Birth Quota of Non-Generic Degeneracy Points

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Weyl points are generic and stable features in the energy spectrum of Hamiltonians that depend on a three-dimensional parameter space. Non-generic isolated two-fold degeneracy points, such as multi-Weyl points, split into Weyl points upon a generic perturbation that removes the fine-tuning or protecting symmetry. The number of the resulting Weyl points is at least $|Q|$, where $Q$ is the topological charge associated to the non-generic degeneracy point. Here, we show that such a non-generic degeneracy point also has a birth quota, i.e., a maximum number of Weyl points that can be born from it upon any perturbation. The birth quota is a local multiplicity associated to the non-generic degeneracy point, an invariant of map germs known from singularity theory. This holds not only for the case of a three-dimensional parameter space with a Hermitian Hamiltonian, but also for the case of a two-dimensional parameter space with a chiral-symmetric Hamiltonian. We illustrate the power of this result for band structures of two- and three-dimensional crystals. Our work establishes a strong and powerful connection between singularity theory and topological band structures, and more broadly, parameter-dependent quantum systems.

Introduction. Weyl semimetals are a class of topological materials whose electronic band structure exhibits pointlike linear band-touchings [1–3]. These Weyl points are stable and generic, requiring no fine-tuning or symmetries. Crystal symmetries, however, can stabilize isolated non-generic two-fold degeneracy points, such as multi-Weyl points, in the electronic band structure of three-dimensional solids [4–7]. If the symmetry is broken, e.g., by changing an external magnetic (Zeeman) field or applying mechanical strain, the non-generic degeneracy point splits into multiple Weyl points [4]. As the symmetry-breaking perturbation is switched on gradually, these newly born Weyl points follow continuous trajectories in the Brillouin zone, originating from the original degeneracy point.

For a given non-generic degeneracy point, how many newborn Weyl points are allowed? From topological charge conservation and the generic character of Weyl points, it follows that the minimum number of newborn Weyl points upon a generic perturbation is the absolute value $|Q|$ of the topological charge $Q$ associated to the non-generic degeneracy point (e.g., the Chern number in 3D). The same consideration implies that the number of newborn Weyl points may also be $|Q| + 2M$ with $M$ being a positive integer, in such a way that $M$ of the excess Weyl points have unit positive charge and $M$ have unit negative charge, hence the sum of the charges of the newborn Weyl points equals $Q$. Is there also a ‘birth quota’, i.e., an upper limit of the number of newborn Weyl points? This is a fundamental question that, to our knowledge, has not been addressed in the context of band structure theory.

In this work, we answer this question positively, and show that such a non-generic degeneracy point does have a birth quota, which turns out to be the so-called local multiplicity known in singularity theory. Our result is not exclusive to Weyl points in three dimensions (3D), we also obtain an analogous result for two-dimensional (2D) crystals with chiral symmetry illustrated on the example of bilayer graphene, as well as a minimal example in 1D (Fig. 1). We showcase the power of these results on quasiparticle (electronic, photonic, phononic) band structures: we compute the birth quota of all four types of two-fold degeneracies stabilised by the 230 crystalline space groups [7] (Table I). However, the notion of the birth quota is more generic: it is applicable to quantum systems controlled by external parameters, such as interacting spin systems [8–12] or quantum circuits [13, 14]; more generally, it is applicable to any physical system that is described by a matrix, e.g., linearly coupled mechanical oscillators or electromagnetic modes.

Example: Bilayer graphene. We exemplify the birth of Weyl points from a non-generic degeneracy point with the well-known example of electrons in A-B-stacked bilayer graphene [15]. For more details and illustrations, see Sec. I of SI.

Bilayer graphene is a two-dimensional crystal, whose simplest band-structure models have chiral (a.k.a. sublattice) symmetry, which protects the generic degeneracies (2D Weyl points) at zero energy in the two-dimensional Brillouin zone. A simple tight-binding model of delocalized electrons in graphene yields an envelope-function Hamiltonian $H(k_x,k_y) \propto (k_x^2 - k_y^2) \sigma_x + 2k_x k_y \sigma_y$, valid in the vicinity of the high-symmetry point $K$ (and $K'$) of the Brillouin zone [15, 16]. Here, $k_{x,y}$ are momentum components measured from $K$, $\sigma_{x,y}$ are Pauli matrices, the matrix structure represents a combined layer-sublattice degree of freedom, and chiral
symmetry forbids the $\sigma_z$ term [17].

This Hamiltonian $H$ exemplifies a non-generic degeneracy point in 2D, located at $(k_x, k_y) = 0$ with a quadratic dispersion $E_{\pm} \propto \pm k^2$. Furthermore, the Hamiltonian $H$ can be reinterpreted as the dimensionless effective Hamiltonian map $h : \mathbb{R}^2 \to \mathbb{R}^2, (k_x, k_y) \mapsto (k_x^2 - k_y^2, 2k_x k_y)$. This map has a ‘winding number’ or ‘topological charge’ $Q_{2D} = +2$, as opposed to 2D Weyl points whose topological charge is $\pm 1$.

One type of perturbation to this degeneracy point is mechanical strain: applying it along $x$ adds a perturbation term $H_s \propto \sigma_x$ to $H$ [15]. The effect of the strain is that the degeneracy point splits into two 2D Weyl points along the $k_x$ axis, both having charge $Q_{2D} = +1$, i.e., the total charge is conserved upon perturbation.

Another type of perturbation appears when the skew interlayer hopping is taken into account, causing trigonal warping [15, 16]. This perturbation term is described by a Hamiltonian $H_{tw} \propto (k_x \sigma_x - k_y \sigma_y)$. The effect of this perturbation is that the non-generic degeneracy point of $H$ splits into four 2D Weyl points: 3 having charge $Q_{2D} = +1$ and 1 having $Q_{2D} = -1$. Again, the charge of the degeneracy point of $H$ is conserved by the perturbation.

The observation that the non-generic degeneracy point at $K$ can split to two or four 2D Weyl points triggers the question: is there a perturbation of $H$ such that the number of newborn 2D Weyl points is different from 2 or 4? For example, is it possible to have 4 newborn Weyl points with $Q_{2D} = +1$ and 2 newborn Weyl points with $Q_{2D} = -1$? One implication of our analysis below is that the answer is ‘no’: the lower bound (2) is governed by topological charge conservation, whereas the upper bound (4), i.e., the ‘birth quota’, follows from our analysis below.

**Minimal 1D model.** First, we consider a minimal mathematical model of the birth quota effect: the birth of generic roots (‘1D Weyl points’) of the polynomial $f : \mathbb{R} \to \mathbb{R}, f(x) = x^3$, from its non-generic root at the origin $x = 0$. Any generic perturbation of the form $f_t(x) = x^3 + t_1 x^2 + t_2 x + t_3$ has one or three real roots, and all of them converge to 0 as the vector of control parameters $t = (t_1, t_2, t_3)$ tends to 0. We draw such perturbations in Fig. 1a, where, for simplicity, we set $(t_1, t_2, t_3) = (0, p, q)$. In the case of three roots (green region), two of them have positive signs (i.e. the function is increasing, charge +1, red dot), and one has negative sign (the function is decreasing, charge −1, blue dot). In the case of one root (orange region), it has positive sign (charge +1). Hence the sum of the charges is +1, same as the charge of the root of the unperturbed function $f$, exemplifying charge conservation.

The number of the real roots changes when the control vector $t$ steps through the zero locus $D = \{(t_1, t_2, t_3) \in \mathbb{R}^3 \mid D(t_1, t_2, t_3) = 0\}$ of the discriminant $D$ of $f$ (see Sec. II. of SL). This **discriminant set** $D$ in the control space is illustrated as the purple solid line in Fig. 1a.

Importantly, when we consider the complexification [18] $f_{C,t} : \mathbb{C} \to \mathbb{C}$, the complex **discriminant set** $D_C$ does not separate different root configurations: one can always find a path between different configurations such that the roots avoid collision in the complex plane. In fact, $f_{C,t}$ has three distinct complex roots for any $t \in \mathbb{C}^3 \setminus D_C$. This is illustrated by Fig. 1b,c,d, displaying the (c) unperturbed map $f_C$ and (b,d) two perturbed maps, and the roots of those $\mathbb{C} \to \mathbb{C}$ maps as red points. The number of complex roots born upon perturbation from the root of $f_C(x) = x^3$ is called the **local multiplicity** $\text{mult}_0 f_C = 3$ of

$$f_{p,q}(x) = x^3 + px + q$$

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**FIG. 1.** Number of generic roots (‘1D Weyl points’) born from the non-generic root of $f(x) = x^3$ is lower-bounded by the charge of the root (which is 1) and upper-bounded by the local multiplicity of the root ($\text{mult}_0 f = 3$). a) Phase diagram of perturbations of $f(x) = x^3$ of the form $f_{p,q}(x) = x^3 + px + q$. Orange: perturbation has one generic root. Green: perturbation has three generic roots. Purple line: perturbation has one generic root and one non-generic root. b) Complexified perturbation $f_{c,p,q}$ with $p = 1, q = 0$. c) Complexified map $f_{C,p,q}$ with $p = 1, q = 0$. c) Complexified map $f_{c,p,q}$ with $p = -1, q = 0$. d) Complexified perturbation $f_{C,p,q}$ with $p = -1, q = 0$. The complex values of the function are represented as arrows, so phase windings can be read off.
of the complexification root of conclude that the number of roots born from the original note the ordinal number of the degenerate levels by \( P \) the \( f \) it produces assume that in the natural wave-vector coordinates of analogous to the function graphene described above. In the rest of this paper, we outline the generalization of this minimal model, and use it to derive the birth quota of non-generic isolated two-fold degeneracy points. **Effective Hamiltonian at a twofold degeneracy point.** The models we study, e.g., tight-binding models of the electronic band structure, are described by a Hamiltonian map \( H : M^m \rightarrow \text{Herm}(N) \). Here, \( M^m \) is an \( m \)-manifold, and \( \text{Herm}(N) \) is the real vector space of \( N \times N \) Hermitian matrices. We focus on the example when \( M^m = \text{BZ} \) is the Brillouin zone of a 3D crystal \( (m = 3) \), but will also comment on the 2D case \( (m = 2) \), relevant for bilayer graphene described above.

A key quantity in our analysis of the birth quota, analogous to the function \( f \) in the minimal model above, is the effective Hamiltonian map \( h \) associated to the non-generic isolated two-fold degeneracy point \( P \in \text{BZ} \). Denote the ordinal number of the degenerate levels by \( i \) and \( i + 1 \). Then, for the eigenvalues of \( H(P) \), it holds that \( E_{i-1} < E_i = E_{i+1} < E_{i+2} \), and \( E_i \not< E_{i+1} \) holds in a neighborhood \( U_P \) of \( P \in \text{BZ} \). The effective Hamiltonian map \( h \) is obtained by an exact Schrieffer–Wolff transformation [19] at \( P \), which provides a map from the neighborhood \( U_P \) of the degeneracy point \( P \) into the space of traceless Hermitian \( 2 \times 2 \) matrices. The latter matrix space is identified with \( \mathbb{R}^3 \) via the standard Pauli-matrix decomposition, \( X \sigma_x + Y \sigma_y + Z \sigma_z \equiv (X,Y,Z) \), hence the Schrieffer–Wolff transformation yields the effective Hamiltonian map \( h : U_P \rightarrow \mathbb{R}^3 \).

The fact that \( P \) is an isolated degeneracy point can be reformulated as \( h^{-1}(0) = \{ P \} \), i.e. the pre-image set of the origin \( 0 \in \mathbb{R}^3 \) contains only one point. We assume that in the natural wave-vector coordinates of the BZ, measured from \( P \) as the reference point, \( h \) is an analytic map, that is, its Taylor series is convergent and it produces \( h \) [20]. This results in an \( h : (\mathbb{R}^3, 0) \rightarrow (\mathbb{R}^3, 0) \) map, consisting of 3 locally convergent power series \( h_i \), \( h_2 \) and \( h_3 \) of 3 variables, fulfilling \( h(0) = 0 \). Our following analysis works for \( m = 3 \) in general, and also for \( m = 2 \) assuming chiral symmetry, when the degeneracy is at zero energy. The latter conditions imply \( h_3 = 0 \) and provide a map \( h : (\mathbb{R}^2, 0) \rightarrow (\mathbb{R}^2, 0) \) [21].

**Birth quota.** Up to now, we converted band-structure features to an \( h : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \) analytic map. This enables us to establish the birth quota of a non-generic degeneracy point using concepts and relations from singularity theory. The local degree \( \deg_0 h \) of the effective Hamiltonian map \( h : (\mathbb{R}^m, 0) \rightarrow (\mathbb{R}^m, 0) \) at 0 is the global degree of the normalised map \( \langle \text{pseudospin texture} \rangle \) \( \tilde{h} = \frac{h}{h_0} : S^{m-1} \rightarrow S^{m-1} \) defined on a sufficiently small sphere \( S^{m-1} \) around the origin, see [22–26] for details. For \( m = 2 \) the local degree is a winding number, and for \( m = 3 \) it agrees with the first Chern number of the eigenstate corresponding to the \( i \)-th eigenvalue, see [17]. For both cases, the local degree is often referred to as the (topological) charge of the degeneracy point. We will also refer to the complexification \( h_C : (\mathbb{C}^m, 0) \rightarrow (\mathbb{C}^m, 0) \) of \( h \), and its local degree \( \deg_0 h_C \).

The effect of a physical perturbation on the crystal electrons, e.g., mechanical strain or a change of the magnetic (Zeeman) field, is described in our framework as a deformation of the effective Hamiltonian map \( h \). An unfolding of \( h \) with \( k \) control parameters is an analytic map \( H : \mathbb{R}^3 \times \mathbb{R}^k \rightarrow \mathbb{R}^3 \times \mathbb{R}^k \) of the special form \( H(x, y, z, t) = (h_t(x, y, z), t) \), where \( t \in \mathbb{R}^k \), such that \( h_0 = h \). For fixed control parameters \( t \), we call \( h_t \) an analytic deformation, or simply deformation, of \( h \). To derive the birth quota of \( h \), we will use the complex generalizations of these concepts: a holomorphic unfolding \( H_C \) and the corresponding complex deformation \( h_{C,t} \) of the complexification \( h_{C,0} = h_C \) are defined similarly to the real case above [23, 26].

We call the points of \( h_{C,0}^{-1}(0) \subset \mathbb{R}^3 \) degeneracy points of \( h_1 \), and the points of \( h_{C,0}^{-1}(0) \subset \mathbb{C}^3 \) complex degeneracy points. A complex degeneracy point \( p \) is generic, and we call it a complex Weyl point, if the Jacobian of \( h_{C,t} \) at \( p \) has maximal rank, i.e., rank 3. A real degeneracy point \( p \) is generic, and we call it a (real) Weyl point, if the Jacobian of \( h_t \) at \( p \) has maximal rank. This happens if and only if \( p \) is generic as a complex degeneracy point. At a real Weyl point \( p \), the local degree is \( \deg_p h_t = \pm 1 \), determined by the sign of the Jacobian determinant, cf. [4]. At a complex Weyl point \( p \), the local degree of \( h_{C,t} \) is always \( \deg_p h_{C,t} = 1 \).

Our goal is to characterize the birth of (real) Weyl points from a non-generic degeneracy point. Hence, we need to distinguish between Weyl points born from the original degeneracy point, and all other Weyl points. This we already noted in the minimal model above, by pointing out that 1D Weyl points can be born at infinity. To make this distinction here, we consider the complex case first. We take a spherical boundary \( S^5 \subset \mathbb{C}^3 \) in the configuration space, centered at the origin, which we call the separator, such that the only degeneracy point of \( h_C \) inside this sphere is the origin. The separator bounds
the closed ball $B^6_0 \subset \mathbb{C}^3$. When a deformation is applied continuously, the degeneracy points $h^{-1}_C(0)$ follow continuous trajectories in the complex configuration space. Therefore, there is a neighborhood $\mathcal{U}_C$ of the origin of the control space such that for all $t \in \mathcal{U}_C$, (i) the degeneracy points born from the original degeneracy point do not reach the separator, and (ii) the degeneracy points of the undeformed map $h_C$ that are outside of the separator do stay outside. For convenience, we take a neighborhood $\mathcal{U}_C$ that is an open ball centered at the origin of the control space. Furthermore, from now on, we restrict the unfolding $h_C$ onto $B^6_0 \times \mathcal{U}_C$.

We define the complex discriminant set $\mathcal{D}_C \subset \mathcal{U}_C$ as those control vectors $t$ for which $h_{C,t}$ has non-generic complex degeneracy points in $B^6_0$. That is, for any control vector $t \in \mathcal{U}_C \ \mathcal{D}_C$, all degeneracy points of $h_{C,t}$ are complex Weyl points. A key observation is that the number of complex Weyl points within $B^6_0$ is the same for any control vector $t \in \mathcal{U}_C \ \mathcal{D}_C$. This is related to the fact that the complex codimension of the discriminant set $\mathcal{D}_C$ is at least 1, and therefore the real codimension is at least 2. This implies that $\mathcal{U}_C \ \mathcal{D}_C$ is path-connected, and hence the number $\# h_{C,t}^{-1}(0)$ of complex Weyl points cannot change along any control trajectory in $\mathcal{U}_C \ \mathcal{D}_C$. For details, we refer to Sec. II.A of SI and Ref. [26]. In conclusion, the number of preimages of 0, $\# h_{C,t}^{-1}(0)$ is a property of $h_C$ and hence a property of $h$. It is called the local multiplicity of $h_C$ (mult$_0 h_C$), and also called the local multiplicity of $h$ (mult$_0 h$).

In the band-structure context, the effective Hamiltonian map $h$ is a real map. We denote the set of real control vectors $t \in \mathbb{R}^k$ in $\mathcal{U}_C$ and $\mathcal{D}_C$ by $\mathcal{U}$ and $\mathcal{D}$, respectively. With these, we can express the key message of this work: the local multiplicity mult$_0 h$ is the birth quota of the original non-generic degeneracy point, i.e., mult$_0 h$ is the upper bound of the number of Weyl points born from the original degeneracy point:

$$\# h_{t}^{-1}(0) \leq \text{mult}_0 h.$$  

Equation (2) is a consequence of the previous paragraph, and the fact that a real Weyl point is also a complex Weyl point.

Methods to calculate the birth quota. We mention three different methods to compute the birth quota mult$_0 h_C$. The first one is the direct application of the definition for the constant deformation $h_{C,q}(x) = h_C - q$ with $q \in \mathbb{C}^3$ close to 0. Note that by Sard’s lemma [22], for almost all values $q$, all degeneracy points of $h_{C,q}$ are generic. By definition, the number of the roots of $h_{C,q}$ inside the ball $B^6_0$ is the local multiplicity. Hence the computation of the birth quota mult$_0 h_C$ reduces to solving the equation $h_C = q$, which, in general, can be done numerically.

Another method is based on the fact that the local multiplicity is equal to the local degree deg$_g h_C$ of the complexification $h_C$, see [26, E.3]. Here, the local degree is understood in the sense described for the minimal model, i.e. it is the local degree of the real-imaginary decomposition (realification) $h_{C,R} : \mathbb{R}^6 \rightarrow \mathbb{R}^6$. The computation of the local degree also allows the use of integral formulas, see e.g. in [17, 27].

We note that an alternative, commonly used definition of the local multiplicity uses algebraic methods: the local multiplicity is defined as the dimension of the so-called local algebra of $h$ at 0, see Sec. III. of SI and Refs. [23, 26]. This definition also provides a practical computational method of the birth quota. In the physical applications below, we computed the birth quotas using deformations, as well as this algebraic method.

Applications. In what follows, we derive the local multiplicity for two different families of isolated twofold degeneracy points: for chiral-symmetric band-structure models of few-layer graphene, and for all stable isolated twofold degeneracy points that arise in time-reversal-symmetric crystals. The results are summarised in Table I.

For bilayer graphene, discussed above, we find that the local multiplicity of the unperturbed effective Hamiltonian map $h$ is 4, confirming that the number of newborn 2D Weyl points upon a generic deformation is either 2 or 4. For chiral-symmetric models of trilayer graphene with ABC stacking, or multi-layer (n-layer) graphene with ABCA... stacking, the local degree of the degeneracy point at the $K$ point is $n$, whereas the local multiplicity is $n^2$, as shown in the top panel of Table I. (For derivation, see Example 2 in Sec. IV. of SI.)

Our methods provide the birth quota for non-generic degeneracy points appearing in 3D crystals as well. We focus on time-reversal-symmetric crystals, which are classified in 230 space groups. It is known [7] that there are four types of isolated twofold degeneracy points in the quasiparticle band structures of such crystals, listed in the bottom panel of Table I.

The charge-1 Weyl point is the generic degeneracy point (called Weyl point throughout this paper), whereas the charge-2, -3, -4 Weyl points are non-generic degeneracy points showing nonlinear dispersion in certain directions. Charge-2 and -3 Weyl points have been proposed in Ref. [4], with effective Hamiltonians in the form $H = \alpha k_x \sigma_y + (bk_x^2 + ck_x^0) \sigma_z + \text{h.c.}$ with $n \in \{2, 3\}$, $|b| \neq |c|$, $k_{\pm} = k_x \pm ik_y$ and $\sigma_{\pm} = \sigma_x \pm i \sigma_y$. The charge-4 Weyl point has been proposed in Ref. [5], and is described by the effective Hamiltonian $H = \mathcal{A} k_x k_y k_z \sigma_z + B \left( k_x^2 + \omega k_y^2 + \omega^2 k_z^2 \right) \sigma_+ + \text{h.c.}$ with $\omega = \exp(-2\pi i/3)$. Note that this map corresponds to the map studied in Ref. [25, Pg. 24], and also that such charge-4 Weyl points have been observed experimentally [28, 29].

We have computed the local multiplicities of these degeneracy points, and list the results in Table I. (Derivations are shown in Example 2 and Example 3 in Sec. IV. of SI.) The table also indicates the number of space groups where the corresponding non-generic degeneracy points are stabilised by symmetries.

Conclusions. We have shown that any isolated twofold non-generic degeneracy point in a 3D configuration space has a birth quota, a maximum number of Weyl
The effective Hamiltonian map associated to the degeneracy point can be computed as the local multiplicity of points that can be born from the degeneracy point. This notion) band structures.

(Without) spin-orbit coupling, e.g. electronic (phononic, photonic) band structures. The label SO (nSO) denotes band structures with symmetries stabilise non-generic degeneracy points, based on Ref. [7]. The label SO (nSO) denotes band structures with (without) spin-orbit coupling, e.g. electronic (phononic, photonic) band structures.

| $\mathbb{R}^2 \to \mathbb{R}^2$ | local degree | local multiplicity |
|-----------------------------|--------------|--------------------|
| monolayer graphene          | 1            | 1                  |
| bilayer graphene (AB)       | 2            | 4                  |
| n-layer graphene (ABC...n)  | $n$          | $n^n$              |
| $\mathbb{R}^3 \to \mathbb{R}^3$ | local degree | local multiplicity | #SG | #SG |
| Charge-1 Weyl point         | 1            | 1                  | 36  | 48  |
| Charge-2 Weyl point         | 2            | 4                  | 26  | 12  |
| Charge-3 Weyl point         | 3            | 9                  | 12  | 15  |
| Charge-4 Weyl point         | 4            | 12                 |     |     |

TABLE I. Local multiplicities of isolated twofold degeneracy points. The upper panel ($\mathbb{R}^2 \to \mathbb{R}^2$) lists the absolute value of the local degree, and the local multiplicity, associated to the electronic quasiparticles that emerge in the simplest chiral-symmetric tight-binding models of mono- or multilayer graphene. The lower panel ($\mathbb{R}^3 \to \mathbb{R}^3$) lists the same invariants, for all four types of isolated two-fold degeneracy points in crystals. The absolute value of the local degree is the minimum number of newborn Weyl points upon a generic deformation. The local multiplicity is the birth quota, i.e., the maximum number of newborn Weyl points. The last two columns of the lower panel indicate the number of space groups where symmetries stabilise non-generic degeneracy points, based on Ref. [7]. The label SO (nSO) denotes band structures with (without) spin-orbit coupling, e.g. electronic (phononic, photonic) band structures.

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[20] Note that our analysis also works in $C^\infty$ (i.e. smooth) category, using the notion of map germs, however the analytic condition simplifies the discussion.

[21] Similarly, spinless $PT$ symmetry restricts the Hamiltonian to be real valued, yielding $h_2 = 0$. Hamiltonians with both chiral and $PT$ symmetry correspond to the case $m = 1$ with effective Hamiltonian map $h : (\mathbb{R}, 0) \to (\mathbb{R}, 0)$. Such symmetric 1D systems can provide a physical realization of the minimal example with $H(k) = f(k)\sigma_x$.

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