Supplementary Information for
"Shift vector as the geometric origin of beam shifts"

Wavepacket peaks from stationary phase analysis

In this section, we detail the standard method of stationary phases used to determine the wavepacket center. Using Eqs. (1), (2), and (3) in the main text, and expressing the Bloch overlaps as $\langle u^{\mathrm{i,r}}(\mathbf{p})|u^{\mathrm{i,r}}(\mathbf{p}+\mathbf{q})\rangle = \exp[-i\mathbf{A}^{\mathrm{i,r}}(\mathbf{p})\cdot\mathbf{q}+\mathcal{O}(q^2)]$, the intensity profiles $|\Psi^{\mathrm{i,r}}(\mathbf{r},z=0)|^2$ on the $z=0$ plane can be expressed as

$$|\Psi^{\mathrm{i,r}}(\mathbf{r},0)|^2 = \int \mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}\, W(\mathbf{p},\mathbf{q})\exp[i\theta^{\mathrm{i,r}}(\mathbf{p},\mathbf{q},\mathbf{r})], \quad \text{(S-1)}$$

where $W(\mathbf{p},\mathbf{q}) = f(\mathbf{p})f(\mathbf{p}+\mathbf{q})\exp[\mathcal{O}(q^2)]$ is a composite amplitude profile, and

$$\theta^{\mathrm{i}}(\mathbf{p},\mathbf{q},\mathbf{r}) = \mathbf{q}\cdot[\mathbf{r}-\mathbf{A}^{\mathrm{i}}(\mathbf{p})]+\mathcal{O}(q^2), \quad \text{(S-2)}$$

$$\theta^{\mathrm{r}}(\mathbf{p},\mathbf{q},\mathbf{r}) = \mathbf{q}\cdot[\mathbf{r}-\mathbf{A}^{\mathrm{r}}(\mathbf{p})]+\phi^{\mathrm{r}}(\mathbf{p}+\mathbf{q})-\phi^{\mathrm{r}}(\mathbf{p})+\mathcal{O}(q^2), \quad \text{(S-3)}$$

are composite phase factors that include both phase information of the superposition of plane waves comprising the beam, as well as the Berry connection $\mathbf{A}^{\mathrm{i,r}}(\mathbf{p}) = \langle u^{\mathrm{i,r}}(\mathbf{p})|i\nabla_{\mathbf{p}}u^{\mathrm{i,r}}(\mathbf{p})\rangle$.

When the amplitude profile $f(\mathbf{p})$ is sharply peaked around $\bar{\mathbf{p}}$, the composite amplitude profile $W(\mathbf{p},\mathbf{q})$ is similarly sharply peaked around $(\bar{\mathbf{p}},\mathbf{0})$. This can be verified by noting $\nabla_{\mathbf{p}}W(\mathbf{p},\mathbf{q})|_{(\bar{\mathbf{p}},\mathbf{0})} = \nabla_{\mathbf{q}}W(\mathbf{p},\mathbf{q})|_{(\bar{\mathbf{p}},\mathbf{0})} = 0$.

The (real-space) peak position $\bar{\mathbf{r}}^{\mathrm{i,r}}$ of $|\Psi^{\mathrm{i,r}}(\mathbf{r},z=0)|^2$ can then be directly determined by the standard stationary phase analysis applied onto Eq. (S-1). In particular, this requires that

$$\nabla_{\mathbf{q}}\theta^{\mathrm{i,r}}[\bar{\mathbf{p}},\mathbf{q},\bar{\mathbf{r}}^{\mathrm{i,r}}]|_{\mathbf{q}\to\mathbf{0}} = 0 \quad \text{(S-4)}$$

yielding a (real-space) peak position for $|\Psi^{\mathrm{i,r}}(\mathbf{r},z=0)|^2$ as

$$\bar{\mathbf{r}}^{\mathrm{i}} = \mathbf{A}^{\mathrm{i}}(\bar{\mathbf{p}}), \quad \bar{\mathbf{r}}^{\mathrm{r}} = \mathbf{A}^{\mathrm{r}}(\bar{\mathbf{p}})-\nabla_{\mathbf{p}}\phi^{\mathrm{r}}(\mathbf{p})|_{\bar{\mathbf{p}}}. \quad \text{(S-5)}$$

This demonstrates that the peak position of Bloch wavepackets depend on both the internal structure of Bloch eigenstates [encoded in $\mathbf{A}^{\mathrm{i,r}}(\bar{\mathbf{p}})$] as well as the superposition phases $\phi(\mathbf{p})$. We note, parenthetically, that $\bar{\mathbf{r}}$ is gauge variant and captures the intra-cell coordinate [29, 30] for a Bloch wave packet, arising from linear combinations of Bloch eigenstates in the unit cell. However, as discussed in the main ext, the difference between $\bar{\mathbf{r}}^{\mathrm{i}}$ and $\bar{\mathbf{r}}^{\mathrm{r}}$ is gauge invariant.

Vanishing of $\Delta\bar{r}^{\mathrm{ext}}_{\mathrm{IF}}$ with mirror symmetry

In the main text, we have shown that $\Delta\bar{r}^{\mathrm{ext}}_{\mathrm{IF}} = 0$ when we have a continuous rotational symmetry (e.g., an emergent continuous rotational symmetry can naturally arise in the low-energy description of many materials).

Beyond this continuous rotational symmetry that emerges at low energy, another example of a vanishing $\Delta\bar{r}^{\mathrm{ext}}_{\mathrm{IF}} = 0$ is when the system has mirror symmetries (a discrete symmetry), which is very common in crystals. If the in-plane incident momentum $\bar{\mathbf{p}} = (\bar{p},0)$ is parallel to the mirror plane, then we have $\mathcal{W}^{\mathrm{ext}}(\bar{p},+q_y) = \mathcal{W}^{\mathrm{ext}}(\bar{p},-q_y)$, and

$$\begin{aligned}\Delta\bar{r}^{\mathrm{ext}}_{\mathrm{IF}} &= \lim\nolimits_{\delta q_y\to 0}\frac{\arg[\mathcal{W}^{\mathrm{ext}}(\bar{p},+\delta q_y)]-\arg[\mathcal{W}^{\mathrm{ext}}(\bar{p},0)]}{+\delta q_y}\\ &= -\lim\nolimits_{\delta q_y\to 0}\frac{\arg[\mathcal{W}^{\mathrm{ext}}(\bar{p},-\delta q_y)]-\arg[\mathcal{W}^{\mathrm{ext}}(\bar{p},0)]}{-\delta q_y}\\ &= -\Delta\bar{r}^{\mathrm{ext}}_{\mathrm{IF}} = 0.\end{aligned} \quad \text{(S-6)}$$

Uniqueness of auxiliary state vector $|v(\mathbf{p})\rangle$

In the main text, we showed that the wavefunction continuity requirement at the boundary leads to $u^{\mathrm{i}}(\mathbf{p})+r(\mathbf{p})u^{\mathrm{r}}(\mathbf{p}) = t(\mathbf{p})w^{\mathrm{t}}(\mathbf{p})$, where $u^{\mathrm{i,r}}(\mathbf{p})$ and $w^{\mathrm{t}}(\mathbf{p})$ are two-component eigenvectors. This equation corresponds to two-band systems [16–20] which has a single reflected (transmitted) channel for a fixed incident frequency. In this case, assuming the transmitted mode is $|w^{\mathrm{t}}(\mathbf{p})\rangle = [w^{\mathrm{t},(1)}(\mathbf{p}),w^{\mathrm{t},(2)}(\mathbf{p})]^T$, then the unique auxiliary state vector is $\langle v(\mathbf{p})| = [w^{\mathrm{t},(2)}(\mathbf{p}),-w^{\mathrm{t},(1)}(\mathbf{p})]$, as can be readily verified: $\langle v(\mathbf{p})|w^{\mathrm{t}}(\mathbf{p})\rangle = 0$. Using the auxiliary state vector $v(\mathbf{p})$, the reflection coefficient reads $r(\mathbf{p}) = -\langle v(\mathbf{p})|u^{\mathrm{i}}(\mathbf{p})\rangle\langle v(\mathbf{p})|u^{\mathrm{r}}(\mathbf{p})\rangle^{-1}$.

We note that one can certainly choose an arbitrary $U(1)$ gauge for $|v(\mathbf{p})\rangle$, but this will not affect the physical result of the shift vector $\Delta\bar{\mathbf{r}}$, because the auxiliary state vector appears in pairs as $|v(\mathbf{p})\rangle\langle v(\mathbf{p})|$ in the Wilson loop [see Eq. (7) in the main text].

Below we use a specific example [20] to concretely illustrate this procedure. We emphasize, however, that the formula for $r(\mathbf{p})$ and the shift in the main text are general. We proceed by considering the following two-band model:

$$H = \begin{bmatrix} p_y & (p_x^2-m_z)-ip_z \\ (p_x^2-m_z)+ip_z & -p_y \end{bmatrix}, \quad \text{(S-7)}$$

in which

$$m_z = \begin{cases} +m_0>0, & z>0, \text{ Weyl media,} \\ -m_1<0, & z<0, \text{ gapped media.}\end{cases} \quad \text{(S-8)}$$

Inside the Weyl media where $z>0$, the dispersion relations for two bands are $\pm[(p_x^2-m_0)^2+p_y^2+p_z^2]$. If we focus on the positive branch, and fix the incident energy to be $\epsilon_0>m_0>0$, the eigenvector $|u^{\mathrm{i,r}}(\mathbf{p})\rangle$ reads

$$|u^{\mathrm{i,r}}(\mathbf{p})\rangle = \begin{pmatrix}\cos[\theta^{\mathrm{i,r}}(\mathbf{p})/2]\\ \sin[\theta^{\mathrm{i,r}}(\mathbf{p})/2]\exp[i\phi^{\mathrm{i,r}}(\mathbf{p})]\end{pmatrix}, \quad \text{(S-9)}$$

where $\cos[\theta^{\mathrm{i,r}}(\mathbf{p})] = p_y/\epsilon_0$, $\tan[\phi^{\mathrm{i,r}}(\mathbf{p})] = \mp p_z(\mathbf{p})/(p_x^2-m_0)$, and $p_z(\mathbf{p}) = [\epsilon_0^2-(p_x^2-m_0)^2-p_y^2]^{1/2}$. We note that the negative branch with a dispersion $-[(p_x^2 - m_0)^2 + p_y^2 + p_z^2]$ cannot support a reflected mode at the incident energy $\epsilon_0 > 0$.

In the gapped media where $z < 0$, the dispersion relation for the two bands are $\pm[(p_x^2 + m_1)^2 + p_y^2 + p_z^2]$. The transmitted eigenvector $|w^{\rm t}(\mathbf{p})\rangle$ with energy $\epsilon_0 > 0$ reads

$$|w^{\rm t}(\mathbf{p})\rangle = \begin{pmatrix} \cos[\theta^{\rm t}(\mathbf{p})/2] \\ \sin[\theta^{\rm t}(\mathbf{p})/2]\exp[i\phi^{\rm t}(\mathbf{p})] \end{pmatrix}, \tag{S-10}$$

where $\cos[\theta^{\rm t}(\mathbf{p})] = p_y/\epsilon_0$, $\tan[\phi^{\rm t}(\mathbf{p})] = -p_z^{\rm t}(\mathbf{p})/(p_x^2 + m_1)$, and $p_z^{\rm t}(\mathbf{p}) = [\epsilon_0^2 - (p_x^2 + m_1)^2 - p_y^2]^{1/2}$. Again, we note that the negative branch with a dispersion $-[(p_x^2 + m_1)^2 + p_y^2 + p_z^2]$ can not support any transmitted mode at the incident energy $\epsilon_0 > 0$.

In this case, the auxiliary state vector reads

$$\langle v(\mathbf{p})| = \big(\sin[\theta^{\rm t}(\mathbf{p})/2]\exp[i\phi^{\rm t}(\mathbf{p})], -\cos[\theta^{\rm t}(\mathbf{p})/2]\big), \tag{S-11}$$

which can be used directly in the formula for the reflection coefficient: $r(\mathbf{p}) = -\langle v(\mathbf{p})|u^{\rm i}(\mathbf{p})\rangle\langle v(\mathbf{p})|u^{\rm r}(\mathbf{p})\rangle^{-1}$. We note that when $\epsilon_0 < m_1$, $p_z^{\rm t}(\mathbf{p}) \to -i\kappa^{\rm t}(\mathbf{p})$ becomes imaginary and total reflection occurs.

This procedure also applies to models with a higher number of bands. For example, four-band models: in Refs. [21, 22], the authors studied the Andreev reflections at metal/superconductor interfaces, the wavefunction continuity requirement at the interface leads to $\psi^{e+} + r\psi^{e-} + r_A\psi^{h-} = t_+\psi_+^{\rm S} + t_-\psi_-^{\rm S}$, where ψ's are four-component state vectors, while r's and t's are reflection and transmission coefficients for two reflected and two transmitted channels. In this case, to extract r_A, a unique four-component auxiliary state vector $|v\rangle$ can be constructed using a Gram-Schmidt process, by satisfying the orthogonal relation $\langle v|\psi^{e-}\rangle = \langle v|\psi_+^{\rm S}\rangle = \langle v|\psi_-^{\rm S}\rangle = 0$.

For both the two-band [16–20] and four-band [21, 22] examples, their wavefunction continuity requirements follow a general form:

$$u^{\rm i}(\mathbf{p}) + \sum_{\mu=1}^{n_1} r_\mu(\mathbf{p})u_\mu^{\rm r}(\mathbf{p}) = \sum_{\nu=1}^{n_2} t_\nu(\mathbf{p})w_\nu^{\rm t}(\mathbf{p}), \tag{S-12}$$

where u's and w's are N-component state vectors, r's and t's are reflection and transmission coefficients, and $n_1 + n_2 = N$ counts the total number of reflected and transmitted channels allowed by energy conservation, with $N = 2$ or $N = 4$ for two-band or four-band models. This reflects the fact that N linear equations [Eq. (S-12)] can determine N unknown variables $\{r_\mu(\mathbf{p}), t_\nu(\mathbf{p})\}$, where $\mu(\nu) = 1, \ldots, n_{1(2)}$. To extract $r_i(\mathbf{p})$ that we are interested in, we can construct the unique state vector $|v(\mathbf{p})\rangle$ using the Gram-Schmidt process described above by satisfying the orthogonal relation $\langle v(\mathbf{p})|u_{\mu\neq i}^{\rm r}(\mathbf{p})\rangle = \langle v(\mathbf{p})|w_\nu^{\rm t}(\mathbf{p})\rangle = 0$ where $\mu(\nu) = 1, \ldots, n_{1(2)}$.

We expect this scheme for constructing a unique auxiliary state vector $|v(\mathbf{p})\rangle$ to obtain the reflection (or indeed, the transmission) coefficient can be readily extend to more general cases, especially for models with an equal number $N/2$ for both conduction bands and valence bands. In this case, the total number of reflected and transmitted channels allowed by energy conservation is N, which is the same as the number of linear equations provided by the wavefunction continuity requirement.