respect to the global chemical potential \( \mu \). We find that the weak link cuts off the divergence of the local compressibility at the transition point and the height of the peak decreases as the ratio \( \Delta_0/\Delta \) deviates from unity (Fig. 3 (a)). In the limit of an open chain, i.e. \( \Delta_0 = t_0 = 0 \), the peak disappears (Fig. 3 (b)). The value of the compressibility close to \( \mu = 2t \) is larger in the clean limit and decreases as the ratio \( \Delta_0/\Delta \) deviates from unity as shown in Fig. 3 (c).

**Local potential:** In the presence of an on-site impurity \( V_i \), there are several interesting features in the behavior of the local particle density and compressibility.

1. For a repulsive potential \( V_i > 0 \), the local density, which is obtained by integrating \( N_i(\omega) \) up to zero, is reduced for all \( \mu \) (Fig. 4 (a)), as expected. This occurs because spectral weight shifts above the Fermi level in the presence of a repulsive potential.

2. The divergences in \( \kappa \) for the clean problem are cut-
(c) show how the non-trivial BS forms.

For positive impurity potential $V_1 < 2t$, the effect is strong close to $\mu = 2t$ (a,b). For $V_1 > 2t$, close the topological phase transition $\mu = 2t$, the local particle density starts to decrease as chemical potential increases and local compressibility becomes negative (c,d). Also, an extra peak appears in the trivial phase. The effect is reversed for negative potential, the same scenario repeats but now for negative $\mu$. (e) The local compressibility for various chemical potentials $\mu$ and the impurity potential strength $V_1$. 

FIG. 4. (Color online) Figures show the local particle density and local chemical potential versus chemical potentials for various local impurity potentials $V_1$ present on site 1. The local impurity potential affects singularities at $\mu = \pm 2t$ non symmetrically. For positive impurity potential $V_1 < 2t$, the effect is strong close to $\mu = 2t$ (a,b). For $V_1 > 2t$, close the topological phase transition $\mu = 2t$, the local particle density starts to decrease as chemical potential increases and local compressibility becomes negative (c,d). Also, an extra peak appears in the trivial phase. The effect is reversed for negative potential, the same scenario repeats but now for negative $\mu$. (e) The local compressibility for various chemical potentials $\mu$ and the impurity potential strength $V_1$.

FIG. 5. (Color online). The local density of states for various values of on-site impurity strength and chemical potential $\mu$. (a,b) show LDOS at quantum critical points $\mu = \pm 2t$ and (c,d) show how the non-trivial BS forms.

off in the presence of disorder; however the singularities in the local $\kappa_1$ are still present at $\mu = \pm 2t$ but are of unequal strengths as seen in Fig. 4(b) for small impurity potential $|V_1| < 2t$. This can be understood from the changes to the local density of states by the presence of the impurity (Fig. 5 (a,b)). While the states for both $\mu = +2t$ and for $\mu = -2t$ are shifted to positive energies, there is a marked difference in the spectra. In particular, the local density of states for $\mu = -2t$ shows a sharpening and the possible formation of a bound state.

(3) For larger impurity strengths $V_1 > 2t$, the effect is quite non-trivial. The local particle density is found to decrease around the topological phase transition (Fig. 4).

(c) even as $\mu$ increases. Correspondingly, the local compressibility $\kappa_i$ becomes negative (Fig. 4(d)) and shows a dip at the transition. The reason for the decrease of the local density and the corresponding negative local compressibility is tied to the formation of an impurity bound state (BS) above zero energy that starts to form close to the topological phase transition.

(4) The bound state formation is induced by the sign change of the order parameter in this unconventional superconductor. As seen in Fig. 5(c), for a small superconducting gap, the bound state is at a finite energy and is broadened into a resonance. For a fixed $V_1$ as $\mu$ increases, the gap increases and the bound state becomes sharper and moves to zero energy at $\mu = V_1$ (Fig. 5(c,d)). At this point the zero energy bound state is detectable as an additional peak in $\kappa_i$.

(5) For a negative impurity potential, the BS forms below the Fermi level and more states shift below the Fermi energy to enhance the local density for all $\mu$. In contrast to the scenario of the positive impurity potential, the BS does contribute to the local particle density for a negative impurity. As the result, the local particle density starts to increase as $\mu$ decreases, until a sharp BS is formed. This once again causes the local compressibility to become negative around the topological phase transition.

Next, we investigate how mid gap bound states develop at the site next to the impurity in the topological phase. With increasing disorder $V_1$, the bound states shift toward zero energy (Fig. 6). In the limit of infinite disorder, the system is equivalent to an open chain and the bound state precursors coincide with the appearance of Majorana fermions and merge at the Fermi level.
Conclusions: Our theoretical proposals based on the compressibility given above can be used to detect the topological phase transition in a 1D Kitaev chain. Specifically in the presence of local defects, the local compressibility can be measured using single-electron transistor (SET) spectroscopies. Ref. 22 in fact used the SET in a different context to measure the inverse compressibility locally on a graphene sample as a function of the back-gate voltage or carrier density. We expect the same technique can be applied to the 1D Kitaev chain to detect the topological phase transition using our predictions.

There are several experimental realizations of the Kitaev chain. Of the two most promising to have addressed the observation of Majorana fermions, one is based on semiconducting quantum wires with strong spin-orbit coupling and the other involves an iron atomic chain deposited on lead.

We discuss the first realization based on the semiconductor wire implementation further, as we believe it is more relevant for our predictions. In the presence of Rashba spin-orbit coupling, the parabolic bands for the two spin projections get separated. In addition, a Zeeman field $h$ opens up a gap leading to an effectively spinless 1D metal when the chemical potential $\mu$ lies in the Zeeman gap. The proximity induced superconductivity with a gap $\Delta$ gives rise to the topological phase when $h > \sqrt{\Delta^2 + \mu^2}$. In this regime, the wire can be realized as a Kitaev chain and should have two Majorana localized zero energy modes at the ends. Upon decreasing the field, the wire undergoes a phase transition at $h_c = \sqrt{\Delta^2 + \mu^2}$ from the topological to trivial s-wave superconducting phase. Even though our predictions are for the topological phase transition in the Kitaev chain where the trivial phase is a p-wave superconductor, we expect certain features that occur close to the transition to remain robust in the semiconductor wire.

Some of the most promising directions to experimentally investigate are:

(a) the peak in the compressibility at the topological phase transition tuned by the Zeeman field in the clean wire, and,

(b) the negative compressibility induced by the on-site impurity.

In general it will be useful to see the interplay between local scanning and local compressibility spectroscopies for giving insights into single particle and collective modes.

ACKNOWLEDGEMENTS

DN and NT were supported by the NSF under Grant No. nsf-dmr1309461

1. C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. D. Sarma, Rev. Mod. Phys. 80, 1083 (2008).
2. F. Wilczek, Nat. Phys. 5, 614 (2009).
3. A. Kitaev, Ann. Phys. 303, 2 (2003).
4. G. Moore and N. Read, Nucl. Phys. B 360, 362 (1991).
5. J. Alicea, Rep. Prog. Phys. 75, 076501 (2012).
6. L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008).
7. J. Linder, Y. Tanaka, T. Yokoyama, A. Sudbø, and N. Nagaosa, Phys. Rev. Lett. 104, 067001 (2010).
8. N. Read and D. Green, Phys. Rev. B 61, 10267 (2000).
9. J. D. Sau, R. M. Lutchyn, S. Tewari, and S. D. Sarma, Phys. Rev. Lett. 104, 040502 (2010).
10. J. Alicea, Phys. Rev. B 81, 125318 (2010).
11. M. Duckheim and P. W. Brouwer, Phys. Rev. B 83, 054513 (2011).
12. S. B. Chung, H.-J. Zhang, X.-L. Qi, and S.-C. Zhang, Phys. Rev. B 84, 060510(R) (2011).
13. A. C. Potter and P. A. Lee, Phys. Rev. B (2012).
14. A. Kitaev, Phys. Usp. 44, 131 (2001).
15. R. M. Lutchyn, J. D. Sau, and S. D. Sarma, Phys. Rev. Lett. 105, 077001 (2010).
16. Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. 105, 177002 (2010).
17. K. Sengupta, I. Zutić, H.-J. Kwon, V. M. Yakovenko, and S. D. Sarma, Phys. Rev. B 63, 144531 (2001).
18. H.-J. Kwon, V. M. Yakovenko, and K. Sengupta, Low Temp. Phys. 30, 613 (2004).
19. V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Science 336, 1003 (2012).
20. L. P. Rokhinson, X. Liu, and J. K. Furdyna, Nat. Phys. 8, 795 (2012).
21. S. Nadj-Perge, I. K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A. H. MacDonald, B. A. Bernevig, and A. Yazdani, Science 340, 602 (2014).
22. J. D. Sau and E. Demler, Phys. Rev. B 88, 205402 (2013).
23. J. Martin, N. Akerman, G. Ulbricht, T. Lohmann, J. H. Smet, K. von Klitzing, and A. Yacoby, Nat. Phys. 4, 144 (2008).
24. A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum, and H. Shtrikman, Nat. Phys. 8, 887 (2012).