Topological quantization in units of the fine structure constant

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Fundamental topological phenomena in condensed matter physics are associated with a quantized electromagnetic response in units of fundamental constants. Recently, it has been predicted theoretically that the time-reversal invariant topological insulator in three dimensions exhibits a topological magneto-electric effect quantized in units of the fine structure constant \(\alpha = e^2/hc\). In this Letter, we propose an optical experiment to directly measure this topological quantization phenomenon, independent of material details. Our proposal also provides a way to measure the half-quantized Hall conductances on the two surfaces of the topological insulator independently of each other.

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Topological phenomena in condensed matter physics are typically characterized by the exact quantization of the electromagnetic response in units of fundamental constants. In a superconductor (SC), the magnetic flux is quantized in units of the flux quantum \(\phi_0 \equiv \frac{\hbar}{2e}\); in the quantum Hall effect (QHE), the Hall conductance is quantized in units of the conductance quantum \(G_0 \equiv \frac{e^2}{h}\). Not only are these fundamental physical phenomena, they also provide the most precise metrological definition of basic physical constants. For instance, the Josephson effect in SC allows the most precise measurement of the flux quantum which, combined with the measurement of the quantized Hall conductance, provides the most accurate determination of Planck’s constant \(\hbar\) to date\textsuperscript{1}. The remarkable observation of such precise quantization phenomena in these imprecise, macroscopic condensed matter systems can be understood from the fact that they are described in the low-energy limit by topological field theories (TFT) with quantized coefficients. For instance, the QHE is described by the topological Chern-Simons theory \textsuperscript{2} in \(2 + 1\) dimensions, with coefficient given by the quantized Hall conductance. SC can be described by the topological \(BF\) theory \textsuperscript{3} with coefficient corresponding to the flux quantum.

More recently, a new topological state in condensed matter physics, the time-reversal (\(T\)) invariant topological insulator (TI), has been investigated extensively\textsuperscript{4,5}. The concept of TI can be defined most generally in terms of the TFT\textsuperscript{7} with effective Lagrangian

\[ L = \frac{1}{8\pi} (\varepsilon E^2 - \frac{1}{\mu} B^2) + \frac{\theta}{2\pi} \frac{\alpha}{2\pi} E \cdot B, \]  

(1)

where \(E\) and \(B\) are the electromagnetic fields, \(\varepsilon\) and \(\mu\) are the dielectric constant and magnetic permeability, respectively, and \(\theta\) is an angular variable known in particle physics as the axion angle \textsuperscript{8}. Under periodic boundary conditions, the partition function and all physical quantities are invariant under shifts of \(\theta\) by any multiple of \(2\pi\). Since \(E \cdot B\) is odd under \(T\), the only values of \(\theta\) allowed by \(T\) are 0 or \(\pi\) (modulo \(2\pi\)). The second term of Eq. (1) thus defines a TFT with coefficient quantized in units of the fine structure constant \(\alpha \equiv e^2/\hbar c\). The TFT is generally valid for interacting systems, and describes a quantized magnetoelectric response denoted topological magneto-electric effect (TME) \textsuperscript{9}. The quantization of the axion angle \(\theta\) depends only on the \(T\) symmetry and the bulk topology; it is therefore universal and independent of any material details. More recently, it has been shown\textsuperscript{9} that the TFT\textsuperscript{7} reduces to the topological band theory (TBT)\textsuperscript{10,11} in the noninteracting limit. Interestingly, the TME is the first topological quantization phenomenon in units of \(\alpha\). It can therefore be combined with the two other known topological phenomena in condensed matter, the QHE and SC, to provide a metrological definition of the three basic physical constants, \(e, \hbar\), and \(c\).

The TME has not yet been observed experimentally. An insight into why this is so can be gained by comparing the \(3 + 1\) dimensional TFT\textsuperscript{11} of TI to the \(2 + 1\) dimensional Chern-Simons TFT of the QHE\textsuperscript{2}. In \(2 + 1\) dimensions, the topological Chern-Simons term is the only term which dominates the long-wavelength behavior of the system, which leads to the universal quantization of the Hall conductance. On the other hand, in \(3 + 1\) dimensions the topological \(\theta\)-term in Eq. (1) and the Maxwell term are equally important in the long wavelength limit. Therefore, one has to be careful when designing an experiment to observe the topological quantization of the TME, in which the dependence on the non-topological materials constants \(\varepsilon\) and \(\mu\) are removed.

In this Letter, we propose an optical experiment to observe the topological quantization of the TME in units of \(\alpha\), independent of material properties of the TI such
as $\varepsilon$ and $\mu$. This experiment could be performed on any of the available TI materials, such as the Bi$_2$Se$_3$, Bi$_2$Te$_3$, Sb$_2$Te$_3$ family or the recently discovered thallium-based compounds [12]. Consider a TI thick film of thickness $\ell$ with optical constants $\varepsilon_2, \mu_2$ and axion angle $\theta$ deposited on a topologically trivial insulating substrate with optical constants $\varepsilon_3, \mu_3$ (Fig. 1). The vacuum outside the TI has $\varepsilon = \mu = 1$ and trivial axion angle $\theta_{\text{vac}} = 0$. The substrate being also topologically trivial, both interfaces at $z = 0$ and $z = \ell$ support a domain wall of $\theta$ giving rise to a surface QHE with half-quantized surface Hall conductance $\sigma^x_H = \left(n + \frac{1}{2}\right) e^2/2h$ with $n \in \mathbb{Z}$ [7]. The factor of $\frac{1}{2}$ is a topological property of the bulk and is protected by the $T$ symmetry. On the other hand, the value of $n$ depends on the details of the interface and may thus be different for the two interfaces. To account for this general case we assign $\theta_{\text{subs}} = 2p\pi$ with $p \in \mathbb{Z}$ to the topologically trivial substrate, corresponding to $\sigma^x_H = \frac{e^2}{2h}$ on the $z = 0$ interface and $\sigma^x_H = (p - \frac{1}{2}) \frac{e^2}{2h}$ on the $z = \ell$ interface. The experiment consists in shining normally incident monochromatic light with frequency $\omega$ on the TI film, and measuring the Kerr angle $\theta_K$ of the reflected light and Faraday angle $\theta_F$ of the transmitted light. However, the effective theory [12] applies only in the regime $\omega \ll E_g/h$ where $E_g$ is the surface gap [7]. Such a surface gap can be opened by a thin magnetic coating on both surfaces of the TI, as first suggested in Ref. [7], or by an applied perpendicular magnetic field $B = B\hat{z}$ (Fig. 1) through the surface Zeeman effect as well as the exchange coupling between surface electrons and the paramagnetic bulk. We discuss the experimentally simpler case of the external magnetic field. For incident light linearly polarized in the $x$ direction $E_{\text{in}} = E_{\text{in}}\hat{x}$, the Kerr and Faraday angles are defined by $\tan \theta_K = E_y^r/E_x^r$ and $\tan \theta_F = E_y^r/E_x^r$, respectively, with $E_x = E_x^t - \hat{x}$ and $E_y = E_y^t + \hat{y}$ the reflected and transmitted electric fields, respectively (Fig. 1). Furthermore, $\theta_K$ and $\theta_F$ are to be measured as a function of $B$. The angles that we discuss in the following are defined as the linear extrapolation of $\theta_K(B)$ and $\theta_F(B)$ as $B \rightarrow 0^+$, in which limit the non-topological bulk contribution to optical rotation is removed [7].

The problem of optical rotation at a TI/trivial insulator interface has been studied before [5, 14, 15]. In general, $\theta_K$ and $\theta_F$ depend on the optical constants $\varepsilon_2, \mu_2$ of the TI. In the thick film geometry considered here, they will also depend in a complicated manner on the optical constants $\varepsilon_3, \mu_3$ of the substrate, the film thickness $\ell$, and the photon frequency $\omega$, due to multiple reflection effects at the two interfaces. It seems therefore dubious that one could extract the exact quantization of the TME from such a measurement. However, we find that these multiple reflection effects can be used for a universal measurement of the TME, with no explicit dependence on $\varepsilon_2, \mu_2, \varepsilon_3, \mu_3, \ell$, and $\omega$.

In Fig. 2(a) we plot the reflectivity $R \equiv |E_x^r|^2/|E_{\text{in}}|^2$ as a function of photon frequency $\omega$ in units of a characteristic frequency $\omega_\ell \equiv \sqrt{\varepsilon_2\mu_2}$, for $\varepsilon_2 = 100$, $\varepsilon_3 = 13$, and $\mu_2 = \mu_3 = 1$, appropriate for a topological Bi$_2$Se$_3$ [16] thin film on a Si substrate [17-19]. We observe that minima in $R$ occur when $\omega/\omega_\ell$ is an integer, corresponding to $\ell$ being an integer multiple of $\lambda_2/2$ with $\lambda_2 = \frac{2\pi c}{\omega\sqrt{\varepsilon_2\mu_2}}$ the photon wavelength inside the TI. For radiation in the terahertz range this corresponds to $\ell \sim 100 \mu m$. When
ω is tuned to any of these minima, we find
\[
\tan \theta_K' = \frac{4\alpha p}{Y_3^2 - 1 + 4\alpha^2 p^2}, \quad \tan \theta_F' = \frac{2\alpha p}{Y_3 + 1},
\]  
(2)

where \( Y_i \equiv \sqrt{\varepsilon_i/\mu_i} \) is the admittance of region \( i \), and the prime indicates rotation angles measured at a reflectivity minimum, i.e. for \( \omega/\omega_0 \in \mathbb{Z} \). We see that \( \theta_K' \) and \( \theta_F' \) are independent of the TI optical constants \( \varepsilon_2, \mu_2 \). Equation (2) corresponds simply to the results of Ref. [7, 14] for a unique interface with axion domain wall \( \Delta \theta = 2\pi \). Moreover, the two angles can be combined \[20\] to obtain a universal result independent of both TI \( \varepsilon_2, \mu_2 \) and substrate \( \varepsilon_3, \mu_3 \) properties,
\[
\frac{\cot \theta_K' + \cot \theta_F'}{1 + \cot^2 \theta_F'} = \alpha p, \quad p \in \mathbb{Z}.
\]  
(3)

Since the rotation angles are measured at a reflectivity minimum, Eq. (3) has no explicit dependence on \( \ell \) or \( \omega \) either. Equation (3) clearly expresses the topological quantization in units of \( \alpha \) solely in terms of experimentally measurable quantities, and is the first important result of this work.

However, neither Eq. (2) nor Eq. (3) depend explicitly on the TI axion angle \( \theta \), and one may ask whether Eq. (3) is at all an indication of nontrivial bulk topology. In fact, Eq. (3) describes the topological quantization of the total Hall conductance of both surfaces
\[
\sigma_H^{\text{tot}} = \sigma_H^{+} + \sigma_H^{-} = \sigma_H^{+} = \frac{e^2}{h},
\]
which holds independently of the possibility \( T \) breaking in the bulk. In the special case that the two surfaces have the same surface Hall conductance, we have \( p = 2\sigma_H^{+} = \ell \) and Eq. (3) is sufficient to determine the bulk axion angle \( \theta \). However, for a TI film on a substrate the two surfaces are generically different and can have different Hall conductance. To obtain the axion angle \( \theta \) in the more general case of different surfaces, we propose another optical measurement performed at reflectivity maxima \( \omega = (n + \frac{1}{2})\omega_0, n \in \mathbb{Z} \) [Fig. 2(a)]. We denote by \( \theta_K'' \) and \( \theta_F'' \) the Kerr and Faraday angles measured at an arbitrary reflectivity maximum. In contrast to \( \theta_K' \) and \( \theta_F' \) [Eq. (2)], these depend on \( \varepsilon_2, \mu_2 \) as well as on \( \varepsilon_3, \mu_3 \),
\[
\tan \theta_K'' = \frac{4\alpha}{Y_3^2 - Y_2^4 + 4\alpha^2} \left( Y_2^2 (p - \frac{\theta}{2\pi}) - \frac{\theta}{2\pi} \right) \left( \frac{\theta}{2\pi} \right)^2,
\]
\[
\tan \theta_F'' = \frac{2\alpha}{Y_3 + Y_2^2 - 4\alpha^2} \frac{\theta}{2\pi} \left( p - \frac{\theta}{2\pi} \right).
\]  
(4)

where we define \( Y_2^2 = Y_2^4 + 4\alpha^2 \left( p - \frac{\theta}{2\pi} \right)^2 \). More importantly, \( \theta_K'' \) and \( \theta_F'' \) depend explicitly on the TI axion angle \( \theta \). It is readily checked that Eq. (4) reduces to Eq. (2) in the single-interface limit \( \theta = 2\pi p, Y_2 = Y_3 = 0, Y_2 = 1 \). In general however, from the knowledge of \( p \) [Eq. (3)] and either \( \theta_K' \) or \( \theta_F' \), we can extract \( Y_3 \) by using

\[
\text{FIG. 3: (color online). (a) Kerr-only measurement setup, with material parameters the same as indicated in Fig. 2(b), (c) and (d): universal function } f_3(\theta) \text{ for different material parameters [same as in Fig. 2(b), (c), (d)]}. \text{ As in Fig. 2(b) the position of the zero crossing is universal and provides an experimental demonstration of the quantized TME.}
\]
the Kerr angle to extract $p$ and $\theta$. We denote by $\theta^{p13}_K$ and $\theta^{p13}_K$ the Kerr angles defined previously in Eq. 2 and 4, respectively. Conversely, we denote by $\theta^{K}_{31}$ and $\theta^{p13}_K$ the Kerr angles for light traveling in the opposite direction, i.e. incident from the substrate [Fig. 3(a)]. As before, the prime and double prime correspond to angles measured at reflectivity minima and maxima, respectively. We find

$$\tan \theta^{p13}_K = -\frac{4\alpha p Y_3}{Y_3^2 - 1 + 4\alpha^2 p^2},$$

$$\tan \theta^{K}_{31} = \frac{4\alpha Y_3 \left[ Y_3^2 \theta^{p13}_K - \gamma \left(p - \frac{\theta^{p13}_K}{2}\right)\right]}{\gamma Y_3^2 + 4\alpha^2 \left[p^2 - \left(\frac{\theta^{p13}_K}{2}\right)^2\right] - Y_3^4 - 8\alpha^2 Y_3^2 \left(\frac{\theta^{p13}_K}{2}\right)^2},$$

where we define $\gamma \equiv 1 + 4\alpha^2 \left(\frac{\theta^{p13}_K}{2}\right)^2$. As previously, $\theta^{K}_{31}$ and $\theta^{p13}_K$ can be combined to eliminate $Y_3$ and provide a universal measure of $p \in \mathbb{Z}$,

$$\cot \theta^{K}_{31} - \text{sgn} p \sqrt{1 + \cot^2 \theta^{p13}_K (1 - \tan^2 \theta^{p13}_K)} = 2\alpha p,$$  

provided $Y_3^2 \equiv \varepsilon_3/\mu_3 > 1 + 4\alpha^2 p^2$, which is satisfied in practice for low $p$ since $\alpha^2 \sim 10^{-4}$. Furthermore, comparing Eq. 5 for $\theta^{p13}_K$ to Eq. 2 for $\theta^{K}_{31}$ we see that $Y_3$ is easily obtained as $Y_3 = -\cot \theta^{p13}_K \tan \theta^{p13}_K$. Finally, to extract the bulk axion angle $\theta$, we need to solve for $Y_3^2$ in Eq. 4 in terms of $\theta^{p13}_K$, and substitute into the resulting expression $Y_3^2 = Y_3^2(\theta)$ into the equation for $\theta^{K}_{31}$ in Eq. 3. The result of this analysis can once again be expressed in the form $f_K(\theta^{13}, \theta^{31}, \theta^{p13}, \theta^{p31}; p, \theta) = 0$, where $f_K$ is a ‘universal’ function which only depends on the measured Kerr angles. As before, we substitute into $f_K$ the experimental values of $\theta^{13}, \theta^{31}, \theta^{p13}, \theta^{p31}$ and $p$ [obtained from Eq. 4] and obtain a function of a single variable $f_K(\theta)$ which crosses zero at the value of the bulk axion angle with no 2\pi ambiguity. In Fig. 3(b), (c) and (d) we plot the universal function $f_K$ for different values of the material parameters $\varepsilon_2, \varepsilon_3, p$ and for a bulk axion angle $\theta = \pi$. The zero crossing point is independent of material parameters and, together with Eq. 6, provides another means to demonstrate experimentally the universal quantization of the TME in the bulk of a TI.

Recent work 22 has addressed the similar problem of optical rotation on a TI film, and found interesting and novel results for the rotation angles. However, these results hold only in certain limits which are less general than the ones discussed in this work. First, Ref. 22 considers a free-standing TI film in vacuum. Most films are grown on a substrate which can affect the physics qualitatively. For instance, the giant Kerr rotation $\theta_K = \tan^{-1}(1/\alpha) \approx \pi/2$ found in Ref. 22 is a special case of our Eq. 2, with $p = 1$ and $\varepsilon_3/\mu_3 = 1$. It is dramatically suppressed when $\varepsilon_3/\mu_3 - 1$ is greater than $\alpha^2 \sim 10^{-4}$, which is typically the case in practice. Second, in Ref. 22 a correction proportional to $\Delta/\epsilon_c$ was introduced to the surface Hall conductance, where $\Delta$ is the $T$-breaking Dirac mass and $\epsilon_c$ is a non-universal high-energy cutoff. According to the general bulk TFT of the TI 7, the surface Hall conductance is always quantized as long as the surface is gapped and the bulk is $T$-invariant (in the $B \rightarrow 0$ limit). Thus we conclude that such a non-universal correction is absent and the requirement $\Delta < \epsilon_c$ is not necessary within the TFT approach 7. This difference clearly demonstrates the power of the TFT approach 7 in predicting universally quantized topological effects in condensed matter physics.

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