

FIG. 1: (Color online) Charge density in our model TI on the cube-shaped lattice with 20^3 sites with a unit monopole at its center, with parameters $t=\lambda$, $\epsilon=4t$, leading to a bulk gap $\Delta=4t$. (a) Charge density $\delta\rho$ of the three closest layers below the monopole, for g=0. (b) The excess charge $\delta Q(r)$ (in units of e) for different Zeeman coupling g. The knee feature seen at r=10 corresponds to the radius at which the sphere used to calculate $\delta Q(r)$ first touches the system boundary. (c) Log-log plot of $\delta Q_g - \delta Q_0$ showing the power-law approach $\sim r^{-\alpha}$ of the accumulated charge to its assymptotic value of 1/2. The least-square fit yields exponents $\alpha=2.85, 3.04, 2.79$ for g=2,6,10, respectively. We attribute the deviations of the numerically determined exponent α from the expected value of 3 to the finite size effect.

charge density $\delta \rho = \rho_0 - \rho_1$ is plotted in Fig. 1a. To determine the total charge bound to the monopole we calculate the excess accumulated charge in a sphere of radius r centered on the monopole, $\delta Q(r) = \sum_{|\mathbf{r}_i| < r} \delta \rho(\mathbf{r}_i)$. We find (Fig. 1b) that it saturates at -e/2 to within 4 significant digits, comparable to the accuracy of our numerics. For q = 0 we find two localized zero modes, one at the monopole and one on the surface. Fractional charge bound to the monopole can be understood in this case by appealing to the standard arguments^{28,29} developed originally to describe charge fractionalization in polyacetylene.³⁰ Briefly, when a topological defect (such as a domain wall in polyacetylene) produces a localized zero mode inside the gap in a particle-hole symmetric system, one can show that the spectral weight of the state contains equal contributions from the valence and the conduction bands. Thus, the valence band shows a net deficit of half a state in the vicinity of the defect. This translates into the defect carrying fractional charge $\pm e/2$, the sign depending on whether the zero mode is empty or occupied.

Like in polyacetylene we find the saturation of charge to be exponential $\sim \exp{(-r/\xi)}$, where $\xi \sim 1/\Delta$ and Δ is the bulk gap.

When g>0, the Zeeman coupling causes changes in the charge distribution near the monopole but the total accumulated charge remains quantized at -e/2. In this case there are no exact zero modes in the spectrum and $\delta Q(r)$ approaches e/2 as a power law with the exponent close to -3 (Fig. 1c).

The power-law dependence can be understood as follows. The Zeeman term acts as an additional time-reversal breaking field which modifies the value of axion θ away from π close to the monopole. This causes non-vanishing $\nabla \theta$ and thus, according to Eq. (2), additional contribution to the effective charge density. The simplest assumption, $\delta \theta \sim \mathbf{B}^2$, gives $\delta \rho \sim \nabla \theta \cdot \mathbf{B} \sim r^{-7}$ and $\delta Q \sim r^{-4}$, a power law but with the exponent not

quite in agreement with our numerical simulation. On further reflection one realizes that in our model $\delta\theta$ cannot be proportional to \mathbf{B}^2 but rather must be proportional to its gradients. This is because in the presence of a uniform Zeeman term the system remains inversion-symmetric. Inversion symmetry dictates quantized value of $\theta=0,\pi$ even when \mathcal{T} is explicitly broken. Help thus, non-vanishing $\delta\theta$ requires spatially varying Zeeman field. The simplest assumption satisfying these requirements is $\nabla\theta\sim\nabla^2\mathbf{B}$. In the vicinity of the monopole one finds $\delta\rho\sim\nabla\theta\cdot\mathbf{B}\sim r^{-6}$ and $\delta Q\sim r^{-3}$ in agreement with our numerical results.

We note that the above considerations are based on the effective axion action (1) and apply on lengthscales large compared to ξ . The power law tail in the fractional charge distribution for g>0 appears on top of a short-lengthscale structure with a roughly exponential profile that is controlled by the properties of the microscopic Hamiltonian and is thus non-universal. At the intermediate lengthscales the interplay of the two contributions can give rise to interesting structures such as the peak in $\delta Q(r)$ at $r\simeq 2.5$ seen in Fig. 1b for g=10.

By the same method described above we have investigated spin density induced by the monopole. We find that there is no net spin $\langle \mathbf{S} \rangle$ attached to the monopole. Thus, in addition to charge fractionalization, a magnetic monopole inserted in a STI constitutes an example of spin-charge separation in three spatial dimensions. This is perhaps not surprising in view of the fact that spin-orbit coupling present in the Hamiltonian (7) breaks the SU(2) spin symmetry and, as a result, electron spin is not a good quantum number in the model describing our system.