Direct Probe of Topological Order for Cold Atoms

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Cold-atom experiments in optical lattices offer a versatile platform to realize various topological quantum phases. A key challenge in those experiments is to unambiguously probe the topological order. We propose a method to directly measure the characteristic topological invariants (order) based on the time-of-flight imaging of cold atoms. The method is generally applicable to detection of topological band insulators in one, two, or three dimensions characterized by integer topological invariants. Using detection of the Chern number for the 2D anomalous quantum Hall states and the Chern-Simons term for the 3D chiral topological insulators as examples, we show that the proposed detection method is practical, robust to typical experimental imperfections such as limited imaging resolution, inhomogeneous trapping potential, and disorder in the system.

The study of topological phases of matter, such as topological band insulators and superconductors, has attracted a lot of interest in recent years [1]. Various topological phases have been found associated with the free-fermion band theory and classified into a periodic table according to the system symmetry and dimensionality [2]. The topology of the band structure is characterized by a topological invariant taking only integer values, which gives the most direct and unambiguous signal of the corresponding topological order. To experimentally probe the topological order, it is desirable to have a way to measure the underlying topological invariant. For some phase, the topological invariant may manifest itself through certain quantized transport property or characteristic edge state behavior [3]. For instance, the quantized Hall conductivity is proportional to the underlying topological Chern number that characterizes the integer quantum Hall states [3, 4]. For many other topological phases in the periodic table, it is not clear yet how to experimentally extract information of the underlying topological invariants.

Cold atoms in optical lattices provide a powerful experimental platform to simulate various quantum states of matter. In particular, recent experimental advance in engineering of spin-orbit coupling and artificial gauge field for cold atoms [5–8] has pushed this system to the forefront for realization of various topological quantum phases [9–12]. The detection method for cold-atom experiments is usually quite different from those for conventional solid-state materials. A number of intriguing proposals have been made for detection of certain topological order in cold-atom experiments, such as those based on the dynamic response [13, 14], the Bragg spectroscopy [15, 16], imaging of the edge states [17], or detection of the Berry phase or curvature [18–21]. Most of these proposals are targeted to detection of the quantum Hall phase. Similar to solid-state systems, it is not clear yet how to probe the topological invariants for various other topological phases in the periodic table.

In this paper, we propose a general method to directly measure the topological invariants in cold-atom experiments based on the state-of-the-art time-of-flight imaging. The method has the following distinctive features: 1) it is applicable to detection of any topological band insulators in one, two, or three dimensions that are characterized by integer topological invariants in the periodic table. 2) The method is not limited by the requirement of a two-band structure for the Hamiltonian [18] or occupation of only the lowest band [19]. Instead, it detects the topological invariants associated with each band for any multi-band Hamiltonians. 3) Our proposed detection method is very robust to practical experimental imperfections. As examples, we numerically simulate two experimental detections: one for the Chern number of the 2D anomalous quantum Hall phase and the other for the Chern-Simons term of the 3D chiral topological insulator. Both simulations show that accurate values of the topological invariants can be obtained experimentally under imaging resolution of a few to a dozen pixels along each spatial dimension, even with inhomogeneous traps and random potentials or interactions.

The topological band insulators are described by effective free-fermion Hamiltonians, typically with complicated spin-orbit couplings. We consider a real-space Hamiltonian with $N$ degrees of freedom in each unit cell, which are referred to as spin states $|m\rangle$ with $m = 1, 2, \ldots, N$. In the momentum $k$ space, the Hamiltonian has $N$ bands and is described by an $N$-by-$N$ Hermitian matrix $H(k)$. The energy spectrum is obtained by solving the Schrödinger equation in the momentum space

$$H(k)|u_b(k)\rangle = E_b(k)|u_b(k)\rangle,$$ (1)

where $b = 1, 2, \ldots, N$ is the band index and $|u_b(k)\rangle$ denotes the corresponding Bloch state with eigen-energy $E_b(k)$. For simplicity, we assume the bands are non-degenerate. Expressed in the original spin basis $|m\rangle$, the
Bloch state has the form
\[ |u_b(k)⟩ = \sum_{m=1}^{N} c_{bm}(k) |m⟩, \]
where \( c_{bm}(k) \) is the Bloch wavefunction with normalization \( \sum_m |c_{bm}(k)|^2 = 1 \).

An topological invariant can be defined for each band, which usually takes the form of the Chern numbers for even spatial dimensions and the Chern-Simons terms for odd spatial dimensions. The Chern numbers (or Chern-Simons terms) for odd spatial dimensions can be obtained as derivatives of the Chern numbers for even spatial dimensions. The Chern numbers (or Chern-Simons terms) can be expressed as momentum-space integrals of the Berry curvature and connection associated with the Bloch state \( |u_b(k)⟩ \). For instance, in 2D \((x, y)\)-plane, the Chern number \( C_b \) for the band \( b \) is defined by
\[ C_b = -\frac{1}{2\pi} \int_{BZ} dk_x dk_y F_{xy}^{(b)}(k), \]
where the Berry curvature \( F_{xy}^{(b)}(k) \equiv \partial_{k_x} A_y^{(b)}(k) - \partial_{k_y} A_x^{(b)}(k) \) and the Berry connection \( A_\mu^{(b)}(k) \equiv \langle u_b(k)|i\hbar \partial_\mu|u_b(k)⟩ \) (\( \mu = x, y \)), and the integration is over the whole Brillouin zone (BZ) which forms a compact manifold.

To probe the topological invariant such as the Chern number in Eq. (3), what we need to measure is the Bloch wave function \( c_{bm}(k) \). The Berry connection and curvature can be obtained as derivatives of \( c_{bm}(k) \) and the Chern number is just a two-fold integration of \( F_{xy}^{(b)}(k) \). For cold atoms in an optical lattice, we can map out the momentum distribution with the conventional time-of-flight imaging and separate different spin components through a magnetic field gradient [22]. Through the band mapping technique employed in experiments [9], populations in different bands are mapped to atomic densities in different spatial regions, so by this measurement we can get information about \( n_{bm}(k) = |c_{bm}(k)|^2 \) for all occupied bands. To extract the wavefunction \( c_{bm}(k) \), it is also crucial to measure the phase information. For this purpose, we apply an impulsive pulse right before the flight of atoms to induce a rotation between different spin components [23]. The rotation should keep the atomic momentum unchanged but mix their spins. For instance, a \( \pi/2 \)-rotation between spin components \( m \) and \( m' \) induces the transition \( c_{bm}(k) \rightarrow [c_{bm}(k) + ic_{bm'}(k)]/\sqrt{2} \) and \( c_{bm'}(k) \rightarrow [-c_{bm}(k) + ic_{bm'}(k)]/\sqrt{2} \), which can be achieved by applying two co-propagating Raman beams or a radio frequency coupling that couples the spin components \( m, m' \) and preserves the momentum \( k \). The pulse is short so that expansion of the atomic cloud is negligible during the pulse. With this prior \( \pi/2 \)-pulse, the time-of-flight (TOF) imaging then measures the densities \( |c_{bm}(k)|^2 \) and \( |c_{bm'}(k)|^2 \), whose difference gives the interference terms \( \text{Re}[c_{bm}(k)c_{bm'}(k)] \). By the same method but with a different phase of the \( \pi/2 \)-pulse, one can similarly measure the imaginary part \( \text{Im}[c_{bm}(k)c_{bm'}(k)] \) between any two spin components \( m \) and \( m' \). The measurement of the population and interference terms \( c_{bm}(k)c_{bm'}(k) \) for all \( m, m' \) fully determines the Bloch wave function \( c_{bm}(k) \) up to arbitrariness of an overall phase \( c_{bm}(k) \rightarrow c_{bm}(k)e^{i\phi(k)} \), where \( \phi(k) \) in general is \( k \)-dependent but independent of the spin index.

In experiments, one needs to discretize the TOF image and measure the density distribution at each pixel of the BZ. The wavefunction \( c_{bm}(k) \) is fixed up to an overall phase \( \varphi(k) \) at each pixel with the above method. This arbitrary \( k \)-dependent phase poses an obstacle to measurement of the topological invariants. To overcome this difficulty, we use a different way to calculate the Berry curvature based on the so-called \( U(1) \)-link defined for each pixel \( k \) of the discrete BZ [24]. The \( U(1) \)-link is defined as \( U_\nu^{(b)}(k) \equiv \langle u_b(k_\nu)|u_b(k_{\nu+\hat{e}})/|\langle u_b(k_\nu)|u_b(k_{\nu+\hat{e}})⟩ \rangle \), where \( \nu = x, y, z \), a unit vector in the corresponding direction. A gauge-independent field is obtained from the \( U(1) \)-link as [24]
\[ \mathcal{F}_{\mu\nu}^{(b)}(k) = i \ln \frac{U_\mu^{(b)}(k_{\nu+\hat{e}})U_\nu^{(b)}(k)}{U_\mu^{(b)}(k_\nu)U_\nu^{(b)}(k_{\nu+\hat{e}})}, \]
where \( \mathcal{F}_{\mu\nu}^{(b)}(k) \in (-\pi, \pi) \) corresponds to a discrete version of the Berry curvature and it reduces to the latter in the large size limit. \( \mathcal{F}_{\mu\nu}^{(b)}(k) \) can be obtained directly from the TOF images associated with the pixel \( k \) of the BZ, independent of the overall phase factor \( \varphi(k) \). The topological invariant can be calculated from \( \mathcal{F}_{\mu\nu}^{(b)}(k) \) by a direct summation over all the pixels of the BZ (instead of \( k \) integration in Eq. (3)). This gives a simple and robust way to experimentally extract the topological invariant from the TOF images.

The detection method described above is general and applicable to various topological phases in different spatial dimensions. To show that the method is robust to experimental imperfections, in the following we numerically simulate detection of two kinds of topological invariants: one is the Chern number associated with the 2D quantum anomalous Hall effect and the other is the Chern-Simons term associated with the 3D chiral topological insulator.

2D quantum anomalous Hall (QAH) effect—The conventional quantum Hall effect requires application of a strong magnetic field. For the QAH effect, a combination of spontaneous magnetization and spin-orbit coupling gives rise to quantized Hall conductivity in the absence of an external magnetic field [25]. In solid-state systems, a recent experiment has observed this peculiar phenomenon in thin films of a magnetically doped topological insulator [26]. A simple square-lattice Hamiltonian which captures the essential physics of the QAH
The method to extract the Chern number through C < 0 rect calculation shows that the topological structure of this model is characterized by a trapped state, where the fermionic atom with pseudospin $a$ is a unit lattice vector along the $y$ direction. The first term in the Hamiltonian describes the spin-orbit coupling. The second and the third terms denote respectively the spin-conserved nearest-neighbor hopping and the Zeeman interaction. It was proposed recently that $H_{\text{QAH}}$ may be realized with cold fermionic atoms trapped in a blue-detuned optical lattice [27].

In momentum space, this Hamiltonian has two Bloch bands. The topological structure of this model is characterized by the Chern number defined in Eq. (3). Direct calculation shows that $C_2 = -C_1 = \text{sign}(h)$ when $0 < |h| < 4t$ and $C_2 = -C_1 = 0$ otherwise. Experimentally, one can measure $F_{\mu \nu}^b(k)$ by our proposed method to extract the Chern number through $C_b \approx -\sum_j F_{xy}^b(k_j)/(2\pi)$, where the band index $b = 1, 2$.

To simulate experiments, we consider a finite-size lattice with open boundary condition. In addition, we add a global harmonic trap of the form $V_T = m_a \omega^2 r^2/2$ for atoms of mass $m_a$ as in real experiments and use $\gamma_T = m_a \omega^2 a^2/2t$ to parameterize the relative strength of the trap, where $a$ denotes the lattice constant. To account for possible experimental noise, we add a random perturbation Hamiltonian of the following general form

$$H_P = \gamma_P t \sum_{(r,s), \alpha, \beta} a_{r,\alpha}^\dagger P_{\alpha \beta} a_{s,\beta}, \quad (6)$$

where $\gamma_P$ is a dimensionless parameter characterizing the strength of random perturbation, $(r,s)$ denotes the neighboring sites, and $P$ is a random Hermitian matrix with its largest eigenvalue normalized to unity. We numerically diagonalize the real-space Hamiltonian on a finite lattice with different number of sites and calculate the corresponding momentum density distributions [28].

An example, in Fig. 1, we show the reconstructed density distribution in two complementary bases $\{|\uparrow\rangle, \{\downarrow\rangle\}$ under open boundary condition with a harmonic trap and random perturbations (more detailed calculation results are shown in the supplement [28]). The Chern numbers for each case are calculated and listed in Table II under choices of different parameters and system sizes. The extracted Chern numbers exactly equal the corresponding theoretical values, even under a small system size and significant disorder potentials. This is so as Chern numbers characterize the topological property, which does not change under perturbations. Furthermore, our detection method through measurement of $F_{\mu \nu}^b(k)$ guarantees an integer value for the extracted Chern number [24], so it automatically corrects small errors due to experimental imperfections.

**3D chiral topological insulator**—Chiral topological insulators (CTIs) are protected by the chiral symmetry (also known as the sub-lattice symmetry) and belong to the AIII class in the periodic table for topological phases [2]. A simple Hamiltonian that supports 3D CTIs has the form [29]:

$$H_{\text{CTI}} = t \sum_{r} \sum_{j=1}^{3} \sum_{\alpha, \beta} [\psi_r^\dagger (iG_{3+j} - G_7) \psi_{r+j, \alpha} + \text{H.c.}] + h \sum_r \psi_r^\dagger G_7 \psi_r,$$

where the operator $\psi_r^\dagger = (a_{r,1}^\dagger, a_{r,2}^\dagger, a_{r,3}^\dagger)$ with $a_{r,\alpha}^\dagger (\alpha =$

| h/t | Size | Periodic | Open | Trap | Pert.+ Trap |
|-----|------|---------|------|------|-------------|
| QAH | 1    | 4^2     | -1   | -1   | -1          |
|     | 1    | 10^2    | -1   | -1   | -1          |
|     | 5    | 10^2    | 0    | 0    | 0           |
| CTI | 2    | 10^3    | 1.041| 1.056| 1.055       |
|     | 2    | 12^3    | 1.031| 1.009| 0.981       |
|     | 4    | 10^3    | 0    | -2*10^{-4}| 1.1*10^{-3}|
|     |      |         |      | 1.2*10^{-3}|

Table I. Simulated detection results of the topological invariants for different lattice sizes under various conditions (Periodic boundary condition, Open boundary condition, with Trap, with both Trap and Perturbation Hamiltonians). For the QAH, the invariant is the Chern number for the first band ($C_1$), whereas for the CTI, it is the Chern-Simons term for the middle flat band ($CS_2/\pi$). Results for both the nontrivial phase ($h/t = 1$ for the QAH and $h/t = 2$ for the CTI) and the trivial phase ($h/t = 5$ for the QAH and $h/t = 4$ for the CTI) are presented. The parameters are the same as in Fig. 1 and Fig. 2.
calculations show that where Hamiltonian with cold fermionic atoms in an optical lattice (b) has been proposed to realize this model in the middle protected by the chiral symmetry. An experimental scheme has been proposed to realize this model in the case of [28]. In the momentum space, this model Hamiltonian does not guarantee the result to be an integer, so numerically simulated experiments are shown in Table II under middle condition for the middle flat band of $H_{\text{CTI}}$ with open boundary condition under lattice size $12 \times 12 \times 12$. Layers corresponding to $k_z = -\pi, -\pi/2, \pi/2$ are displayed. The parameters are $\hbar = 2t$, $\gamma_T = 0.001t$, $\gamma_P = 0.1t$.

In summary, we have proposed a general method to numerically simulate the experimental imperfections (traps and random perturbation Hamiltonians change the result by less than $3\%$).

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SUPPLEMENTARY MATERIAL: DIRECT PROBE OF TOPOLOGICAL ORDER FOR COLD ATOMS

This supplementary material gives more details on numerical simulation of the experimental detection and extraction of the topological invariants. In section I, we show how to numerically calculate the atomic momentum distribution by solving the real-space Hamiltonians under open boundary condition. In section II, we provide details on how the random perturbation and harmonic trapping potential are incorporated into the simulation. In Sec. III, we include more detailed results from the numerical simulations as well as an explicit definition of the Gell-Mann matrices used in the main text.

MOMENTUM DENSITY DISTRIBUTIONS WITH OPEN BOUNDARY CONDITIONS

In the main text, we have numerically simulated the momentum density distribution of an actual ultracold atomic experiment with finite-size lattices and possible imperfections under an open boundary condition. Here, we provide more details on how the momentum density distribution is calculated. Consider a generic quadratic Hamiltonian in real space without any particle interactions:

$$ H = \sum_{\mathbf{r}, \mathbf{s}, \alpha, \beta} a_{\mathbf{r}, \alpha}^\dagger \mathcal{H}_{\mathbf{r}, \alpha} a_{\mathbf{s}, \beta}, $$ (9)

where $a_{\mathbf{r}, \alpha}^\dagger$ ($a_{\mathbf{s}, \beta}$) creates (annihilates) a particle at lattice site $\mathbf{r}$ ($\mathbf{s}$) with pseudospin $\alpha$ ($\beta$). One can solve the Schrödinger equation $\mathcal{H} \Psi = \epsilon \Psi$ to obtain the single-particle energy spectrum. In matrix form, one can diagonalize $\mathcal{H}$ by a unitary matrix $U$: $\mathcal{H} = U^\dagger \mathcal{E} U$, and find the single-particle eigenmodes $b_{\mathbf{r}, \alpha} = \sum_{\mathbf{s}, \beta} \mathcal{H}_{\mathbf{r}, \alpha} a_{\mathbf{s}, \beta}$. Here $\mathcal{E} = \text{diag}(\epsilon_1, \epsilon_2, \cdots)$ is a diagonal matrix. For a free fermionic system described by Eq. (9), the total particle number $\mathcal{N} = \sum_{\mathbf{r}, \alpha} a_{\mathbf{r}, \alpha}^\dagger a_{\mathbf{r}, \alpha}$ is a conserved quantity [H, $\mathcal{N}$] = 0. These $\mathcal{N}$ particles will occupy the first $\mathcal{N}$ eigenmodes with lowest eigenenergies.
Consequently, the ground state of the system reads

$$|G\rangle = \prod_{i=1}^{N} b_i^\dagger |0\rangle,$$  \hfill (10)

where we suppress r and α into a single index i for the occupied eigenmodes, and |0⟩ is the vacuum state without any particles. The density distribution in momentum space can then be obtained:

$$n_\alpha(k) = \langle G | a_\alpha^\dagger(k) a_\alpha(k) | G \rangle,$$  \hfill (11)

where $a_\alpha(k)$ relates to $a_{r,\alpha}$ by a Fourier transform,

$$n_\alpha(k) = \langle G | \frac{1}{\sqrt{L}} \sum_r e^{i k \cdot r} a_{r,\alpha}^\dagger \frac{1}{\sqrt{L}} \sum_{r'} e^{-i k \cdot r'} a_{r',\alpha} | G \rangle$$

$$= \frac{1}{L} \sum_{r, r'} \langle G | a_{r,\alpha}^\dagger a_{r',\alpha} | G \rangle e^{i (r - r')},$$ \hfill (12)

where L denotes the number of lattice sites. As $a_{r,\alpha} = \sum_{s,\beta} (U^\dagger)_{r\alpha,s\beta} b_{s,\beta}$, the quantity $\langle G | a_{r,\alpha}^\dagger a_{r',\alpha} | G \rangle$ can be further simplified:

$$\langle G | a_{r,\alpha}^\dagger a_{r',\alpha} | G \rangle = \langle G | \sum_{s,\beta} (U^\dagger)_{r\alpha,s\beta} b_{s,\beta}^\dagger \sum_{s',\beta'} (U^\dagger)_{r',\beta's'} b_{s',\beta'} | G \rangle$$

$$= \sum_{s,\beta,s',\beta'} \langle G | b_{s,\beta}^\dagger b_{s',\beta'} | G \rangle (U^\dagger)_{r\alpha,s\beta} (U^\dagger)_{r',\beta's'}$$

$$= \sum_i (U^\dagger)_{r\alpha,i} (U^\dagger)_{r',i,i}.$$

In the last step of Eq. (13), we have used the following equation

$$\langle G | b_{s,\beta}^\dagger b_{s',\beta'} | G \rangle = \begin{cases} 1 & \text{if } s = s', \beta = \beta' \text{ and the eigen-mode } b_{s,\beta} \text{ is occupied} \\ 0 & \text{otherwise}. \end{cases}$$

Combining Eq. (13) and Eq. (12), we can obtain the momentum density distribution for each pseudospin component from a generic quadratic real-space Hamiltonian with a specific filling number (the filling number is defined as the total particle number divided by the lattice site number: $f = N/L$). Analogously, one can rotate the pseudospin and use the same method to compute the momentum density distribution of a superposition state $n_{a|\alpha\rangle + \beta|\beta\rangle(k)}$.

**RANDOM PERTURBATION AND HARMONIC TRAPPING POTENTIAL**

As discussed in the main text, a typical optical lattice experiment includes a weak harmonic trapping potential,

$$V_T = \frac{1}{2} m \omega^2 \sum_{r,\alpha} \frac{d_r^2}{2} a_{r,\alpha}^\dagger a_{r,\alpha},$$ \hfill (14)

where $d_r$ is the distance from the center of the trap to the lattice site r, m is the atomic mass, and $\omega$ is the trap frequency. In our numerical simulation, we use $\gamma_T = \frac{m \omega^2 a^2}{2t}$ to parametrize the influence of this trapping potential. Here a is the lattice constant and $t$ is the hopping rate. For a typical experiment, $t/h \sim 1$kHz, $a \sim 400$ nm, and $\gamma_T$ ranges from $10^{-3}$ ($^6$Li with $\omega/2\pi = 60$ Hz) to $2 \times 10^{-2}$ ($^{40}$K with $\omega/2\pi = 100$ Hz) [18]. To account for other possible experimental noise, we also add a weak random perturbation term

$$H_P = \gamma_P t \sum_{r,s,\alpha,\beta} a_{r,\alpha}^\dagger a_{r,\alpha} \mathcal{P}_{r,s,\alpha,\beta} a_{s,\beta},$$ \hfill (15)

where $\mathcal{P}$ is a random Hermitian matrix with its largest eigenvalue normalized to unity.

In the numerical simulation, we add both $V_T$ and $H_P$ into the original Hamiltonians and calculate the momentum density distributions using the method described in Sec. I. Although only partial results are included in Fig. 1, Fig. 2 and Table I of the main text, we have done substantial calculations with a number of different choices of parameters ($\gamma_T, \gamma_P$) for both the 2D quantum anomalous Hall effect (QAH) and 3D chiral topological insulators (CTIs). Our results consistently show that topological invariants extracted from time-of-flight (TOF) measurements will be very robust to the trapping potential and random perturbations.
Figure 3. (color online). Density distributions in momentum space for the first band with lattice size $10 \times 10$. (a), (c) and (e) correspond to the periodic boundary condition without perturbation and trapping potential; (b), (d), and (f) correspond to open boundary conditions with random perturbations and harmonic trapping (subfigures (b) and (d) are repeated from the main text for clarity and completeness). The parameters used in the calculations are chosen to be $\lambda_{\text{SO}}^{(x)} / t = \lambda_{\text{SO}}^{(y)} / t = 1$, $h / t = 1$, $\gamma_T / t = 0.1$, and $\gamma_P / t = 0.01$. The resulted first Chern number is $C_1 = -1$ for both open and periodic boundary conditions.

Figure 4. (color online). Relative phase factors in momentum space for the first band of the Hamiltonian $H_{\text{QAH}}$ with lattice size $10 \times 10$. (a) Periodic boundary condition without perturbations and the trapping potential. (b) Open boundary conditions with random perturbations and a harmonic trap. The parameters are chosen to be the same as in Fig. 1 of the main text.
Figure 5. (color online). Momentum density distributions and relative phase factors for the middle flat band with open boundary conditions for $H_{\text{CTI}}$ including a harmonic trap and some random perturbations. The lattice size is $12 \times 12 \times 12$. Layers corresponding to $k_z = -\pi, -\pi/4, \pi/2$ are displayed. The parameters are chosen to be the same as in Fig. 2 of the main text.

MORE RESULTS ON THE NUMERICAL SIMULATION

In this section, we provide more numerical results for both the 2D QAH and 3D CTI cases.

2D QAH effect — In the Fig. 1 of the main text, we have plotted two momentum density distributions of the first band. Here, we present more plots of the density distributions in Fig. 3, considering both periodic and open boundary conditions. From this figure, it is obvious that the open boundary condition and the added trapping potential and random perturbations only have a minimal effect on the momentum density distributions. As a consequence, the extracted first Chern number is the same for open and periodic boundary conditions. As discussed in the main text, we are able to extract the desired Chern number the first band is determined up to a momentum dependent overall phase. Using the method introduced in the main text:

$$2n_{i\uparrow\downarrow}(\mathbf{k}) = 1 + 2\sqrt{n_{\uparrow}(\mathbf{k}) \times (1 - n_{\downarrow}(\mathbf{k})) \cos(\phi(\mathbf{k}))}$$  \hspace{2cm} (16)

$$2n_{i\uparrow\downarrow}(\mathbf{k}) = 1 + 2\sqrt{n_{\uparrow}(\mathbf{k}) \times (1 - n_{\downarrow}(\mathbf{k})) \sin(\phi(\mathbf{k}))}.$$  \hspace{2cm} (17)

Plugging the density distributions observed from TOF measurements into the above equations, one obtains the relative phase. We performed the calculations for both periodic and open boundary conditions and the corresponding relative phase factors are shown in Fig. 4. With the relative phases and the density distributions, the Bloch wavefunction for the first band is determined up to a momentum dependent overall phase. Using the method introduced in the main text, we are able to extract the desired Chern number $C_1 = -1$.

3D CTI — Let us first write down explicitly the four Gell-Mann matrices used in the Hamiltonian $H_{\text{CTI}}$ in the main text:

$$G_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad G_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad G_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad G_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}. $$
Table II. The Chern-Simons terms of the first and third bands for the Hamiltonian $H_{\text{CTI}}$. The parameters are chosen to be the same as in Fig. 2b of the main text.

| Size | $h/t$ | Periodic $\psi_{\text{CTI}}^{\text{CS}_1/\pi}$ | Open $\psi_{\text{CTI}}^{\text{CS}_1/\pi}$ | Trap $\psi_{\text{CTI}}^{\text{CS}_1/\pi}$ | Pert. + Trap $\psi_{\text{CTI}}^{\text{CS}_1/\pi}$ |
|------|------|--------------------------------|--------------------------------|-----------------|-------------------------------|
| $10^3$ | 2 | 0.246 | 0.228 | 0.231 | 0.231 |
| $12^3$ | 2 | 0.248 | 0.228 | 0.235 | 0.235 |
| $10^3$ | 4 | $5.8 \times 10^{-5}$ | $8.6 \times 10^{-5}$ | $1.5 \times 10^{-4}$ | $1.4 \times 10^{-4}$ |

CTI ($CS_3/\pi$)

| Size | $h/t$ | Periodic $\psi_{\text{CTI}}^{\text{CS}_3/\pi}$ | Open $\psi_{\text{CTI}}^{\text{CS}_3/\pi}$ | Trap $\psi_{\text{CTI}}^{\text{CS}_3/\pi}$ | Pert. + Trap $\psi_{\text{CTI}}^{\text{CS}_3/\pi}$ |
|------|------|--------------------------------|--------------------------------|-----------------|-------------------------------|
| $10^3$ | 2 | 0.246 | 0.226 | 0.227 | 0.227 |
| $12^3$ | 2 | 0.248 | 0.229 | 0.230 | 0.231 |
| $10^3$ | 4 | $5.8 \times 10^{-5}$ | $5.0 \times 10^{-5}$ | $1.7 \times 10^{-4}$ | $1.8 \times 10^{-4}$ |

A Fourier transform brings $H_{\text{CTI}}$ to momentum space [29, 30]:

$$H_{\text{CTI}} = \sum_k \psi_k^\dagger \mathcal{H}_{\text{CTI}}(\mathbf{k}) \psi_k,$$

where $\psi_k^\dagger = (a_{\mathbf{k},1}^\dagger, a_{\mathbf{k},2}^\dagger, a_{\mathbf{k},3}^\dagger)$ and $\mathcal{H}_{\text{CTI}}(\mathbf{k}) = \sum_{j=1}^4 G_{j+4} q_j(\mathbf{k})$ with $[q_1(\mathbf{k}), q_2(\mathbf{k}), q_3(\mathbf{k}), q_4(\mathbf{k})] = [\sin k_x, \sin k_y, \sin k_z, m - \cos k_x - \cos k_y - \cos k_z]$. One can easily check that this Hamiltonian indeed has a chiral symmetry represented by $SH_{\text{CTI}}(\mathbf{k})S^{-1} = -H_{\text{CTI}}(\mathbf{k})$, where $S \equiv \text{diag}(1, 1, -1)$ is a unitary matrix. This chiral symmetry leads to an exact zero-energy flat band as discussed in Ref. [29, 30].

In the main text, we plotted some of the momentum density distributions of the middle flat band in Fig. 2(b). Here we include more results of the density distributions and the relative phases in Fig. 5. Analogous to the case of QAH effect, the momentum density distributions can be directly observed from the layered TOF measurements and the relative phases can be calculated from the observed density distributions. After all density distributions are observed in an actual experiment, the Chern-Simons term characterizing the topological structure of the Bloch band can be readily extracted with the method described in the main text.

Besides the Chern-Simons term for the middle flat band shown in Table I of the main text, we have also calculated it for both the first (lowest) and third (highest) bands. Our results are recorded in Table I here. From this table, the extracted Chern-Simons terms converge to the expected theoretical value $CS_1/\pi = CS_3/\pi = 1/4$ rapidly as we increase the lattice size.