Supplementary Information for "Geometric photon-drag effect and nonlinear shift current in centrosymmetric crystals"

A. NONLINEAR RESPONSE THEORY AND DERIVATION OF PHOTON-DRAG SHIFT CURRENT

In this section, we will provide a full quantum mechanical derivation of the photon-drag shift current. We begin with the Hamiltonian describing the material and its interaction with incident electro-magnetic (EM) irradiation with a finite wavevector [21]

$$\mathcal{H} = \mathcal{H}^{(0)} + \mathcal{V}, \quad \mathcal{V} = -e\boldsymbol{\mathcal{A}}(\mathbf{r},t)\cdot\mathbf{v}^{(0)}e^{\eta t}, \quad \mathbf{v}^{(0)} = (i/\hbar)[\mathcal{H}^{(0)},\mathbf{r}], \tag{S-1}$$

where $\mathcal{H}^{(0)}(\mathbf{r})$ is the hamiltonian of the material in the absence of light-matter interaction, $\mathcal{V}$ describes the finite wavevector (EM) light-matter interaction [21]. We note that Eq. (S-1) has recently been used to describe non-vertical transitions in a hybrid semiconductor-plasmonic heterostructure [21]; $\mathcal{V}$ can be obtained directly from the bare hamiltonian via minimal coupling and employing the velocity gauge [18, 21]. $\boldsymbol{\mathcal{A}}(\mathbf{r},t)$ is the vector potential of the incident EM irradiation, e is the carrier charge, and $\eta \to 0^+$ ensures that the EM/light-matter interaction is turned on adiabatically. The EM irradiation can comprise (oblique) incident light as well as the enhanced electromagnetic fields of polaritons (e.g., plasmons).

The bare Hamiltonian is diagonalized by the quantum states $|\psi_\alpha\rangle$:

$$\mathcal{H}^{(0)}|\psi_\alpha\rangle = \epsilon_\alpha|\psi_\alpha\rangle, \quad \epsilon_\alpha = \hbar\omega_\alpha, \tag{S-2}$$

where α (greek letter index) is a shorthand for $\alpha = n_\alpha, \mathbf{p}_\alpha$ that depend on the quantum numbers in the material, e.g., band index n_α, wave vector $\mathbf{p}_\alpha$. Where appropriate, we will switch to explicitly identifying the quantum numbers.

As we will see below, the finite wavevector of the irradiation [captured in $\boldsymbol{\mathcal{A}}(\mathbf{r},t)$] enables non-vertical transitions and the photon-drag shift current discussed in the main text. For concreteness, we will consider incident EM fields: $\boldsymbol{\mathcal{E}}(\mathbf{r},t) = (1/2)(\mathbf{E}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + \text{c.c.})$ with $\mathbf{E}$ the electric field amplitude. Using these fields, we have

$$\langle\psi_\alpha|\mathcal{V}|\psi_\beta\rangle \equiv \frac{1}{2}e^{\eta t}\sum_{\zeta=\pm1}\mathcal{V}^{\zeta}_{\alpha\beta}(\mathbf{k})e^{-i\zeta\omega t}, \quad \mathcal{V}^{\zeta}_{\alpha\beta}(\mathbf{k}) = \frac{e}{i\zeta\omega}\mathbf{E}^{(\zeta)}\cdot\langle\psi_\alpha|e^{i\zeta\mathbf{k}\cdot\mathbf{r}}\mathbf{v}^{(0)}|\psi_\beta\rangle, \tag{S-3}$$

where $\mathbf{E}^{(+1)} = \mathbf{E}$ and $\mathbf{E}^{(-1)} = \mathbf{E}^*$, and the latter matrix element imposes quasi-momentum conservation (modulo reciprocal lattice vector). Indeed, writing out the form of the eigenstates in a crystal $|\psi_\alpha\rangle, |\psi_\beta\rangle$ yields $\mathcal{V}^{\zeta}_{\alpha\beta}(\mathbf{k}) = (e/i\zeta\omega)\mathbf{E}^{(\zeta)}\cdot\langle u_{n_\alpha}(\mathbf{p}_\alpha)|\hat{\boldsymbol{\nu}}|u_{n_\beta}(\mathbf{p}_\beta)\rangle\delta_{\mathbf{p}_\beta+\zeta\mathbf{k};\mathbf{p}_\alpha}$, where $|u_n(\mathbf{p})\rangle$ are Bloch (periodic) states. Here the velocity operator is $\hat{\boldsymbol{\nu}} = \partial H(\mathbf{p})/\hbar\partial\mathbf{p}$, where $H(\mathbf{p})$ is the Bloch hamiltonian. Throughout our main text and the Supplementary Information, $\mathbf{p}$ denotes wavevector instead of momentum. For simplicity, and because the wavevector of light as well as that of other polaritons are much smaller than the size of a Brillouin zone, we will confine ourselves to transitions within the first Brillouin zone. Here we used $\partial_t\boldsymbol{\mathcal{A}}(\mathbf{r},t) = \boldsymbol{\mathcal{E}}(\mathbf{r},t)$ and we have set $c = 1$ without loss of generality throughout.

We now proceed to derive the photon-drag shift current from nonlinear response theory. In so doing, we first note that the equation of motion for the density matrix, $\varrho(t)$, is

$$\frac{\partial}{\partial t}\varrho = -\frac{i}{\hbar}[\mathcal{H},\varrho] \tag{S-4}$$

and can be expanded order by order (in successive powers of the perturbation $\mathcal{V}$)

$$\varrho(t) = \varrho^{(0)} + \varrho^{(1)}(t) + \varrho^{(2)}(t) + \cdots \tag{S-5}$$

where $\varrho^{(0)}$ is the zeroth order density matrix (i.e. the equilibrium density matrix in the absence perturbation) that is purely diagonal in α: $\varrho^{(0)}_{\alpha\beta} = \langle\alpha|\varrho^{(0)}|\beta\rangle = \delta_{\alpha\beta}f(\epsilon_\alpha)$ with $f(\epsilon_\alpha) = [1+\exp\{\beta(\epsilon_\alpha-\mu)\}]^{-1}$ the Fermi distribution function.

Using Eq. (S-3) above, the higher order density matrices can be obtained iteratively from Eq. (S-4) [8]. For instance, the first order density matrix is

$$\varrho^{(1)}_{\alpha\beta}(t) = \langle\alpha|\varrho^{(1)}(t)|\beta\rangle = \frac{e^{\eta t}}{2}\sum_{\zeta=\pm1}\frac{\mathcal{V}^{\zeta}_{\alpha\beta}(\mathbf{k})}{\hbar}(\varrho^{(0)}_{\alpha\alpha} - \varrho^{(0)}_{\beta\beta})\frac{e^{-i\zeta\omega t}}{\omega_{\alpha\beta} - \zeta\omega - i\eta} \tag{S-6}$$

where $\omega_{\alpha\beta} = \omega_\alpha - \omega_\beta$, and the greek indices denote the eigenstates of the bare hamiltonian as in Eq. (S-2).

In the same fashion, we obtain the second order density matrix as

$$\varrho^{(2)}_{\alpha\beta}(t) = \langle\alpha|\varrho^{(2)}(t)|\beta\rangle = \frac{-1}{4\hbar^2}\sum_{\gamma}\sum_{\zeta_1,\zeta_2=\pm1}\Big(\frac{\mathcal{V}^{\zeta_1}_{\alpha\gamma}(\mathbf{k})\mathcal{V}^{\zeta_2}_{\gamma\beta}(\mathbf{k})}{\omega_{\alpha\beta}-(\zeta_1+\zeta_2)\omega-i2\eta}\frac{\varrho^{(0)}_{\gamma\gamma}-\varrho^{(0)}_{\beta\beta}}{\omega_{\gamma\beta}-\zeta_2\omega-i\eta} - \frac{\mathcal{V}^{\zeta_2}_{\alpha\gamma}(\mathbf{k})\mathcal{V}^{\zeta_1}_{\gamma\beta}(\mathbf{k})}{\omega_{\alpha\beta}-(\zeta_1+\zeta_2)\omega-i2\eta}\frac{\varrho^{(0)}_{\alpha\alpha}-\varrho^{(0)}_{\gamma\gamma}}{\omega_{\alpha\gamma}-\zeta_2\omega-i\eta}\Big)e^{-i(\zeta_1+\zeta_2)\omega t}e^{2\eta t}. \tag{S-7}$$

where ζ_1,ζ_2 capture the contributions in Eq. (S-3).

The induced current density (response) can be obtained by taking traces with the density matrix: $\mathbf{j}(t) = \mathrm{Tr}[\varrho(t)\,\mathbf{J}] = \sum_{\alpha\beta}\varrho_{\alpha\beta}(t)\mathbf{J}_{\beta\alpha}$, where $\mathbf{J} = e(i/\hbar)[\mathcal{H},\mathbf{r}]$ and $\mathbf{J}_{\beta\alpha} = \langle\beta|\mathbf{J}|\alpha\rangle$ is the current density matrix element. As is customary in the literature [8, 9, 17, 18], it will be useful to delineate the induced current density into two sources, namely off-diagonal and on-diagonal currents (see explanation below):

$$\mathbf{j}(t) = \mathbf{j}_{\rm off-diag}(t) + \mathbf{j}_{\rm on-diag}(t), \quad \mathbf{j}_{\rm off-diag}(t) = \sum_{\alpha\neq\beta}\varrho_{\alpha\beta}(t)\mathbf{J}_{\beta\alpha}, \quad \mathbf{j}_{\rm on-diag}(t) = \sum_{\alpha}\varrho_{\alpha\alpha}(t)\mathbf{J}_{\alpha\alpha}. \tag{S-8}$$

Bulk photovoltaic currents arise as the DC contribution to $\mathbf{j}(t)$ at second order in the applied EM fields, $\boldsymbol{\mathcal{E}}$. We denote these DC bulk photovoltaic currents as $\mathbf{j}^{(2)}$ [8, 9, 17, 18]. Indeed, as we will see below, the resonant contributions to the (second order) off-diagonal current, $\mathbf{j}^{(2)}_{\rm off-diag}$, is called the **shift photocurrent** (the subject of our main text) [8, 9, 17]; similarly, the resonant contributions to the (second order) on-diagonal current, $\mathbf{j}^{(2)}_{\rm on-diag}$, is called the injection current [9, 17]. Recently, off-resonant contributions to bulk photovoltaic currents have also been discussed [18]. We will analyze each of them in turn.

A1. Photon-drag Shift Current

We now turn to analyzing the photon-drag shift current. In so doing, we first collect the DC contributions of $\mathbf{j}_{\rm off-diag}$ that are second order in the EM fields $\boldsymbol{\mathcal{E}}$ in Eq. (S-8) [i.e. $\zeta_1+\zeta_2=0$]. Performing momentum conservation and expressing the matrix elements in terms of band indices and wavevectors with the states $|\alpha\rangle = |n,\mathbf{p}+\zeta\mathbf{k}/2\rangle$ and $|\beta\rangle = |m,\mathbf{p}-\zeta\mathbf{k}/2\rangle$, the second order off-diagonal current reads as

$$\mathbf{j}^{(2)}_{\rm off-diag} = \frac{e}{4\hbar^2}\lim_{\eta\to0^+}\sum_{n,m,\zeta=\pm1,\mathbf{p}}\frac{f^{\zeta}_{nm}(\mathbf{p},\mathbf{k})}{\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k})-\zeta\omega-i\eta}\Big[V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})\nabla_{\mathbf{p}}V^{-\zeta}_{mn}(\mathbf{p},\mathbf{k}) + i\mathbf{A}^{\zeta}_{nm}(\mathbf{p},\mathbf{k})V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})V^{-\zeta}_{mn}(\mathbf{p},\mathbf{k})\Big], \tag{S-9}$$

where $f^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) = f[\epsilon_n(\mathbf{p}+\zeta\mathbf{k}/2)] - f[\epsilon_m(\mathbf{p}-\zeta\mathbf{k}/2)]$ is the difference between Fermi functions, $\hbar\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) = \epsilon_n(\mathbf{p}+\zeta\mathbf{k}/2)-\epsilon_m(\mathbf{p}-\zeta\mathbf{k}/2)$, the short-hand notation for Berry connection *difference* $\mathbf{A}^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) \equiv \mathbf{A}_n(\mathbf{p}+\zeta\mathbf{k}/2)-\mathbf{A}_m(\mathbf{p}-\zeta\mathbf{k}/2)$, and the (roman typeset) $V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})$ matrix element is

$$V^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) = (e/i\zeta\omega)\mathbf{E}^{(\zeta)}\cdot\langle u_n(\mathbf{p}+\zeta\mathbf{k}/2)|\hat{\boldsymbol{\nu}}|u_m(\mathbf{p}-\zeta\mathbf{k}/2)\rangle. \tag{S-10}$$

In obtaining Eq. (S-9), we have used the Bloch state identity [8]:

$$\sum_{l\neq n}\frac{|u_l(\mathbf{p})\rangle\langle u_l(\mathbf{p})|\hat{\boldsymbol{\nu}}|u_n(\mathbf{p})\rangle}{\omega_n(\mathbf{p})-\omega_l(\mathbf{p})} = |\nabla_{\mathbf{p}}u_n(\mathbf{p})\rangle - |u_n(\mathbf{p})\rangle\langle u_n(\mathbf{p})|\nabla_{\mathbf{p}}|u_n(\mathbf{p})\rangle. \tag{S-11}$$

An explicit proof of Eq. (S-11) can be found later in the supplementary information, see section "Useful Identities". We note, parenthetically, that $\mathbf{j}^{(2)}_{\rm off-diag}$ is not only DC, but also uniform in space. This is because when $\zeta_1+\zeta_2=0$, the $-\omega,\mathbf{k}$ and $\omega,-\mathbf{k}$ matrix elements [Eq. (S-3)] appear in pairs in the off-diagonal current density.

Noting that $V^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) = [V^{-\zeta}_{mn}(\mathbf{p},\mathbf{k})]^*$, and using the identity $\lim_{\eta\to0^+}(x-i\eta)^{-1} = i\pi\delta(x)+P(1/x)$ in Eq. (S-9), we obtain the resonant contribution to the off-diagonal current (i.e. the shift photocurrent) as

$$\mathbf{j}^s(\mathbf{k}) = -\frac{e\pi}{4\hbar^2}\sum_{n,m,\zeta=\pm1,\mathbf{p}}f^{\zeta}_{nm}(\mathbf{p},\mathbf{k})\delta\big(\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k})-\zeta\omega\big)|V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})|^2\mathbf{r}_{nm}(\mathbf{p},\zeta\mathbf{k}),$$
$$\mathbf{r}_{nm}(\mathbf{p},\zeta\mathbf{k}) = \mathbf{A}_n(\mathbf{p}+\zeta\mathbf{k}/2)-\mathbf{A}_m(\mathbf{p}-\zeta\mathbf{k}/2)-\nabla_{\mathbf{p}}\arg[V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})], \tag{S-12}$$

where the resonant contribution is identified as the current density that arises from real transitions between $|m,\mathbf{p}-\zeta\mathbf{k}/2\rangle$ and $|n,\mathbf{p}+\zeta\mathbf{k}/2\rangle$ captured by the delta-function $\delta\big(\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k})-\zeta\omega\big)$. In obtaining Eq. (S-12) we have also recalled that for a complex valued function $z_p = |z_p|\exp[i\phi_p]$, the derivative $z_p\partial_p[z_p]^* = (1/2)[\partial_p|z_p|^2] - i|z_p|^2[\partial_p\phi_p]$.

For the simple two-band system illustrated in the main text, where $n, m \in \{\mathrm{c}, \mathrm{v}\}$ are conduction and valence band states, and summing over the available bands, we find Eq. (S-12) reduces to Eq. (3) of the main text. In so doing, we have substituted Eq. (S-10), and written $\mathbf{E} = E\mathbf{e}$ where $E = |\mathbf{E}|$ and $\mathbf{e}$ denotes the light polarization. Eq. (3) of the main text provides a physically intuitive picture for the photon-drag shift current: it arises from the real-space displacements of particles as they (non-vertically) transition from valence band to the conduction band. We note that when the material has more than two bands, Eq. (S-12) also captures the full (photon-drag) shift current. Similar to that described above for the two-band case, this shift current can be understood as arising from transitions between pairs of bands (n, m) with $\mathbf{r}_{nm}(\mathbf{p}, \zeta\mathbf{k})$ as the real-space displacement when a particle transitions between such pairs of bands. The full shift current is the sum of all such transitions between the pairs as captured by Eq. (S-12).

Several comments are in order. First, we emphasize that Eq. (S-12) generalizes the traditional shift current [8, 9, 17, 18] (wherein only vertical transitions were considered) to include photon drag processes (non-vertical transitions). Additionally, we note that Eq. (S-12) can be used for arbitrary polarizations. This is because $V^{\zeta}_{nm}(\mathbf{p}, \mathbf{k})$ captures incident EM radiation with arbitrary polarizations in its (complex) electric field amplitude $\mathbf{E}$. We note that when $\mathbf{k} = 0$, Eq. (S-12) also reproduces the well-known shift current [8], for an explicit discussion, see section "Nonlinear susceptibility for photon drag shift current" below. Lastly, we note that Eq. (S-9) can also possess an (off-resonant) part arising from $P(1/x)$. As we will see below, this will contribute to the off-resonant bulk photovoltaic current density.

A2. Injection Current and Photon Drag

For comprehensiveness, we now proceed to discuss the on-diagonal bulk photovoltaic currents. Following the method described for obtaining Eq. (S-9) above, the DC current from $\mathbf{j}_{\mathrm{on-diag}}$ at second order in $\boldsymbol{\mathcal{E}}$ is

$$\mathbf{j}^{(2)}_{\mathrm{on-diag}} = -\frac{e}{4\hbar^2}\lim_{\eta\to 0^+}\left(\left[\frac{e^{2\eta t}}{2i\eta}\right]\sum_{n,m,\zeta=\pm1,\mathbf{p}}\frac{f^{\zeta}_{nm}(\mathbf{p},\mathbf{k})}{\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) - \zeta\omega - i\eta}V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})V^{-\zeta}_{mn}(\mathbf{p},\mathbf{k})\,\boldsymbol{v}^{\zeta}_{nm}(\mathbf{p},\mathbf{k})\right), \tag{S-13}$$

where we expressed the on-diagonal velocity *difference* as $\boldsymbol{v}^{\zeta}_{nm} \equiv \langle u_n(\mathbf{p}+\zeta\mathbf{k}/2)|\hat{\boldsymbol{\nu}}|u_n(\mathbf{p}+\zeta\mathbf{k}/2)\rangle - \langle u_m(\mathbf{p}-\zeta\mathbf{k}/2)|\hat{\boldsymbol{\nu}}|u_m(\mathbf{p}-\zeta\mathbf{k}/2)\rangle$. To proceed, we first note the identity

$$\lim_{\eta\to 0^+}\frac{1}{i\eta}\frac{1}{x - i\eta} = \lim_{\eta\to 0^+}\left(\frac{\pi}{\eta}\delta(x) + P\frac{1}{x^2} - \frac{i}{\eta}P\frac{1}{x}\right). \tag{S-14}$$

An explicit proof of Eq. (S-14) is provided later in the supplementary information, see section "Useful Identities".

The injection current corresponds to the resonant contribution to the on-diagonal current in Eq. (S-13) [9, 17, 18]. This can be obtained as the contribution that goes as $\delta(x)$ when applying the identity Eq. (S-14) to Eq. (S-13) yielding the injection current injection rate as $\mathrm{d}\mathbf{j}^{\mathrm{inj}}/\mathrm{d}t$

$$\frac{\mathrm{d}\mathbf{j}^{\mathrm{inj}}(\mathbf{k})}{\mathrm{d}t} = -\frac{e\pi}{4\hbar^2}\sum_{n,m,\zeta=\pm1,\mathbf{p}} f^{\zeta}_{nm}(\mathbf{p},\mathbf{k})\delta\big(\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) - \zeta\omega\big)|V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})|^2\,\boldsymbol{v}^{\zeta}_{nm}(\mathbf{p},\mathbf{k}). \tag{S-15}$$

Eq. (S-15) generalizes the injection rate (for injection currents) to include photon drag processes. It naturally reduces to the conventional injection rate when $\mathbf{k} = 0$ [17, 18].

We note that in addition to the resonant contribution to the (second-order) on-diagonal contribution there also exist off-resonant contributions, e.g., arising from the second and third terms of Eq. (S-14) when applied to Eq. (S-13). Crucially, the third term of Eq. (S-14) [corresponding to $-(i/\eta)P(1/x)$] trivially vanishes when we swap the dummy indexes $\alpha \leftrightarrow \beta$ and $\zeta \leftrightarrow -\zeta$ [18]. However, the second term of Eq. (S-14) [corresponding to $P(1/x^2)$] does not. We will discuss this off-resonant contribution below.

A3. Off-resonant Contributions

In the previous sections, we discussed the resonant contributions to the bulk photovoltaic currents. The off-resonant contributions to Eq. (S-9) and Eq. (S-13) are

$$\mathbf{j}^{\mathrm{off-res}}(\mathbf{k}) = \frac{e}{8\hbar^2}\sum_{n,m,\zeta=\pm1,\mathbf{p}} f^{\zeta}_{nm}(\mathbf{p},\mathbf{k})\left\{\frac{1}{\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) - \zeta\omega}\nabla_{\mathbf{p}}|V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})|^2 + |V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})|^2\nabla_{\mathbf{p}}\Big(\frac{1}{\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k}) - \zeta\omega}\Big)\right\}, \tag{S-16}$$

where the first and second terms of Eq. (S-16) correspond to the off-resonant contributions of Eq. (S-9) and Eq. (S-13) respectively. Integrating by parts and noting the periodicity of the Brillouin zone, one obtains

$$\mathbf{j}^{\mathrm{off-res}}(\mathbf{k}) = -\frac{e}{8\hbar^2}\sum_{n,m,\zeta=\pm1,\mathbf{p}}\frac{|V^{\zeta}_{nm}(\mathbf{p},\mathbf{k})|^2}{\omega^{\zeta}_{nm}(\mathbf{p},\mathbf{k})-\zeta\omega}\nabla_{\mathbf{p}}f^{\zeta}_{nm}(\mathbf{p},\mathbf{k}), \tag{S-17}$$

We note that when $\mathbf{k}=0$, Eq. (S-17) produces the intrinsic Fermi surface bulk photovoltaic currents recently discussed in the context of the circularly photogalvanic currents [18].

B. FERMI'S GOLDEN RULE DERIVATION OF PHOTON DRAG SHIFT CURRENT

The photon drag shift current, derived in the previous section using non-linear response theory, can also be obtained from a physically intuitive semiclassical approach [17]. This can be done by considering the real-space displacements produced by non-vertical processes and their transition rates using Fermi's Golden Rule, viz. Eq. (1) of the main text, reproduced here for the convenience of the reader, as [17]

$$\mathbf{j}^{\mathrm{s}} = e\sum_{i\to f}W_{i\to f}\mathbf{r}_{i\to f}, \tag{S-18}$$

where $W_{i\to f}$ is the transition rate from an initial i to a final f state, and $\mathbf{r}_{i\to f}$ is the real-space displacement when a particle transitions from i to f. This provides a physically intuitive description of the shift current: it arises due to a real-space displacement of particles as they transition (with rate $W_{i\to f}$) from i to f.

For the EM field irradiation (captured by $\mathcal{V}$) in Eq. (S-1), the rate of transition from a state β to a state α is given by Fermi's golden rule (and vice versa) as [21]

$$W_{\beta\to\alpha} = \frac{2\pi}{\hbar}|\mathcal{V}^{\zeta=1}_{\alpha\beta}(\mathbf{k})|^2\delta(\omega_{\alpha\beta}-\omega)f(\epsilon_\beta)\big[1-f(\epsilon_\alpha)\big],\quad W_{\alpha\to\beta} = \frac{2\pi}{\hbar}|\mathcal{V}^{\zeta=-1}_{\beta\alpha}(\mathbf{k})|^2\delta(\omega_{\beta\alpha}+\omega)f(\epsilon_\alpha)\big[1-f(\epsilon_\beta)\big]. \tag{S-19}$$

This takes into account the non-vertical transition process arising from a finite photon/polariton momentum $\mathbf{k}$. Recently, the rate of such non-vertical transition were modelled in Ref. [21] in a hybrid semiconductor-plasmonic heterostructure in the same fashion.

Similarly, for $\mathcal{V}$ in Eq. (S-1), the real-space displacement in transitioning from state β to state α (and vice versa) is given by the generalized (gauge-invariant) shift vector [34, 35]

$$\mathbf{r}_{\beta\to\alpha} = \mathbf{A}_\alpha - \mathbf{A}_\beta - \nabla_{\mathbf{p}}\mathrm{arg}[\mathcal{V}^{\zeta=1}_{\alpha\beta}(\mathbf{k})],\quad \mathbf{r}_{\alpha\to\beta} = \mathbf{A}_\beta - \mathbf{A}_\alpha - \nabla_{\mathbf{p}}\mathrm{arg}[\mathcal{V}^{\zeta=-1}_{\beta\alpha}(\mathbf{k})], \tag{S-20}$$

This form can be obtained by considering the motion of wavepackets as they scatter off a perturbation [34, 35].

Summing up all initial and final states (that the non-vertical transition allows), we obtain the photon-drag shift current as

$$\mathbf{j}^{s}(\mathbf{k}) = -\frac{e\pi}{2\hbar^2}\sum_{n,m,\mathbf{p}}f_{nm}(\mathbf{p},\mathbf{k})\delta\big(\omega_{nm}(\mathbf{p},\mathbf{k})-\omega\big)|V^{(1)}_{nm}(\mathbf{p},\mathbf{k})|^2\mathbf{r}_{nm}(\mathbf{p},\mathbf{k}), \tag{S-21}$$

where we substituted Eq. (S-3), accounted for momentum conservation, as well as noted $V^{(1)}_{nm}(\mathbf{p},\mathbf{k}) = [V^{(-1)}_{mn}(\mathbf{p},\mathbf{k})]^*$ [see Eq. (S-10)]. In the above expression, we have used the short-hand notation $f_{nm}(\mathbf{p},\mathbf{k}) = f^{\zeta=1}_{nm}(\mathbf{p},\mathbf{k})$ and $\omega_{nm}(\mathbf{p},\mathbf{k}) = \omega^{\zeta=1}_{nm}(\mathbf{p},\mathbf{k})$. We note that Eq. (S-21) reproduces the same form for the photon-drag shift current in Eq. (S-12), which was derived using non-linear response theory, after both $\zeta=+1$ and $\zeta=-1$ transitions in Eq. (S-12) are summed over. Indeed, when $\mathbf{k}=0$, it also reproduces the expression for the standard (vertical transition) shift current [8–10, 17], see discussion below.

C. USEFUL IDENTITIES

In this section, we discuss the well-known identities Eq. (S-11) and Eq. (S-14) that we used above. These identities are extensively used in the literature, e.g., Eq. (S-11) is used in Ref. [8] and Eq. (S-14) is used in Ref. [18] to name a few instances. For the convenience of the reader, here we provide explicit proofs for both of them.

(1) We first consider the identity in Eq. (S-11), which, for the convenience of reader, is reproduced below

$$\sum_{l\neq n}\frac{|u_l(\mathbf{p})\rangle\langle u_l(\mathbf{p})|\hat{\boldsymbol{\nu}}|u_n(\mathbf{p})\rangle}{\omega_n(\mathbf{p})-\omega_l(\mathbf{p})} = |\nabla_{\mathbf{p}}u_n(\mathbf{p})\rangle - |u_n(\mathbf{p})\rangle\langle u_n(\mathbf{p})|\nabla_{\mathbf{p}}|u_n(\mathbf{p})\rangle. \tag{S-22}$$

To proceed, we note that applying $\nabla_{\mathbf{p}}$ on to $\langle u_l(\mathbf{p})|H(\mathbf{p})|u_n(\mathbf{p})\rangle$ for $n \neq l$ bands, produces

$$\langle u_l(\mathbf{p})|\nabla_{\mathbf{p}} H(\mathbf{p})|u_n(\mathbf{p})\rangle = (\epsilon_n(\mathbf{p}) - \epsilon_l(\mathbf{p}))\langle u_l(\mathbf{p})|\nabla_{\mathbf{p}} u_n(\mathbf{p})\rangle, \quad n \neq l \tag{S-23}$$

where we have noted that $\langle \nabla_{\mathbf{p}} u_l(\mathbf{p})|u_n(\mathbf{p})\rangle = -\langle u_l(\mathbf{p})|\nabla_{\mathbf{p}} u_n(\mathbf{p})\rangle$. Here $H(\mathbf{p})$ is the Bloch hamiltonian. Noting that $\hat{\boldsymbol{\nu}} = \nabla_{\mathbf{p}} H(\mathbf{p})/\hbar$ and inserting Eq. (S-23) in the left hand side of Eq. (S-22) results in

$$\begin{aligned}\sum_{l\neq n} \frac{|u_l(\mathbf{p})\rangle\langle u_l(\mathbf{p})|\hat{\boldsymbol{\nu}}|u_n(\mathbf{p})\rangle}{\omega_n(\mathbf{p}) - \omega_l(\mathbf{p})} &= \Big[\sum_{l\neq n} |u_l(\mathbf{p})\rangle\langle u_l(\mathbf{p})|\nabla_{\mathbf{p}} u_n(\mathbf{p})\rangle\Big] + |u_n(\mathbf{p})\rangle\langle u_n(\mathbf{p})|\nabla_{\mathbf{p}} u_n(\mathbf{p})\rangle - |u_n(\mathbf{p})\rangle\langle u_n(\mathbf{p})|\nabla_{\mathbf{p}} u_n(\mathbf{p})\rangle \\ &= |\nabla_{\mathbf{p}} u_n(\mathbf{p})\rangle - |u_n(\mathbf{p})\rangle\langle u_n(\mathbf{p})|\nabla_{\mathbf{p}}|u_n(\mathbf{p})\rangle. \end{aligned} \tag{S-24}$$

where in the last line we have noted the resolution of the identity. This proves the identity Eq. (S-11).

(2) We now move on to the identity in Eq. (S-14), which, for the convenience of reader, is reproduced below

$$\lim_{\eta\to 0^+} \frac{1}{i\eta}\frac{1}{x - i\eta} = \lim_{\eta\to 0^+} \left(\frac{\pi}{\eta}\delta(x) + P\frac{1}{x^2} - \frac{i}{\eta}P\frac{1}{x}\right). \tag{S-25}$$

It will be useful to introduce a smooth "test" function $f(x)$ that is regular in the neighborhood of the origin, such that we can track the action of the left-hand side of Eq. (S-25) on a funcion as:

$$\int_{-\infty}^{\infty} \lim_{\eta\to 0^+}\left[\frac{1}{i\eta}\frac{1}{x - i\eta} f(x)\right] \mathrm{d}x = -\int_{-\infty}^{\infty} \lim_{\eta\to 0^+}\left[\frac{i}{\eta}\frac{x}{x^2+\eta^2} f(x)\right]\mathrm{d}x + \int_{-\infty}^{\infty} \lim_{\eta\to 0^+}\left[\frac{f(x)}{x^2+\eta^2}\right]\mathrm{d}x. \tag{S-26}$$

To proceed, we observe the following:

$$\int_{-\delta}^{\delta} \frac{x}{x^2+\eta^2}\mathrm{d}x = 0, \quad \int_{-\delta}^{\delta} \frac{1}{x^2+\eta^2}\mathrm{d}x = \frac{2}{\eta}\arctan(\delta/\eta), \tag{S-27}$$

where $\delta > 0$. Next we note that

$$\int_{-\infty}^{\infty} \lim_{\eta\to 0^+}\left[\frac{x}{x^2+\eta^2} f(x)\right]\mathrm{d}x = \lim_{\delta\to 0}\left[\int_{-\infty}^{-\delta}\frac{f(x)}{x}\mathrm{d}x + \int_{\delta}^{\infty}\frac{f(x)}{x}\mathrm{d}x\right] = P\int_{-\infty}^{\infty}\frac{f(x)}{x}\mathrm{d}x, \tag{S-28}$$

where in going from the first to second equality, we have noted that for a small enough δ, we can approximate $f(x) \approx f(0)$ for values of $|x| < \delta$ enabling to apply the first equation of Eq. (S-27). Here P denotes the principal part. Similarly, we have

$$\begin{aligned}\int_{-\infty}^{\infty} \lim_{\eta\to 0^+}\left[\frac{f(x)}{x^2+\eta^2}\right]\mathrm{d}x &= \lim_{\delta\to 0}\left[\int_{-\infty}^{-\delta}\frac{f(x)}{x^2}\mathrm{d}x + \int_{\delta}^{\infty}\frac{f(x)}{x^2}\mathrm{d}x\right] + \lim_{\delta\to 0}\lim_{\eta\to 0^+}\frac{2}{\eta}\arctan(\delta/\eta) f(0) \\ &= P\int_{-\infty}^{\infty}\frac{f(x)}{x^2}\mathrm{d}x + \lim_{\eta\to 0^+}\frac{\pi}{\eta} f(0)\end{aligned} \tag{S-29}$$

By plugging Eq. (S-28) and Eq. (S-29) into the right-hand side of Eq. (S-26), and comparing with its left-hand side, we arrive at the identity in Eq. (S-14).

D. NONLINEAR SUSCEPTIBILITY FOR PHOTON-DRAG SHIFT CURRENT

When EM-radiation of a general polarization is incident on a material, it is sometimes useful to express the total shift photocurrent in terms of its nonlinear susceptibility

$$[\mathbf{j}^s(\mathbf{k})]_c = \sum_{a,b} \sigma^c_{ab}(\mathbf{k}) E_a E_b^* \tag{S-30}$$

where a, b, c are x, y, z components of the current and electric field (note E_a is the "a" component of the electric field amplitude $\mathbf{E}$), and $\sigma^c_{ab}(\mathbf{k})$ is the nonlinear susceptibility associated with photon-drag shift current. For an electric field $\boldsymbol{\mathcal{E}}(\mathbf{r}, t) = (1/2)(\mathbf{E}e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} + \text{c.c.})$ with $\mathbf{E}$ the electric field amplitude, using Eq. (S-9) and Eq. (S-10), the nonlinear susceptibility can be expressed as

$$\sigma^c_{ab}(\mathbf{k}) = -\frac{\pi e^3}{4\hbar^2\omega^2}\sum_{n,m,\mathbf{p}} f_{nm}(\mathbf{p},\mathbf{k})\delta\big(\omega_{nm}(\mathbf{p},\mathbf{k}) - \omega\big) v^a_{nm}(\mathbf{p},\mathbf{k}) v^b_{mn}(\mathbf{p},-\mathbf{k})\big[R^{c,a}_{nm}(\mathbf{p},\mathbf{k}) - R^{c,b}_{mn}(\mathbf{p},-\mathbf{k})\big], \tag{S-31}$$

where

$$R^{c;a}_{nm}(\mathbf{p},\mathbf{k}) = A_{n,c}(\mathbf{p}+\mathbf{k}/2) - A_{m,c}(\mathbf{p}-\mathbf{k}/2) + i\partial_{p_c}\log[v^a_{nm}(\mathbf{p},\mathbf{k})], \tag{S-32}$$

and $v^a_{nm}(\mathbf{p},\mathbf{k}) = \langle u_n(\mathbf{p}+\mathbf{k}/2)|\hat{\nu}_a|u_m(\mathbf{p}-\mathbf{k}/2)\rangle$ and $\hat{\nu}_a$ is the velocity operator along the a-direction. The Berry connection along the c direction is $A_{n,c}(\mathbf{p}) = \langle u_n(\mathbf{p})|i\partial_{p_c}|u_n(\mathbf{p})\rangle$. Here we have used the shorthand $f_{nm}(\mathbf{p},\mathbf{k}) = f^{\zeta=1}_{nm}(\mathbf{p},\mathbf{k})$ and $\omega_{nm}(\mathbf{p},\mathbf{k}) = \omega^{\zeta=1}_{nm}(\mathbf{p},\mathbf{k})$.

When $\mathbf{k}=0$, Eq. (S-31) for the nonlinear susceptibility (of the photon-drag shift current) can be reduced to a compact form. To do this we recall the identity

$$[r^{(0)}_{nm}(\mathbf{p})]^a \equiv \frac{\langle n,\mathbf{p}|\hat{v}_a|m,\mathbf{p}\rangle}{i\omega^{(0)}_{nm}(\mathbf{p})}, \tag{S-33}$$

where $\hbar\omega^{(0)}_{nm}(\mathbf{p}) = \epsilon_n(\mathbf{p}) - \epsilon_m(\mathbf{p})$. Substituting into Eq. (S-31) when $\mathbf{k}=0$ yields the conventional ($\mathbf{k}=0$) shift current nonlinear susceptibility [17]

$$\sigma^c_{ab}(\mathbf{k}=0) = \frac{\pi e^3}{4\hbar^2}\sum_{n,m,\mathbf{p}}\left[f[\epsilon_m(\mathbf{p})] - f[\epsilon_n(\mathbf{p})]\right]\delta(\omega^{(0)}_{nm}(\mathbf{p})-\omega)[r^{(0)}_{nm}(\mathbf{p})]^a[r^{(0)}_{mn}(\mathbf{p})]^b\left[\tilde{R}^{c,a}_{nm}(\mathbf{p}) - \tilde{R}^{c,b}_{mn}(\mathbf{p})\right], \tag{S-34}$$

where $\tilde{R}^{c,a}_{nm}(\mathbf{p}) = A_{n,c}(\mathbf{p}) - A_{m,c}(\mathbf{p}) + i\partial_{p_c}\log[r^{(0)}_{nm}(\mathbf{p})]^i$. This is consistent with Eq. (4) of Ref. [17]; we note, however, that we have used particles with charge e and a field $\boldsymbol{\mathcal{E}}(\mathbf{r},t) = (1/2)(\mathbf{E}e^{\eta t}e^{-i\omega t} + \text{c.c.})$ instead.

E. WILSON LOOP FORMALISM AND SYMMETRY PROPERTIES FOR THE SHIFT VECTOR

This section describes the symmetry properties of the shift vector. In order to clearly display its symmetry properties, we directly show how the shift vector proceeds from phases accumulated during transition processes described in the main text. We begin by noting that the Berry connection in the Bloch band n, $\mathbf{A}_n(\mathbf{p})$ in Eq. (4) essentially encodes phases between different Bloch eigenstates $\langle u_n(\mathbf{p})|u_n(\mathbf{p}+\mathbf{q})\rangle = \exp[-i\mathbf{A}_n(\mathbf{p})\cdot\mathbf{q} + O(q^2)]$, and can be expressed as $\mathbf{A}_n(\mathbf{p}) = -\lim_{\mathbf{q}\to 0}\nabla_{\mathbf{q}}\arg[\langle u_n(\mathbf{p})|u_n(\mathbf{p}+\mathbf{q})\rangle]|$. Using this, we can rewrite $\mathbf{r}(\mathbf{p},\mathbf{k})$ in Eq. (4) as the gradient of a (Pacharatnam-Berry) geometric phase [34, 35]

$$\mathbf{r}_{nm}(\mathbf{p},\mathbf{k}) = \lim_{\mathbf{q}\to\mathbf{0}}\nabla_{\mathbf{q}}\arg[\mathcal{W}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})], \tag{S-35}$$

with the Wilson loop $\mathcal{W}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})$

$$\begin{aligned}\mathcal{W}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k}) = &\langle u_m(\mathbf{p}-\mathbf{k}/2)|u_m(\mathbf{p}+\mathbf{q}-\mathbf{k}/2)\rangle\langle u_m(\mathbf{p}+\mathbf{q}-\mathbf{k}/2)|\hat{\boldsymbol{\nu}}\cdot\mathbf{e}|u_n(\mathbf{p}+\mathbf{q}+\mathbf{k}/2)\rangle\\ &\cdot\langle u_n(\mathbf{p}+\mathbf{q}+\mathbf{k}/2)|u_n(\mathbf{p}+\mathbf{k}/2)\rangle\langle u_n(\mathbf{p}+\mathbf{k}/2)|u_m(\mathbf{p}-\mathbf{k}/2)\rangle,\end{aligned} \tag{S-36}$$

encoding the transition process $u_m(\mathbf{p}-\mathbf{k}/2)\to u_m(\mathbf{p}+\mathbf{q}-\mathbf{k}/2)\to\hat{\boldsymbol{\nu}}\cdot\mathbf{e}\to u_n(\mathbf{p}+\mathbf{q}+\mathbf{k}/2)\to u_n(\mathbf{p}+\mathbf{k}/2)$. In obtaining Eq. (S-36) we have added $\langle u_n(\mathbf{p}+\mathbf{k}/2)|u_m(\mathbf{p}-\mathbf{k}/2)\rangle$ (last term) that is $\mathbf{q}$-independent to create a closed loop; its contribution to $\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})$ vanishes under the action of $\nabla_{\mathbf{q}}$ in Eq. (S-35). We note that even without the last term, the first four terms of Eq. (S-36) give a Wilson line that under the action of $\nabla_{\mathbf{q}}$ remains gauge invariant as all Bloch state vectors containing $\mathbf{q}$ always appear in pairs. The symmetry properties of $\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})$ are therefore determined by those of $\mathcal{W}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})$.

The conventional shift vector, $\mathbf{r}^{(0)}_{nm}(\mathbf{p})$ (valid for vertical transitions), can also be directly obtained from Eq. (S-35) as

$$\mathbf{r}^{(0)}_{nm}(\mathbf{p}) \equiv \mathbf{r}_{nm}(\mathbf{p},\mathbf{0}) = \lim_{\mathbf{k},\mathbf{q}\to\mathbf{0}}\nabla_{\mathbf{q}}\arg[\mathcal{W}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})]. \tag{S-37}$$

This emphasizes the gauge invariant nature of $\mathbf{r}^{(0)}_{nm}(\mathbf{p})$ being a gradient of the phase obtained in the closed loop.

We note that the shift vector, $\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})$, and the Wilson loop, $\mathcal{W}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})$, in general have Bloch band indices n,m. For clarity in the main text, we focussed on a two band model with only two bands, i.e. a conduction band, c, and a valance band, v. To simplify the presentation and the notation in the main text, we have used shift vectors where the band indices are dropped (used only in the main text) to denote

$$\mathbf{r}(\mathbf{p},\mathbf{k}) = \mathbf{r}_{\rm cv}(\mathbf{p},\mathbf{k}), \quad \mathbf{r}^{(0)}(\mathbf{p}) = \mathbf{r}^{(0)}_{\rm cv}(\mathbf{p}) \tag{S-38}$$

For the convenience of the reader, these are also defined explicitly in the main text. For comprehensiveness, in what follows in the supplementary information we will specify the band indices explicitly.

E1. Symmetry properties of the shift vector

As discussed in the main text, we will focus on centrosymmetric crystals with additional symmetries such as time reversal symmetry or mirror symmetry. For clarity and brevity, in what follows we will concentrate on light polarization directed along a high symmetry axes of the crystal, so that $\hat{\boldsymbol{\nu}} \cdot \mathbf{e} = \nu_x$.

(1) When a crystal has inversion symmetry, its full Hamiltonian in real-space $\mathcal{H}(\mathbf{r})$ obeys the commutation relation $[\mathcal{H}(\mathbf{r}), \mathcal{I}] = 0$; here $\mathcal{I}$ is the inversion operator. The Bloch Hamiltonian $H(\mathbf{p}) = e^{-i\mathbf{p}\cdot\mathbf{r}}\mathcal{H}(\mathbf{r})e^{i\mathbf{p}\cdot\mathbf{r}}$ then satisfies

$$\mathcal{I}H(\mathbf{p})\mathcal{I}^{-1} = H(-\mathbf{p}). \tag{S-39}$$

As a result, the (Bloch) periodic eigenstates $|u_n^\sigma(\mathbf{p})\rangle$ ($\sigma = \uparrow, \downarrow$) of $H(\mathbf{p})$ also inherit corresponding symmetry properties; here n is a general Bloch band index. To see this, we apply the inversion operator $\mathcal{I}$ on $\epsilon_{n,\mathbf{p}}^\sigma|u_n^\sigma(\mathbf{p})$ and obtain

$$\mathcal{I}[\epsilon_{n,\mathbf{p}}^\sigma|u_n^\sigma(\mathbf{p})] = \mathcal{I}[H(\mathbf{p})|u_n^\sigma(\mathbf{p})] = \mathcal{I}H(\mathbf{p})\mathcal{I}^{-1}|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle = H(-\mathbf{p})|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle, \tag{S-40}$$

where we used the symmetry relation Eq. (S-39). On the other hand we have $\mathcal{I}[\epsilon_{n,\mathbf{p}}^\sigma|u_n^\sigma(\mathbf{p})] = \epsilon_{n,\mathbf{p}}^\sigma|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle$ since $\epsilon_{n,\mathbf{p}}^\sigma$ is a real scalar. Together with Eq. (S-40) we must have

$$H(-\mathbf{p})|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle = \epsilon_{n,\mathbf{p}}^\sigma|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle, \tag{S-41}$$

that leads to

$$|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle = |u_n^\sigma(-\mathbf{p})\rangle, \quad \epsilon_{n,\mathbf{p}}^\sigma = \epsilon_{n,-\mathbf{p}}^\sigma. \tag{S-42}$$

Using Eq. (S-42), we can readily see that

$$\langle u_{n_1}^{\sigma_1}(\mathbf{v}_1)|u_{n_2}^{\sigma_2}(\mathbf{v}_2)\rangle = \langle u_{n_1}^{\sigma_1}(\mathbf{v}_1)|\mathcal{I}^{-1}\mathcal{I}|u_{n_2}^{\sigma_2}(\mathbf{v}_2)\rangle = \langle \mathcal{I}u_{n_1}^{\sigma_1}(\mathbf{v}_1)|\mathcal{I}u_{n_2}^{\sigma_2}(\mathbf{v}_2)\rangle = \langle u_{n_1}^{\sigma_1}(-\mathbf{v}_1)|u_{n_2}^{\sigma_2}(-\mathbf{v}_2)\rangle, \tag{S-43}$$

and similarly,

$$\langle u_{n_1}^{\sigma_1}(\mathbf{v}_1)|\nu_x|u_{n_2}^{\sigma_2}(\mathbf{v}_2)\rangle = -\langle u_{n_1}^{\sigma_1}(-\mathbf{v}_1)|\nu_x|u_{n_2}^{\sigma_2}(-\mathbf{v}_2)\rangle, \tag{S-44}$$

where we have used the fact that $\mathcal{I}\nu_x\mathcal{I}^{-1} = \mathcal{I}[\partial H(\mathbf{p})/\hbar\partial p_x]\mathcal{I}^{-1} = \partial H(-\mathbf{p})/\partial p_x = -\nu_x$, as readily obtained from Eq. (S-39).

Eqs. (S-43) and (S-44) guarantee that

$$\arg[\mathcal{W}_{nm}^\sigma(\mathbf{p}, \mathbf{q}, \mathbf{k})] = \arg[\mathcal{W}_{nm}^\sigma(-\mathbf{p}, -\mathbf{q}, -\mathbf{k})] + \pi, \tag{S-45}$$

where the argument function $\arg[z]$ here and below is defined within the interval $(-\pi, \pi]$. As a result, we find

$$[\mathbf{r}_{nm}(\mathbf{p}, \mathbf{k})]^\sigma = -[\mathbf{r}_{nm}(-\mathbf{p}, -\mathbf{k})]^\sigma, \tag{S-46}$$

And in the $\mathbf{k} = \mathbf{0}$ limit,

$$[\mathbf{r}_{nm}^{(0)}(\mathbf{p})]^\sigma = -[\mathbf{r}_{nm}^{(0)}(-\mathbf{p})]^\sigma. \tag{S-47}$$

(2) When the crystal has both inversion symmetry $\mathcal{I}$ and time reversal symmetry $\mathcal{T} = -i\sigma_y K$, then we have

$$\mathcal{I}H(\mathbf{p})\mathcal{I}^{-1} = H(-\mathbf{p}), \quad \mathcal{T}H(\mathbf{p})\mathcal{T}^{-1} = H(-\mathbf{p}). \tag{S-48}$$

Following similar analysis as above we have relations between (Bloch) periodic eigenstates

$$|\mathcal{I}u_n^\sigma(\mathbf{p})\rangle = |u_n^\sigma(-\mathbf{p})\rangle, \quad |\mathcal{T}u_n^\sigma(\mathbf{p})\rangle = |u_n^{-\sigma}(-\mathbf{p})\rangle^*. \tag{S-49}$$

as well as

$$\langle u_{n_1}^{\sigma_1}(\mathbf{v}_1)|u_{n_2}^{\sigma_2}(\mathbf{v}_2)\rangle = [\langle u_{n_1}^{-\sigma_1}(\mathbf{v}_1)|u_{n_2}^{-\sigma_2}(\mathbf{v}_2)\rangle]^*, \quad \langle u_{n_1}^{\sigma_1}(\mathbf{v}_1)|\nu_x|u_{n_2}^{\sigma_2}(\mathbf{v}_2)\rangle = [\langle u_{n_1}^{-\sigma_1}(\mathbf{v}_1)|\nu_x|u_{n_2}^{-\sigma_2}(\mathbf{v}_2)\rangle]^*, \tag{S-50}$$

where we have consecutively carried out inversion and time reversal operations, used the fact that $\mathcal{I}\nu_x\mathcal{I}^{-1} = -\nu_x$ discussed above, and $\mathcal{T}\nu_x\mathcal{T}^{-1} = \mathcal{T}[\partial H(\mathbf{p})/\hbar\partial p_x]\mathcal{T}^{-1} = \partial H(-\mathbf{p})/\hbar\partial p_x = -\nu_x$ obtained from Eq. (S-48). Applying Eq. (S-50) in Eq. (S-36), we see the spin-resolved Wilson loops obey

$$\arg[\mathcal{W}^{\sigma}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})] = \arg\left([\mathcal{W}^{-\sigma}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})]^*\right) = -\arg[\mathcal{W}^{-\sigma}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})], \tag{S-51}$$

and the relation between the spin-resolved shift vectors

$$[\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})]^{\sigma} = -[\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})]^{-\sigma}, \tag{S-52}$$

as well as in the $\mathbf{k} = \mathbf{0}$ limit

$$[\mathbf{r}^{(0)}_{nm}(\mathbf{p})]^{\sigma} = -[\mathbf{r}^{(0)}_{nm}(\mathbf{p})]^{-\sigma}. \tag{S-53}$$

(3) When the crystal has inversion symmetry $\mathcal{I}$, time reversal symmetry $\mathcal{T}$, and mirror symmetry $\mathcal{M}_y$, we have

$$|\mathcal{I}u^{\sigma}_n(\mathbf{p})\rangle = |u^{\sigma}_n(-\mathbf{p})\rangle, \quad |\mathcal{T}u^{\sigma}_n(\mathbf{p})\rangle = |u^{-\sigma}_n(-\mathbf{p})\rangle^*, \quad |\mathcal{M}_y u^{\sigma}_n(\mathbf{p})\rangle = |u^{-\sigma}_n(\mathcal{M}_y\mathbf{p})\rangle, \tag{S-54}$$

and

$$\langle u^{\sigma_1}_{n_1}(\mathbf{v}_1)|u^{\sigma_2}_{n_2}(\mathbf{v}_2)\rangle = [\langle u^{\sigma_1}_{n_1}(\mathcal{M}_y\mathbf{v}_1)|u^{\sigma_2}_{n_2}(\mathcal{M}_y\mathbf{v}_2)\rangle]^*, \quad \langle u^{\sigma_1}_{n_1}(\mathbf{v}_1)|\nu_x|u^{\sigma_2}_{n_2}(\mathbf{v}_2)\rangle = [\langle u^{\sigma_1}_{n_1}(\mathcal{M}_y\mathbf{v}_1)|\nu_x|u^{\sigma_2}_{n_2}(\mathcal{M}_y\mathbf{v}_2)\rangle]^*, \tag{S-55}$$

where we have consecutively carried out inversion, time reversal, and mirror ($\mathcal{M}_y$) operations, used the fact that $\mathcal{I}\nu_x\mathcal{I}^{-1} = -\nu_x$ and $\mathcal{T}\nu_x\mathcal{T}^{-1} = -\nu_x$ discussed above, and $\mathcal{M}_y\nu_x\mathcal{M}_y^{-1} = \nu_x$. In the same way as detailed above, Eq. (S-55) applied on Eq. (S-36) leads to

$$\arg[\mathcal{W}^{\sigma}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})] = -\arg[\mathcal{W}^{\sigma}_{nm}(\mathcal{M}_y\mathbf{p},\mathcal{M}_y\mathbf{q},\mathcal{M}_y\mathbf{k})], \tag{S-56}$$

and

$$[r_{nm}(\mathbf{p},\mathbf{k})]^{\sigma}_x = -[r_{nm}(\mathcal{M}_y\mathbf{p},\mathcal{M}_y\mathbf{k})]^{\sigma}_x, \quad [r_{nm}(\mathbf{p},\mathbf{k})]^{\sigma}_y = [r_{nm}(\mathcal{M}_y\mathbf{p},\mathcal{M}_y\mathbf{k})]^{\sigma}_y, \tag{S-57}$$

where the subscript $[\cdots]_{x,y}$ indicate the x and y components respectively. In the $\mathbf{k} = \mathbf{0}$ limit,

$$[r^{(0)}_{nm}(\mathbf{p})]^{\sigma}_x = -[r^{(0)}_{nm}(\mathcal{M}_y\mathbf{p})]^{\sigma}_x, \quad [r^{(0)}_{nm}(\mathbf{p})]^{\sigma}_y = [r^{(0)}_{nm}(\mathcal{M}_y\mathbf{p})]^{\sigma}_y, \tag{S-58}$$

which means that spin-resolved shift vectors are pseudo vectors with respect to the mirror plane. In deriving Eq. (S-57), we used $\mathcal{M}_y(q_x, q_y) = (q_x, -q_y)$ and Eq. (S-37).

For the convenience of the reader, we note that Eq. (S-57) readily reproduces Eq. (8) of the main text when the evenness of the *square* of the velocity matrix element under the combined action of MS, IS, and TRS (see above). In so doing, we have also noted the notation defined in Eq. (S-38).

(4) When an external field breaks both TRS and MS, but preserves the inversion symmetry $\mathcal{I}$ and a composite symmetry $\mathcal{S} = \mathcal{M}_y\mathcal{T}$, then we have

$$\mathcal{I}H(\mathbf{p})\mathcal{I}^{-1} = H(-\mathbf{p}), \quad \mathcal{S}H(\mathbf{p})\mathcal{S}^{-1} = H(-\mathcal{M}_y\mathbf{p}), \tag{S-59}$$

and the relations between periodic eigenstates

$$|\mathcal{I}u^{\sigma}_n(\mathbf{p})\rangle = |u^{\sigma}_n(-\mathbf{p})\rangle, \quad |\mathcal{S}u^{\sigma}_n(\mathbf{p})\rangle = |u^{\sigma}_n(-\mathcal{M}_y\mathbf{p})\rangle^*. \tag{S-60}$$

Together with $\mathcal{I}\nu_x\mathcal{I}^{-1} = -\nu_x$ and $\mathcal{S}\nu_x\mathcal{S}^{-1} = -\nu_x$ which can be derived from Eq. (S-59), following the same way as detailed above, we arrive at the same results in case **(3)**:

$$\arg[\mathcal{W}^{\sigma}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})] = -\arg[\mathcal{W}^{\sigma}_{nm}(\mathcal{M}_y\mathbf{p},\mathcal{M}_y\mathbf{q},\mathcal{M}_y\mathbf{k})], \tag{S-61}$$

and

$$[r_{nm}(\mathbf{p},\mathbf{k})]^{\sigma}_x = -[r_{nm}(\mathcal{M}_y\mathbf{p},\mathcal{M}_y\mathbf{k})]^{\sigma}_x, \quad [r_{nm}(\mathbf{p},\mathbf{k})]^{\sigma}_y = [r_{nm}(\mathcal{M}_y\mathbf{p},\mathcal{M}_y\mathbf{k})]^{\sigma}_y. \tag{S-62}$$

In the $\mathbf{k} = \mathbf{0}$ limit

$$[r^{(0)}_{nm}(\mathbf{p})]^{\sigma}_x = -[r^{(0)}_{nm}(\mathcal{M}_y\mathbf{p})]^{\sigma}_x, \quad [r^{(0)}_{nm}(\mathbf{p})]^{\sigma}_y = [r^{(0)}_{nm}(\mathcal{M}_y\mathbf{p})]^{\sigma}_y. \tag{S-63}$$

The pseudo-vector nature of $\mathbf{r}^{\sigma}(\mathbf{p})$ persists when inversion symmetry $\mathcal{I}$ and the composite symmetry $\mathcal{S} = \mathcal{M}_y\mathcal{T}$ are preserved.

F. DERIVATION OF $d_a^\rho(\mathbf{p})$ IN THE MAIN TEXT

In this section, we will explicitly calculate $d_a^\rho(\mathbf{p})$, that can be expressed as $d_a^\rho(\mathbf{p}) = [\partial\rho(\mathbf{p},\mathbf{k})/\partial k_a]_{\mathbf{k}=\mathbf{0}}$, where

$$\rho(\mathbf{p},\mathbf{k}) = [f(\epsilon_{\mathrm{v},\mathbf{p}-\mathbf{k}/2}) - f(\epsilon_{\mathrm{c},\mathbf{p}+\mathbf{k}/2})]\delta(\omega_{\mathrm{c},\mathbf{p}+\mathbf{k}/2} - \omega_{\mathrm{v},\mathbf{p}-\mathbf{k}/2} - \omega). \tag{S-64}$$

To proceed, we expand $\rho(\mathbf{p},\mathbf{k})$ in terms of k_a. The first part of $\rho(\mathbf{p},\mathbf{k})$ can expanded out as

$$[f(\epsilon_{\mathrm{v},\mathbf{p}-\mathbf{k}/2}) - f(\epsilon_{\mathrm{c},\mathbf{p}+\mathbf{k}/2})] = [f(\epsilon_{\mathrm{v},\mathbf{p}}) - f(\epsilon_{\mathrm{c},\mathbf{p}})] - \frac{k_a}{2}\frac{\partial(f_{\mathrm{v},\mathbf{p}} + f_{\mathrm{c},\mathbf{p}})}{\partial p_a} + O(k^2). \tag{S-65}$$

To expand the second part of $\rho(\mathbf{p},\mathbf{k})$, i.e., $\delta(\omega_{\mathrm{c},\mathbf{p}+\mathbf{k}/2} - \omega_{\mathrm{v},\mathbf{p}-\mathbf{k}/2} - \omega)$, we introduce an auxiliary symmetrization:

$$\omega_{\mathrm{c},\mathbf{p}} = \omega_{\mathbf{p}}^{\mathrm{av}} + \tilde{\omega}_{\mathrm{c},\mathbf{p}}, \quad \omega_{\mathrm{v},\mathbf{p}} = \omega_{\mathbf{p}}^{\mathrm{av}} + \tilde{\omega}_{\mathrm{v},\mathbf{p}}, \tag{S-66}$$

where $\omega_{\mathbf{p}}^{\mathrm{av}} = (\omega_{\mathrm{c},\mathbf{p}} + \omega_{\mathrm{v},\mathbf{p}})/2$ is the the shared kinetic part, while $\tilde{\omega}_{\mathrm{c},\mathbf{p}} = (\omega_{\mathrm{c},\mathbf{p}} - \omega_{\mathrm{v},\mathbf{p}})/2$ and $\tilde{\omega}_{\mathrm{v},\mathbf{p}} = -(\omega_{\mathrm{c},\mathbf{p}} - \omega_{\mathrm{v},\mathbf{p}})/2$ are symmetrized conduction and valence band dispersions. Using this auxiliary symmetrization, we have

$$\delta(\omega_{\mathrm{c},\mathbf{p}+\mathbf{k}/2} - \omega_{\mathrm{v},\mathbf{p}-\mathbf{k}/2} - \omega) = \delta(\tilde{\omega}_{\mathrm{c},\mathbf{p}+\mathbf{k}/2} - \tilde{\omega}_{\mathrm{v},\mathbf{p}-\mathbf{k}/2} - \omega) = \delta(\omega_{\mathbf{p}}^{\mathrm{cv}} - \omega) + O(k^2), \quad \omega_{\mathbf{p}}^{\mathrm{cv}} = \omega_{\mathrm{c},\mathbf{p}} - \omega_{\mathrm{v},\mathbf{p}}, \tag{S-67}$$

where we used $\tilde{\omega}_{\mathrm{c},\mathbf{p}} = -\tilde{\omega}_{\mathrm{v},\mathbf{p}}$ in the second equation. Combining the terms in Eqs. (S-65) and (S-67), up to the first order of k_α, we have

$$\rho(\mathbf{p},\mathbf{k}) = \rho(\mathbf{p},\mathbf{0}) + k_a d_a^\rho(\mathbf{p}) + O(k^2), \tag{S-68}$$

where

$$\rho(\mathbf{p},\mathbf{0}) = [f(\epsilon_{\mathrm{v},\mathbf{p}}) - f(\epsilon_{\mathrm{c},\mathbf{p}})]\delta(\omega_{\mathbf{p}}^{\mathrm{cv}} - \omega), \tag{S-69}$$

that gives a vanishing shift current in a centrosymmetric crystal, and

$$d_a^\rho(\mathbf{p}) = -\frac{1}{2}\frac{\partial(f_{\mathrm{v},\mathbf{p}} + f_{\mathrm{c},\mathbf{p}})}{\partial p_a}\,\delta(\omega_{\mathbf{p}}^{\mathrm{cv}} - \omega), \tag{S-70}$$

which is Eq. (7) in the main text.

G. CHARGE CONJUGATION SYMMETRY AND VANISHING OF d_{ab}^R

In the main text, we noted that the spin-up branch $H_0^\uparrow$ in Eq. (10) possess an emergent charge conjugation symmetry (CCS). Below we discuss its consequences on the generalized shift vector.

For a generic two-band Hamiltonian (repeated indices are implicitly summed over)

$$H(\mathbf{p}) = h_i(\mathbf{p})\tau_i, \quad (i = x, y, z) \tag{S-71}$$

where τ_i denote orbital degrees of freedom. $H(\mathbf{p})$ in Eq. (S-71) have eigenenergies $\epsilon_{\mathrm{c,v}}(\mathbf{p}) = \pm\sqrt{h_i(\mathbf{p})h_i(\mathbf{p})}$ and eigenstates

$$|u_{\mathrm{c}}(\mathbf{p})\rangle = \begin{bmatrix}\cos(\theta_{\mathbf{p}}/2)e^{-i\phi_{\mathbf{p}}/2}\\ \sin(\theta_{\mathbf{p}}/2)e^{i\phi_{\mathbf{p}}/2}\end{bmatrix}, \quad |u_{\mathrm{v}}(\mathbf{p})\rangle = \begin{bmatrix}\sin(\theta_{\mathbf{p}}/2)e^{-i\phi_{\mathbf{p}}/2}\\ -\cos(\theta_{\mathbf{p}}/2)e^{i\phi_{\mathbf{p}}/2}\end{bmatrix}, \tag{S-72}$$

where $\cos\theta_{\mathbf{p}} = h_z(\mathbf{p})/[h_x^2(\mathbf{p}) + h_y^2(\mathbf{p})]^{1/2}$ and $\tan\phi_{\mathbf{p}} = h_y(\mathbf{p})/h_x(\mathbf{p})$. Such a system possesses CCS : $\mathcal{P}H(\mathbf{p})\mathcal{P}^{-1} = -H(\mathbf{p})$; $\mathcal{P} = i\tau_y\mathcal{K}$ is the charge conjugation operation, where $\mathcal{K}$ is the complex conjugation, and τ denotes the orbital degrees of freedom. It also relates the eigenstates of conduction and valence bands:

$$\mathcal{P}|u_{\mathrm{v,c}}(\mathbf{p})\rangle = i\tau_y\mathcal{K}|u_{\mathrm{v,c}}(\mathbf{p})\rangle = |u_{\mathrm{c,v}}(\mathbf{p})\rangle. \tag{S-73}$$

In other words, each eigenstate $|u_{\mathrm{v,c}}(\mathbf{p})\rangle$ at energy $\epsilon_{\mathrm{v,c}}(\mathbf{p})$ has a copy $\mathcal{P}|u_{\mathrm{v,c}}(\mathbf{p})\rangle = |u_{\mathrm{c,v}}(\mathbf{p})\rangle$ at energy $\epsilon_{\mathrm{c,v}}(\mathbf{p})$.

Due to the CCS possessed between the Bloch states $|u_{\rm c,v}(\mathbf{p})\rangle = i\tau_y\mathcal{K}|u_{\rm v,c}(\mathbf{p})\rangle$, we arrive at the following relation [recalling the notation of the main text, also described in Eq. (S-38)]

$$\begin{aligned}
\mathbf{r}(\mathbf{p},-\mathbf{k}) &= +\mathbf{A}_{\rm c}(\mathbf{p}-\mathbf{k}/2) - \mathbf{A}_{\rm v}(\mathbf{p}+\mathbf{k}/2) - \nabla_{\mathbf{p}}\arg[\langle u_{\rm c}(\mathbf{p}-\mathbf{k}/2)|\nu_x|u_{\rm v}(\mathbf{p}+\mathbf{k}/2)\rangle] \\
&= -\mathbf{A}_{\rm v}(\mathbf{p}-\mathbf{k}/2) + \mathbf{A}_{\rm c}(\mathbf{p}+\mathbf{k}/2) - \nabla_{\mathbf{p}}\arg[\langle (i\tau_y)\mathcal{K}u_{\rm v}(\mathbf{p}-\mathbf{k}/2)|\nu_x|(i\tau_y)\mathcal{K}u_{\rm c}(\mathbf{p}+\mathbf{k}/2)\rangle] \\
&= +\mathbf{A}_{\rm c}(\mathbf{p}+\mathbf{k}/2) - \mathbf{A}_{\rm v}(\mathbf{p}-\mathbf{k}/2) - \nabla_{\mathbf{p}}\arg[\langle \mathcal{K}u_{\rm v}(\mathbf{p}-\mathbf{k}/2)|\nu_x|\mathcal{K}u_{\rm c}(\mathbf{p}+\mathbf{k}/2)\rangle] \\
&= +\mathbf{A}_{\rm c}(\mathbf{p}+\mathbf{k}/2) - \mathbf{A}_{\rm v}(\mathbf{p}-\mathbf{k}/2) - \nabla_{\mathbf{p}}\arg[\langle u_{\rm c}(\mathbf{p}+\mathbf{k}/2)|\nu_x|u_{\rm v}(\mathbf{p}-\mathbf{k}/2)\rangle] = \mathbf{r}(\mathbf{p},\mathbf{k}),
\end{aligned} \tag{S-74}$$

where we have used

$$\begin{aligned}
\mathbf{A}_{\rm c,v}(\mathbf{p}) &= i\langle u_{\rm c,v}(\mathbf{p})|\nabla_{\mathbf{p}}|u_{\rm c,v}(\mathbf{p})\rangle = i\langle (i\tau_y)\mathcal{K}u_{\rm v,c}(\mathbf{p})|\nabla_{\mathbf{p}}|(i\tau_y)\mathcal{K}u_{\rm v,c}(\mathbf{p})\rangle \\
&= i\langle \mathcal{K}u_{\rm v,c}(\mathbf{p})|\nabla_{\mathbf{p}}|\mathcal{K}u_{\rm v,c}(\mathbf{p})\rangle = -i\langle u_{\rm v,c}(\mathbf{p})|\nabla_{\mathbf{p}}|u_{\rm v,c}(\mathbf{p})\rangle = -\mathbf{A}_{\rm v,c}(\mathbf{p}),
\end{aligned} \tag{S-75}$$

and the fact that $\langle u_{\rm v,c}(\mathbf{p})|\nabla_{\mathbf{p}}|u_{\rm v,c}(\mathbf{p})\rangle$ is purely imaginary. Eq. (S-74) shows that $\mathbf{r}(\mathbf{p},\mathbf{k}) = \mathbf{r}(\mathbf{p},-\mathbf{k})$ is even with respect to $\mathbf{k}$. In the meantime, as already shown in Eq. (S-74), we also have $|\langle u_{\rm c}(\mathbf{p}-\mathbf{k}/2)|\nu_x|u_{\rm v}(\mathbf{p}+\mathbf{k}/2)\rangle|^2 = |\langle u_{\rm c}(\mathbf{p}+\mathbf{k}/2)|\nu_x|u_{\rm v}(\mathbf{p}-\mathbf{k}/2)\rangle|^2$, i.e., $|\nu(\mathbf{p},\mathbf{k})|^2 = |\nu(\mathbf{p},-\mathbf{k})|^2$. The above two equations about $\mathbf{r}(\mathbf{p},\mathbf{k})$ and $|\nu(\mathbf{p},\mathbf{k})|^2$ give rise to $\mathbf{R}(\mathbf{p},\mathbf{k}) = \mathbf{R}(\mathbf{p},-\mathbf{k})$ when CCS is present.

H. SYMMETRY AND SHIFT CURRENT FOR CIRCULAR POLARIZATION

We now turn to the behavior of the photon drag shift current for circularly polarized EM irradiation. To do this, we consider specific left-handed (L) or right-handed (R) circularly polarized EM irradiations with opposite chirality, described by $\boldsymbol{\mathcal{E}}_{\rm L,R}(\mathbf{r},t) = (1/2)\left[\mathbf{E}^{\rm L,R}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + \text{c.c.}\right]$, in which $\mathbf{E}^{\rm L,R} = E(\hat{\mathbf{e}}_1 \pm i\hat{\mathbf{e}}_2)$ with directional unit vectors $\hat{\mathbf{e}}_1 \perp \hat{\mathbf{e}}_2$. While the total photon-drag shift current comprises contributions from multiple elements of the nonlinear susceptibility tensor in Eq. (S-31) [see also Eq. (S-30)], it is interesting to isolate the part of the photon-drag shift current that depends only on the chirality of the incident L and R irradiation by studying the difference

$$\delta\mathbf{j}^s(\mathbf{k}) = \mathbf{j}^s_{\rm L}(\mathbf{k}) - \mathbf{j}^s_{\rm R}(\mathbf{k}), \tag{S-76}$$

where $\mathbf{j}^s_{\rm L,R}(\mathbf{k})$ denotes the photon-drag shift current obtained for (obliquely incident, captured by $\mathbf{k}$) circularly polarized irradiation $\boldsymbol{\mathcal{E}}_{\rm L,R}(\mathbf{r},t)$ respectively. From its definition, the chirality-dependent photon drag shift current $\delta\mathbf{j}^s(\mathbf{k})$ reverses sign when we flip the chirality of $\boldsymbol{\mathcal{E}}_{\rm L,R}(\mathbf{r},t)$ (i.e. L $\to$ R). Apart from this obvious chirality dependence, we can also investigate the properties of $\delta\mathbf{j}^s(\mathbf{k})$ in the presence of various symmetries. To start with, we write down $\mathbf{j}^s_{\rm L,R}(\mathbf{k})$ explicitly using Eq. (S-12) as

$$\mathbf{j}^s_{\rm L,R}(\mathbf{k}) = \frac{e\pi}{2\hbar^2}\sum_{n,m,\mathbf{p}}\rho_{nm}(\mathbf{p},\mathbf{k})\mathbf{R}^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k}), \quad \mathbf{R}^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k}) = |V^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k})|^2\mathbf{r}^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k}), \tag{S-77}$$

in which $\rho_{nm}(\mathbf{p},\mathbf{k}) = [f(\epsilon_{m,\mathbf{p}-\mathbf{k}/2}) - f(\epsilon_{n,\mathbf{p}+\mathbf{k}/2})]\delta(\omega_{n,\mathbf{p}+\mathbf{k}/2} - \omega_{m,\mathbf{p}-\mathbf{k}/2} - \omega)$, $V^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k}) = (e/i\omega)\mathbf{E}^{\rm L,R}\cdot\langle u_n(\mathbf{p}+\mathbf{k}/2)|\hat{\boldsymbol{\nu}}|u_m(\mathbf{p}-\mathbf{k}/2)\rangle$, and $\mathbf{r}^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k}) = \mathbf{A}_n(\mathbf{p}+\mathbf{k}/2) - \mathbf{A}_m(\mathbf{p}-\mathbf{k}/2) - \nabla_{\mathbf{p}}\arg[V^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k})]$. Below we will analyze the symmetry properties of $\rho_{nm}(\mathbf{p},\mathbf{k})$ and $\mathbf{R}^{\rm L,R}_{nm}(\mathbf{p},\mathbf{k})$ using the Wilson loop formalism discussed previously.

(1) When a crystal has inversion symmetry, then we have $\epsilon^\sigma_{n,\mathbf{p}} = \epsilon^\sigma_{n,-\mathbf{p}}$, $|\mathcal{I}u^\sigma_n(\mathbf{p})\rangle = |u^\sigma_n(-\mathbf{p})\rangle$, and $\mathcal{I}\nu^{\rm L,R}\mathcal{I}^{-1} = -\nu^{\rm L,R}$. These leads to $\arg[\mathcal{W}^\sigma_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})]_{\rm L,R} = \arg[\mathcal{W}^\sigma_{nm}(-\mathbf{p},-\mathbf{q},-\mathbf{k})]_{\rm L,R} + \pi$, and

$$[\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})]^\sigma_{\rm L,R} = -[\mathbf{r}_{nm}(-\mathbf{p},-\mathbf{k})]^\sigma_{\rm L,R}, \quad \rho^\sigma_{nm}(\mathbf{p},\mathbf{k}) = \rho^\sigma_{nm}(-\mathbf{p},-\mathbf{k}), \tag{S-78}$$

where the $[\cdots]_{\rm L,R}$ subscripts denote left-hand polarization and right-hand polarization (see above) respectively. Together with Eq. (S-76) and Eq. (S-77) and, we obtain

$$[\delta\mathbf{j}^s(\mathbf{k})]^\sigma = -[\delta\mathbf{j}^s(-\mathbf{k})]^\sigma. \tag{S-79}$$

We note that this shows that the chirality-dependent circular photon drag shift current switches sign when the photon wavevector switches sign. As a sanity check, we can consider the limit $\mathbf{k} \to 0$. Using Eq. (S-79) shows that when $\mathbf{k} = 0$ we have $[\delta\mathbf{j}^s(\mathbf{k}=0)]^\sigma = -[\delta\mathbf{j}^s(\mathbf{k}=0)]^\sigma$ implying that the chirality dependent (normal incident) circular shift current *vanishes* in an IS preserving system, as expected. Photon-drag unblocks this requirement by having a finite $\mathbf{k}$.

(2) When a crystal has time reversal symmetry $\mathcal{T} = -i\sigma_y K$, then we have $\epsilon^{\sigma}_{n,\mathbf{p}} = \epsilon^{-\sigma}_{n,-\mathbf{p}}$, $|\mathcal{T} u^{\sigma}_n(\mathbf{p})\rangle = |u^{-\sigma}_n(-\mathbf{p})\rangle^*$, and $\mathcal{T}\nu^{\mathrm{L,R}}\mathcal{T}^{-1} = -\nu^{\mathrm{R,L}}$. These give rise to $\arg[\mathcal{W}^{\sigma}_{nm}(\mathbf{p},\mathbf{q},\mathbf{k})]_{\mathrm{L,R}} = -\arg[\mathcal{W}^{-\sigma}_{nm}(-\mathbf{p},-\mathbf{q},-\mathbf{k})]_{\mathrm{R,L}}$,

$$[\mathbf{r}_{nm}(\mathbf{p},\mathbf{k})]^{\sigma}_{\mathrm{L,R}} = [\mathbf{r}_{nm}(-\mathbf{p},-\mathbf{k})]^{-\sigma}_{\mathrm{R,L}}, \quad \rho^{\sigma}_{nm}(\mathbf{p},\mathbf{k}) = \rho^{-\sigma}_{nm}(-\mathbf{p},-\mathbf{k}), \tag{S-80}$$

where we have noted that the time reversal operation flips spin $\sigma \to -\sigma$. In the same fashion as above, we substitute Eq. (S-80) into Eq. (S-76) and Eq. (S-77), and obtain

$$[\delta \mathbf{j}^s(\mathbf{k})]^{\sigma} = -[\delta \mathbf{j}^s(-\mathbf{k})]^{-\sigma}. \tag{S-81}$$

This demonstrates that the chirality-dependent circular photon drag shift current switches sign when both the photon wavevector and the spin switch sign. It is instructive to consider the limit of zero photon drag $\mathbf{k} = 0$ (i.e. normally incident light). This shows that the chirality-dependent circular shift current for spin σ has the opposite sign from $-\sigma$. Summing both spins, we find that the *charge* chirality-dependent circular shift current vanishes in a TRS preserving system. This is consistent with the odd parity of the charge circular shift current under time reversal recently discussed in Ref. [17]. Eq. (S-81) shows that photon drag processes unblocks this requirement by having a finite $\mathbf{k}$.