Selection rules for quasiparticle interference with internal nonsymmorphic symmetries

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Introduction — Symmetry plays a pivotal role in band theory for the determination of the global features of energy bands, even in the absence of details of the microscopic Hamiltonian $H$. Symmetry characterizes electronic bands by assigning them quantum numbers that label the representation under which they transform. It induces a block diagonalization of the Hilbert space, possibly leading to stable or enforced band crossings in the Brillouin zone (BZ) [6–11]. In these cases, exotic relativistic fermions can be found on the lattice, dominating the transport properties when close to the Fermi level [12]. Even though the experimental inspection of the global symmetry character of Bloch electrons is of unquestioned interest, it is not an easy task. It is notably challenging when the symmetries are nonsymmorphic. These are unique to crystalline environments, combining a point-group action with fractional lattice translations. Direct experimental probes, such as tunneling or photoemission spectroscopy couple directly with either momentum ($\mathbf{p}$) or position ($\mathbf{r}$) eigenvalues and therefore cannot preserve nonsymmorphic symmetries. One would naively think that consequently their eigenvalues cannot be measured by these techniques. In this work, we see that this is indeed not true. There are precise symmetry signatures in the response to spectroscopic probes, which may be relevant for the measurement of crystalline topological materials, for example in Ref. [13].

Our strategy is to find universal, symmetry-enforced, selection rules in the interference pattern created by elastically scattered electrons due to dilute impurities. Fourier-transformed STM, or QPI [14,13], measures fluctuations of the density of states $N(\mathbf{r})$ through a differential conductance map around an isolated impurity. Through a Fourier transformation, it is possible to identify the contribution of elastic scattering events according to a fixed momentum transfer $\mathbf{q}$. The relative intensity of the differential conductance peaks depends on unknown details of the impurity and tunneling elements of the measuring tip, obscuring the interpretation of a QPI pattern. Here we offer an argument based solely on symmetry to extract information from relative peak intensities, remarkably evident in the presence of nonsymmorphic symmetries. Simply put,

$$N_{\nu',\nu}(\mathbf{q}) = 0, \quad \text{if} \quad \omega^{\nu'-\nu}+\beta = 1.$$  (1)

where $\omega$ is a phase that characterizes the unitary symmetry, whose eigenvalues at the $\Gamma$-point are $\omega^\nu$ with $\nu$ an integer; $\alpha$ counts the number of times $\mathbf{q}$ crosses the BZ boundary along the direction of the fractional translation. QPI replications are labelled by different $\alpha$ along the nonsymmorphic direction. Finally, $\beta$ is determined by the properties of the tunneling tip. Even though $\beta$ is not generally fixed, a single measurement can strongly favor one.

Equation (1) gives us a necessary condition for a $\beta$-tip to observe QPI amplitude from a transition between two energy eigenstates with symmetry flavors $\nu$ and $\nu'$ through a momentum transfer of $\mathbf{q}$, when $\mathbf{q}$ crosses the BZ boundary $\alpha$ times. In the following sections we prove this statement by expressing the eigenstates as a function of the local degrees of freedom, position $\mathbf{r}$ and eigenstates of the point group $\tilde{R}$, resolving how the symmetry is manifested when the system is coupled to a local tunneling tip $M$. We find a decomposition of the energy eigenstates relating the Bloch component and the $\tilde{R}$ eigenvalue, leading to scattering selection rules that depend on $\mathbf{q}$.

Eigenstates and internal symmetries — We restrict our study to cases where the symmetry involves internal degrees of freedom, eigenvalues of a local operator $\tilde{O}$. This operator labels the atomic orbitals, $\phi_n(\mathbf{r})$ by a quantum number $n$. It can refer to spin or any representation of the local point group. The form of $\phi_n(r)$ is determined by microscopic details of the Hamiltonian, but nevertheless highly constrained by the symmetries. An energy eigenstate is generally written as

$$|\psi^{\nu_k}_b\rangle = \sum_o \int d\mathbf{r} \phi_o^{\nu_k,b}(\mathbf{r}) |o(\mathbf{r})\rangle ,$$  (2)

where $\nu$ labels the symmetry eigenvalue, $k$ the crystal momentum and $b$ a band index, omitted in the following. The combined notation $|o(\mathbf{r})\rangle \equiv |o\rangle \otimes |\mathbf{r}\rangle$ stands for eigenstates...
of both $\hat{O}$ and $\hat{r}$, forming a basis that satisfies $\langle o; r|o'; r'\rangle = \delta_{o o'} \delta(r - r')$.

We consider a discrete internal transformation, say a rotation, that respects $\hat{R}^n = 1$. Its possible eigenvalues are given by the integer powers of $\omega = \exp\{2\pi i/n\}$, with matrix representation $\rho$ in the orbital basis. Since $\hat{R}$ acts on internal degrees of freedom, such as spin or a direction perpendicular to the lattice plane, it acts trivially on the position eigenstates and commutes with lattice translations $\hat{T}_j|o; r\rangle = |o; r+j\rangle$. Examples to such symmetries are abundant in low dimensional or layered materials.

While for a symmorphic symmetry $\hat{R}$ commutes with the Hamiltonian, in a nonsymmorphic symmetry $\hat{R}$ only commutes with the Hamiltonian when combined with a fractional translation $\hat{T}_{e/n}$ along a unit cell vector $e$ [10] [19]. The combined action $\hat{R}\hat{T}_{e/n}$ relates different points in the unit cell creating a Wyckoff orbit of multiplicity $n$ that ends shifted by a full lattice translation, $(\hat{R}\hat{T}_{e/n})^n = \hat{T}_e$. This fixes the eigenvalues of the nonsymmorphic symmetry to be $\omega^n e^{i\kappa e/n}$. Finally, the energy eigenstates find their coefficients conditioned by lattice translation symmetry and the nonsymmetric symmetry to satisfy

$$\phi^\nu_{\alpha}(r) = e^{i\kappa r} \phi^\nu_{\alpha}(r + j) = \omega^n e^{i\kappa r} \rho^\nu_{\alpha} \phi^\nu_{\alpha}(r + e/n).$$

It is illuminating to first see what [3] implies on the form of the energy eigenstates in real and momentum space. Consider $\hat{R}$ a shift in $o$ by one. We can decompose the position $r$ to be $\bar{r} = a e/n - j$, where $a = 0, ..., n - 1$. Then $\bar{r}$ is defined in one fraction of the unit cell. Then,

$$\langle \psi^\nu_{\kappa} \rangle = \sum_{\alpha j} e^{i\kappa r} \omega^n \int_{\bar{r}} \phi^\nu_{\alpha}(\bar{r})|o - \alpha/n; \bar{r} + a e - j\rangle,$$

Here $\phi_{\alpha}(\bar{r})$ is fixed by the details of the Hamiltonian which are not symmetry dictated. The relationship between contributions of different orbital and position eigenstates is, on the other hand, fixed by symmetry. We can look at a simple one-dimensional example with $n = 2$ and $\rho = \sigma_x$. The band structure, shown Fig.1(a), corresponds to a hopping tight-binding Hamiltonian $H(k) = \sin(k/2) \sigma_x$. With only two bands, there is a perfect locking between the orbital (depicted as upwards and downwards droplets) and the atomic position in the unit cell.

Alternatively, in the eigenbasis of $\hat{R}$ (with eigenvalue $\omega^\lambda$) and momentum $\hat{p} = -i\partial_r$ (with an eigenvalue $p$), Eq. (4) is translated to a restriction on the Fourier coefficients of each Bloch state,

$$\bar{\phi}^\nu_{\lambda}(p) \propto \delta\left(e^{ip} - e^{ik}\right) \delta(\omega^\lambda e^{i\lambda p} - \omega^{\nu}),$$

The first $\delta$-function implies momentum is fixed to differ from $k$ by a reciprocal lattice vector $G$ respecting $\exp\{i\bar{G} \cdot j\} = 1$, which is the essence of Bloch’s theorem. Importantly, the second $\delta$-function implies that $G$ fixes the eigenvalue of the point group, $\lambda$. In the diagonal basis, $|\lambda; p\rangle$ then

$$|\psi^\nu_{\kappa}\rangle = \sum_{\lambda} \phi^\nu_{\lambda - \gamma}(k + G)|\nu - \gamma; k + G\rangle,$$

where we define the shorthand $\gamma = G \cdot e/2\pi \mod n$.

Note that each Bloch component in (6) is characterized by a different point group eigenvalue. From this it follows how bands with different $\nu$’s meet at the boundaries of the BZ: Changing smoothly $k \rightarrow k + G \cdot e$ implies $\gamma \rightarrow \gamma + 1$, and consequently $\nu \rightarrow \nu - 1$ after one cycle. That is, there is an adiabatic connection between states of different $\nu$ at different boundaries of the BZ, which leads to enforced band crossings and justifies the large number of degeneracies present in nonsymmorphic materials [8] [20] [21].

Quasiparticle interference — QPI is a direct measurement of the elastic scattering due to dilute impurities. It is ideal to study symmetry allowed scattering, and it has been extensively used to study topological insulators [22] [27], graphene [28] [29], and high temperature superconductors [17] [30] [34]. An impurity located at $r_0$ that creates (for example) a Gaussian-shaped potential $v(r, r_0) \propto \exp\{-\frac{1}{2}(r - r_0)^2/\xi^2\}$, adds the operator $\hat{\hat{V}} = \int v(r, r_0)\hat{\hat{V}}(r)$, where $\hat{\hat{V}}$ acts on the $\hat{R}$ subspace, to the electron’s Hamiltonian. It is generally not diagonal, and assumed to be random. The tunneling tip can be similarly described by $\hat{M}(r) = |r\rangle\langle r|$, where $\hat{M}$ contains the tunneling elements in orbital space. Finally, the measured local density of states is compactly written as $\hat{N}(r) = -\text{im} \Lambda(r)/\pi$ with

$$\Lambda(r) = Tr \hat{M}(r)\hat{G}\hat{V}\hat{G},$$

where $\hat{G}$ is the retarded Green’s function, and the trace is taken over the quantum numbers $\nu$ and $k$. Performing a Fourier transformation we write $\hat{M}(q) = \int P(|p|\hat{M}(p - q)$, and
\( \hat{V} = \int d^3r \, v(q, r_0) |p - q| \). The phase associated with the impurity position remains as an overall prefactor, as addressed in Ref. [35]. As we show in the supplementary material [36], the block diagonalization of the eigenstates \( |\psi_i\rangle \), and the consequent diagonalization of \( \mathcal{G} \), implies that in Fourier space \( \Lambda(q) \) can be decomposed in a sum of contributions of the form

\[
\Lambda^{\nu\nu'}_{kk'}(q, Q) = T^{\nu\nu'}_{kk'}(q, Q) \mathbf{m}^{\nu'-\gamma} \delta(q - k' + k + Q),
\]

(8)

with \( \alpha \equiv Q \cdot e/2\pi \mod n \). Each summand in (8) describes the interference of incoming and outgoing waves, weighted by a nonuniversal intensity function \( T \). The lattice periodicity determines that all processes satisfy \( q - k' + k = Q \), with \( Q \) a reciprocal lattice vector, fixed by the restriction of \( k \) and \( k' \) to the first BZ. Symmetries within the unit cell impose further conditions, and suppress contributions to the QPI as encoded in the matrix elements of \( \mathbf{m} \). In the nonsymmorphic case, these suppressed contributions depend on \( Q \). More precisely they depend on \( \alpha \), since it indicates whether momentum is transferred along \( e \), see Fig. [1].

The function \( T \), whose explicit form is given in the supplementary material, includes the nonuniversal details that modulate the intensity of the QPI signal. Those include features associated with the impurity, which is only a tool in the experiment, and features associated with the Bloch coefficients, that are dependent on the non symmetry dictated details of the Hamiltonian. The former include the impurity matrix elements, spatial distribution and energy dependence. The exact form of the potential exerted by the impurity may limit the visibility of certain features of the interfering wavefunctions. The latter is determined by the charge distribution within the unit cell. Generally, the first Bloch component is favored and \( \alpha = 0 \) dominates the QPI, but frequently other values of \( \alpha \) are observed as well.

We now focus on what the matrix elements of \( \mathbf{m} \) can tell us about the symmetry dictated features of the interfering electrons, both in the symmorphic and non-symmorphic cases. In the symmorphic case the matrix element in (8) is substituted by \( \mathbf{m}^{\nu'} \nu \). This implies that Eq. (1) is satisfied with \( \alpha = 0 \), provided the \( \mathbf{m} \) respects

\[
\mathbf{m} \hat{R} = \omega^\beta \hat{R} \mathbf{m},
\]

(9)

If, for example, \( \mathbf{m} \) is diagonal in the eigenspace of \( \hat{R} \), the QPI will manifest only scattering between states of equal eigenvalue \( \nu \). This is relevant, for example, in the study of surface states of topological insulators [23, 24], where \( \nu \) relates to spin, and \( \beta \) to the polarization of a magnetic tunneling tip. In contrast is the nonsymmorphic case, due to the correlation between the amplitude of the momentum \( k + G \) in the interfering Bloch states and the quantum state of the intracellular degrees of freedom. The observed channels satisfy Eq. (1), which allows for all scattering channels at all \( \beta \). However, different channels are manifested at different replications, that is, at different \( \alpha \). In Fig. [1(b)] the two replicated signals will be subject to distinct matrix element effects, and thus strongly vary in intensity.

Even though a general measurement will consist of a superposition of \( \beta \) and will generally not be able to fully suppress replications, the relative intensity of different \( \alpha \) contains information about the band representations. There are two ways of retrieving this information. First, in the presence of internal nonsymmorphic symmetries matrix elements will alternate along \( Q_\epsilon \). If the impurity is sharply localized, allowing for the observation of many replications, the alternating intensity of QPI peaks along a preferred direction is a strong indicator of a nonsymmorphic structure. Second, \( \beta \) can be used as a tuning knob, varying the intensity of different \( \alpha \) channels. Experimentally, this can be achieved by combining data of distinct measurements around an impurity, differing in the tip’s position within the unit cell. Since all Hermitian operators can be decomposed as a sum of operators satisfying (9), combining distinct measurements can be used to isolate \( \beta \). To clarify the latter proposal consider the idealized example presented in Fig.2(b-inset), with \( \rho = \sigma_z \) in the orbital basis. Measuring a single orbital is represented by \( m_\pm = \sigma_0 \pm \sigma_z \). Then \( m_\beta \) can be constructed by \( m_0 = m_+ + m_- \) and \( m_1 = m_+ - m_- \). Realistically, a fine tuned superposition is needed, but we note
that intracell spatial resolution has been successfully used to highlight surface states in TaAs [38–40].

**Model calculations** — We calculate the QPI numerically for two one-dimensional tight-binding models [37], a symmorphic and a nonsymmorphic chain and a two-dimensional nonsymmorphic semimetal corresponding to an effective model for ZrSiS [41, 42]. In all cases \( \omega = -1 \).

First, we look at Fig. 2. In the symmorphic case (panels a, c and e), we show a two-orbital model with first and second neighbour hopping. The two bands, which carry different eigenvalues of \( \hat{t} \), cross forming two distinct Dirac points in the BZ. The QPI (panels c and e) depends crucially on \( \tilde{m} \) as expected from (1) but \( \alpha \) plays no role. This implies that the crossing of replications at \( q = \pi \) is only present in panel (c), and the Dirac points can only be seen in panel (e) at both \( q = 0 \) and \( q = 2\pi \). For the nonsymmorphic chain (b, d and f) we consider a four-band model, with two orbitals at each site. We show the QPI for the two lower energy bands. In contrast with the symmorphic case, here \( \beta \) defines which \( \alpha \) signal is observed. This is an evidence for the locking between momentum and \( \hat{R} \) eigenvalues. We find in panels (d) and (f) only two lines, and not four. The crossing at \( q = \pi \) in (d) is absent, and the evidence for the Dirac point appears only either at \( q = 0 \) (d) or at \( q = 2\pi \) (f) but not both. A Dirac point with equal \( \nu \) is typical at the boundaries of the BZ in time-reversal symmetric nonsymmorphic systems.

Now we consider the two-dimensional model in Fig. 3. It can be generally applied to layered nonsymmorphic materials with a glide plane along the surface, with \( e = \hat{x} + \hat{y} \). The relevant physics is well described by a four-band model, with two sets of bands, \( b = 0, 1 \), distinguished by a symmorphic symmetry, protecting a Dirac ring at the Fermi level. The nonsymmorphic symmetry acts on each set separately. Since we are interested in the scattering selection rules for different \( \nu \), we choose to show the QPI of a single set \( b = 0 \). Physically, different bands can occupy different regions in the unit cell, and the impurity position can induce scattering primarily in one set. Consequently, the results are blind to the Dirac ring. We show the density of states (panels a-d) at constant energy \( \nu \), \( \beta \) for the \( b = 0 \) band at different energies. The dashed lines (blue and red) guide the eye to the contributions from different \( \alpha \). The selection rule (1) implies that \( \nu - \nu ' = \beta - \alpha \mod 2 \) is satisfied, resulting in the complete suppression of one \( \nu \) QPI channel, and a remarkable qualitative change in the pattern due to the internal glide symmetry. (1-m) QPI at fixed \( q_x \).

**Conclusion** — In this letter we propose a set of measurement-based selection rules to explore the symmetry aspects of Bloch electrons with STM. We do so by expressing the Green’s function in eigenstates of the point-group and momentum operators. When a nonsymmorphic symmetry is present, this decomposition must be performed at each Bloch component of the energy eigenstates independently. We show that two factors are crucial to define universal selection rules. First, how the tunneling tip couples with the local orbital degrees of freedom (\( \beta \)). Second, whether the momentum transfer between energy eigenstates crosses the boundaries of the BZ along the direction of the fractional translation (\( \alpha \)). The two factors play an analogous role, evident in Eq. (1) and in the similarity of Figs. 2 (d) and (f). Independently of the impurity potential, we show that the relative intensity of QPI replication of different \( \alpha \) contains information about the symmetry representation of Bloch bands and can be revealed by data analysis. That is, to find a signature of internal nonsymmorphic symmetries we should compare QPI peaks of different Brillouin zones. We further propose that in order to overcome measuring limitations imposed by the finite extent of the atomic orbitals and impurities, we can alternatively explore the spatial resolution of STM. Performing distinct measure-
ments around the same impurity, thereby varying the tunneling elements in orbital space, it is possible to select the tip character $\beta$. If the symmetry is nonsymmorphic the two approaches yield similar results. The effect on non-local spatial symmetries and extensions to other experimental techniques will be the focus of future research.

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1. M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, Group theory (2008).
2. C. Bradley and A. Cracknell, The mathematical theory of symmetry in solids: representation theory for point groups and space groups (2010).
3. B. Bradlyn, L. Elcoro, J. Cano, M. Vergniory, Z. Wang, C. Felser, M. Aroyo, and B. Bernevig, Nature 547, 298 (2017).
4. J. Kruthoff, J. d. Boer, J. v. Wezel, C. L. Kane, and R.-J. Slager, Physical Review X 7, 041069 (2017).
5. H. Po, A. Vishwanath, and H. Watanabe, Nature Communications 8, 50 (2017).
6. J. Zakeri, Phys Rev B 26, 3010 (1982).
7. M. Young and C. L. Kane, Phys Rev Lett 115, 126803 (2015).
8. H. Po, H. Watanabe, M. P. Zaletel, and A. Vishwanath, Sci Adv 2, e1501782 (2016).
9. A. Alexandradinata, Z. Wang, and A. B. Bernevig, Phys Rev X 6, 021008 (2016).
10. B. Bradlyn, J. Cano, Z. Wang, M. Vergniory, C. Felser, R. Cava, and B. Bernevig, Science 353, aaf5037 (2016).
11. T. Wehling, B. A.M., and A. Balatsky, Adv Phys 63, 1 (2014).
12. J. Ma, C. Yi, B. Lv, Z. Wang, S. Nie, L. Wang, L. Kong, Y. Huang, P. Richard, P. Zhang, K. Yaji, K. Kuroda, S. Shin, H. Weng, B. Bernevig, Y. Shi, T. Qian, and H. Ding, Nature 363, 0162415 (2017).
13. M. Crommie, C. Lutz, and D. Eigler, Nature 363, 36524a0 (1993).
14. L. Petersen, S. Spring, P. Hofmann, E. Liegsgaard, B. Briner, M. Doering, P. H. Rust, A. Bradshaw, F. Beshenbacher, and E. Plummer, Phys Rev B 57, R6858 (1998).
15. L. Capriotti, D. Scalapino, and R. Sedgewick, Phys Rev B 68, 104508 (2003).
16. T. Pereg-Barnea and M. Franz, Phys Rev B 68, 180506 (2003).
17. Q. Wang and D. Lee, Phys Rev B 67, 020511 (2003).
18. H. Hiller, Am Math Mon 93, 765 (1986).
19. Y. Zhao and A. P. Schnyder, Phys Rev B 94 (2016).
20. S. Young, S. Zaheer, J. Teo, C. Kane, E. Mele, and A. Rappe, Phys Rev Lett 108, 140405 (2012).
21. X. Zhou, C. Fang, W. Tsai, and J. Hu, Phys Rev B 80 (2009).
22. M. H. Guo and M. Franz, Phys Rev B 81 (2010), 10.1103/Phys Rev B.81.041102.
23. J. S. Hofmann, R. Queiroz, and A. P. Schnyder, Phys Rev B 88, 134505 (2013).
24. F. Roushan, J. Seo, C. V. Parker, Y. Hor, D. Hsieh, D. Qian, A. Richardella, M. Hasan, R. Cava, and A. Yazdani, Nature 460, 1106 (2009).
25. H. Beidenkopf, P. Roushan, J. Seo, L. Gorman, I. Drozdov, Y. Hor, R. Cava, and A. Yazdani, Nat Phys 7, 939 (2011).
26. Z. Alpichshev, J. Analytis, J. Chu, I. Fisher, Y. Chen, Z. Shen, A. Fang, and A. Kapitulnik, Phys Rev Lett 104, 016401 (2010).
27. G. Rutter, J. Crain, N. Guisinger, T. L. P. First, and J. Stroscio, Science 317, 219 (2007).
28. T. Pereg-Barnea and A. MacDonald, Phys Rev B 78, 014201 (2008).
29. J. Hoffman, M. K. D. Lee, K. Lang, H. Eisaki, S. Uchida, and J. Davis, Science 297, 1148 (2002).
30. J. Hoffman, E. Hudson, K. Lang, V. Madhavan, H. Eisaki, S. Uchida, and J. Davis, Science 295, 466 (2002).
31. T. Hanaguri, S. Nii, and K. Uchida, Science 328, 474 (2010).
32. D. Podolsky, E. Demler, K. Damle, and B. I. Halperin, Physical Review B 67, 094514 (2003).
33. K. Fujita, M. H. Hamidian, S. D. Edkins, C. K. Kim, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, H. Eisaki, S.-i. Uchida, A. Allais, M. J. Lawler, E.-A. Kim, S. Sachdev, and J. C. S. Davis, Proceedings of the National Academy of Sciences 111, E3026 (2014).
34. E. G. D. Torre, Y. He, and E. Demler, Nature Physics 12, 1052 (2016).
35. Supplementary material available at ......
36. In the numerical calculations we use $H(k) = (3 \cos k + \sin(2k))/4 - 1)(3\sigma_z - 1)$ and $H(k) = (3 + \cos k)\sigma_z + \cos(k/2)\tau_x(2\sigma_z - 1) - \sin(k/2)\tau_z\tau_x$ for the symmorphic and nonsymmorphic chains, respectively.
37. R. Batavaly, N. Morali, N. Avraham, Y. Sun, M. Schmidt, C. Felser, A. Stern, B. Yan, and H. Beidenkopf, Sci Adv 2, e1600709 (2016).
38. H. Inoue, A. Gynis, Z. Wang, J. Li, S. Oh, S. Jiang, N. Ni, A. B. Bernevig, and A. Yazdani, Science 351, 1184 (2016).
39. A. Gynis, H. Inoue, S. Jeon, B. B. Zhou, B. E. Feldman, Z. Wang, J. Li, S. Jiang, Q. D. Gibson, S. K. Kushwaha, J. W. Krizan, N. Ni, R. J. Cava, A. B. Bernevig, and A. Yazdani, New J Phys 18, 105003 (2016).
40. A. Topp, Y. Queiroz, A. Grünies, L. Müchler, A. W. Rost, A. Varykhalov, D. Marchenko, M. Krivenkov, F. Rodolakis, J. L. McChesney, B. V. Lotsch, L. M. Schoop, and C. R. Ast, Phys Rev X 7, 041073 (2017).
41. L. M. Schoop, M. N. Ali, C. Sträßer, A. Topp, A. Varykhalov, D. Marchenko, V. Duppel, S. S. Parkin, B. V. Lotsch, and C. R. Ast, Nat Commun 7, ncomms11696 (2016).
DERIVATION OF THE QUASIPARTICLE INTERFERENCE AMPLITUDE

To analyze the quasiparticle interference pattern, as well as other physical responses, it is convenient to block diagonalize the the Green’s function with respect to the crystal momentum \( k \) and symmetry flavor \( \nu \),

\[
G^\nu_k(E) = \frac{|\psi^\nu_k\rangle \langle \psi^\nu_k|}{(E - i0^+) - \varepsilon^\nu_k} \tag{10}
\]

Here \( \varepsilon^\nu_k \) is the band energy, and we omit the explicit dependence in energy, \( E \), to avoid cluttering. Using the eigenstate decomposition in the main text, Eq. (6), we find,

\[
G^\nu_k = \sum_{G'} |\nu - \gamma; k + G\rangle I^{\nu k}(G, G') |\nu - \gamma'; k + G'\rangle, \tag{11}
\]

where \( \gamma = G \cdot e/2\pi \mod n \) and \( G \) is a reciprocal lattice vector. The relative intensity of each Bloch component takes the explicit form

\[
I^{\nu k}(G, G') = \sum_b \frac{\tilde{\delta}_{\nu - \gamma}^b(k + G)\tilde{\delta}_{\nu - \gamma'}^b(k + G')}{(E - i0^+) - \varepsilon^\nu_k}. \tag{12}
\]

While the divergence from the denominator only depends on \( k \), \( I^{\nu k}(G, G') \) exponentially decays with \( G \) as a consequence of the spatial width of the atomic wavefunctions.

We calculate the quasiparticle interference amplitude by Fourier transforming the local density of states, which is given by

\[
N(r) = -\frac{1}{\pi} \text{Im} \Lambda(r), \quad \Lambda(r) = \text{Tr} \tilde{M}(r)\tilde{G}\tilde{V}\tilde{G}, \tag{13}
\]

where the trace is taken over the internal degrees of freedom of the energy eigenstates \( \nu \) and \( k \). In Fourier space it is translated to

\[
N(q) = \frac{1}{2\pi}\left\{ \Lambda^*(-q) - \Lambda(q) \right\}, \quad \Lambda(q) = \text{Tr} \tilde{M}(q)\tilde{G}\tilde{V}\tilde{G}. \tag{14}
\]

Substituting in (14) the tip and impurity operators

\[
\tilde{M}(q) = \int |\lambda; p\rangle \tilde{m}_\lambda \langle \lambda'; p - q|, \quad \tilde{V} = \int_{p,q} v(q, r_0)|\lambda; p\rangle |\lambda'; p - q|, \tag{15}
\]

as well as the diagonalized Green’s function (11), we find that the QPI amplitude decomposes in

\[
\Lambda(q) = \sum_{\nu, \nu', k,k'} \sum_{G,G',Q,Q'} v(q + Q + Q', r_0) I^{\nu k}(G, G') I^{\nu' k'}(G + Q, G' + Q') \tilde{m}_{\nu - \gamma - \alpha} \tilde{v}_{\nu' - \gamma' - \alpha'} \delta(q - k' + k + Q), \tag{16}
\]

with \( \alpha = Q \cdot e/2\pi \mod n \) and \( \alpha' = Q' \cdot e/2\pi \mod n \) which dictate whether \( Q \) or \( Q' \) crosses the Brillouin zone boundary along the nonsymmetric direction \( e \). The summands in (16) can be combined into

\[
\Lambda(q) = \sum_{\nu, \nu', k,k'; Q, \gamma} \tilde{t}_{\nu k k' \gamma}^{\nu'}(q, Q), \quad \tilde{t}_{\nu k k' \gamma}^{\nu'}(q, Q) = \mathcal{I}_{\nu k k' \gamma}^{\nu'}(q, Q) \tilde{m}_{\nu - \gamma - \alpha} \delta(q - k' + k + Q), \tag{17}
\]

by carrying out the sum over the internal variables

\[
\mathcal{I}_{\nu k k' \gamma}^{\nu'}(q, Q) = \sum_{G,G',Q'} v(q + Q + Q', r_0) I^{\nu k}(G, G') I^{\nu' k'}(G + Q, G' + Q') \tilde{v}_{\nu' - \gamma' - \alpha'} \delta_{\omega_{\nu' - \gamma' - \alpha'} \omega_{\nu - \gamma - \alpha}.} \tag{18}
\]

Note that \( Q \), and consequently \( \alpha \), is fully determined by \( q \) and the crystal momentum \( k \) and \( k' \), since the latter are only defined in the first Brillouin zone. On the other hand \( Q' \), and consequently \( \alpha' \), is summed over. This the a key ingredient to factor out the matrix elements of \( \tilde{m} \). Once we fix the relation,

\[
\tilde{m} \tilde{R} = \omega^\beta \tilde{R} \tilde{m} \tag{19}
\]

it implies that \( \tilde{m}^{\lambda \lambda'} = 0 \) unless \( \omega^{\lambda - \lambda'} = \omega^\beta \). This means that \( \tilde{t}_{\nu k k' \gamma}^{\nu'}(q, Q) \) vanishes unless \( \omega^{\nu' - \nu + \alpha} = \omega^\beta \), for all \( \gamma \). This is the selection rule presented in the main text.

We point out that the matrix elements introduced by \( \tilde{v} \) include \( \alpha' \), not fixed by \( q \). Therefore, they will not enter in the selection
rule for \( N(q) \) if the symmetry is nonsymmorphic. If, on the other hand, the symmetry flavor \( \nu \) is symmorphic, we find that the matrix elements are independent of \( \gamma \) or \( \alpha \). That is, when we decompose the QPI amplitude we find the matrix elements to be independent of the Brillouin zone distance \( Q \),

\[
\Lambda(q) = \sum_{\nu,\nu',k,k'} \sum_Q \Lambda^{\nu\nu'}_{kk'}(q, Q), \quad \Lambda^{\nu\nu'}_{kk'}(q, Q) = \mathcal{I}^{\nu\nu'}_{kk'}(q, Q) \bar{m}^{\nu'}_{\nu} \bar{v}^{\nu'}_{\nu} \delta(q - k' + k + Q),
\]

with

\[
\mathcal{I}^{\nu\nu'}_{kk'}(q, Q) = \sum_{G, G', Q} \nu(q + Q + Q', r_0) \mathcal{I}^{\nu k}_{G, G'} \mathcal{I}^{\nu' k'}_{G + Q, G' + Q'}. \tag{21}
\]

That is, the matrix elements of the impurity factor out and become as relevant as the tip matrix elements. Only for probing symmorphic symmetries the impurity and the tip have an interchangeable role.

Finally, we note that the impurity can be invisible to given bands, and in this way further suppress QPI signals, both in the symmorphic and the nonsymmorphic cases.