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Hidden quasi-symmetries stabilize non-trivial quantum oscillations in CoSi

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Unlocking the exotic properties promised to occur in topologically non-trivial semi-metals currently requires significant fine-tuning. Crystalline symmetry restricts the location of topological defects to isolated points (0D) or lines (1D), as formalized by the Wigner-Von Neumann theorem. The scarcity of materials in which these anomalies occur at the chemical potential is a major obstacle towards their applications. Here we show how non-crystalline quasi-symmetries stabilize near-degeneracies of bands over extended regions in en-

11 **ergy and in the Brillouin zone. Specifically, a quasi-symmetry is an exact sym-**
 12 **metry of a $k \cdot p$ Hamiltonian to lower-order that is broken by higher-order**
 13 **terms. Hence quasi-symmetric points are gapped, yet the gap is parametrically**
 14 **small and therefore does not influence the physical properties of the system.**
 15 **We demonstrate that in the eV-bandwidth semi-metal CoSi an internal quasi-**
 16 **symmetry stabilizes gaps in the 1-2 meV range over a large near-degenerate**
 17 **plane (2D). This quasi-symmetry is key to explaining the surprising simplicity**
 18 **of the experimentally observed quantum oscillations of four interpenetrating**
 19 **Fermi surfaces around the R-point. Untethered from the limitations of crys-**
 20 **talline symmetry, quasi-symmetries eliminate the need for fine-tuning as they**
 21 **enforce sources of large Berry curvature to occur at the chemical potential,**
 22 **and thereby lead to new Wigner-Von Neumann classifications of solids. Quasi-**
 23 **symmetries arise from a comparable splitting of degenerate states by spin-**
 24 **orbit coupling and by orbital dispersion - suggesting a hidden classification**
 25 **framework for symmetry groups and materials in which quasi-symmetries are**
 26 **critical to understand the low-energy physics.**

27 The introduction of concepts of topology in the past years into the field of electronic dis-
 28 persions has captured the imagination of condensed matter physics and sparked a flurry of new
 29 research directions in the past years. At its core is the realization that the electronic wave-
 30 forms constituting a material cannot always be derived from an entirely local description. In
 31 these topologically non-trivial metals, the wavefunctions are inherently non-local, and as such
 32 novel electronic states are expected and observed at the crystal surface terminating them (*1–10*).
 33 Beyond these surface properties, interesting anomalies in the bulk dispersion lead to novel phys-
 34 ical phenomena, such as the emergence of quasiparticles mimicking ultra-relativistic Weyl- and
 35 Dirac-Fermions in 3D; a solid-state analogon of the Adler-Bell-Jackiw anomaly; a planar Hall

effect; topological piezoelectric effect; second harmonic generation in Weyl semimetals; or strong Berry curvature that impacts the semi-classical and quantum dynamics of quasiparticles (11–19).

Given the wealth of new phenomena and potential applications, it is important to identify such "ideal" Weyl-, Dirac- or nodal-line semi-metals in which a priori unrelated chemical potential and the topological anomaly coincide. That such a coincidence is rather rare can be understood from the Wigner-Von Neumann theorem, which states that a two-level crossing generally requires three tuning parameters (24, 25). Any two-level model can be expanded as $H = \epsilon_0 + \sum_i d_i \sigma_i$ where $i = x, y, z$ and ϵ_0 is an offset, while the momenta k_i take the role of the generic tuning parameters d_i in this discussion. Thus to obtain a two level degeneracy, all 3 tuning parameters are required to achieve $d_x = d_y = d_z = 0$ (codimension 3). Such a point would generally only coincide with the Fermi level accidentally. To stabilize crossings of more than two bands or achieve higher dimensional degeneracies (nodal lines, planes), additional crystalline symmetries must provide further constraints on the form of the Hamiltonian, such as two-fold screw axis for the nodal plane in MnSi (26) or rotational symmetries for the fourfold Dirac points in the 3D Dirac semi-metals Cd_3As_2 and Na_3Bi (6, 7). As symmetry and topology are inseparably intertwined, it is natural that symmetry should guide our search for interesting materials.

Here we refine this picture, and argue for the importance of approximate symmetries as an additional concept [Fig. 1(a)] that can generate interesting measurable quantum phenomena. A crystalline symmetry operation, M , commutes with the Hamiltonian of the system, $[H(k), M] = 0$. The well-known representation theory dictates that low-symmetry points, such as generic k-point in the Brillouin zone, usually support only one-dimensional representations, and hence bands anti-cross at these points. It may further be possible, however, that at these low symmetry points *approximate* symmetries emerge and can even be k-dependent. They are

not exact symmetries of the material yet 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. They already naturally occur when exact symmetries are weakly broken, such as tiny monoclinic distortions weakly removing a rotational symmetry that otherwise stabilizes a band crossing point. Graphene could be considered as an alternative example in the spin channel, as its Dirac point is weakly gapped when spin-orbit coupling is considered, turning spin-rotation into an approximate symmetry (27). However, as approximate symmetries leave the bounds set by crystalline point-groups, more exciting hidden approximate symmetries may emerge that have no counterpart in the crystal symmetry. A famous example of a hidden symmetry is the Laplace–Runge–Lenz vector in classical gravitation. It is the conserved quantity stabilized by the hidden SO(4) symmetry of the r^{-1} potential of the Kepler problem that enforces strictly closed classical gravitational orbits. Weak perturbations, such as $r^{-1+\epsilon}$, mathematically reduce the symmetry to SO(3), yet the almost closed orbits for small ϵ evidence that the system senses the proximity to that hidden 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_{eff} that 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 a 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 which pin a source of Berry curvature to the Fermi level (Fig. 1). Excitingly, it falls into the latter category of hidden quasi-symmetries that are unrelated to approximate point-group symmetries, but can be treated as a 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 k -dependent and forms a

part of the Hamiltonian. It has remarkable consequences on the quantum oscillation spectrum, which we here present as the first experimental observation of material properties critically defined by quasi-symmetries.

CoSi crystallizes in a chiral cubic structure of space group $P2_13$ without an inversion center [Fig. 2(a)]. Recent studies revealed the existence of exceptionally long Fermi arcs which connect the sixfold and fourfold band degenerate points (9, 29–31). These two degenerate points correspond to two branches of Fermi surfaces located at the Γ - and R-point, respectively, yet only the R-point pockets are observed in quantum oscillation experiments. Band structure calculations reveal four split bands due to spin-orbit coupling which correspond to four Fermi surfaces at R, which we label as 1^+ , 1^- , 2^+ , 2^- , representing the orbital and spin degree of freedom respectively. 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 (5). The spin-orbit coupling and the orbital gap are both small yet similar in magnitude, which explains how four slightly degenerate, interpenetrating spheroids make up a surprisingly rich internal structure of the Fermi surfaces.

CoSi single crystals resemble octahedra, indicating a dominant growth along the [111] direction (see supplement for growth details). The quality of the single-phase crystallinity was checked by Laue and single crystal X-Ray diffraction. These crystals were fabricated into microstructures using focused-ion-beam machining (32) (see supplement) to increase the current path homogeneity and signal of Shubnikov-de Haas oscillations. The resistivity as well as the large residual resistivity ratio in the samples agrees well with previous bulk measurements (34), indicating an unchanged material quality during fabrication (Fig. 3). Hence not surprisingly, large quantum oscillations of the magnetoresistance are readily observed at low fields. Subtracting a polynomial background uncovers strong oscillations that resemble a beating pattern of two frequencies around $F_1 \sim 550$ T and $F_2 \sim 660$ T. These two, and their harmonics, are the

only frequencies observed in our as well as previous experiments (33–36). The temperature dependence of the oscillations follows well the Lifshitz-Kosevich form, leading to a low cyclotron effective mass of $m_c \sim 0.84 m_e$.

In light of the complexity of the self-intersecting Fermi surfaces it appears at first surprising that the quantum oscillation spectrum is tantalizingly simple, with only two frequencies that, most importantly, only weakly depend on the direction of the applied magnetic field (Fig. 4). 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 centered around the 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 (26, 36) on the planes of Brillouin zone boundary [marked pink in Fig. 4(a)] .

Yet the orbits further intersect at low-symmetry points at which a gap must open [marked blue in Fig. 4(a)]. Neither the frequencies nor their angle dependence obtained from DFT calculations match the data if this gap is considered to separate the orbits via significant avoided-crossing. As the gap is small, the quasiparticle may tunnel across it continuing on the original trajectory, a phenomenon known as magnetic breakdown (37–40). Based on estimations of the gap from DFT and further analytical calculations, vanishingly small breakdown fields fall below 0.11 T for any field orientation, and hence the experimental data is always obtained in an extreme breakdown regime (see supplement for details). Thus the wavefunctions propagate through these points at perfect transmission, and indeed an excellent match of frequencies and their angle dispersion between theory and experiment is found (Fig. 4).

The oscillation spectrum thus can be completely rationalized a priori without quasi-symmetries. However one overlooks a key question about the structure of the wavefunctions, namely why in a metal with eV bandwidth two bands anti-cross with a gap no larger than 2 meV over the

entire Fermi surface. To obtain such a parametrically small gap accidentally, an unreasonable degree of fine-tuning is required that acts simultaneously at many k-points, as well as at a wide range of energies as we will show. Instead, a hidden quasi-symmetry enforces the smallness of the gap at these points, and thus explains why magnetic breakdown at full transparency occurs at any arbitrary angle.

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

$$\mathcal{H}_R = \mathcal{H}_0(\mathbf{k}) + \mathcal{H}_{soc} + \mathcal{H}_{k^2}(\mathbf{k}), \quad (1)$$

where $\mathcal{H}_0(\mathbf{k}) = C_0 + 2A_1(\mathbf{k} \cdot \mathbf{L})$ is the lower-order expansion of the spin-independent Hamiltonian, and three 4-by-4 matrices $\mathbf{L}$ form an emergent angular momentum algebra $[L_i, L_j] = i\varepsilon_{ijk}L_k$ with Levi-Civita symbol ε_{ijk} and $i, j, k = x, y, z$. The SOC term is given by $\mathcal{H}_{soc} = 2\lambda_0(\mathbf{s} \cdot \mathbf{L})$, where $\mathbf{s}$ is the spin operator. $\mathcal{H}_{k^2}(\mathbf{k})$ is the higher-order spin-independent term with its form given in the supplement. Here $\mathcal{H}_0(k) + \mathcal{H}_{k^2}(k)$ is the SOC-free expanded Hamiltonian to second order. By choosing appropriate parameters such as C_0, A_1, λ_0 , the energy dispersion of $\mathcal{H}_R$ well reproduces that from the DFT calculations (see supplement).

A striking feature in the Hamiltonian $\mathcal{H}_R$ is that the SOC term $\mathcal{H}_{soc}$ takes a similar form as the linear-momentum term, just by replacing the momentum $\mathbf{k}$ by spin $\mathbf{s}$. 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 eigen-states is parallel or anti-parallel to the momen-

tum $\mathbf{k}$ and thus we can label the spin states of these bands by $\pm$ in Fig. 1(e). We derive an effective Hamiltonian for the near degenerate bands. This can be done by first projecting the full Hamiltonian $\mathcal{H}_R$ into the 4 closest bands ($1^\pm$ and $2^\pm$ bands) to get a 4-band model and then constructing a 2-band model for the 1^- and 2^+ bands, as discussed in supplement. Up to the first-order perturbation, the 2-band Hamiltonian takes the form $H_{eff} = \epsilon_0 + d_z(\mathbf{k})\sigma_z$, where $d_z(\mathbf{k}) = \lambda_0 - \sqrt{3}\tilde{C}\frac{|k_x k_y k_z|}{k}$ and the form of the function ϵ_0 is given in supplement. Here σ_z is the Pauli matrix on the basis of 1^- and 2^+ bands, λ_0 term comes from the SOC Hamiltonian $\mathcal{H}_{soc}$ and the $\tilde{C}$ term from $\mathcal{H}_{k^2}(\mathbf{k})$. It is striking to see that the operator $\mathcal{M}_{eff} = \sigma_z$ commutes with H_{eff} and thus serves as an *exact* symmetry at the first-order expansion. The existence of $\mathcal{M}_{eff}$ forbids any terms that are coupled to $\sigma_{x,y}$ in the effective Hamiltonian, thus reducing the codimension of a two-level crossing from 3 to 1 and stabilizing a nodal plane, which is defined by the equation $\lambda_0 = \sqrt{3}\tilde{C}\frac{|k_x k_y k_z|}{k}$ in this two-band model. A more accurate and complete description around the Fermi energy is the 4-band model, which shares a similar $\mathbf{k}$ -dependent hidden quasi-symmetry and is essential in deriving the 2-band model (see supplement), and the whole perturbation theory reveals a striking hierarchy structure (41). Higher-order perturbation expansion breaks $\mathcal{M}_{eff}$ through inducing additional terms coupled to $\sigma_{x,y}$ in the effective model and thus leads to a small gap opening of this nodal plane (See supplement). Therefore, $\mathcal{M}_{eff}$ 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 low-symmetry regions of the Brillouin zone, in contrast to symmetry-enforced exact degeneracies. It is this combined structure of symmetry and quasi-symmetry induced degeneracies that forms the basis of the complex structure of the Fermi surface centered at R, and reduces the complexity of the quantum orbits in magnetic fields to two, angle-independent frequencies.

Compared to the exact degeneracy due to symmetry, near degeneracies from quasi-symmetry have unique implications in the Berry curvature distribution in momentum space [Fig. 1(e)].

The U(1) Berry curvature is not well-defined at a degeneracy, while for near-degeneracy, the small gap concentrates significant Berry curvature. In our model, 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 physical phenomena that are related to local Berry curvature, including intrinsic spin Hall effect (42, 43) and quantum non-linear Hall effect (44). The strong Berry curvature is focused into the near-degeneracy, where the quasiparticle tunneling occurs. It will be interesting to explore how this Berry curvature modifies the tunneling conditions in magnetic breakdowns at such quasi-symmetry given near-degeneracies (45).

The observation of quasi-symmetries raises new questions on how wave functions can be woven together in condensed matter systems. The most practical concerns finding the main ingredients for quasi-symmetries to occur in actual materials. The novelty of separating them from crystalline symmetries equally presents a challenge in that a detailed and rigorous analysis of the electronic bands at all low-symmetry k-points is required to identify them. Search programs based on symmetry analysis will not find this type of anomaly without further guideline. It is natural, however, to suspect related compounds crystallizing in the same structure to share this feature, such as e.g. PtGa, PtAl, RhSi and the magnetic MnSi where the influence of magnetism can be explored. (26, 46–54). At the same time, it 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 due to the hidden proximity of the system to a topological state. Here, quantum oscillation experiments may provide guidance by pointing to materials with similarly extreme magnetic breakdown on extended regions on the Fermi surface, which a quasi-symmetry would naturally explain without further fine-tuning. On the theoretical side, it will be critical to elucidate further the physical meaning

of the M_{eff} in CoSi and to evolve the understanding of the mathematical structure behind it. These developments are expected to hold an interesting future for the role of topology. A consensus of high-throughput efforts emerges that 20-30% of materials are topological (20–23). Yet it appears that crystal symmetry may not hold up as the strict barrier it was thought to be, and via quasi-symmetries concepts of topology may reach even further than these estimates predict.

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³⁷⁷ **Competing Interests** The authors declare that they have no competing financial interests.

Figure 1: Illustration of quasi-symmetry. (a) If a crystalline symmetry operation commutes with the Hamiltonian system, the band crossing point is therefore symmetry-protected. (b) In this case the Hamiltonian itself does not commute with the symmetry operation yet its first order perturbation does. This lead to the situation where though the band crossing is numerically avoided but the resulted gap size is negligible for the physical properties of the system. This type of symmetry is called quasi-symmetry. (c) 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 lost of topological character. (d) Quasi-symmetry and crystalline-symmetry protected degenerate planes. (e) The Berry curvature distribution of the 1^- -band [see Fig. 2(e)] at different Fermi energy calculated from the model Hamiltonian Eq. (1).

Figure 2: (a) Crystal structure of CoSi. Co and Si atoms are presented as red and blue spheres respectively. (b) Optical microscope image of a CoSi single crystal sample. (c) Laue diffraction pattern of the grown CoSi single crystal, superimposed with a theoretically simulated one confirming high crystalline quality. (d) Ab-initio-calculated band structure of CoSi. (e) Enlarged section of band structure around R-point. Here 1/2 denotes orbital character while +/- stands for the spin character of the band. (f) 3D view of all Fermi surfaces, which are centered around either R- or Γ - point of the Brillouin zone. (g) 3D view of Fermi surfaces centered around R-point with a quadrant cut.

Figure 3: (a) Scanning electron microscope image of CoSi microdevice. A long bar along [100] direction with a 6 by 6 μm^2 cross section is fabricated by FIB. (b) Temperature dependence of resistivity measured from 300 K to 50 mK. (c) Transverse and longitudinal magnetoresistivity as a function of magnetic field. (d) Temperature-dependent SdH oscillations with field applied along [100] axis. Here $\rho_{osc} = \Delta\rho/\rho_{BG}$, with $\Delta\rho$ the oscillatory part of the magnetoresistivity, and ρ_{BG} the background obtained from a 3rd-order polynomial fit to the magnetoresistivity. (e) Fast-Fourier-transformation spectrum of the SdH oscillations presented in (d) with the field window of 3 to 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. (f) Lifshitz-Kosevich fit to the temperature dependence of cyclotron mass. The fitting yields a cyclotron mass $m_c \sim 0.84 m_e$, comparable to the previously reported values (34–36).

Figure 4: (a) (011)-orbit with symmetry-protected (pink) and quasi-symmetry protected (blue) degenerate points encircled. The symmetry-protected degenerate points always locate at the high symmetry plane while the quasi-symmetry protected crossings are positioned at arbitrary low-symmetry point. (b) Fast-fourier-transformation spectrum of angle-dependent quantum oscillations measured at $T = 2$ K. Here the magnetic field is rotated within (100) plane and the angle is defined between the field direction and $[001]$ axis. (c) Landau orbits and corresponding FFT spectrum for Quasi-symmetry and avoided-crossing scenarios. It is clear that only the quasi-symmetry scenario reproduces FFT peaks that match perfectly well with the experimental data. For the avoided crossing case the predicted frequency is far off. (d) Summary of angular dependence of oscillation frequencies. The contrast between two different scenario again clearly demonstrates that quasi-symmetry is the only option to explain the experimental results of nearly angle-independent oscillation frequencies.

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