Four-dimensional topological lattices without gauge fields

Hannah M. Price
School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom

Thanks to recent advances, the 4D quantum Hall (QH) effect is becoming experimentally accessible in ultracold atoms and photonics. In this paper, we propose a new type of 4D topological system that, unlike other 2D and 4D QH models, does not require (artificial) gauge fields and/or time-reversal symmetry breaking. Instead, we show that there are 4D QH systems that can be engineered for spinless particles by designing the lattice connectivity, and we explain how this physics can be intuitively understood in analogy with the 2D Haldane model. We illustrate our discussion with a specific 4D lattice proposal, inspired by the widely-studied 2D honeycomb and brickwall lattice geometries. As well as a minimal model for the 4D QH effect, this is also an experimental proposal for a topological system in Class AI, which supports nontrivial topological band invariants only in four spatial dimensions or higher.

Topological concepts provide a powerful way to discover and classify different phases of matter [1–3]. Within this paradigm, topological states are characterised by topological invariants and classified according to symmetries and spatial dimensionality [4–6]. As topological invariants are integer-valued, these states can exhibit remarkably robust phenomena, such as quantized transport and surface modes, unaffected by small perturbations.

A notable example of a topological phase of matter is a 2D quantum Hall (QH) system, which has energy bands indexed by the 1st Chern number (1CN) [7]. The 1CN is a 2D topological invariant that is only non-zero if time-reversal symmetry (TRS) is broken, and which underlies the precise quantization of Hall conductance in the 2D QH effect. Although this effect was first discovered for electrons in a magnetic field [8], such 2D QH states have recently been realised for neutral particles, such as cold atoms [9, 10] and photons [11–13], thanks to the development of artificial gauge fields.

The engineering of topology for cold atoms and photons has also opened up opportunities to explore topological physics predicted in higher spatial dimensions. This includes the 4D QH effect, which is a quantized current response, like its 2D cousin, but now due to a 4D topological invariant, called the 2nd Chern number (2CN) [14–20]. Very recently, this 4D QH effect has been probed using 2D “topological pumps” of atoms [21] and photons [22], exploiting a mapping from higher-dimensional topological systems to lower-dimensional time-dependent pumps [23–33]. It has also been proposed to directly engineer 4D QH atomic or photonic systems [34–36] by using “synthetic dimensions”, where sets of internal states are coupled to mimic the connectivity of extra spatial dimensions [37–41].

By bringing 4D topology into the laboratory, these advances give us access to a surprisingly rich variety of different topological phases of matter. Unlike the 2D QH effect, the 4D QH effect is associated with several distinct symmetry classes [4], as the 2CN does not necessarily vanish with TRS. Indeed, this effect has been studied both for Class AII systems [17, 18, 27, 18, 50], where TRS for spinful fermions is preserved (as in the 2D quantum spin Hall effect), as well as for Class A systems [21, 22, 27, 31, 34–36], where TRS is broken (as in the 2D QH effect). Physically, such models can correspond to spinful particles in non-Abelian gauge fields and spinless particles in magnetic fields, respectively.

In this paper, we explore a third 4D topological class of systems, which do not require gauge fields, but which can be realised using the lattice connectivity. These systems have non-zero 2CNs and exhibit a 4D QH effect, but unlike previous proposals, are in Class AI, where TRS for spinless or bosonic particles is preserved. This is important for several reasons: firstly, nontrivial topological bands in Class AI only arise in 4D and higher, and so this provides a way to explore robust topological models in this symmetry class. Secondly, the absence of lower topological invariants can simplify the 4D QH effect, by isolating the 2CN response. Thirdly, the 4D topological characteristics in this class are different to previous models as the 2CN only takes even integer values (instead of any integer values), indicating that surface states always come in pairs. Finally, relevant experimental set-ups, e.g. with photons, bosonic atoms or spin-polarized fermionic atoms, naturally have this TRS, avoiding the need to either artificially engineer or break the symmetry.

To introduce our proposal, we review how to construct minimal 2D QH models, such as the 2D Haldane model [51]. We then discuss how to generalise these ideas into four spatial dimensions to engineer Class AI energy bands with nontrivial 2CNs. As an illustration, we introduce a specific lattice model, which extends the widely-studied 2D honeycomb/brickwall lattice [52] into 4D. This is a minimal 4D QH model without gauge fields.

Minimal 2D QH Models– As topological invariants are integers, they do not change continuously but instead jump through topological phase transitions, where energy gaps between bands close and re-open. An intuitive approach for constructing topological models is therefore to focus on how such transitions can be induced by tuning the parameters of a Hamiltonian.

Minimal 2D QH models can be constructed from
two energy bands, as described generically by the momentum-space Hamiltonian \[3\]:

\[ H(k) = \varepsilon(k) \hat{I} + d(k) \cdot \sigma, \]

where \( \hat{I} \) is the 2 \( \times \) 2 identity, \( k \) is the momentum and \( \sigma \) is the vector of Pauli matrices. We focus on spinless models, where \( \sigma \) represents a pseudo-spin degree of freedom, such as a sublattice basis. The two bands are given by: \( E_{\pm}(k) = \varepsilon(k) \pm \sqrt{\mathbf{d}(k) \cdot \mathbf{d}(k)} \), where \( \mathbf{d}(k) \) is a three-component vector and \( \varepsilon(k) \) is an overall energy shift, neglected without loss of generality hereafter. When the two bands are gapped, the topological 1CN (of the lower band) is given by \[3\]:

\[ \nu_{-}^{(1)} = \frac{1}{2\pi} \int_{\text{BZ}} \Omega_{-} = \frac{1}{4\pi} \int_{\text{BZ}} d^{2}k \epsilon^{abc} \partial_{a} \partial_{b} \partial_{d} \partial_{c}, \]

where the integrals run over the 2D Brillouin zone (BZ), \( \epsilon^{abc} \) is the 3D Levi-Civita symbol, \( \mathbf{d} = \mathbf{d} / |\mathbf{d}| \) and \( \Omega_{-} \) is the Berry curvature two-form of the lower band \[2\]. The RHS is reached by calculating \( \Omega_{-} \) for the eigenstates of Eq. 1. In this form, the 1CN of a two-band model can be interpreted as the “winding number”, counting how many times \( \mathbf{d}(k) \) covers the unit Bloch sphere, \( S^{2} \), across the 2D BZ \[2\].

As introduced above, the 1CN only changes via topological phase transitions, where the band-gap closes and re-opens. In the simplest case, the two bands touch, at the transition, at a set of isolated Dirac points in the BZ. Around each Dirac point, Eq. 1 can be expanded linearly such that, locally (up to a rotation), \( \mathbf{d}(\mathbf{q}) \approx (v_x q_x, v_y q_y, m) \), where \( \mathbf{q} \) is the momentum relative to the Dirac point, and \( v_x (v_y) \) is the dispersion slope with respect to \( q_x (q_y) \). The mass, \( m \), smoothly tunes across the transition, as the Dirac point closes and re-opens as \( m \) changes sign.

Crucially, flipping the sign of \( m \) also flips the sign of the Berry curvature (as \( d_{3} \approx m \) in Eq. 2). Indeed, it can be shown that each isolated Dirac point that closes and opens changes the 1CN by \( \pm 1 \) \[3\]. However, the sign of this change depends on the signs of the other two components, \( d_{1} \approx v_x q_x \) and \( d_{2} \approx v_y q_y \). If they have the same (opposite) sign, the Dirac point increases (decreases) the 1CN as \( m \) goes from negative to positive. Whether a transition is topological then depends on how many Dirac points of each type there are.

This argument has important consequences for the construction of simple 2D QH models. For spinless systems, TRS implies that there are equal numbers of Dirac points of both types in the BZ. This is because the spinless TRS operator is \( \mathcal{T} = \mathcal{K} \), where \( \mathcal{K} \) is complex conjugation, and so when TRS is present, \( \mathcal{T} H(k) \mathcal{T}^{-1} = H(-k) \), then \( d_{1}(k) = d_{1}(-k) \), \( d_{2}(k) = -d_{2}(-k) \), \( d_{3}(k) = d_{3}(-k) \). A Dirac point at momentum \( \mathbf{K} \) is therefore paired with another Dirac point of the opposite type (as \( d_{2} \) must flip sign) at momentum \( -\mathbf{K} \). These constraints also rule out unpaired Dirac points at TRS-invariant momenta, \( \mathbf{k} = -\mathbf{k} \). Any transition that preserves TRS is therefore topologically trivial in 2D. Note that if \( \sigma \) represents a real spin, the TRS operator and the constraints are different, such that the two bands are only gapped if TRS is broken \[3\].

To design a spinless topological model, we need to separate out the Dirac points in each pair by breaking TRS. This is beautifully illustrated by the Haldane model \[51\], based on a 2D honeycomb lattice, such as graphene, or equivalently, a brickwall lattice, as in cold atom experiments \[53\]. Both lattices have two sites per unit cell, and can be modelled by a two-band Hamiltonian like Eq. 4 where \( \sigma \) is a sublattice basis \[52\]. If only nearest-neighbour hoppings are present, there is one pair of Dirac points in the BZ, which can be gapped out together by a momentum-independent mass, \( m \sigma_{3} \). Physically, this corresponds to adding an energy offset between the two sites, breaking inversion symmetry and preserving TRS.

In the Haldane model, TRS is broken by also including complex next-nearest-neighbour hoppings \[51\]. These hoppings are designed such that, close to the two Dirac points, the local vector \( d_{3} \approx m \pm m_{1} \), where \( m_{1} \) depends on the geometry, complex hopping phase and amplitude. Then, one Dirac point closes and re-opens at \( m = m_{1} \) and the other at \( m = -m_{1} \), such that the Haldane model has a 1CN of \( \pm 1 \) for \( m < |m_{1}| \), as experimentally probed in ultracold atoms \[53, 54\].

4D Class AI Topological Models– We now show how extending these ideas can lead to 4D QH models with nontrivial topological 2CNs, which do not require TRS-breaking or (artificial) gauge fields. In 4D, minimal QH systems can be constructed from four-band models of the form \[52\]:

\[ H(k) = \varepsilon(k) \Gamma_{0} + d(k) \cdot \Gamma, \]

where \( \Gamma_{0} \) is the 4 \( \times \) 4 identity; \( \mathbf{d}(k) \) is a five-component vector; \( \varepsilon(k) \) is an overall energy shift, neglected without loss of generality hereafter; and \( \Gamma \) is a vector of 4 \( \times \) 4 Dirac matrices, chosen as \( \Gamma_{1} = \sigma_{1} \otimes \sigma_{3}, \Gamma_{2} = 2 \sigma_{0} \otimes 1, \Gamma_{3} = \sigma_{1} \otimes 1, \Gamma_{4} = 1 \otimes \sigma_{2}, \Gamma_{5} = 1 \otimes 1 \) \[56\]. Note that, unlike a two-band model, the decomposition in Eq. 3 is not generic, and the energy bands are doubly-degenerate: \( E_{\pm} = \varepsilon(k) \pm \sqrt{\mathbf{d}(k) \cdot \mathbf{d}(k)} \). The 2CN for the lower pair of bands is \[14, 53\]:

\[ \nu_{-}^{(2)} = \frac{1}{8\pi^{2}} \int_{\text{BZ}} \text{tr} (\Omega_{-} \wedge \Omega_{-}), \]

\[ = \frac{3}{8\pi} \int_{\text{BZ}} d^{4}k \epsilon^{abcde} \partial_{a} \partial_{b} \partial_{c} \partial_{d} \partial_{e}, \]

where the trace runs over the Berry curvature wedge product of the lower band pair. The integral is over the 4D BZ, with \( \epsilon^{abcde} \) being the 5D Levi-Civita symbol, and \( \mathbf{d} = \mathbf{d} / |\mathbf{d}| \) as above. In such a four-band model, the 2CN is again a “winding number”, but now counting how often \( \mathbf{d}(k) \) covers the unit sphere, \( S^{4} \), across the 4D BZ.
As in 2D, the topological invariant changes via topo- logical phase transitions where band gaps close and re- open. In the simplest case, the four bands touch at an isolated set of Dirac points in the BZ, around each of which \( d(\mathbf{q}) \approx (v_x q_x, v_y q_y, v_z q_z, v_w q_w, m) \), where \( v_z(\nu_w) \) is the dispersion slope with respect to \( q_z(q_w) \). As before, the mass, \( m \), smoothly tunes across the transition, with the integrand of Eq. 4 flipping sign as \( d_s \approx m \) changes sign. Each isolated point that closes and opens changes the 2CN by \( \pm 1 \). Again, this divides the Dirac points into two types; the first (second) type has an even (odd) number of minus signs within the other components \( \{d_1, d_2, d_3, d_4\} \) such that the 2CN increases (decreases) as \( m \) goes from negative to positive values.

Importantly, in 4D, preserving TRS for spinless systems does not imply equal numbers of the two types of Dirac points. This is because when spinless or bosonic TRS is present, \( d_1(\mathbf{k}) = d_1(-\mathbf{k}) \), \( d_3(\mathbf{k}) = d_3(-\mathbf{k}) \) and \( d_5(\mathbf{k}) = d_5(-\mathbf{k}) \) are even, while \( d_2(\mathbf{k}) = -d_2(-\mathbf{k}) \) and \( d_4(\mathbf{k}) = -d_4(-\mathbf{k}) \) are odd. Then, a Dirac point at \( \mathbf{K} \) is again paired with another Dirac point at \( -\mathbf{K} \), but now these Dirac points are of the same type, as both \( d_2 \) and \( d_4 \) flip sign. As a result, each TRS pair of Dirac points will change the 2CN by \( \pm 2 \) across a transition.

Unlike 2D, it is therefore possible to have spinless 4D QH models with TRS, where the 2CNs take only even integer values, \( 2Z \). This is a key difference from previously-studied 4D systems in Class A (with broken TRS) and Class AII (with fermionic TRS), where the 2CN takes any integer values, \( Z \). For a four-band Class AII model, for example, the different TRS constraints allow unpaired Dirac points at TRS-invariant momenta, so that the 2CN can change by \( \pm 1 \). Physically, the latter may describe a lattice of particles in spatially-varying, spin-dependent gauge fields, which is challenging to realise with current technology. Instead, as we now illustrate, a suitable four-band model in Class AII could be engineered for spinless particles by exploiting lattice connectivity.

Proposal for 4D Model—Inspired by the 2D Hal- dane model, our 4D proposal extends the honeycomb/brickwall lattice into 4D. As introduced above, these lattices are topologically-equivalent, having two sites per unit cell and a single pair of Dirac points in the BZ. Hereafter, we focus on the brickwall geometry, which is most natural for synthetic dimensions, but note that similar arguments apply to the honeycomb geometry.

To realise a four-band model like Eq. 3 we construct a 4D lattice [see Fig. S1(a)], with a four-site unit cell and the connectivity of a 2D brickwall lattice in both \( x-y \) and \( z-w \) planes. The Hamiltonian is:

\[
H(\mathbf{k}) = J[(2 \cos k_x + \cos k_y) \Gamma_1 + \sin k_y \Gamma_2 + (2 \cos k_z + \cos k_w) \Gamma_3 + \sin k_w \Gamma_4 + m \Gamma_5],
\]

where \( J \) is the hopping amplitude, the lattice spacing \( a = 1 \), and \( m \) is an energy offset between the \( A, B, C, D \) sites. Note that the real-space hoppings between \( B \) and \( D \) sites need to have an opposite sign compared to other hoppings, as indicated in Fig. S1(a), in order to realise the required \( \Gamma \) matrix structure [54].

When \( m = 0 \), this model has four 4D Dirac points in the BZ, as shown in Fig. S1(b). The points at \( \mathbf{K}_{1,2} = (\mp 2\pi/3, 0, \mp 2\pi/3, 0) \) are time-reversal pair of the first type, while those at \( \mathbf{K}_{3,4} = (\pm 2\pi/3, 0, \mp 2\pi/3, 0) \) are a pair of the second type. Therefore, this model is still topologically trivial, as shown, for example, in Fig. S1(c), for a cut at \( k_y = k_w = 0 \) and \( m = -J/2 \), where the contributions to the 2CN (Eq. 4) cancel out for the two pairs.

As in the 2D Haldane model, another ingredient is needed to separate out the two types of Dirac points and engineer topological bands. In particular, we need a mass-like term, proportional to \( \Gamma_5 \), which distinguishes between the two pairs of Dirac points. In this model, there are many possible terms that achieve this, corresponding to different long-range hoppings between alike-sites (e.g. \( A \rightarrow A \) [56]). As an example, we consider long-range hoppings in the \( x-z \) plane along \( \mathbf{r}' = (\pm 2a, 0, \pm 2a, 0) \) and \( \mathbf{r}'' = (\pm 2a, 0, \mp 2a, 0) \) (e.g. see Fig. S2(a)), giving:

\[
H'(\mathbf{k}) = [2 J' \cos(2k_x + 2k_z) + 2 J'' \cos(2k_x - 2k_z)] \Gamma_5,
\]

where \( J' (J'') \) is the hopping amplitude along \( \mathbf{r}' (\mathbf{r}'') \). As a result, the first closes at \( m = J' - 2J'' \) and the
second at \( m = J'' - 2J' \) (see Fig. 2(c)\&(d)). Provided that \( J' \neq J'' \), these are topological transitions; for example, if \( J'' = 0 \) and \( J' > 0 \), this model has a 2CN of -2 for \(-2J' < m < J'\), and is trivial otherwise, as can also be confirmed numerically [1]. Note that the above terms preserve TRS and so all 1CNs vanish by symmetry. Adding TRS-breaking terms will separate the Dirac points within a pair; this can give a 4D QH model, but in Class AI where the 1CNs can be non-zero [21, 22, 27, 34].

4D QH Effect and 3D Surface States–Bands with non-zero 2CNs support a 4D QH response, as could be probed, for example, in the current density [17, 55], in the center-of-mass motion of a cloud [34, 58, 59] or in the displacement of a driven-dissipative steady state [33, 60]. As the 1CNs vanish in Class AI, this QH response will stem purely from the 2CN and so will be easier to isolate than in Class A models where the 1CN response can dominate [21, 22, 34]. There is also a one-to-one correspondence between the bulk topological invariant and the number of topological surface states [1, 23, 55]. For Class AI models, the 2CN takes even integer values, as discussed above, and so surface states come in pairs. In the 3D BZ of our model, these correspond to pairs of Weyl points with the same chirality. The existence of such surface states could be probed in ultracold atomic [4, 10] and photonic experiments [11, 13].

**Experimental Remarks**–Our proposal avoids the need to control (artificial) gauge fields in a 4D geometry, by constructing a 4D QH model using the lattice connectivity. The tuneability of lattice connectivity is a well-established tool in lower dimensions, with the 2D honeycomb/brickwall lattices having been engineered experimentally in atomic [61, 62] and photonic set-ups [63, 66].

To realise the specific 4D lattice in Fig. S1(a), a 2D honeycomb/brickwall lattice can be extended by a third spatial dimension \( (z) \) and a synthetic dimension \( (w) \) [35, 57, 58]. To create the \( z-w \) brickwall connectivity, only a subset of states in the synthetic dimension should be coupled at each site along \( z \); this could be achieved, for example, by engineering states to have two alternating energy-level spacings, such that different transitions can be addressed at alternating sites. Furthermore, the sign of certain hoppings along real dimensions can be flipped, as required in Eq. S4, by employing different orbitals or modes at different sites [47], or by driving the system [68]. Longer-range hoppings like in Fig. 2(a) can be controlled, e.g., by designing the shape of an optical lattice potential for atoms or through arrangement of photonic resonators. However, care must be taken to design these terms to dominate over other long-range hoppings [56]. Alternatively, as this proposal relies on the lattice connectivity, it could be implemented as a 4D network model [69].

**Conclusions**–We have proposed how to realise 4D topological systems without gauge fields, by designing the lattice connectivity. These are systems in Class AI, corresponding to spinless or bosonic models with TRS and even-valued 2CNs. To illustrate this, we have designed a minimal 4D lattice model which exhibits the 4D QH effect and hosts pairs of chiral Weyl surface states. As this model could be realised using ultracold atoms or photons, it opens the way towards the exploration of a new class of systems with nontrivial band invariants only in four dimensions or higher.

**Note:** In preparation of this manuscript, we became aware of a recent proposal for an eight-band 4D crystalline topological insulator, which has bosonic TRS [70], but which is instead topologically-protected by reflection symmetry and which relies on spin-orbit couplings.

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Supplemental Materials: “Four-dimensional topological lattices without gauge fields”

In this Supplemental Material, we derive the momentum-space Hamiltonian for the proposed model, as stated in the main text, beginning from the real-space tight-binding model for the lattice. As shown in Fig. S1, our lattice has four sites, denoted by \((A, B, C, D)\). The corresponding set of lattice vectors are: \(R_1 = (1, -1, 0, 0)\), \(R_2 = (1, 1, 0, 0)\), \(R_3 = (0, 0, 1, -1)\) \(R_4 = (0, 0, 1, 1)\), with \(a = 1\) being the distance between any two nearest-neighbour lattice sites.

The full real-space tight-binding Hamiltonian is given by:

\[
H = H_x + H_y + H_z + H_w + H_{\text{on-site}},
\]

\[
H_x = J \sum_{m,n,j,l} (c_{m,n,j,l}^\dagger a_{m,n,j,l} + a_{m+1,n+1,j,l}^\dagger c_{m,n,j,l} - b_{m,n,j,l}^\dagger d_{m,n,j,l} - d_{m+1,n+1,j,l}^\dagger b_{m,n,j,l} + \text{h.c})
\]

\[
H_y = J \sum_{m,n,j,l} (c_{m-1,n,j,l}^\dagger a_{m,n,j,l} - b_{m-1,n,j,l}^\dagger d_{m,n,j,l} + \text{h.c})
\]

\[
H_z = J \sum_{m,n,j,l} (d_{m,n,j,l}^\dagger a_{m,n,j,l} + a_{m,n,j+1,l+1}^\dagger d_{m,n,j,l} + b_{m,n,j,l}^\dagger c_{m,n,j,l} + c_{m,n,j+1,l+1}^\dagger b_{m,n,j,l} + \text{h.c})
\]

\[
H_w = J \sum_{m,n,j,l} (d_{m,n,j-1,l}^\dagger a_{m,n,j,l} + b_{m,n,j-1,l}^\dagger c_{m,n,j,l} + \text{h.c})
\]

\[
H_{\text{on-site}} = m \sum_{m,n,j,l} (a_{m,n,j,l}^\dagger a_{m,n,j,l} + b_{m,n,j,l}^\dagger b_{m,n,j,l} - c_{m,n,j,l}^\dagger c_{m,n,j,l} + d_{m,n,j,l}^\dagger d_{m,n,j,l})
\]  

(S1)

where we have split the Hamiltonian into hopping terms along each direction, and where the index \((m, n, j, l)\) indicates a particular unit cell with respect to lattice vectors \((R_1, R_2, R_3, R_4)\). We have also introduced the operators \(\alpha_{m,n,j,l}\) \((\alpha_{m,n,j,l}^\dagger)\) which annihilate (create) a particle on an \(\alpha\)-site in the \((m, n, j, l)\) unit cell. Fourier-transforming these

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**FIG. S1.** The 4D brickwall lattice, shown for (a) the A-C slices in the x-y plane, (b) the B-D slice in the x-y plane, (c) the A-D slices in the z-w plane, (d) the B-C slices in the z-w plane, and (d) the x-z plane, where the four-site unit cell is highlighted. The set of lattice vectors are labelled: \(R_1 = (1, -1, 0, 0)\), \(R_2 = (1, 1, 0, 0)\), \(R_3 = (0, 0, 1, -1)\) \(R_4 = (0, 0, 1, 1)\), and the indices \((m, n, j, l)\) label a given unit cell with respect to these lattice vectors.
operators as:

\[
a_{m,n,j,l} = \frac{1}{\sqrt{N}} \sum_k a_k e^{-i[mk \mathbf{R}_1 + nk \mathbf{R}_2 + jk \mathbf{R}_3 + lk \mathbf{R}_4]} \\
b_{m,n,j,l} = \frac{1}{\sqrt{N}} \sum_k b_k e^{-i[mk \mathbf{R}_1 + nk \mathbf{R}_2 + jk \mathbf{R}_3 + lk \mathbf{R}_4]} e^{-ik(\mathbf{R}_1 + \mathbf{R}_3 + \mathbf{R}_2 + \mathbf{R}_4)/2} \\
c_{m,n,j,l} = \frac{1}{\sqrt{N}} \sum_k c_k e^{-i[mk \mathbf{R}_1 + nk \mathbf{R}_2 + jk \mathbf{R}_3 + lk \mathbf{R}_4]} e^{-ik(\mathbf{R}_1 + \mathbf{R}_2)/2} \\
d_{m,n,j,l} = \frac{1}{\sqrt{N}} \sum_k d_k e^{-i[mk \mathbf{R}_1 + nk \mathbf{R}_2 + jk \mathbf{R}_3 + lk \mathbf{R}_4]} e^{-ik(\mathbf{R}_3 + \mathbf{R}_4)/2}
\]

where \(N\) is the number of cells and where the sum runs over all momenta in the BZ, we find:

\[
H_x = \sum_k \begin{pmatrix} a_k^t & b_k^t & c_k^t & d_k^t \end{pmatrix} \begin{pmatrix} 0 & 0 & 2J \cos k_x & 0 \\ 0 & 0 & 0 & -2J \cos k_x \\ 2J \cos k_x & 0 & 0 & 0 \\ 0 & -2J \cos k_x & 0 & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \\ c_k \\ d_k \end{pmatrix},
\]

\[
H_y = \sum_k \begin{pmatrix} a_k^t & b_k^t & c_k^t & d_k^t \end{pmatrix} \begin{pmatrix} 0 & 0 & J e^{-ik_y} & 0 \\ 0 & 0 & 0 & -J e^{ik_y} \\ J e^{ik_y} & 0 & 0 & 0 \\ 0 & -J e^{-ik_y} & 0 & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \\ c_k \\ d_k \end{pmatrix},
\]

\[
H_z = \sum_k \begin{pmatrix} a_k^t & b_k^t & c_k^t & d_k^t \end{pmatrix} \begin{pmatrix} 0 & 0 & 2J \cos k_z & 0 \\ 0 & 0 & 0 & 2J \cos k_z \\ 2J \cos k_z & 0 & 0 & 0 \\ 0 & 2J \cos k_z & 0 & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \\ c_k \\ d_k \end{pmatrix},
\]

\[
H_w = \sum_k \begin{pmatrix} a_k^t & b_k^t & c_k^t & d_k^t \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & J e^{-ik_w} \\ 0 & 0 & J e^{-ik_w} & 0 \\ 0 & J e^{ik_w} & 0 & 0 \\ J e^{ik_w} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \\ c_k \\ d_k \end{pmatrix},
\]

\[
H_{\text{on-site}} = \sum_k \begin{pmatrix} a_k^t & b_k^t & c_k^t & d_k^t \end{pmatrix} \begin{pmatrix} m & 0 & 0 & 0 \\ 0 & m & 0 & 0 \\ 0 & 0 & -m & 0 \\ 0 & 0 & 0 & -m \end{pmatrix} \begin{pmatrix} a_k \\ b_k \\ c_k \\ d_k \end{pmatrix}
\]

Introducing the Dirac matrices:

\[
\Gamma_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & -i & 0 \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad \Gamma_3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_4 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad \Gamma_5 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},
\]

the above expressions can be combined and written compactly as:

\[
H = \sum_k \begin{pmatrix} a_k^t & b_k^t & c_k^t & d_k^t \end{pmatrix} H(k) \begin{pmatrix} a_k \\ b_k \\ c_k \\ d_k \end{pmatrix},
\]

\[
H(k) = J \left[ (2 \cos k_x + \cos k_y) \Gamma_1 + \sin k_y \Gamma_2 + (2 \cos k_z + \cos k_w) \Gamma_3 + \sin k_w \Gamma_4 + m \Gamma_5 \right],
\]

as stated in the main text.

To engineer a topological phase transition, we also need to add longer-range hoppings that can separate out the Dirac points of the two types. In the main text, we give the example of a hoppings in the \(x - z\) plane along \(r' = (\pm 2a, 0, \pm 2a, 0)\) and \(r'' = (\pm 2a, 0, \mp 2a, 0)\). In terms of the tight-binding real-space model, this would correspond
to adding terms:

\[ H_1 = J' \sum_{m,n,j,l} (a_{m+1,n+1,j+1,l+1}^\dagger a_{m,n,j,l} + b_{m+1,n+1,j+1,l+1}^\dagger b_{m,n,j,l} - c_{m+1,n+1,j+1,l+1}^\dagger c_{m,n,j,l} - d_{m+1,n+1,j+1,l+1}^\dagger d_{m,n,j,l} + h.c) \]

\[ + J'' \sum_{m,n,j,l} (a_{m-1,n-1,j-1,l-1}^\dagger a_{m,n,j,l} + b_{m-1,n-1,j-1,l-1}^\dagger b_{m,n,j,l} - c_{m-1,n-1,j-1,l-1}^\dagger c_{m,n,j,l} - d_{m-1,n-1,j-1,l-1}^\dagger d_{m,n,j,l} + h.c) \]

\[ + J''' \sum_{m,n,j,l} (a_{m+1,n+1,j-1,l-1}^\dagger a_{m,n,j,l} + b_{m+1,n+1,j-1,l-1}^\dagger b_{m,n,j,l} - c_{m+1,n+1,j-1,l-1}^\dagger c_{m,n,j,l} - d_{m+1,n+1,j-1,l-1}^\dagger d_{m,n,j,l} + h.c) \]

where we have allowed for the hoppings along \( \mathbf{r}' = (\pm 2a, 0, \pm 2a, 0) \) to have amplitude \( J' \) and those along \( \mathbf{r}'' = (\pm 2a, 0, \mp 2a, 0) \) to have amplitude \( J'' \). Such terms could be tuned in practice, for example, through the design of the optical lattice potential for cold atoms or through the arrangement of photonic resonators. Applying Eq. S2 as above, the long-range hoppings lead to a momentum-space Hamiltonian of the form:

\[
H_{\text{on-site}}(\mathbf{k}) = (2J' \cos(2k_x + 2k_z) + 2J'' \cos(2k_x - 2k_z)) \Gamma_5,
\]

as discussed in the main text. Note also that the hoppings from \( A \to A \), \( B \to B \) have different signs to those from \( C \to C \), \( D \to D \) to get the required matrix structure in this momentum-space equation.

We emphasise that the above is only one choice of long-range hoppings that will lead to topological bands. Indeed, all that is required are hoppings between similar sites chosen such that the effective mass-term in momentum-space is proportional to \( \Gamma_5 \) and has a momentum-dependence such that it distinguishes between the first Dirac pair at \( \mathbf{K}_1 \) and \( \mathbf{K}_2 \) as compared to the second pair at \( \mathbf{K}_3 \) and \( \mathbf{K}_4 \). To give just a few other examples of appropriate terms:

1. hoppings along \( \mathbf{r}''' = (a, a, 2a, 0) \) and similar, leading to momentum-space terms \( \propto \cos(k_x + k_y + 2k_z) \Gamma_5 \) etc,

2. hoppings along \( \mathbf{r}''' = (a, a, a, a) \) and similar, leading to momentum-space terms \( \propto \cos(k_x + k_y + k_z + k_w) \Gamma_5 \) etc.

In each case, a suitable design of these hoppings will lead to a similar topological phase diagram that has a topological phase with a 2CN of [2] within certain parameters, and a trivial topological phase otherwise. As there is considerable freedom therefore in choosing the long-range hopping terms, the most suitable choice may depend on the specific experimental implementation.

In practice, there may also be other long-range hopping terms present experimentally which are not of the desired type. However, the topological phase of this model will be robust, provided that these unwanted terms are sufficiently small. We note that those terms which cannot be expressed in terms of the five \( \Gamma \) matrices introduced above will also break the double-degeneracy of the energy bands. While this may complicate the simple picture for counting Dirac points, the 2CN can still be calculated numerically according to the algorithm of Ref. [S1].

[S1] M. Mochol-Grzelak, A. Dauphin, A. Celi, and M. Lewenstein, arXiv:1803.07003