Quasi-symmetry-protected topology in a semi-metal

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The crystal symmetry of a material dictates the type of topological band structure it may host, and therefore, symmetry is the guiding principle to find topological materials. Here we introduce an alternative guiding principle, which we call 'quasi-symmetry'. This is the situation where a Hamiltonian has exact symmetry at a lower order that is broken by higher-order perturbation terms. This enforces finite but parametrically small gaps at some low-symmetry points in momentum space. Untethered from the restraints of symmetry, quasi-symmetries eliminate the need for fine tuning as they enforce that sources of large Berry curvature occur at arbitrary chemical potentials. We demonstrate that quasi-symmetry in the semi-metal CoSi stabilizes gaps below 2 meV over a large near-degenerate plane that can be measured in the quantum oscillation spectrum. The application of in-plane strain breaks the crystal symmetry and gaps the degenerate point, observable by new magnetic breakdown orbits. The quasi-symmetry, however, does not depend on spatial symmetries and hence transmission remains fully coherent. These results demonstrate a class of topological materials with increased resilience to perturbations such as strain-induced crystalline symmetry breaking, which may lead to robust topological applications as well as unexpected topology beyond the usual space group classifications.

Therefore, crystalline symmetry and band topology are intertwined, and it is natural that symmetry should guide our search for materials. Here we refine this picture and argue for the importance of approximate symmetries as an additional concept (Fig. 1), with clearly observable experimental consequences. Suppose that a crystalline symmetry operation $M$ commutes with the Hamiltonian of the system, namely, $[H(k),M]=0$. The well-known representation theory dictates that low-symmetry points usually support only one-dimensional representations and hence bands anti-cross at these points. It may be possible, however, that at these low-symmetry points, 'approximate' symmetries emerge. They are not exact symmetries of the crystal, yet they still commute with a dominant part of the Hamiltonian. Such approximate symmetries would stabilize almost linear band crossings by enforcing finite yet perturbatively small energy gaps. A trivial example is a weak lattice distortion that removes a spatial symmetry that otherwise stabilizes a band crossing. Graphene could be considered as an alternative example in the spin channel, as its Dirac point is weakly gapped when spin–orbit coupling (SOC) is considered, turning spin rotation into an approximate symmetry $^{23,24}$. However, as approximate symmetries leave the bounds set by crystalline point groups, more exciting approximate symmetries may emerge that have no counterpart in the crystal symmetry.

We adopt the term 'quasi-symmetry' to denote a special type of approximate symmetry of electronic band structures that emerges from the hierarchy of a $k\cdot p$ type of perturbation expansion around a high-symmetry point. Quasi-symmetries are operators $M_{\text{eff}}$ that


Fig. 1 | General concept of quasi-symmetry. a, Illustration of a mirror symmetry operation, which consistently acts at the whole object. b, In contrast to mirror symmetry, the quasi-symmetry operation acts differently on different parts of the system. c, If a crystalline symmetry operation commutes with the Hamiltonian system, the band-crossing point is therefore symmetry protected. d, In this case, the Hamiltonian itself does not commute with the symmetry operation, yet its first-order perturbation does. This leads to the situation where although the band crossing is numerically avoided, the resulting gap size is negligible for the physical properties of the system. This type of symmetry is called quasi-symmetry. e, If the symmetry operation does not commute with the Hamiltonian to any order of perturbation of the system, the crossing is not protected by any symmetry. This will result in a sizeable gap and loss of topological character.

are the exact symmetries of the lower-order expansion but not of higher-order perturbation terms. The main goal of this paper is to show such quasi-symmetry exists in the semi-metal CoSi as well as a large set of similar materials, and that it enforces a low-symmetry plane of near-degeneracies spanning the Brillouin zone that pin a source of Berry curvature to the Fermi level (Fig. 2). This falls into the latter category of quasi-symmetries that are unrelated to approximate point-group symmetries, but can be treated as the symmetry of internal degrees of freedom, akin to spin in graphene. Unlike graphene, however, the form of quasi-symmetry is non-trivial as the corresponding symmetry operator is generally \( k \) dependent and forms a part of the Hamiltonian. The key distinction is that although a proper crystal symmetry uniformly acts on all the atomic coordinates, the quasi-symmetry operation acts on different subsets of inequivalent Co sites in different manners. A simplified example may be an incomplete mirror image (Fig. 1a,b), in which the mirror operation acts only on parts of the object but not consistently on the whole.

CoSi crystallizes in a chiral cubic structure of space group \( \text{P} \text{2}_\text{1} \text{3} \) without an inversion centre (Fig. 2). Recent studies revealed the existence of exceptionally long Fermi arcs that connect the sixfold and fourfold band degenerate points\(^{25-27}\). These two degenerate points correspond to two branches of Fermi surfaces located at the \( \Gamma \) and \( \text{R} \) points, respectively; yet, only the \( \text{R} \)-point pockets are observed in quantum oscillation experiments. Band structure calculations reveal four split bands due to SOC that correspond to four Fermi surfaces at \( \text{R} \), which are labelled as \( 1^*, 1^*, 2^* \) and \( 2^* \), representing the orbital and spin degrees of freedom. States at the boundary of the Brillouin zone are doubly degenerate due to crystalline symmetry; hence, the non-degenerate Fermi surfaces are enforced to touch there\(^3\). Both SOC and orbital gap are small yet similar in magnitude, which explains how four slightly degenerate, interpenetrating spheroids make up a rich internal structure of the Fermi surfaces.

CoSi single crystals resemble octahedra, indicating a dominant growth along the [111] direction (Supplementary Section IA provides the growth details). These crystals were fabricated into microstructures using focused-ion-beam (FIB) machining\(^9\) (Supplementary Section IB) to increase the current path homogeneity and signal of Shubnikov–de Haas (SdH) oscillations. This microfabrication will be the key to study the effects of unidirectional strain. The resistivity and large residual resistivity ratio in the samples agree well with previous bulk measurements\(^29\), indicating an unchanged material quality during fabrication (Supplementary Fig. 1). Hence, not surprisingly, large quantum oscillations of the magnetoresistance are readily observed at low fields (Fig. 3). Subtracting a polynomial background uncovers strong oscillations that resemble a beating pattern of two frequencies around \( F_1 \approx 550 \text{T} \) and \( F_2 \approx 660 \text{T} \), in good agreement with the existing literature\(^20\). The temperature dependence of the oscillations effectively follows the Lifshitz–Kosevich form, leading to a cyclotron effective mass of \( m_e \approx 0.84m_0 \) (Supplementary Fig. 14) with \( m_0 \) the free electron mass.

Although the self-intersecting Fermi surfaces are fairly complex, the quantum oscillation spectrum is relatively simple, with only two frequencies that—most importantly—only weakly depend on the direction of the applied magnetic field (Fig. 3). When magnetic quantum oscillations arise from such highly degenerate Fermi surfaces, the main question is which, if any, possible trajectories become quantum coherent. As the Fermi surface is centred around the \( \text{R} \) point, any orbit necessarily crosses the symmetry-enforced degeneracies at the Brillouin zone boundary multiple times. This has been argued to stabilize band degeneracies pinned to the Fermi level in this crystal structure\(^25,26\) on the planes of the Brillouin zone boundary (Fig. 4f, purple).

Yet, the orbits further intersect at low-symmetry points at which a gap must open (Fig. 4f, blue). Neither the frequencies nor their angle dependence obtained from density functional theory (DFT) calculations match the data if this gap is considered to separate the branches. The angle dependence obtained from density functional theory (DFT) calculations match the data if this gap is considered to separate the branches. The gap accidentally, an unreasonable degree of fine tuning is required for either the Fermi level to pin to these states or the degeneracies to be accidental at certain angles of the Brillouin zone. To obtain such a parametrically small gap, a very special trajectory is required that simultaneously acts at many \( k \) points, as well as in a wide range of energies (as shown later). Instead, quasi-symmetry enforces the uniform smallness of this gap and thus explains why magnetic breakdown at full transparency occurs at any arbitrary angle.
Fig. 2 | Structural and electronic properties of CoSi. a, Crystal structure of CoSi. Co and Si atoms are represented as red and blue spheres, respectively. b, Ab initio calculated band structure of CoSi around the R point. Here 1/2 denotes the orbital character, whereas ± stands for the spin character of the band. c, Three-dimensional view of all the Fermi surfaces, which are centred around either the R or Γ point of the Brillouin zone. d, Three-dimensional view of the Fermi surfaces centred around the R point with a quadrant cut. e, Quasi-symmetry- and crystalline-symmetry-protected degenerate planes. f, Berry curvature distribution of the 1− band defined in b at different Fermi energies calculated from the model Hamiltonian (equation (1)).

Fig. 3 | Temperature and angle-dependent quantum oscillations of CoSi. a, Temperature-dependent SdH oscillations with field and current applied along the [100] axis. Here $\rho_{osc} = \Delta \rho / \rho_{bg}$, where $\Delta \rho$ is the oscillatory part of the magnetoresistivity and $\rho_{bg}$ is the background obtained from a third-order polynomial fit to the magnetoresistivity. b, Fast Fourier transform (FFT) spectrum of the SdH oscillations presented in a with a field window of 3–14 T. Two main peaks, as well as their higher-harmonic components, can be clearly observed. The suppression of peak amplitude with increasing temperature is due to the thermal damping effect. c, FFT spectrum of angle-dependent quantum oscillations measured at $T = 2$ K. Here the magnetic field is rotated within the (100) plane and the angle is defined between the field direction and [001] axis. d, Summary of angular dependence of oscillation frequencies. Here the fitting is generated by calculating the orbital area based on the band structure calculations and taking into account the extreme magnetic breakdown due to quasi-symmetry (Supplementary Information). The near-perfect fitting clearly demonstrates that quasi-symmetry is the only option to explain the experimental results of nearly angle-independent oscillation frequencies.
Fig. 4 | Resilience of quasi-symmetry to lattice distortion. a, Scanning electron microscopy image of the CoSi microdevice. A long bar roughly along the \([110]\) direction with a cross section of \(2.5 \times 2.4 \mu \text{m}^2\) is fabricated by FIB. b, Illustration of tensile strain along the \([110]\) direction that breaks the \(C_3\) rotational symmetry of the crystal structure. c, SdH oscillations with both field and current applied along the fabricated bar direction at \(T = 50 \text{ mK}\). d, Logarithmic-scaled FFT spectrum of SdH oscillations displayed in c. The main peaks are always accompanied by satellite peaks up to the third harmonic. e, Enlarged view of the satellite peaks corresponding to the first- to third-harmonic oscillations. The red, purple and blue vertical lines correspond to the calculated FFT spectra produced by the fully symmetric, crystalline-symmetry-preserved and quasi-symmetry-preserved scenarios, respectively. f, Corresponding Landau orbits for three different scenarios. Here the coloured area illustrates the difference in orbital area compared with the fully symmetric case, and the black crosses represent the degeneracies that are lifted in different scenarios. Only the quasi-symmetry-preserved scenario reproduces FFT peaks that match with the experimental data.

To understand this quasi-symmetry, we next consider an effective model around the R point. Without SOC, all the bands are eight-fold degenerate at R due to the combination of twofold screw-axis symmetries along the \(x\) and \(y\) directions and time-reversal symmetry. Including spin doubles the degeneracy, and SOC splits the eight-fold degenerate states into sixfold and twofold degenerate states at the R point. An effective model for these eight bands around the R point can be constructed as

\[
\mathcal{H}(k) = \mathcal{H}_0(k) + \mathcal{H}_\text{soc} + \mathcal{H}_\text{LZ}(k),
\]

where \(\mathcal{H}_0(k) = C_0 + 2A_1(k \cdot L)\) is the lower-order expansion of the spin-independent Hamiltonian and three \(4 \times 4\) matrices \(L\) form an emergent angular momentum algebra \([L_i, L_j] = i \epsilon_{ijk} L_k\) with the Levi-Civita symbol \(\epsilon_{ijk}\) and \(i, j, k = x, y, z\). The SOC term is given by \(\mathcal{H}_\text{soc} = 2\lambda_0 (s \cdot L)\), where \(s\) is the spin operator. Further, \(\mathcal{H}_\text{LZ}(k)\) is the higher-order spin-independent term, with its form given in the Supplementary Information. Here \(\mathcal{H}_0(k) + \mathcal{H}_\text{LZ}(k)\) is the SOC-free expanded Hamiltonian to the second order. By choosing appropriate parameters such as \(C_0, A_1\) and \(\lambda_0\), the energy dispersion of \(\mathcal{H}(k)\) effectively reproduces that from the DFT calculations (Supplementary Section VII).

One feature in the Hamiltonian \(\mathcal{H}(k)\) is that the SOC term \(\mathcal{H}_\text{soc}\) takes a similar form as the linear momentum term, just by replacing momentum \(k\) by spin \(s\). This is because spin, as a pseudo-vector, behaves exactly the same as a vector due to the lack of inversion, mirror or other roto-inversion symmetries for a chiral crystal. Due to this similarity, up to the first-order perturbation, we find that the spin of the eigenstates is parallel or anti-parallel to momentum \(k\) and thus we can label the spin states of these bands by \(\pm\) (Fig. 2b). We derive an effective Hamiltonian for the near-degenerate bands. This can be done by first projecting the full Hamiltonian \(\mathcal{H}(k)\) into the four closest bands (\(1^\text{st}\) and \(2^\text{nd}\) bands) to get a four-band model and then constructing a two-band model for the \(1^\text{st}\) and \(2^\text{nd}\) bands (Supplementary Information). Up to the first-order perturbation, the two-band Hamiltonian takes the form \(\mathcal{H}_\text{eff}(k) = \epsilon_0 + \Delta_0(k)\sigma_z\), where \(\Delta_0(k) = \lambda_0 - \sqrt{3}C(k)l(k)k_z\) and the form of function \(\epsilon_0\) is given in the Supplementary Information. Here \(\sigma_z\) is the Pauli matrix on the basis of the \(1^\text{st}\) and \(2^\text{nd}\) bands, the \(\lambda_0\) term comes from SOC Hamiltonian \(\mathcal{H}_\text{soc}\) and the \(C\) term comes from \(\mathcal{H}_\text{LZ}(k)\). It is striking to see that this operator \(\mathcal{M}_\text{eff} = \sigma_z\) commutes with \(\mathcal{H}_\text{eff}\) and thus serves as exact symmetry at the first-order expansion. The existence of \(\mathcal{M}_\text{eff}\) forbids any terms that are coupled to \(\sigma_z\) in the effective Hamiltonian, thus reducing the co-dimension of a two-level crossing from 3 to 1 and stabilizing a nodal plane, which is defined by the equation \(\lambda_0 = \sqrt{3}C(k)l(k)k_z\) in this two-band model. A more accurate and complete description around the Fermi energy is the four-band model, which shares a similar \(k\)-dependent hidden quasi-symmetry and is essential in deriving the two-band model (Supplementary Section VII), and the whole perturbation theory reveals a striking hierarchy structure. Higher-order perturbation expansion breaks \(\mathcal{M}_\text{eff}\) by inducing additional terms coupled to \(\sigma_z\) in the effective model and thus leads to a small gap opening in this nodal plane (Supplementary Information). Therefore, \(\mathcal{M}_\text{eff}\) is not a symmetry of the system, but an emergent quasi-symmetry in the sense of low-energy effective theory. Importantly, this curved nodal plane spans the low-symmetry regions of the Brillouin zone, in contrast to symmetry-enforced exact degeneracies. This combined structure of symmetry- and quasi-symmetry-induced degeneracies forms the basis of the complex structure of the Fermi surface centred at \(R\), and reduces the complexity of the quantum orbits in magnetic fields to two angle-independent frequencies.

Physically, quasi-symmetry is linked to the orbital structure of the wavefunctions, and its operation only interchanges the orbitals at different atomic sites (internal degrees). Thus, unlike crystalline symmetries, they remain robust against symmetry-breaking lattice distortions (Fig. 4). This is experimentally probed by the application of tensile strain to a bar cut approximately along the [110] direction. The low-symmetry distortion removes the critical
screw symmetries at the zone boundaries, and gaps the otherwise symmetry-protected crossing points. Experimentally, such strain can be easily applied by thinning the transport bar by FIB milling, thus reducing its effective spring constant and increasing the total distortion under equal force. The microstructures are coupled to a sapphire substrate and their differential thermal contraction generates the desired tensile strain along the bar (Supplementary Information and ref. 33). As such strain lifts the screw symmetry protecting the degeneracy, one expects the sample to gradually leave the magnetic breakdown regime as the strain is increased and a collection of sum frequencies to emerge that correspond to all the possible area differences between the orbits42–46. Indeed, the strained bar exhibits pronounced satellite peaks that are symmetrically offset from the main peaks by $\Delta F = 32T$ for all harmonics. This exactly matches with the calculated difference in area between the crystalline symmetry-protected points, explaining the observed spectrum. However, those areas associated with quasiparticle tunnelling at a quasi-symmetry-protected point are not observed, implying that the magnetic breakdown field associated with that gap remains much smaller than the lowest field at which quantum oscillations are observed. This is direct experimental proof that quasi-symmetry protection is insensitive to the breaking of crystalline symmetries, a notion that can be corroborated by calculations (Fig. 4). This resilience clearly distinguishes symmetry- and quasi-symmetry-enforced topological band anomalies.

Their implications for the Berry curvature distribution in momentum space are another key characteristic of the topological character of near-degeneracies enforced by quasi-symmetry, compared with the exact degeneracies due to symmetry (Fig. 2f). The Berry curvature almost vanishes in the vicinity of the exact degenerate plane, yet it is concentrated to a ring on the near-nodal plane at any fixed energy. This large Berry curvature around the near-nodal lines, which always occurs at the Fermi energy, may strongly affect the physical phenomena that are related to the local Berry curvature, including the intrinsic spin Hall effect47–49 and quantum nonlinear Hall effect30.

The quasi-symmetry is the mathematical and physical framework behind the simple, strain-resistant quantum oscillation spectrum of CoSi. It is, however, just one example of a large class of materials in which quasi-symmetries can exist. Clearly, this new class of near-degenerate manifolds at low-symmetry k points is not found by current search programs for topological materials based on crystalline symmetry without further guideline. To search for materials with quasi-symmetries, a systematic expansion of the k-p-type effective Hamiltonian in an order-by-order manner is required for all the space groups, which is, in principle, feasible11. Typically, lower-order terms with higher symmetries than the crystalline symmetry itself possess larger prefactors than the higher-order terms with lower symmetries12, and a symmetry hierarchy is expected for the terms of different orders in the k-p-type Hamiltonian. Further interesting flavours of quasi-symmetry may exist, which emerge when higher-order terms with additional symmetries become dominant. Experimentally, we propose that quantum oscillations may provide guidance by pointing to materials with similarly extreme magnetic breakdown on extended regions on the Fermi surface, which quasi-symmetry would naturally explain. Although the search methods described here need to be implemented in the future, it is natural to anticipate quasi-symmetries in related compounds crystallizing in the same structure, such as PtGa, PtAl, RhSi and magnetic MnSi, where the influence of magnetism can be explored12,43–45. Our DFT calculations indeed reveal similar energy dispersions and Fermi surface shapes with quasi-symmetry-induced near-degeneracies in PtAl, PtGa and RhSi (Supplementary Section VI). The concept of quasi-symmetry raises the interesting prospect that even those materials in which crystalline symmetries do not allow stable band crossings may still host exotic quasiparticles and strong Berry curvature at the Fermi level. If such features at the Fermi level are desired, the current approach of automated symmetry classifications may not prove to lead to the most practical materials. Without the necessity of crystalline symmetry protecting higher-order band-crossing points, quasi-symmetries hold an advantage for topological applications. Often, topological anomalies in real materials are far away from the Fermi level; in the thin-film form, they are exposed to mismatch strains inherent to the heterostructures. These key bottlenecks of topological materials do not restrict quasi-symmetric materials. A consensus of high-throughput efforts emerges that 20–30% materials are topological2–46, yet it appears that crystal symmetry may not hold up as the strict barrier it was thought to be; furthermore, via quasi-symmetry concepts, topology may reach even further than predicted by these estimates.

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Data availability
Source data are available for this paper. Other data that support the findings of this study are available at Zenodo: https://doi.org/10.5281/zenodo.6336000.

Code availability
MATLAB code used for this study is available at Zenodo: https://doi.org/10.5281/zenodo.6336013.

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Author contributions
The crystals were synthesized and characterized by K.M., C.S. and C.F. The experimental design, FIB microstructuring and magnetotransport measurements were performed by C.G., C.P., J.D., X.H. and P.J.W.M. L.H., C.L. and B.A.B. developed and applied the general theoretical framework, and the analysis of experimental results was done by C.G., C.P. and P.J.W.M. The band structures were calculated by Y.S., F.-R.F. and C.F. All the authors were involved in writing the paper.

Competing interests
The authors declare no competing interests.

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