Momentum-dependent spin selection rule in photoemission with glide symmetry

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We present a comprehensive theory on the spin- and angle-resolved photoemission spectroscopy (SARPES) of materials with glide-mirror symmetry, focusing on the role of glide symmetry on the spin selection rule. In the glide-symmetric SARPES configuration, where the surface of a material, the incoming light and the outgoing photoelectrons are invariant under a glide reflection, the spin polarization of photoelectrons is determined by the glide eigenvalue of the initial state, which makes SARPES a powerful tool for studying topological phases protected by glide symmetry. We also show that, due to the nonsymmorphic character of glide symmetry, the spin polarization of a photoelectron whose momentum is in the second surface Brillouin zone is the opposite of the spin polarization of a photoelectron which is ejected from the same initial Bloch state but whose momentum is in the first zone. This momentum dependence of spin selection rule clearly distinguishes glide symmetry from mirror symmetry and is particularly important if the Bloch wavevector of the initial state is close to the first surface Brillouin zone boundary. As a proof of principle, we simulate the SARPES from the surface states of KHgSb (010) and investigate how the spin selection rule imposed by the glide symmetry manifests itself in a real material.

I. INTRODUCTION

In study of a crystal possessing a certain set of symmetries, the electronic band energies and wavefunctions at symmetry-invariant crystal momenta provide valuable information on the electronic structure over the whole Brillouin zone. The representation of wavefunctions at a symmetry-invariant $k$ point alone greatly restricts the form of the electronic structure at all the nearby $k$-points. For example, the effective Hamiltonian of the Bi$_2$Se$_3$ (111) surface is nearly isotropic with respect to the crystal momentum $k$ around $\Gamma$ with its leading correction proportional to $k^3$ yielding the hexagonal warping of the Fermi circle thanks to the $C_{3v}$ symmetry at $\Gamma$. In addition to the local information near the high-symmetry points or lines, analysis of symmetry representations at symmetry-invariant $k$ points reveals topological aspects of the electronic structure throughout the entire Brillouin zone. For example, a glide-symmetric two-dimensional material hosts at least one Dirac point along the glidesymmetric line of the Brillouin zone regardless of the strength of the spin-orbit coupling (SOC). Also, the three-dimensional Dirac point of Na$_3$Bi which resides on its fourfold rotation axis is robust against any deformation of the crystal structure as long as the symmetry is preserved.

On the other hand, simulating the photocurrent intensity in angle-resolved photoemission spectroscopy (ARPES) from first principles is quite subtle due to the effects of elastic multiple scattering by ions, inelastic scattering by various collective excitations in a solid (and the finite inelastic lifetime and the inner potential thereby induced), and the change in the electric field of light when the light penetrates the surface of a material. In particular, neglecting the multiple scattering effect by the lattice potential and assuming a photoelectron state to be a plane-wave state even inside the material may often fail to provide accurate values of photocurrent intensities which are necessary to simulate the circular or linear dichroism and the spin polarization of photoelectrons from first principles.

As an important example, if we assume that final states in a photoemission process are plane-wave states, then the dipole matrix element $\langle k' \mid A \cdot p \mid i \rangle = A \cdot k' / \langle k' \mid i \rangle$ vanishes when light polarization $A$ and the momentum of the photoelectron $k'$ are perpendicular to each other. Here, $i$ is the initial electronic state and $|k'\rangle$ the (plane-wave) final state. Similarly, if we assume that final states in spin- and angle-resolved photoemission spectroscopy (SARPES) are the direct product of the plane wave $|k'\rangle$ and a constant spinor $|\sigma^f\rangle (\sigma^f = \pm 1)$, the ratio between the spin-up and spin-down photoelectron intensities would be $\langle k', 1 \mid i \rangle / \langle k', -1 \mid i \rangle$, which cannot explain the dependence of the spin polarization of photoelectrons on $A$ observed in experiments. To avoid this difficulty while retaining the simplicity of the plane-wave approximation for the final states, one may assume that the relevant part of the final state in photoemission processes is the Bloch sum of the atomic orbitals whose phase factor is similar to the plane wave. This approach yields the light-polarization dependence of the spin polarization of photoelectrons which was absent in the simple plane-wave approximation. Still, however, the accurate description of the photon-energy dependence of the ARPES intensities requires a better treatment of final states.

Remarkably, the analysis of ARPES at symmetry-invariant $k$ points can bypass this difficulty and provide useful guidance for interpreting ARPES. The symmetry group of the ARPES configuration including the direction of the light polarization, the momentum of photoelectrons, and the surface of a solid is smaller than the symmetry group of the surface alone in general. However, when the symmetry group of the ARPES configuration is the same as that of the surface, ARPES reflects the rich information on the underlying electronic struc-
metrics, apart from one complex-valued parameter which is a photoelectron state whose momentum is in the first surface Brillouin zone is the momentum dependence in the selection rule imposed by glide symmetry to ARPES, when SOC is negligible, has been studied in several papers. Due to the fractional translational direction of the glide reflection, the spin polarization of the photoelectron whose momentum is in the first surface Brillouin zone is invariant under glide reflection (Fig. 2b); thus, \( k_y^i = k_y^f = 0 \). (Especially, we will only refer to the line node \( k_y^i = 0 \) in the surface Brillouin zone as the glide-invariant line hereafter and will not consider states with \( k_y^i = \pi/c \), which yield photoelectrons breaking the glide symmetry.) Due to the lattice symmetry, the in-plane components of the initial and final states, \( k_y^i = (0, 0, k_z^i) \) and \( k_y^f = (0, 0, k_z^f) \), satisfy

\[
k_y^f - k_y^i = G_y = n(2\pi/c)\hat{\sigma},
\]

where \( G_y \) is a surface reciprocal lattice vector parallel to the glide plane and \( n \) is an integer.

We used the dipole approximation to describe the photoemission. Then the spin polarization of the photoelectron is given by \( \mathbf{P}^f = \langle \chi |2\mathbf{S}|\chi\rangle/\langle\chi|\chi\rangle \) with \( \langle\chi|\chi\rangle = \sum_\sigma |\sigma\rangle\langle f, \sigma|\mathbf{A} \cdot \mathbf{p}|i\rangle \), where \( \mathbf{S} \) denotes the spin operator in unit of \( \hbar \), \( \mathbf{A} \) a constant vector parallel to the glide plane from a mirror plane. Our paper develops a unified and comprehensive theory to explain the photoelectric effect from materials with mirror or glide symmetry. For demonstration purposes, we apply our theory to the SARPES from the so-called hourglass surface states of KHgSb (010).
light polarization, and \( |\sigma \hat{y}\rangle \) the constant two-component spinor fully polarized along \( \sigma \hat{y} \).

After deriving the SARPES selection rule imposed by the glide symmetry, we numerically demonstrated the validity of the selection rule by simulating the SARPES of the surface bands of KHgSb (010). In order to simulate the electronic structure of KHgSb, we used an \textit{ab initio} tight binding method. We used Quantum Espresso package for density-functional-theory (DFT) calculations of the bulk material\cite{27} with the PBEsol functional\cite{28} for the exchange-correlation energy. The energy cutoff for wavefunctions was set to 80 Ry and the Brillouin zone was sampled on a uniform \( 8 \times 8 \times 8 \) grid.

We constructed maximally localized Wannier functions which accurately describe the bands near the band gap using Wannier90 package\cite{29}. From those Wannier functions, which mainly consist of Hg 6s orbitals and Sb 5p orbitals, we extracted the hopping integrals of the tight-binding model for the surface calculation.

III. RESULTS AND DISCUSSION

Let \( \hat{M}_y \) be the glide operation which acts on a spinor as \( e^{i\pi s_y} \). Since \( k^f \) is on the glide-invariant line, the initial state is an eigenstate of \( \hat{M}_y \):

\[
\hat{M}_y |i\rangle = i\lambda \exp[-ik_z^f c/2] |i\rangle \quad (\lambda = \pm 1).
\]

As is well-known, compared with the eigenvalue of an ordinary mirror operation, the eigenvalue of the glide reflection contains an additional phase factor \( \exp[-ik_z^f c/2] \) which depends on \( k^f \).

Similarly, the final state \( |f, \sigma \hat{y}\rangle \) is also an eigenstate of \( \hat{M}_y \). Since the final state in the asymptotic vacuum is the product of a plane wave \( |ik^f \cdot r\rangle \) and a constant spinor \( |\sigma \hat{y}\rangle \) \textit{no matter how complicated the wavefunction is near or inside the crystal}, the eigenvalue of \( |f, \sigma \hat{y}\rangle \) with respect to the glide symmetry is \( i\sigma \exp[-ik_z^f c/2] \).

When the light is \( p \)-polarized, i.e., the light polarization is parallel to the glide plane, \( \hat{M}_y (A \cdot p) \hat{M}_y^{-1} = -A \cdot p \). Therefore, in this case, the photoemission is allowed only if the glide eigenvalues of the initial and final states are equal:

\[
i\lambda \exp[-ik_z^f c/2] = i\sigma \exp[-ik_z^f c/2].
\]

Using Eq. 1, we see that the photoemission is allowed only if

\[
\sigma = (-1)^n \lambda \quad (p\text{-polarized light}).
\]

Hence, the photoelectrons ejected by \( p \)-polarized light from the initial state with glide eigenvalue \( i\lambda \exp[-ik_z^f c/2] \) is fully spin-polarized along \( \sigma \hat{y} = (-1)^n \lambda \hat{y} \).

Similarly, when the light is \( s \)-polarized, the light polarization is perpendicular to the glide plane, \( \hat{M}_y (A \cdot p) \hat{M}_y^{-1} = -A \cdot p \) and thus the photoemission is allowed only if

\[
\sigma = (-1)^{n+1} \lambda \quad (s\text{-polarized light}).
\]

Thus the photoelectrons ejected by \( p \) and \( s \)-polarized light are fully spin-polarized in the opposite directions. Equations (3), (4) and (5) are the key results of our paper.

The selection rule derived above for a glide-symmetric configuration is clearly different from the selection rule for a mirror-symmetric configuration. If a system is invariant with respect to ordinary mirror reflection \( (x, y, z) \rightarrow (x, -y, z) \) instead of glide reflection, then the mirror eigenvalues of the initial and final states are \( i\lambda \) and \( i\sigma \), respectively, which are \( k \)-independent. Therefore, \( p \)-polarized light allows the transition with \( \sigma = \lambda \) and \( s \)-polarized light allows \( \sigma = -\lambda \) regardless of \( k^f \) or \( k^f \). However, in the glide-symmetric configuration, the glide eigenvalue of the initial state has a \( k^f \)-dependent phase factor while the eigenvalue of the final state contains a \( k^f \)-dependent factor. These two different phase factors do not cancel out, introducing an additional element \( \exp[i(k_f^f - k_z^f)c/2] \) to the selection rule. Therefore, in the glide-symmetric configuration, the photoelectron with momentum \((\sqrt{2mEf}/\hbar^2 - (k_f^f)^2, 0, k_f^f + 2\pi/\ell)\) ejected from the same initial surface state \( |i\rangle \) by the same light are fully spin-polarized in the directions opposite to each other.

We remark that our theory on the glide selection rule is valid for any non-degenerate initial states of a glide-symmetric surface, regardless of the time-reversal symmetry. In the case of a two-dimensional glide-symmetric material, the theory is applicable except only when the material is invariant under \( PT \), the combination of the spatial inversion and the time reversal, which would make every energy band doubly degenerate. Despite its generality, we demonstrate our theory using non-magnetic materials.

Figure 1 shows a typical behavior of the spin polarization of photoelectrons from SARPES on the glide-invariant line of the surface Brillouin zone when the light is \( p \)-polarized, assuming the material is non-magnetic. Since the time-reversal and glide-reflection operators commute, every Kramer pair at \( k_z = 0 \) or \( \pi/\ell \) is composed of two states the glide eigenvalues of which are complex conjugates of each other. Therefore, the glide eigenvalues of a Kramer pair [Eq. 2] at \( k_z = 0 \) must be different from each other \((\pm i)\) while at \( k_z = \pi/\ell \) they must be the same, either 1 or -1. This fact implies that, in Fig. 1, two bands connected to a single Kramer pair at \( k_z = 0 \) have different glide eigenvalues and thus the photoelectrons ejected from those two bands are spin-polarized in opposite directions. Near \( k_z^f = \pi/\ell \), on the other hand, two bands which are degenerate at \( k_z = \pi/\ell \) have the same glide eigenvalue and the spin polarization of the photoelectrons ejected from those two bands are the same.

More importantly, due to the dependence of the glide eigenvalue on the momentum of photoelectrons [Eq. 2],
TABLE I. The selection rules determining the spin polarization of photoelectrons. Here \( n \) is the integer satisfying \( k^{\parallel}_{c} - k^{\parallel}_{s} = n(2\pi/c)\hat{z} \) [see Eq. (1)] and \( \sigma \) denotes the spin of the final state along \( \hat{y} \).

|       | \( p \)-pol. light | \( s \)-pol. light |
|-------|---------------------|---------------------|
| Glide-symmetric: \( M_{p}|i\rangle = i\lambda e^{-ik^{\parallel}_{c}c/2}|i\rangle \) | \( \sigma = \lambda \) | \( \sigma = -\lambda \) |
| Even \( n \) | \( \sigma = \lambda \) | \( \sigma = -\lambda \) |
| Odd \( n \) | \( \sigma = -\lambda \) | \( \sigma = \lambda \) |
| Mirror-symmetric: \( M_{p}|i\rangle = i\lambda|i\rangle \) | \( \sigma = \lambda \) | \( \sigma = -\lambda \) |

The difference in the SARPES behaviors between glide-symmetric and mirror-symmetric configurations is quite remarkable since many physical quantities such as electrical conductivity, Raman tensor, and stiffness tensor in elasticity theory depend only on the point group of the crystal rather than the full space group \( \text{28,29} \). In SARPES, however, due to its momentum resolution, the translation part of a nonsymmorphic symmetry operation plays an important role in determining the spin polarization of photoelectrons, and thus SARPES provides a way to distinguish glide symmetry from mirror symmetry.

Having established the glide-symmetry selection rule, we simulate spin-dependent photoemission from the surface bands of a glide-invariant material KHgSb \((010)\) (Fig. 2) and investigate the manifestation of the glide-symmetry selection rule in this numerical simulation. The \((010)\) surface of KHgSb hosts four branches of the metallic surface bands with the hourglass-like energy-momentum dispersion inside the bulk band gap \( \text{23,24,30,31} \). Due to its large SOC, KHgSb is an appropriate test bed for verifying the spin-selection rule imposed by glide symmetry in the spin-dependent photoemission.

We constructed the Wannier functions from \textit{ab initio} calculation of the bulk material without considering SOC and extracted the hopping integrals among them (Fig. 3a). Together with an on-site spin-orbit coupling term \( \alpha_{\text{SO}} L \cdot S/\hbar^{2} \) with \( \alpha_{\text{SO}} = 0.56 \text{ eV} \) for the 5p-like orbitals at Sb atoms, the resulting tight-binding Hamiltonian well describes the \textit{ab initio} calculation of the bulk where SOC is fully taken into account near the Fermi energy (Fig. 3b). We then constructed a surface slab containing 60 bulk unit cells along the surface normal direction and calculated the surface band structure (Fig. 4), which shows four hourglass surface bands partially buried in bulk bands. We remark that our theory applies to any surface bands on a glide-invariant material KHgSb \((010)\) face bands of a glide-invariant material KHgSb \((010)\) and investigate the manifestation of the glide-symmetry selection rule in this numerical simulation. The \((010)\) surface of KHgSb hosts four branches of the metallic surface bands with the hourglass-like energy-momentum dispersion inside the bulk band gap \( \text{23,24,30,31} \). Due to its large SOC, KHgSb is an appropriate test bed for verifying the spin-selection rule imposed by glide symmetry in the spin-dependent photoemission.

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Since the purpose of our paper is not to accurately calculate the photocurrent intensity in ARPES but to demonstrate the selection rule imposed by glide symmetry, it is not necessary to calculate the photoemission final state exactly. (Nevertheless, as discussed below, a single complex parameter – the ratio of the dipole ma-
The electronic band structure of bulk KHgSb without [(a)] and with [(b)] SOC. Black dots denote the energy eigenvalues obtained from DFT calculations, and solid red curves denote the results obtained from ab initio tight binding models containing Hg 6s and Sb 5p orbitals.

Fig. 4. (a) The electronic band structure of KHgSb (100). (b) Zoom-in of (a) on the hourglass surface bands.

The final state inside the material can be described as the Bloch sum of atomic orbitals:

$$|f, \sigma \hat{y}\rangle = \sum_{\alpha, R} c_{R\alpha} e^{i \mathbf{k} \cdot \mathbf{R}_{\alpha} - R_{\alpha} \cdot \mathbf{y}/2} |\phi_{R\alpha}\rangle.$$  

Here \(\alpha\) denotes the combined index of the atom, orbital and spin in the surface unit cell, \(\mathbf{R}_{\alpha}\) the position of the \(\alpha\)-th atom in the unit cell displaced by the surface lattice vector \(\mathbf{R}\), \(|\phi_{R\alpha}\rangle\) the state representing the \(\alpha\)-th atomic orbital located at \(\mathbf{R}_{\alpha}\), and \(l\) the inelastic mean free path of the final state. We set \(l = 10\) Å and the final state energy \(E' = 13.6\) eV in the calculation below.

Since the surface state is mainly composed of Sb 5p and Hg 6s orbitals, the relevant atomic transition is \(p \rightarrow s\) transition at Sb and \(s \rightarrow p\) transition at Hg by the atomic dipole selection rule. Having this fact in mind, we consider the following three simplified cases: (i) the \(p \rightarrow s\) transition at Sb is dominant and the effect of SOC on the final state is negligible, in which case \(c_{R\alpha}\) in Eq. (6) is a nonzero constant for 5s orbitals at Sb with \(s_y = \sigma/2\) and zero otherwise; (ii) the \(s \rightarrow p\) transition at Hg is dominant, the effect of SOC is very strong, and \(c_{R\alpha}\) is a nonzero constant for 5p_{1/2} orbitals (i.e., 5p orbitals with total angular momentum \(j=1/2\)) at Hg with \(j_y = \sigma/2\) and zero otherwise; (iii) \(c_{R\alpha}\) is taken so that the final states in the preceding two cases are superposed.

For those final states, we show in Fig. 5 the spin polarization of the photoelectrons ejected from the surface state denoted by \(\mathbf{P}\) in Fig. 4, with crystal momentum \(\mathbf{k}^f = (0, 0, 0.45(2\pi/c))\), as a function of the direction of the linear light polarization. Irrespective of the final state (Fig. 5a-5c), the spin polarization of photoelectrons whose momentum is in the first surface Brillouin zone \((\mathbf{k}^f = 0.45(2\pi/c)\hat{\epsilon})\) is along \(-\hat{y}\) when ejected by s-polarized light \((\theta_{ph} = 0^\circ)\) and is along \(+\hat{y}\) when ejected by p-polarized light \((\theta_{ph} = 90^\circ)\). On the contrary, the spin polarization of photoelectrons whose momentum is in the second Brillouin zone (Fig. 5d-5f, \(\mathbf{k}^f = -0.55(2\pi/c)\hat{\epsilon})\) is along \(+\hat{y}\) when ejected by s-polarized light. This result is a direct consequence of the glide symmetry.

When the light is neither s- nor p-polarized, the photoemission configuration breaks the glide symmetry, i.e., \(\mathbf{A} \cdot \mathbf{p}\) is not invariant under the glide reflection. Even in this case, however, any light polarization \(\mathbf{A}\) is a linear combination of s- and p-polarizations \(\mathbf{A}_s\) and \(\mathbf{A}_p\). For example, when the light polarization is rotated from the s polarization by \(\theta_{ph}\), the photoemission matrix element is \(\langle f \sigma | \mathbf{A}_s \cdot \mathbf{p} | i \rangle = \cos \theta_{ph} \langle f \sigma | \mathbf{A}_s | i \rangle + \sin \theta_{ph} \langle f \sigma | \mathbf{A}_p | i \rangle\). (We have suppressed \(\hat{y}\) for simplicity.) Therefore, similar to the mirror-symmetric case, \(\mathbf{A}\), a single complex parameter, namely, the ratio between the matrix elements for s-polarized light \((f(-\sigma) | \mathbf{A}_s \cdot \mathbf{p} | i)\) and for p-polarized light \((f \sigma | \mathbf{A}_p \cdot \mathbf{p} | i)\) with \(\sigma = (-1)^n \lambda\) determines the relative photoemission intensity and the spin polarization of photoelectrons ejected with arbitrary light polarization. Conversely, by measuring the spin polarizations of photoelectrons ejected by light with a few different polarizations, we can obtain the ratio of the matrix elements.
FIG. 5. Spin polarizations of photoelectrons with \( \mathbf{k}^f = (0, 0, 0.45(2\pi/c)) \), ejected from the initial state denoted by P in Fig. 4 assuming that the final state is composed of (a) Sb 5s orbitals, (b) Hg 6p orbitals with \( j = 1/2 \), and (c) a coherent superposition of both. (d-f) The same quantities as (a-c) for photoelectrons with \( \mathbf{k}^f = (0, 0, -0.55(2\pi/c)) \).

Moreover, we claim that the magnitude of that complex parameter is an indicator of tunability of the spin direction of a possible spin-polarized photocathode using glide- or mirror-symmetric materials. If \( |\langle f (\sigma) | \mathbf{A}_s \cdot \mathbf{p} | i \rangle| \ll |\langle f \sigma | \mathbf{A}_p \cdot \mathbf{p} | i \rangle| \), then the SARPES behavior is mostly determined by the \( p \)-polarization component of the light and the spin polarization of photoelectrons will be close to \( \sigma \hat{y} \) unless the \( p \)-polarization component is very small. Even in this case, the photoemission intensity is low due to the small magnitude of \( |\langle f (\sigma) | \mathbf{A}_s \cdot \mathbf{p} | i \rangle|^2 \). A similar argument holds for the case \( |\langle f (\sigma) | \mathbf{A}_s \cdot \mathbf{p} | i \rangle| \gg |\langle f \sigma | \mathbf{A}_p \cdot \mathbf{p} | i \rangle| \). Therefore, the magnitudes of the two matrix elements must be similar in order for the spin polarization of photoelectrons to be tuned easily by changing the light polarization.

IV. CONCLUSIONS

In summary, we have studied spin-resolved ARPES of materials with glide symmetry where the propagating directions of the incident light and outgoing electrons are also in the glide plane. When the light polarization is parallel or perpendicular to the glide plane (say, \( z \bar{x} \) plane), the spin polarization of photoelectrons is \( \pm \hat{y} \), which is perpendicular to the glide plane. Whether the spin polarization is \( +\hat{y} \) or \( -\hat{y} \) is determined by (i) the glide eigenvalue of the initial surface state and (ii) the in-plane momentum of photoelectrons. Regarding (ii), even if the photoelectrons are ejected from a single initial state by the same light, when the in-plane momentum of photoelectrons change by the smallest surface reciprocal lattice vector, the spin of photoelectrons is reversed. In particular, when the momentum of photoelectrons are near the first surface zone boundary, the spin polarizations of the photoelectron and the initial state are either parallel or antiparallel to each other depending on whether the momentum of photoelectrons is near one zone boundary or the other. This momentum-dependent spin selection distinguishes glide symmetry from mirror symmetry. Not only do these results manifest the nonsymmorphic character of glide reflection, they also show that the spin-resolved ARPES is a powerful tool in studying the topo-
logical phases protected by glide symmetry because it directly measures the glide eigenvalue of the initial states. We also have shown that the spin of photoelectrons are fully controlled by a single complex parameter due to glide symmetry and the magnitude of that complex parameter measures the tuning power of the spin of electrons using light.

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For example, consider the Kubo formula for the optical conductivity tensor: \( \sigma_{\alpha\beta}(\omega) \propto \int_0^\beta d\tau \int_0^\infty dt \langle [J_\alpha(-i\hbar\tau), J_\beta(t)] \rangle \), where the angular bracket \( \langle \cdots \rangle \) denotes the thermal ensemble average at a given temperature and \( J \) the total current operator proportional to the sum of the momenta of all electrons inside the material. Since \( J \) is a vector operator invariant with respect to translation, if the crystal has a symmetry \( \mathbf{r} \mapsto A\mathbf{r} + \mathbf{b} \) for some orthogonal matrix \( A \), then \( A^{-1} \sigma(\omega)A = \sigma(\omega) \). This proves that the optical conductivity is invariant under the action of the point group, which is the quotient of the space group by its translational subgroup. In particular, mirror and glide symmetries impose the same constraint on \( \sigma(\omega) \) as long as their invariant plane is the same.

C. Ma, J. and 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. A. Bernevig, Y. Shi, T. Qian, and H. Ding, “Experimental evidence of hourglass fermion in the candidate nonsymmorphic topological insulator KHgSb,” Sci. Adv. 3 (2017).