Tomography of band-insulators from quench dynamics

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We propose a simple scheme for a complete tomography of band-insulating states in one- and two-dimensional optical lattices with two sublattice states. In particular, the proposed scheme allows for mapping out the Berry curvature in the entire Brillion zone and to extract topological invariants such as the Chern number. The measurement simply relies on observing—via time-of-flight imaging—the dynamics following a sudden quench in the band structure. We illustrate the performance of the scheme in noisy settings with limited resolution by considering two examples of experimental relevance: the Harper model with π-flux and the Haldane model on a honeycomb lattice.

The concept of topological order has profoundly changed the understanding and the classification of states of matter. Topological quantum numbers, such as the Chern index or the $Z_2$ invariant, separate even “simple” band-insulating states into classes with fundamentally different behaviour [1, 2], some of which support chiral or helical edge modes [3, 4]. Only recently, first evidence of such topological insulators has been found in solid-state materials [5–7] and photonic systems [8]. The recent creation of artificial gauge fields in optical lattices [9–16] makes it seem likely that topological insulators will be realized in the near future also in highly tunable systems of ultracold atoms. However, the experimental characterization of apparently structureless band insulators poses a challenge. So far, there are schemes that are designed to measure specific topological properties of the system. For example, recently Zak’s phase, i.e., the Berry phase acquired during the adiabatic motion along a path through the Brillouin zone (BZ), has been measured [12]. Other proposed schemes are designed to directly measure either the Chern number (from density profiles [17], wave-packet dynamics [12, 18–21], time-of-flight (TOF) imaging [21,22], or unidirectional TOF imaging with single-site resolution [23]) or to probe the presence of chiral edge modes (via transport measurements [25,26] or Bragg-scattering [20,22]). A method allowing for a full tomography of a band insulator has so far only been proposed for a specific experimental realization of a topological insulator based on spin-dependent hexagonal optical lattices [33].

Here, we propose a simple scheme for the complete tomography of band-insulating states in one-dimensional (1D) and two-dimensional (2D) optical lattices that is not restricted to a specific system. In particular, the scheme allows for mapping-out the Berry curvature as a function of quasimomentum and for measuring the Chern number. Our scheme is based on the momentum-resolved monitoring—via TOF imaging—of the dynamics following an abrupt quench in the band structure (a different quench-based measurement scheme, relying on the observation of real-space dynamics, has been introduced only recently for the detection of chiral equilibrium currents [26,27]). In the following, we first introduce the basic protocol underlying our method, and then discuss two relevant applications: the π-flux Harper model [31,35] and the Haldane model [36].

Scheme for the tomography of band insulators. — Consider spin-polarized (i.e., non-interacting) fermions in a 2D optical lattice. In each elementary cell $\ell$, the lattice shall have two sublattice states $s = A, B$, located at $r_{\ell s}$ [see Fig. 1(a), left]. The corresponding tight-binding Hamiltonian is characterized by matrix elements $h_{v'v,\ell s}$ that obey the translational symmetry of the lattice. The diagonal terms refer to on-site potentials, $h_{\ell s,\ell s} \equiv v_s$, and the off-diagonal matrix elements describe tunneling between near neighbors. Thanks to the translational symmetry, the Hamiltonian is diagonal in quasimomentum, $k$. With respect to the basis states $|ks\rangle \propto \sum_{\ell} e^{-i\mathbf{k} \cdot \mathbf{r}_\ell} |\ell s\rangle$ it is represented by a $k$-dependent $2 \times 2$ matrix $H_{v'v,\ell s} = \sum_{v'} h_{v'v,\ell s} e^{-i(r_{\ell v'}-r_{\ell s})} k^v$, which we decompose as $h_{v'v,\ell s}(k) \equiv h_0(k) \delta_{v'v,s} + h(k) \sigma_{v'v,s}$. Here, $\sigma_{v'v,s}$ denotes the vector of Pauli matrices in sublattice space. At every point $k$ in quasimomentum, the two-dimensional sublattice space defines a Bloch sphere, with north and south pole given by $|kA\rangle$ and $|kB\rangle$, respectively. The two eigenstates $|k\pm\rangle$ lie at $+\hbar(k)$ on this Bloch sphere, where $\hbar(k) \equiv h_0(k) / |h(k)| \equiv (\sin(\vartheta_k) \cos(\varphi_k), \sin(\vartheta_k) \sin(\varphi_k), \cos(\vartheta_k))$. Their energies $\mathcal{E}_\pm(k) = h_0(k) \pm |h(k)|$ define the band structure of the lattice.

We are interested in the situation where the system is in a band-insulating state characterized by complete occupation of the single-particle states of the lower band,
whose oscillatory time dependence directly reveals both $\varphi_{k}$ and $\sin(\theta_{k}) = 1 - |\hat{h}_{z}(k)|^2$. The time-dependence of $n(k, t)$ allows us to reconstruct $\hat{h}_{z}(k)$, $\hat{h}_{y}(k)$, as well as $|\hat{h}_{z}(k)|$ from the amplitude and the phase of the oscillations. (The Wannier envelope $f(k)$ does not spoil the measurement as it just gives an irrelevant overall prefactor for each value of $k$.) For a full tomography, it remains to reveal the sign of $\hat{h}_{z}(k)$. Since the overall sign is not important, one has to determine those lines in $k$-space where $\hat{h}_{z}(k)$ changes sign. These lines can be clearly identified by a characteristic cusp-like behavior of $|\hat{h}_{z}(k)|$ when crossing them, $|\hat{h}_{z}(k)| \propto |k - k_{\text{sign-change}}|$, which sharply contrasts with the smooth variation of $\hat{h}_{z}(k)$ on the scale of the inverse lattice constant as it results from tunneling between near neighbors.

**Edge states in the Harper model with $\pi$-flux.** — Once $\hat{h}(k)$ is reconstructed, one can infer whether the system supports edge modes or not by invoking the bulk-boundary correspondence. According to the procedure derived in Ref. [37], for that purpose one has to identify a closed path $k(\lambda)$ in $k$-space such that $\hat{h}(k(\lambda))$ lies in a plane $E$ that contains the origin. We can now distinguish between two topologically distinct scenarios: if the unit vector $\hat{h}$ describes a closed circle around the origin when moving along the path, the system does possess zero-energy edge modes; if not, it does not.

Motivated by recent experiments [15, 16], let us consider the example of a square lattice with nearest-neighbor tunneling and with a flux of $\pi$ (half a flux quantum) per plaquette, which can be generated via laser-assisted tunneling or lattice shaking [38]. We consider a gauge where the tunneling matrix elements in $y$-direction alternate between $-J_{\text{d}}$ and $+J$ when moving through the lattice in $x$-direction, giving two inequivalent sublattices $s = A, B$. Additionally, we assume different on-site energies $v_{A} = \Delta/2$ and $v_{B} = -\Delta/2$ and that the tunneling matrix element in $x$-direction alternates between $-J_{\text{d}}$ and $-J$ [Fig. 1(a)]; both can be achieved by a superlattice in $x$-direction. The extent of the first BZ is given by $\pi (2\pi)$ in $k_{x}$ ($k_{y}$) direction. The momentum-space Hamiltonian of this model is characterized by

$$\hat{h}(k) = (-J - J' \cos(2k_{x}), J' \sin(2k_{x}), -J \cos(k_{y}) + \Delta).$$

(2)

The two parameters $\Delta/J$ and $J'/J$ allow us to explore various situations with qualitatively different band structures. Most notably, for $J = J'$ and $\Delta < 2J$, one finds two Dirac cones (i.e., band touching points with a cone-like linear dispersion relation) lying at $k_{z} = \pm \pi/2$ and $k_{y} = \arccos(\Delta/2J)$. For imbalanced tunneling matrix elements $J' \neq J$, a band gap opens at the Dirac points and edge states appear if $J' > J$. We focus here on the case $\Delta = 0$ (we discuss $\Delta \neq 0$ in the Appendix [A] where also the evolution of spectrum and edge states may be found).

In this case, by choosing $k_{y}^{0}/2 = \pi/2 \left( \hat{h}_{z} = 0 \right)$, we can confine $\hat{h}_{k}(k_{x})$ to a plane that contains the origin of $\hat{h}$'s Bloch sphere, a necessary condition for observing edge
modes at zero energy [37]. Edge states (in the equivalent system with open boundary conditions in x-direction) do appear if the origin is encircled by $\hat{h}_y(k_x)$ [37].

In an experiment, we wish to reconstruct $\hat{h}_y(k_x)$ from the dynamics following a sublattice quench in order to conclude whether the system possesses edge states or not. Assuming a mediocre experimental resolution of 21 points in $k_x$ and 41 time points, (e-f) If edge states are supported, the temporal maximum as a function of quasimomentum winds around the period once (panels a,b), and $\hat{h}_y(k_x) = (h_x, h_y, 0)$ describes a unit circle around the origin (e,f), contrary to when no edge state is supported (c,d and g,h, respectively). Red line: exact case. Bullets: values extracted from the noisy data of the upper row, using Eq. 4 [k_x from 0 (light) to $\pi$ (dark)].

FIG. 2. (a-d) Time-resolved TOF images for the $\pi$-flux Harper model ($\Delta = 0$ and $k_y^0 = \pi/2$). To mimic a realistic experiment, we added normal-distributed noise with a standard deviation of 0.1 of the average signal and assumed a limited resolution of 21 points along $k_x$ and 41 time points.

Note that the origin is encircled by $\hat{h}_y(k_x)$, expected for the two plots on $k$-space. The resulting system with open boundary conditions in $x$ and $y$ appears if the origin is encircled by $\hat{h}_y(k_x)$, where we plot $n(k,t)$ for $J'/J > J' > J$, where for $J' = J$ both Dirac cones merge. This is illustrated in Appendix A, where we also directly compute the emergence of edge modes for open boundary conditions.

Measuring Berry curvature and Chern number in a Haldane-like system. — Edge currents are topologically protected only if the associated integer Chern number, given by the integral of the Berry curvature over the whole BZ, is finite. In the above example, this is not the case, since the edge modes always appear in counter-propagating pairs located at the two Dirac cones. We now turn to a lattice model where a finite Chern number can be found and demonstrate how our scheme can be used to map out the Berry curvature in quasimomentum.

The Berry curvature of the lower band is given by

$$\Omega_-(k) = \frac{1}{2} \left( \partial_{k_x} \hat{h} \times \partial_{k_y} \hat{h} \right) \cdot \hat{h},$$

and is readily obtained from $\hat{h}(k)$. It describes the polarization [39] and the anomalous Hall conductivity [40] of the system also at lower filling. The Chern number reads

$$w_- = \frac{1}{2\pi} \int d^2k \Omega_-(k).$$

It counts how often $\hat{h}(k)$ wraps around the Bloch sphere when $k$ covers the full first BZ. It is proportional to the Hall conductivity of the completely filled band and indicates the presence of robust chiral edge modes [3].

Let us consider the concrete example given by the Haldane-like model sketched in Fig. 3(a) with the lower band completely filled. The atoms live on a honeycomb lattice with real tunneling matrix elements $J$ between nearest neighbors (NNs) and complex tunneling matrix elements $J' e^{i\theta}$ with Peierls phase $\theta$ between next-nearest neighbors (NNNs). The model can be realized, e.g., in a shaken optical lattice [41]. For $J' = 0$, the vector $\hat{h}(k)$ lies in the $xy$-plane. The band structure possesses two Dirac points where $\hat{h}(k) = 0$. For finite NNN tunneling, $J' > 0$, $\hat{h}_z(k)$ acquires a finite value and a direct band gap opens at the Dirac cones (though one still has an indirect band touching). While for $J' = 0$ the unit vector $\hat{h}(k)$ was confined to the equator of the Bloch sphere, when approaching the Dirac points it will now visit either the north or the south pole, depending on the sign of $\hat{h}_z(k)$. The unit vector $\hat{h}(k)$ can only wrap around the Bloch sphere, as required for a finite Chern number, if $\hat{h}_z(k)$ has opposite sign at the two Dirac points such that it visits both poles. We find that, while for $|\theta| < \theta_c$, the system is a trivial band insulator, it becomes a topological Chern insulator, characterized by a Chern number $|w_-| = 1$, once $|\theta| > \theta_c$, with the transition happening at $\theta_c = 0.18\pi$. In the following, we will illustrate how this transition can be observed within our scheme.

As exemplified in Fig. 3(b) for an initial state in the topological phase ($\theta = \pi/2$), $n(k,t)$ changes its pattern strongly as a function of time. From this dynamics we can extract the position of $\hat{h}_z(k)$ on the Bloch sphere [Fig. 3(c-e)]. The sign change of $\hat{h}_z$ for $\theta/\pi > 0.18$ [Fig. 3(e)] between the two Dirac cones identifies a finite Chern number $|w_-| = 1$. Although within our scheme one can directly measure only the absolute value $|w_-|$.
from the pronounced kink where a reciprocal lattice points.

\[
\hat{h}_z = \left| \hat{h}_z \right| \cos \theta
\]

The white circles mark the position of the two Dirac points. (c) The winding of the phase \( \hat{\varphi}_k \) is opposite around the two Dirac points (independent of \( \theta \)). (d,e) In the topologically trivial phase (d, \( J' = 0.3J \) and \( \theta = 0 \)), the plotted quantity \( \hat{h}_z \) has the same sign at the two Dirac cones, while in the topological phase (d, \( J' = 0.3J \) and \( \theta = \pi/2 \)) it has opposite sign; this sign change is clearly visible as a kink in the measured quantity \( \left| \hat{h}_z \right| \) (lower plots showing \( \left| \hat{h}_z \right| \) along the dashed lines). (f) The coarse-grained Chern number computed following Ref. [42] reproduces the exact result already for 4 \times 4 reciprocal lattice points.

In a realistic situation, the resolution of \( n(k,t) \) in TOF images will be restricted. A common approach for such cases is to approximate the Chern number [4] by a sum over differences. This method yields reasonable results deep within each many-body phase, but is unreliable close to the topological transition (see Appendix [3]). Much better results can be obtained by the gauge-invariant description in terms of effective field strengths developed by Fukui et al. [12]. In Appendix [3] we show how their formula can be expressed in terms of \( \hat{h} \). Since this method enforces an integer result, it gives the exact answer already for very small numbers of reciprocal lattice points. To mimic a realistic experimental situation, we coarse grain \( n(k) \) over 4 \times 4 pixels in the first BZ and take only 10 time steps. We again obtain \( \sin \theta_k \) from the difference between the minimal and maximal data point, and \( \varphi_k \) from the position of the maximum. Remarkably, as seen in Fig. [3](f), even for this extremely coarse-grained situation, the Chern number can be reproduced accurately.

**Discussion, conclusion, and outlook.** — A natural question arising in the context of an optical lattice experiment concerns the role of the trapping potential and the resulting non-uniform density profile. We address this issue in Appendix [C] where we show that the effect of the trap is not detrimental. The robust and simple method for the tomography of band-insulators described here is not restricted to the two concrete examples that we discussed. It can be applied to any 1D or 2D band-insulator with two states per elementary lattice cell—interesting examples include the Su–Schrieffer–Heeger [43] or Rice–Mele model [11], which has recently been realized in an optical lattice [12]. Here an interesting application would be to measure the state of a topological charge pump [15] at different times during its cycle and to extract the Chern number quantizing the transport of matter. Moreover, the method can also be employed to measure systems with the lowest band only partially filled, and it provides a means to validate Hamiltonians synthesized for the purpose of quantum simulation. As an outlook, it will be interesting to generalize the scheme to lattices with more than two sublattice states and to include internal atomic states.

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In this Appendix, (i) we provide additional information on how the topological phase transitions in the Harper and Haldane models may be observed, (ii) we adapt the method of Ref. [42] to compute Chern numbers directly from the Hamiltonian in quasimomentum representation, using only a small number of grid points, and (iii) we discuss why a possible harmonic trapping potential is not detrimental to the proposed scheme.

A. Possible observation of topological phase transitions in the π-flux Harper model

Here, we discuss the possibility of observing the topological phase transitions supported by the Harper model at half a flux quantum [as given by Eq. (2) of the main text]. We first describe under which circumstances zero-energy edge states are to be expected. Afterwards, we turn to the question how these can be detected using the quench-based band tomography.

The spectrum of the Harper model with π flux is exemplified in Fig. 4, upper row, for several values of $J'/J$ and $\Delta/J$ (we consider an infinite lattice in $y$-direction, $\pi$-flux in $x$-direction, leading to a vanishing Chern number. When $J' = J$, a band gap opens. In these spectra, edge modes can clearly be distinguished as lines that are separated from the bands. The lower row of Fig. 4 shows the joint occupation of the two modes that come closest to zero energy (for $L = 30$ for better visibility). These are the two edge modes at the opposite ends of the sample, if any edge states exist. In the absence of edge modes, the plotted modes are the bulk modes at the band boundary. As these figures show, at any $J' \neq J$, a band gap opens. Edge states appear on both boundaries when $J' > J$, i.e., when the edge is connected to the bulk by a weak link. Associated to each Dirac cone and boundary, there is exactly one edge mode with finite energy. When the edge is connected to the bulk by a weak link. Associated to each Dirac cone and boundary, there is exactly one edge mode with finite energy.
in the π-flux Harper model, for a cylindric geometry (open boundaries in x-direction with even number of sites, periodic in y-direction). Upper row: Spectrum. Lower row: Occupation probability as a function of kx, ky. Shown is the combined probability for the two modes closest to \( \epsilon = 0 \) (for increased visibility, the color map is rescaled for each figure). Edge states appear when \( J'/J > 1 \). At \( \Delta = 2J \), the two points of minimal direct gap (the Dirac cones if \( J' = J \)) merge, and as a result possible edge modes do not lie at zero energy for any \( \Delta > 2J \).

FIG. 5. Topological phase transitions in the π-flux Harper model. Upper row (a,c,e): Edge modes at \( k_y^0 \) are supported if \( \hat{h}_{k_x}(k_y) \) encloses a circle around the origin. Whether the circle is closed can be quantified by \( \min |\varphi_{k_x,k_y}| \), even for noisy ‘data’ similar to Fig. 2. Bottom row (b,d,f): The edge states are only at zero-energy if \( h_z = 0 \) (i.e., the parametric curve \( \hat{h}_{k_x}(k_y) \) encloses \( h = 0 \)). The solid line represents the ideal prediction and the dots simulate a noisy experiment (which measures only the absolute value of \( h_z \)). (a,b) As a function of \( J'/J \), at \( \Delta = 0 \) and \( k_y^0 = \pi/2 \): zero-energy edge modes appear for \( J'/J > 1 \). (c,d) As a function of \( k_y^0 \), at \( J'/J = 2 \) and \( \Delta = 0 \): although edge modes may be supported at any \( k_y^0 \), their energy vanishes only at the position of the Dirac cone. (e,f) As a function of \( \Delta \), at \( J'/J = 2 \) and \( k_y^0 \) at the position of one of the Dirac points: when \( \Delta > 2J \), no zero-energy edge modes are supported.

\( \Delta > 2J \), the Dirac cones merge at \( k_y^0 = 0 \), and as a result the edge modes do not cross the band gap. They approach the bulk energy bands with increasing \( \Delta \).

We now turn to the question how these topological transitions can be observed using the proposed scheme. We proceed analogous to Fig. 2 of the main text. First, we use Eq. (2) to compute \( n(k,t) \) on a finite grid in time and quasimomentum space. To mimic a realistic experimental situation, we again add noise with standard deviation of 10% of the average value. We use Eq. (1) to extract from this data the characteristics of \( \hat{h}(k) \) along a path in \( k \)-space with fixed \( k_y^0 \). The results are summarized in Fig. 6.

According to Ref. [37], the system supports zero-energy edge modes if the path \( \hat{h}_{k_y}(k_x) \) is (i) closed and (ii) encircles \( \hat{h}(k) = 0 \). In the considered model, the second condition can only be fulfilled if \( \hat{h}_z(k_x,k_y^0) = 0 \), i.e., if \( \Delta < 2J \) and \( k_y^0 = \arccos(\Delta/2J) \). Otherwise, the system may still support edge modes, but these then do not lie at zero energy. The fulfilment of the first condition, the closing of the curve, can be identified by a small value of \( \min |\varphi_{k_x,k_y}| \) [see Figs. 2(e-h) for examples].

Indeed, in the entire topological phase at \( J'/J > 1 \), we find \( \min |\varphi_{k_x,k_y}| \approx 0 \) [shown in Fig. 5(a)], where \( \Delta = 0 \) and \( k_y^0 = \pi/2 \). For these parameters, we moreover find \( |h_z| \approx 0 \), indicating that the edge states lie at zero energy [Fig. 5(b)].

As Fig. 5(c) exemplifies for the point \( \Delta = 0 \) and \( J'/J = 2 \), edge modes actually exist for all \( k_y^0 \) as long as \( J'/J > J \) and \( \Delta < 2J \) (see Fig. 4). However, these modes lie at zero energy only at the Dirac point, which can be seen by a sharp kink of \( |h_z| \) as a function of \( k_y^0 \) [Fig. 5(d)].

As illustrated in Fig. 5(e,f) for \( J'/J = 2 \), when increasing \( \Delta \) to values larger than \( 2J \), we find \( |h_z| > 0 \): the Dirac cones have merged and, although edge states still exist, they are no longer at zero energy.

**B. Chern numbers in a Haldane-like model, extracted from discrete k-space grids**

In a realistic TOF image of \( h(k) \), the resolution will be restricted. If data is available only on a discrete mesh \{\( k_{x,n} \)\} of the BZ, one would typically approximate the integral in Eq. (4) by a discrete sum, and the derivatives...
The formulation in the second line corresponds to a Wilson loop [6]. The Chern number can be approximated as
\[
\tilde{F}_{xy}(k) = \ln \left[ \frac{\text{Tr} (P_k P_{k+\hat{x}} P_{k+\hat{y}} P_{k+\hat{y}+\hat{x}})}{N_x(k) N_y(k+\hat{x}) N_x(k+\hat{y}) N_y(k)} \right],
\]
with \(N_k(\mu) = \sqrt{\text{Tr} (P_k P_{k+\mu})} \). This formula is generally valid for non-Abelian Berry connections. It has the advantage that the projectors can be easily expressed in terms of the original Hamiltonian. For lattices with two sublattice states as they are considered here, the projectors are given by \(P_k^{\pm \mu} = \frac{1}{2} (1 \pm \hat{h}(k) \cdot \sigma) \). Therefore, knowledge of \(\hat{h}(k)\) allows to immediately compute the Chern number. The result is presented in Fig. 3(f) of the main text (where we assumed that the additional information of the sign change of \(\hat{h}_z\) is known).

C. Influence of a harmonic trap

To estimate the influence of a trap on the proposed scheme, we employ a local density approximation. Within this approximation, for shallow traps and for short times, the signal will be approximately modified by a factor
\[
\propto \frac{r_{\text{max}}^4(k)}{R^4} \left( 1 - \frac{1}{12} \left( \frac{\hbar}{2 m \omega_{tr}^2 r_{\text{max}}^2(k) t} \right)^2 \right). \tag{9}
\]
Here, \(\omega_{tr}\) is the trap frequency, \(m\) the atom mass, \(R\) the size of the sample, and \(r_{\text{max}}(k)\) the maximal radius at which the mode \(k\) is still populated. Within the local density approximation, \(r_{\text{max}}(k)\) is the radius where the potential energy due to the trap reaches the band energy of mode \(k\). The assumption of short time scales requires \(\frac{1}{2} m \omega_{tr}^2 r_{\text{max}}^2(k) t \ll 1\). For larger times, the proportionality factor becomes
\[
\propto \frac{\sin(\frac{1}{2} m \omega_{tr}^2 r_{\text{max}}^2(k) t)}{\left( \frac{1}{2} m \omega_{tr}^2 R^2 t \right)^2}. \tag{10}
\]
For small \(\omega_{tr}\), the influence of the trap will be small, and by knowing the above prefactors it can be entirely subtracted.

Additionally, the trap in principle admixes terms with \(k \neq k\) to the contribution at \(k\), but in shallow traps this effect is negligible. Moreover, the corresponding contributions are strongly oscillating functions of \(|k' - k| r_{\text{max}}(k)\) so that for large \(r_{\text{max}}(k)\) (shallow traps) their effect cancels out. Therefore, the presence of a harmonic trapping potential will only have minor effects on the measurement results.