Microscopic theory of spin-orbit torque and spin memory loss from interfacial spin-orbit coupling

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Despite extensive efforts it has remained elusive how the spin-relaxation and spin-precession processes influence the spin-orbit torque and spin memory loss at heavy metal (HM)–ferromagnetic insulator (FI) heterostructure. Here, we study the spin transport of the spin-orbit-coupled ferromagnets based on the SU(2) gauge field theory and reveal that the interfacial spin-orbit coupling is responsible for (i) noncollinear spin exchange, (ii) anisotropic spin relaxation, and (iii) interfacial magnetic field. We show that the noncollinear spin exchange can tune the damping- and field-like torques. The spin-loss conductance is analytically derived by considering interfacial Rashba, Dresselhaus, and strain-induced spin-orbit couplings. Our theory offers a deep understanding of the spin transport across the HM|FI interface.

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I. INTRODUCTION

The interplay of the spin-orbit coupling (SOC) and the spin-exchange coupling (SEC) is currently a subject of particular interest in spintronics [1–16], because it can lead to many peculiar phenomena including anomalous Hall effect [1], spin swapping effect [2–4], and spin-orbit torques [5–16]. This interplay is ubiquitous, for example, at the magnetic interface [16–19], in van der Waals (vdW) ferromagnets [20–23], and even at the interface of two nonmagnetic materials [24,25]. The atomically thin vdW ferromagnets, owing to sizable SOC, possess high-quality perpendicular magnetic anisotropy up to room temperature [26–28]. Thus, these ultrathin vdW ferromagnets emerge as prime candidates for practical spintronic applications [29] especially offering unprecedented opportunities for the spin-orbit torque [13]. It has been speculated that both SOC and SEC can lead to the spin relaxation and spin precession, but it remains unclear how the interfacial SOC interacts with the SEC to tune the spin-orbit torque across the heavy metal (HM)–ferromagnetic insulator (FI) interface [30,31].

Recent theoretical efforts reveal the possible relevance of the interfacial SOC to the spin-orbit torque [5–8] and assume a full transfer of the perpendicular component of the interfacial spin current into the local moment of FI via the damping-like torque [9–11]. However, the unavoidable spin relaxation from the interfacial SOC substantially reduces the spin current arising from the spin Hall effect in the HM and hence suppresses the torque exerted on the local moment of FI [32], resulting in spin memory loss [32–37]. The computation of the spin memory loss was thought to be an arduous task which could only be carried out by the first-principle scattering calculations [35–37]. Moreover, the previous spin drift-diffusion formalism [7,8] used for spin-orbit torque omits the spin density-to-current conversion—a direct conversion of nonequilibrium spin density to spin current via the SU(2) gauge field of the interfacial SOC [38–41]. Consequently, it is desirable to develop a microscopic theory to unify the spin-orbit torque and spin memory loss in the presence of interfacial SOC.

In this paper, we analytically study how interfacial SOC generates the noncollinear SEC and tunes the damping- and field-like torques from a microscopic perspective. We explore the spin-orbit torque efficiency after considering several sources of the spin memory effect quantified by the spin-loss conductance that has been analytically derived by considering interfacial Rashba, Dresselhaus, and strain-induced SOC. Importantly, we demonstrate exotic spin-loss conductance zero-, first-, and second-order to the interfacial SOC, resulting in the spin relaxation and precession of the interfacial spin density.

We organize the remainder of this paper as follows. In Sec. II, we not only give the system Hamiltonian of the HM–FI heterostructure (Sec. II A) but also study the spin transport of the itinerant electrons based on the SU(2) gauge field theory (Sec. II B). In Sec. III, we derive the HM|FI interface spin current (Sec. III A), which is responsible for spin-orbit torque (Sec. III B) and spin memory loss (Sec. III C). Section IV summarizes our findings. Finally, Appendix A presents the derivation of SU(2) gauge fields from the interfacial SOC, Appendix B presents the detailed derivations of the quantum kinetic equation of the spin-orbit-coupled ferromagnet,

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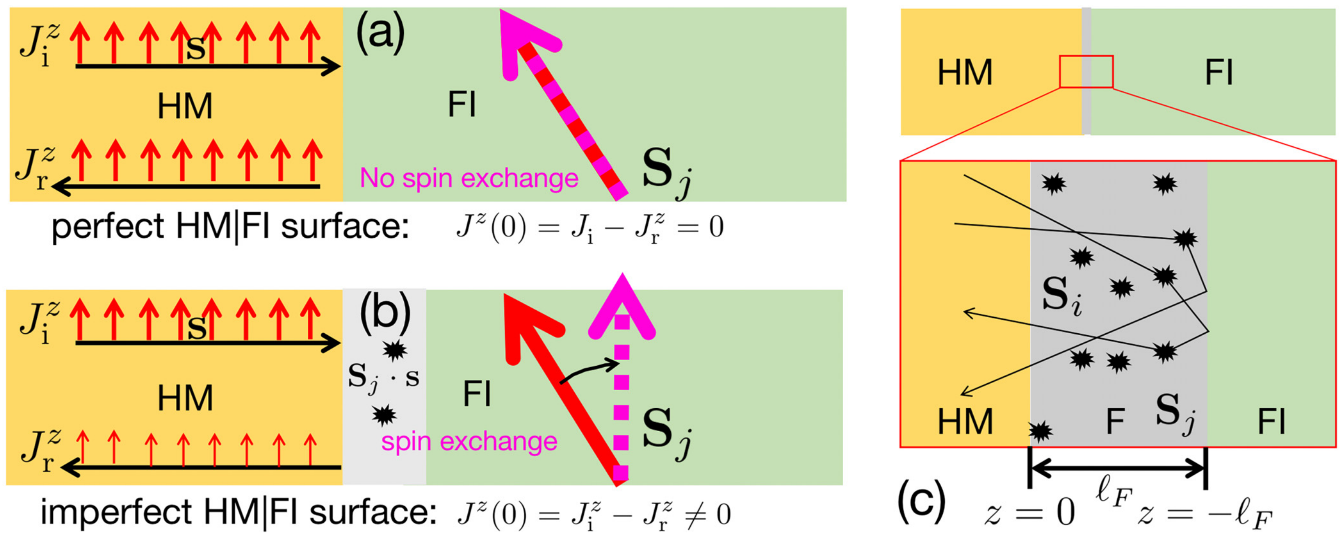

FIG. 1. [(a), (b)] Reflections of spin current at heavy metal (HM) | ferromagnetic insulator (FI) interface. For a perfect HM|FI interface (a), the injected spin current J^z_i is fully reflected, i.e., $J^z_r = J^z_i$, because electron is not able to enter a perfect insulator. Thus, no net spin current is injected into FI to control the magnetization of FI. For an imperfect HM|FI interface (b), there is not a clear boundary between HM and FI. Electron can interact with the *interfacial* local moments of the FI and lose its spin due to its exchange with local moments (black sparks). The reflected spin current is smaller than the injected one, i.e., $J^z_r < J^z_i$. Therefore, the spin-orbit torque can be captured by the nonzero net spin current at HM|FI interface $J^z(0) = J^z_i - J^z_r \neq 0$, whose intrinsic magnetic moments is transferred into the magnetization of the FI. (c) The sketch of a HM-FI heterostructure. We assume the HM|FI interface to be a ferromagnet (F) of thickness ℓ_F.

Appendix C gives the detailed derivations of the noncollinear SEC, and Appendix D shows the interfacial SOC dependence of the spin conductance.

II. MODEL AND THEORY

We consider the HM-FI heterostructure (Fig. 1), for instance, EuS/Pt [42]. The intrinsic magnetic moments of the *interfacial* spin current injected from HM via the spin Hall effect transmit to the local moments of FI [Fig. 1(b)]. Thus, spin-orbit torque and spin memory loss are captured by the interfacial spin current [43] and illustrated by the reflections of spin current at HM|FI interface [Figs. 1(a) and 1(b)]. For an ideal HM|FI interface [Fig. 1(a)], the injected spin current is fully reflected because an electron cannot enter an *insulator*. As a result, no net spin current is injected into the FI to change its magnetization. For an imperfect HM|FI interface [Fig. 1(b)], the electron can interact with the interfacial local moments of the FI and lose its spin due to its exchange with the local moments. Then, the reflected spin current is smaller than the injected spin current. Therefore, the nonzero net spin current, whose intrinsic magnetic moments transmit to the FI's magnetization, captures the spin-orbit torque at the HM|FI interface.

The purpose of this paper is to understand how the interfacial SOC affects spin-orbit torque and spin memory loss. We treat the HM|FI interface as a spin-orbit-coupled ferromagnet (F) of thickness ℓ_F [gray region in Fig. 1(c)], where local moments and itinerant electrons coexist and interact via the SEC [14,44]. In this picture, F acquires magnetization from the intrinsic magnetic moments of the *interfacial* spin current and transfers its magnetization into the FI via the spin-exchange coupling between F and FI. Notably, the FI itself can be an atomically thin vdW ferromagnet, and our theory is also applicable for the state-of-the-art Fe_3GeTe_2/Pt heterostructure [45]. Also, our theory works on other magnetic configurations, for instance, $Gd_3Ga_5O_{12}/Pt$ [46] and $Y_3Fe_5O_{12}/Pt$ [47].

A. System Hamiltonian

The spin exchange (loss) responsible for the spin-orbit torque (spin memory loss) happens at the spin-orbit-coupled F of thickness ℓ_F, as shown by the gray region in Fig. 1. Thus, we consider an F consisting of itinerant electrons and local moments whose total Hamiltonian is given by

$$H = H_m + H_\mathrm{int} + \int \mathcal{H}_e(\boldsymbol{r})d\boldsymbol{r}. \tag{1}$$

To distinguish different magnetic configurations of the FI, we assume that the local moments of the F, i.e., the interfacial local moments of the FI, maintain the similar magnetic configurations as the FI and therefore can be described by the Heisenberg Hamiltonian

$$H_m = \mathrm{g}_n \mu_B \boldsymbol{B} \cdot \boldsymbol{S}_n - \frac{1}{2}\sum_{n,m} J_{nm} \boldsymbol{S}_n \cdot \boldsymbol{S}_m, \tag{2}$$

where $\mathrm{g}_n \simeq 2$ is the g factor, μ_B is the Bohr magneton, and $\boldsymbol{B}$ is a uniform external magnetic field in $\hat{\boldsymbol{B}}^0 = \boldsymbol{B}^0/B^0$ direction. $\mathbf{S}_n = (S^x_n, S^y_n, S^z_n)$ is the spin-S^o operator situated on unit cell n and J_{nm} is the exchange coupling constant between two local moment spins $\mathbf{S}_n$ and $\mathbf{S}_m$, including nearest-neighbor, next-nearest-neighbor spin exchanges and so on.

The SEC responsible for the spin-orbit torque can be modeled by the so-called Kondo coupling—a collinear spin exchange between local moments and itinerant electrons [Fig. 2(a)]. As shown in Fig. 2(b), the Peierls substitution reveals that itinerant electron spin rotates along the spin-orbit

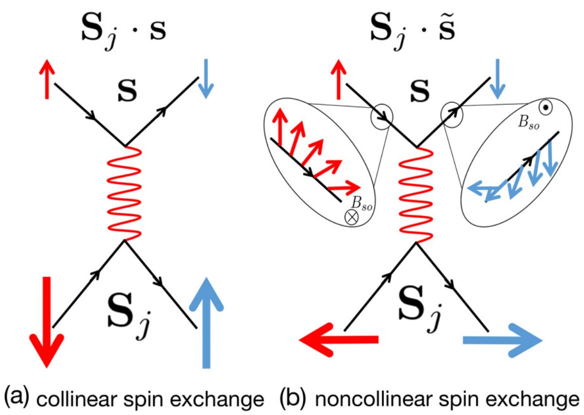

FIG. 2. The sketches of (a) collinear and (b) noncollinear spin exchange between local moments ($\mathbf{S}_j$, thick arrows) and itinerant electrons ($\mathbf{s}$, thin arrows), i.e., Eq. (3). The red (blue) arrows are spins before (after) exchange. The spin rotation of the itinerant electron along the spin-orbit magnetic field (B_{so}) leads to a noncollinear spin exchange between local moments and itinerant electrons (b).

magnetic field during the exchange and therefore we reach a noncollinear SEC between local moments and itinerant electrons via the Schrieffer-Wolff transformation [48–50] (see detailed derivations in Appendix C)

$$H_{\rm int} = -\sum_n K_s \mathbf{S}_n \cdot \tilde{\mathbf{s}}\delta(\boldsymbol{r}-\boldsymbol{r}_n), \tag{3}$$

where K_s describes the noncollinear spin-exchange coupling strength between the itinerant electron and the local moment. The tilde spin operator $\tilde{s}^a = R_{ab}s^b$ is described by a spin rotation matrix R relative to the SOC [49,50] (see derivation in Appendix C). To use powerful single-scattering and disorder-averaging techniques to calculate the spin-relaxation time inside the F layer, the local moments in the F is required to be randomly distributed as a result of the imperfect magnetic interface in real experiments. The F is strongly disordered, such that the mean-free path l is much smaller than both the thickness of the F ℓ_F and the spin-relaxation length ℓ_F^a. Thus, the itinerant electrons in the F undergo a *diffusive* motion and the events of interaction with the local moments located on the F appear as spikes of short duration, randomly distributed along the semiclassical trajectory of the electron [14]. The noncollinear SEC (3) rotates the longitudinal ($s^{\parallel} = \tilde{\mathbf{s}}\cdot\hat{\boldsymbol{B}}^0$) and transverse ($\boldsymbol{s}^{\perp} = \hat{\boldsymbol{B}}^0 \times \tilde{\mathbf{s}} \times \hat{\boldsymbol{B}}^0$) spin components, whose relaxation time, within the Born-Markov and the Weiss-field approximations, reads [14,44]

$$\frac{1}{\tau_{\parallel}^m} = \frac{2\pi}{\hbar} n_m \nu_F K_s^2 \beta\epsilon_L n_B(\epsilon_L)[1+n_B(\epsilon_L)]|\langle S^{\parallel}\rangle|, \tag{4}$$

$$\frac{1}{\tau_{\perp}^m} = \frac{1}{2\tau_{\parallel}^m} + \frac{\pi}{\hbar} n_m \nu_F K_s^2 \langle S^{\parallel} S^{\parallel}\rangle. \tag{5}$$

Here, ν_F is the density of state at Fermi energy, $S^{\parallel}$ is a spin operator along the magnetic-field direction, n_m is the density of local moments, and $n_B(\epsilon_L) = 1/(e^{\beta\epsilon_L}-1)$ is the Bose-Einstein distribution function at effective Larmor frequency $\epsilon_L = g\mu_B B^0 - \sum_n J_{nm}\langle S_n^{\parallel}\rangle$, including the contributions from the nearest-neighbor, next-nearest-neighbor spin exchanges and so on. Note that the Born-Markov approximation requires the Kondo coupling (3) to be a perturbation, and hence $n_m K_s$ should be much smaller than the effective Zeeman energy ϵ_L.

The itinerant electron Hamiltonian [third term of Eq. (1)] can be rewritten into $U(1)\otimes SU(2)$ form [51–57] (see details in Appendix A),

$$\mathcal{H}_e(\boldsymbol{r}) = v_0 e\hat{A}_0(x_\eta) + \frac{\hbar^2}{2m}\hat{\partial}_a\hat{\partial}_a, \tag{6}$$

where e is the charge of electron, $\hbar$ is the reduced Planck constant, m is the effective mass of the ferromagnet, $x^\eta = (v_0 t, \boldsymbol{x})$ is four-vector coordinate, and v_0 is the speed of light. Hereafter, the Greek superscript η sums over four components, the Latin subscripts a refer to the spatial components, and the repeated indices imply summation. The hat derivative contains the non-Abelian gauge fields

$$\hat{\partial}_\eta = \frac{\partial}{\partial x^\eta} + \frac{ie}{\hbar}[\hat{A}_\eta(x^\eta), \cdot]. \tag{7}$$

The SOC and magnetic exchange field are recognized as the spatial and temporal non-Abelian SU(2) gauge fields of itinerant electrons [54,56,57]

$$\hat{A}_\eta(x^n) = \left[\frac{1}{v_0}\Phi^0(x^n) + \frac{1}{v_0}\Phi^a(x^n)\hat{s}^a, -\boldsymbol{A}^0(x^n) - \boldsymbol{A}^a(x^n)\hat{s}^a\right]. \tag{8}$$

The generators of $SU(2)\hat{s}^a$ satisfy $[\hat{s}^a, \hat{s}^b] = i\epsilon^{abc}\hat{s}^c$ and $\mathrm{tr}\{\hat{s}^a, \hat{s}^b\} = \delta_{ab}$, where ϵ^{abc} is the Levi-Civita antisymmetric tensor and δ_{ab} is the Dirac delta function. The scalar $[\Phi^0(x_n)]$ and vector $[\boldsymbol{A}^0(x_n)]$ potentials account for the temporal and spatial components of the Abelian U(1) Maxwell gauge fields, while the Zeeman $[\Phi^a(x_n)]$ and spin-orbit $[\boldsymbol{A}^a(x_n)]$ interactions correspond the temporal and spatial components of the non-Abelian SU(2) Yang–Mills gauge fields [58,59]. The natural lack of inversion symmetry at the HM|FI interface produces sizable Rashba and Dresselhaus SOC [60–62], as well as strain-induced SOC [63–65], whose spatial gauge fields are given by

$$\hat{A}^x = A^x + \frac{2m}{e}[-\beta\hat{s}^1 + (\alpha - u_{xy}\lambda)\hat{s}^2 + u_{zx}\lambda\hat{s}^3], \tag{9}$$

$$\hat{A}^y = A^y + \frac{2m}{e}[+(-\alpha + u_{xy}\lambda)\hat{s}^1 + \beta\hat{s}^2 - u_{yz}\lambda\hat{s}^3], \tag{10}$$

$$\hat{A}^z = A^z + \frac{2m}{e}[-u_{zx}\lambda\hat{s}^1 + u_{yz}\lambda\hat{s}^2]. \tag{11}$$

Here, α, β, and λ are the constants of Rashba, Dresselhaus, and strain-induced SOC, respectively, with u_{ij} being elements of the strain tensor [63].

B. Spin drift-diffusion-gauge formalism

To explore how the interfacial SOC affects the HM|FI interface spin current, we are required to derive the spin drift-diffusion-gauge formalism of the itinerant electrons with $U(1)\otimes SU(2)$ Hamiltonian (6). The equation of motion of the two-time density matrix for itinerant electrons $\hat{\rho}(t_1,t_2) = |\hat{\psi}(t_1)\rangle\langle\hat{\psi}(t_2)|$ [66], derived from the Schrödinger equation, is given by

$$\left[\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}\right]\hat{\rho}(t_1,t_2) = \frac{i}{\hbar}[\hat{\rho}(t_1,t_2), \mathcal{H}_e]. \tag{12}$$

In a position representation we have wave function $\hat{\psi}(x_n) = \langle \boldsymbol{r}_n | \hat{\psi}(t_n) \rangle$ and density matrix $\hat{\varrho}(x_1, x_2) = \hat{\psi}(x_1)\hat{\psi}^+(x_2)$. Then, the two-time master equation (12) becomes

$$\hat{\mathcal{G}}(x_1)\hat{\varrho}(x_1, x_2) - \hat{\varrho}(x_1, x_2)\hat{\mathcal{G}}^+(x_2) = 0. \quad (13)$$

The propagator has U(1) ⊗ SU(2) form [51–57]

$$\hat{\mathcal{G}}(x_n) = i\hbar v_0 \hat{\partial}_0 + \frac{\hbar^2}{2m}\hat{\partial}_a\hat{\partial}_a. \quad (14)$$

The Zeeman magnetic field [first term of Eq. (6)] includes the correction from local moments

$$e\Phi^a(x) = g\mu_B B^{0a} - (n_m K_s/2)\langle \tilde{S}^a \rangle, \quad (15)$$

and combines the time derivative of Eq. (12) to generate temporal covariant derivative—the first term of propagator (14).

Next, we work on the quantum kinetic equation for $\hat{\varrho}_{\boldsymbol{k}}(X)$—the gauge-invariant Wigner transformation of the two-time density matrix $\hat{\varrho}(x_1, x_2)$ (see detailed definition and derivations in Appendix B)

$$v_k^\nu \hat{\partial}_\nu \hat{\varrho}_{\boldsymbol{k}}(X) + \frac{e v_k^\mu}{2\hbar}\{\hat{F}_{j\mu}, \partial_{k_j}\hat{\varrho}_{\boldsymbol{k}}(X)\} = 0, \quad (16)$$

with

$$\hat{F}_{\mu\nu} = \frac{\partial \hat{A}_\nu}{\partial X^\mu} - \frac{\partial \hat{A}_\mu}{\partial X^\nu} + \frac{ie}{\hbar}[\hat{A}_\mu, \hat{A}_\nu], \quad (17)$$

where $x = (x_1 - x_2)$ and $X = (x_1 + x_2)/2$. Notably, the SU(2) technology does not require the translation invariance, and hence $\boldsymbol{k}$, as the gauge-invariant Fourier transformation of $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, is not a good quantum number. Here, we have removed the higher-order terms $\partial_{k_\alpha}\partial_{k_\beta}\hat{\varrho}$, $\partial_{X^\mu}\partial_{X^\mu}\hat{\varrho}$, and $\partial_{X^\mu}\partial_{k_\beta}\hat{\varrho}$ for simplicity [67], which results in the approximation that the velocity of the itinerant electron is independent of the SOC, i.e., $v_k^\nu = (c, \frac{\hbar k^j}{m})$. Our quantum kinetic equation (16) coincides with the Green's function method [51–57,67,68].

We then explore the *nonequilibrium* physics of the itinerant electrons in the presence of the external electric field $E_{\rm ex}^{j0}$. The equilibrium density matrix $\hat{\varrho}_{\boldsymbol{k}}^{\rm eq}$ is defined from quantum kinetic equation (16) at zero external electric field ($E_{\rm ex}^{j0} = 0$),

$$c\hat{\partial}_0\hat{\varrho}_{\boldsymbol{k}}^{\rm eq} + \frac{e v_{\boldsymbol{k}}^i}{\hbar}\epsilon^{ilj}B^l\partial_{k^j}\hat{\varrho}_{\boldsymbol{k}}^{\rm eq} + v_{\boldsymbol{k}}^j\hat{\partial}_j\hat{\varrho}_{\boldsymbol{k}}^{\rm eq} + \frac{e v_{\boldsymbol{k}}^i}{2\hbar}\epsilon^{ilj} B^{la}\{\hat{s}^a, \partial_{k^j}\hat{\varrho}_{\boldsymbol{k}}^{\rm eq}\} + \frac{e}{2}\{(E_{\rm in}^{j0} + E^{ja}\hat{s}^a), \partial_{k_j}\hat{\varrho}_{\boldsymbol{k}}^{\rm eq}\} = 0, \quad (18)$$

and is determined by both $\Phi^\mu(x_n)\hat{s}^\mu$ and $\boldsymbol{A}^\mu(x_n)$. Here, we have used the following relations $E^{ja} = cF_{0j}^a$ and $F_{ji}^\nu = -\epsilon^{jil}B^{l\nu}$. The equilibrium drift term includes both the intrinsic electric force $e\boldsymbol{E}_{\rm in}^0$ responsible for charge current and the spin electric forces $e\boldsymbol{E}^a$ in charge of the spin currents, which cause equilibrium charge and spin accumulations, respectively. We are not required to solve the complicated equilibrium density matrix defined in Eq. (18), because we are only interested in nonequilibrium physics. Introducing the nonequilibrium density matrix $\delta\hat{\varrho}_{\boldsymbol{k}} = \hat{\varrho}_{\boldsymbol{k}} - \hat{\varrho}_{\boldsymbol{k}}^{\rm eq}$, we reach the *linear* nonequilibrium quantum transport equation

$$v_0\hat{\partial}_0\delta\hat{\varrho}_{\boldsymbol{k}} + \frac{e v_{\boldsymbol{k}}^i}{\hbar}\epsilon^{ilj}B^{l0}\partial_{k^j}\delta\hat{\varrho}_{\boldsymbol{k}} + v_{\boldsymbol{k}}^j\hat{\partial}_j\delta\hat{\varrho}_{\boldsymbol{k}} + \frac{e v_{\boldsymbol{k}}^i}{2\hbar}\epsilon^{ilj}B^{la}\{\hat{s}^a, \partial_{k^j}\delta\hat{\varrho}_{\boldsymbol{k}}\} + eE_{\rm ex}^{j0}\partial_{k_j}\hat{\varrho}_{\boldsymbol{k}}^{\rm eq} = -\frac{1}{\tau}\delta\hat{\varrho}_{\boldsymbol{k}}. \quad (19)$$

We have worked in the diffusive regime and used the relaxation time approximation with τ being the momentum relaxation time from nonmagnetic impurities. The Hanle effect results from the temporal covariant derivative [$\eta = 0$ of Eq. (7)], which includes the temporal gauge field $\hat{A}_0$, whereas the spatial covariant derivative [$\eta \neq 0$ of Eq. (7)] containing the spatial gauge fields $\hat{A}_j$ results in the spin density-current conversion [Eqs. (27) and (32)]. The second term is the ordinary magnetic force $e\boldsymbol{v}_{\boldsymbol{k}} \times \boldsymbol{B}^0$, which is responsible for the ordinary Hall effect, and the fourth is the spin magnetic force $e\boldsymbol{v}_{\boldsymbol{k}} \times \boldsymbol{B}^a$, which is in charge of the spin Hall effects [69,70].

The nonequilibrium density tensor can be expressed in terms of the nonequilibrium density matrix $\delta\hat{\varrho}_{\boldsymbol{k}}(X)$

$$\hat{N}(X) = \int \frac{d\boldsymbol{k}}{(2\pi)^3}\delta\hat{\varrho}_{\boldsymbol{k}}(X), \quad (20)$$

Derived from Eq. (19), we obtain the generalized continuity equation [71–73]—the time evolution of the nonequilibrium density tensor (20)

$$v_0\hat{\partial}_0\hat{N}(X) + \hat{\partial}_a\hat{J}^a(X) = 0. \quad (21)$$

The expression of the nonequilibrium spin current tensor is given by

$$\hat{\boldsymbol{J}}(X) = \int \frac{d\boldsymbol{k}}{(2\pi)^3}\boldsymbol{v}_{\boldsymbol{k}}\delta\hat{\varrho}_{\boldsymbol{k}}(X), \quad (22)$$

to have the covariant continuity equation (21). Note that the nonequilibrium density matrix $\delta\hat{\varrho}_{\boldsymbol{k}}(X)$ in Eqs. (20) and (22) is proportional to the drift term—the last term of the left-hand side of Eq. (19) linear in $E_{\rm ex}^{j0}$, which, in principle, includes the information of gauge fields in equilibrium density matrix $\hat{\varrho}_{\boldsymbol{k}}^{\rm eq}$ defined in Eq. (18). To simplify, we excluded the influence of the spatial gauge fields on the equilibrium density matrix by assuming $\hat{\varrho}_{\boldsymbol{k}}^{\rm eq} = f(\epsilon_{\boldsymbol{k}} + e\Phi^a\hat{s}^a)$ such that the equilibrium spin density can be finite but the equilibrium spin current is always zero. Here, $\epsilon_{\boldsymbol{k}} = \frac{\hbar^2\boldsymbol{k}^2}{2m}$ and $f(\epsilon) = 1/[e^{\beta(\epsilon-\mu_F)} + 1]$ is the Fermi-Dirac distribution at the absolute temperature T and global chemical potential μ_F. The solution to Eq. (19), can be obtained by applying the ansatz [74]

$$\delta\hat{\varrho}_{\boldsymbol{k}} \simeq -f'(\epsilon_{\boldsymbol{k}})\hat{s}^\mu v_\mu^\nu k^\nu. \quad (23)$$

The fields v^j and v^0k^0 correspond to the drift velocity and the local chemical potential of the itinerant electrons, respectively. Both are proportional to the external electric field. Then, the nonequilibrium spin density and current, Eqs. (20) and (22), at zero temperature, reduce to

$$N^\mu = k^0\nu_F v^{0\mu}, \quad (24)$$

$$J^{i\mu} = v_F k_F \nu_F v^{i\mu}/d, \quad (25)$$

where ν_F and v_F are the density of state and the velocity at Fermi energy for the d dimensional system. Here, we have assumed $v_{\boldsymbol{k}}^i = v_F k^i/|\boldsymbol{k}|$.

Next, we derive the constitutive equations—the time evolution of the nonequilibrium currents. By substitutions of Eqs. (20) and (22), we can derive a set of constitutive equations from the *linear* nonequilibrium quantum transport equation (19) [38,75],

$$\boldsymbol{J}^0 + \boldsymbol{\theta}_C^0 \times \boldsymbol{J}^0 + \boldsymbol{\theta}_C^a \times \boldsymbol{J}^a = \sigma \boldsymbol{\mathcal{E}}^0 - D\nabla N^0, \tag{26}$$

$$\boldsymbol{J}^a - \epsilon^{abc}\theta_L^b \boldsymbol{J}^c + \boldsymbol{\theta}_C^0 \times \boldsymbol{J}^a + \boldsymbol{\theta}_C^a \times \boldsymbol{J}^0 = \sigma \boldsymbol{\mathcal{E}}^a - D\Big(\nabla N^a + \frac{e}{\hbar}\epsilon^{abc}\boldsymbol{A}^b N^c\Big), \tag{27}$$

where N^c is the density polarized in c direction, $J^{i\eta}$ is the current polarized in η direction and flowing in i direction. Each current $\boldsymbol{J}^\eta$ has its mechanical force $e\boldsymbol{\mathcal{E}}^\eta$ linear to the external electric field $\boldsymbol{E}_{\text{ex}}$, where the charge (spin) electric field $\boldsymbol{\mathcal{E}}^0 = \kappa_0 \boldsymbol{E}_{\text{ex}}$ ($\boldsymbol{\mathcal{E}}^a = \kappa_a \boldsymbol{E}_{\text{ex}}$) accounts for nonequilibrium drift charge (spin) current. The dimensionless coefficients κ_a describe the drift charge-to-spin conversion efficiency, and are derived from the equilibrium density matrix $f'(\mu_F + e\Phi^a\hat{s}^a) \equiv f'(\mu_F)\kappa_\mu \hat{s}^\mu$. The Drude conductivity is $\sigma = e\nu_F D$, where $D = v_F^2\tau/d$ is the diffusion coefficient. For simplicity, σ and D are assumed to be the same for all currents. The Larmor precession of spin currents caused by the Zeeman magnetic field (15) is described by

$$\boldsymbol{\theta}_L = e\boldsymbol{\Phi}\tau/\hbar. \tag{28}$$

Ordinary and spin Hall angles owing to orbital and spin-orbit magnetic fields are

$$\boldsymbol{\theta}_C^0 = \frac{e v_F \tau}{\hbar k_F}\boldsymbol{B}^0, \tag{29}$$

$$\boldsymbol{\theta}_C^a = \frac{e v_F \tau}{\hbar k_F}\boldsymbol{B}^a, \tag{30}$$

proportional to ordinary and spin magnetic forces, respectively. Solving the system of equations (26) and (27), we express $\hat{\boldsymbol{J}}$ in terms of a covariant derivative with $\hat{N}$ and generalize the nonequilibrium drift-diffusion equation [7] into the following nonequilibrium drift-diffusion-gauge equation [38,66]

$$J^{i\eta} = \Theta_{j\nu}^{i\eta}\sigma\mathcal{E}^{j\nu} - \Theta_{j\nu}^{i\eta}D\partial_j N^\nu - \Theta_{j\nu}^{i\eta}D\frac{e}{\hbar}\epsilon^{\nu bc}A^{jb}N^c. \tag{31}$$

The first, second, and third terms, respectively, correspond to the standard Ohm's, Fick's laws, and the spin density-to-current conversion [39,40]. The conversion of different currents is described by a drift-diffusion-gauge tensor $\Theta_{j\nu}^{i\eta}$ that is determined by spin-precession ($\boldsymbol{\theta}_L$), ordinary Hall ($\boldsymbol{\theta}_C^0$), and spin Hall ($\boldsymbol{\theta}_C^a$) angles after inverting the system of equations (26) and (27). Although the derivation of the explicit expressions of the drift-diffusion-gauge tensor is a challenging task, we can iteratively calculate it from Eqs. (26) and (27). Note that there is a long-standing issue in the definition of spin current in the absence of spin conservation due to the SOC [72,73,76–79]. Equations (20) and (22) are consistent with their microscopic definitions [54,55,67]. The covariant expression of current (31) is an alternative of N^η, consistent with both diffusion equation (21) and boundary conditions [71,73]. We can always express the spin transport relevant to the SOC by spin density—the quantity directly measured in experiments.

III. RESULTS AND DISCUSSIONS

A. Ferromagnetic interface spin current

Note that both spin-orbit torque and spin memory loss can be derived from the spin current at the HM|FI interface [14,43]. Microscopically, the ferromagnetic interface spin current is derived from the continuity equation [14]. Thus, we study how the interfacial SOC modifies the continuity equation through the noncollinear SEC (3) and gauge fields (8). The spin-a components of the generalized continuity equation (21), in steady state, are

$$\nabla\cdot\boldsymbol{J}^a = -\frac{1}{\tau_a^m}N^a + \frac{e}{\hbar}\epsilon^{abc}\Phi^b N^c - \frac{e}{\hbar}\epsilon^{abc}\boldsymbol{A}^b\cdot\boldsymbol{J}^c, \tag{32}$$

where we have added the spin relaxation of the itinerant electrons τ_a^m due to its noncollinear SEC with the local moments [Eqs. (4) and (5)]. Hereafter, we assume that the gauge fields (8) are uniform along the z-axis direction in ferromagnet and hybrid system is uniform in the (x, y) plane. Then, we calculate the spin current at the HM|F interface ($z = 0$) by integrating $\partial_3 J^{3a}$ in Eq. (32) over the F ($z \in [-\ell_F, 0]$),

$$J^{za} = -\frac{1}{\tau_a^m}\bar{N}^a + \frac{e}{\hbar}\epsilon^{abc}\Phi^b\bar{N}^c - \frac{e}{\hbar}\epsilon^{abc}\boldsymbol{A}^b\cdot\bar{\boldsymbol{J}}^c, \tag{33}$$

where $\bar{X} = \int_{-\ell_F}^0 X dz$ and we have used the fact that the *nonequilibrium* spin density and current at F|FI surface ($z = -\ell_F$) are zero, that is, $N^a(-\ell_F) = 0$ and $J^{za}(-\ell_F) = 0$. The spin density at F approximately decays according to $N^a(z) \simeq N^a(0)e^{+z/\ell_F^a}$, where ℓ_F^a is the spin-a diffusion length of the itinerant electron in the ferromagnet, arising from both SEC and SOC (see detailed expressions in Appendix D). Thus, we have

$$\bar{N}^a \simeq \tilde{\ell}_F^a N^a(0) \simeq \begin{cases} \ell_F^a N^a(0), & \ell_F \gg \ell_F^a \\ \ell_F N^a(0), & \ell_F \ll \ell_F^a \end{cases}. \tag{34}$$

The interfacial SOC modulation of the interfacial spin current i.e., spin-orbit torque and spin memory loss, is also through ℓ_F^a and becomes more obvious for $\ell_F \gg \ell_F^a$. Thus, hereafter, we consider the case of $\ell_F \gg \ell_F^a$.

Substituting Eq. (31) into Eq. (33), we obtain the boundary condition

$$J^{za} \simeq -\left(\frac{\ell_F^a}{\tau_a^m} + \Omega_+^{aa} + \Gamma_+^{aa}\right)N^a - |\epsilon^{abc}|(\Omega_+^{ac} + \Gamma_+^{ac})N^c + \epsilon^{abc}\left(\frac{e\ell_F^c}{\hbar}\Phi^b - \Omega_-^{ac} - \Gamma_-^{ac}\right)N^c - \sigma\frac{e}{\hbar}\epsilon^{ab\nu}A^{ib}\Theta_{jc}^{i\nu}\bar{\mathcal{E}}^{jc}. \tag{35}$$

The tensors $\Omega_\pm^{ac} = (\Omega^{ac} \pm \Omega^{ca})/2$ and $\Gamma_\pm^{ac} = (\Gamma^{ac} \pm \Gamma^{ca})/2$ show how the spin relaxation and precession of the interfacial spin density, due to the interfacial SOC, control the ferromagnetic interface spin current with

$$\Omega^{ac} = -\frac{e^2\ell_F^c D}{\hbar^2}\epsilon^{ab\mu}\epsilon^{\nu dc}A^{ib}\Theta_{j\nu}^{i\mu}A^{jd}, \tag{36}$$

$$\Gamma^{ac} = -D\frac{e}{\hbar}\epsilon^{abv}A^{ib}\Theta^{iv}_{3c}. \tag{37}$$

The diagonal terms of the tensors ($a = c$) renormalize the spin relaxation time (Ω^{aa}_{+}, Γ^{aa}_{+}), while the off-diagonal ones ($a \neq c$) not only renormalize the interfacial magnetic exchange field (Ω^{ac}_{-}, Γ^{ac}_{-}) but also cause a symmetric coupling (Ω^{ac}_{+}, Γ^{ac}_{+}). Besides, the interfacial spin drift current is *linearly* modified by the gauge fields [last term of Eq. (35)]. Notably, the presence of $\Theta^{i\eta}_{j\nu}$ in the continuity equation (35) includes the feedback of the Hanle ($\boldsymbol{\theta}_L$), ordinary ($\boldsymbol{\theta}^0_C$), and spin ($\boldsymbol{\theta}^a_C$) Hall effects on the spin relaxation. $1/\tau^m_a$ (Ω^{aa}_{+}) term has been extensively studied for the spin-dependent (-loss) conductance [14] ([43]). So far, little attention is paid to the fruitful new terms [Eqs. (36) and (37)] derived from the SU(2) gauge field theory.

Hereafter, we consider the strong ordinary Hall effect ($\theta^0_C \gg \theta_L, \theta^a_C$). Up to the first order of θ^0_C, the spin drift-diffusion-gauge tensor becomes

$$\Theta^{ia}_{jb} \simeq \delta_{ab}\left(\delta_{ij} - \epsilon^{ikj}\theta^{k0}_C\right), \tag{38}$$

which excludes the Hanle effect and spin Hall effect in F. Expressing the nonequilibrium spin density at ferromagnetic interface by spin electrochemical potentials $\boldsymbol{\mu} = \frac{1}{k_F v_F}(N^1, N^2, N^3)$, Eq. (35) becomes

$$\boldsymbol{J}^z = \boldsymbol{J}^M + \boldsymbol{J}^L + \boldsymbol{J}^S + \boldsymbol{J}^A + \boldsymbol{J}^E, \tag{39}$$

where $\boldsymbol{J}^p = (J^{p1}, J^{p2}, J^{p3})$ with $p = (z, M, L, S, A, E)$. The interfacial drift spin current $J^{Ea} = -\sigma\frac{e}{\hbar}\epsilon^{abv}A^{ib}\Theta^{iv}_{jc}\bar{\mathcal{E}}^{jc}$ is determined by both the spatial gauge fields and generalized spin electric fields [last term of Eq. (35)].

B. Spin-orbit torques

First, $\boldsymbol{J}^M$ is the interfacial spin current of the itinerant electrons owing to its noncollinear SEC with the local moments [τ^m_a and Φ^b terms in Eq. (35)]

$$e\boldsymbol{J}^M \simeq G^m_s\boldsymbol{\mu} + G^m_r\tilde{\mathbf{m}} \times (\tilde{\mathbf{m}} \times \boldsymbol{\mu}) + G^m_i\tilde{\mathbf{m}} \times \boldsymbol{\mu}. \tag{40}$$

It exerts a torque on the local moment by transferring its angular momentum, which is quantified by spin-sink conductance G_s [80], and spin-mixing conductance $G_{\uparrow\downarrow} = G^m_r + iG^m_i$ [81] with

$$G^m_s = -e^2\nu_F\ell^{\parallel}_F/\tau^m_{\parallel}, \tag{41}$$

$$G^m_r = e^2\nu_F(\ell^{\perp}_F/\tau^m_{\perp} - \ell^{\parallel}_F/\tau^m_{\parallel}), \tag{42}$$

$$G^m_i = -\frac{e^2}{\hbar}\nu_F\ell^{\perp}_F n_m K_s\langle\hat{S}_{\parallel}\rangle. \tag{43}$$

where G^m_r and G^m_i arise from the interfacial anisotropic spin relaxation and magnetic exchange field, respectively. Note that ℓ^a_F includes the contributions from both the SEC and the interfacial SOC, resulting in the modulation of the spin-orbit torque with the interfacial SOC. The damping- (field-) like torque is directly (inversely) proportional to the interfacial SOC for the SOC-dominated ℓ^a_F and becomes independent of the interfacial SOC for the SEC-dominated ℓ^a_F (see Appendix D). This might explain the recent experiment [16] that finds the interfacial SOC linearly tunes the damping-like spin-orbit torque. G^m_s and $G^m_s - G^m_r$, in the order of $10^{12}\ \Omega^{-1}\,\mathrm{m}^{-2}$ in EuS/Pt [42], respectively, show how fast longitudinal (μ^3) and transverse ($\mu^{1,2}$) components of the interfacial spin density are transferred to the local moments of the ferromagnet. G_i ($\sim 10^{13}\ \Omega^{-1}\,\mathrm{m}^{-2}$ in EuS/Pt [42]) exerts a field-like torque that causes the spin precession of the local moments ($\tilde{\mathbf{m}}$) along $\boldsymbol{\mu}$ direction. Therefore, we demonstrate that the interfacial SOC rotates $\mathbf{m} = \langle\mathbf{S}\rangle/\langle\hat{S}_{\parallel}\rangle$ [Fig. 3(a)] into $\tilde{\mathbf{m}} = \langle\tilde{\mathbf{S}}\rangle/\langle\hat{S}_{\parallel}\rangle$ [Fig. 3(b)]. However, not all intrinsic local moments of the interfacial spin current can be transferred into the local moments of the ferromagnet [10,32,34,36]. The spin-orbit torque efficiency can be reduced by the spin relaxation from the interfacial SOC.

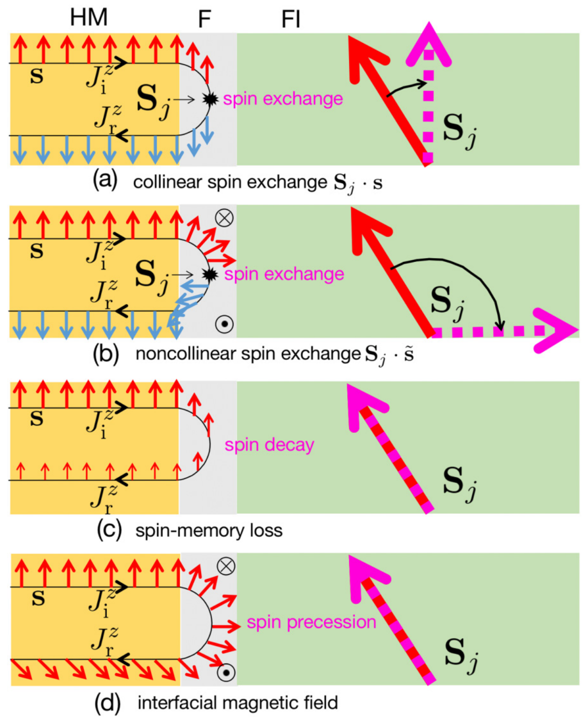

FIG. 3. Spin-orbit torques and spin memory loss. The thin arrows show the evolution of interfacial spin current during the reflection at HM|FI interface. [(a), (b)] The spin exchange between itinerant electrons and local moments. Panels (a) and (b) plot the spin-orbit torques from the collinear and the noncollinear spin exchange between local moments and itinerant electrons [Eqs. (41) and (42)]. Although the spatial gauge fields can cause spin decay [Eqs. (45) and (46)], the corresponding spin loss can not be transferred into the local moments, as shown in panel (c). In addition, the in-plane interfacial spin-orbit magnetic fields [Eqs. (49) and (50)] merely induces the spin precession of the interfacial spin density of itinerant electrons, as shown in panel (d).

C. Spin memory loss

Next, we present the possible spin memory loss from the spin decay and precession of the interfacial SOC. $\boldsymbol{J}^L$ is the interfacial spin current arising from the interaction of the spatial gauge fields [Ω^{aa}_{+} and Ω^{ac}_{-} terms in Eq. (35)]

$$e\boldsymbol{J}^L \simeq G^l_s\boldsymbol{\mu} + G^l_r\hat{\mathbf{z}} \times (\hat{\mathbf{z}} \times \boldsymbol{\mu}) + G^l_i\hat{\mathbf{z}} \times \boldsymbol{\mu} + G^l_j\hat{\mathbf{x}} \times \boldsymbol{\mu} + G^l_j\hat{\mathbf{y}} \times \boldsymbol{\mu}. \tag{44}$$

The spin memory loss is quantified by the spin-loss conductance [43] quadratic to gauge fields [Ω_+^{aa} terms in Eq. (35)]

$$G_s^l = -e^2\nu_F\Omega_{+,0}^{zz}, \tag{45}$$

$$G_r^l = e^2\nu_F\left(\Omega_{+,0}^{xx} - \Omega_{+,0}^{zz}\right), \tag{46}$$

with

$$\Omega_{+,0}^{zz} = \frac{2\ell_F^{\parallel}Dm^2}{\hbar^2}[(\alpha - u_\parallel\lambda)^2 + \beta^2 + u_\perp^2\lambda^2], \tag{47}$$

$$\Omega_{+,0}^{xx} = \frac{\ell_F^{\perp}Dm^2}{\hbar^2}[(\alpha - u_\parallel\lambda)^2 + \beta^2 + 3u_\perp^2\lambda^2], \tag{48}$$

where the subscript l of $\Omega_{\pm,l}$ means l order in ordinary Hall angle. We have presumed a strain configuration in which $u_{yz} = u_{zx} = u_\perp$ and $u_{xy} = u_\parallel$. Both G_s^l and G_r^l account for the spin relaxation of itinerant electrons and hence can also be induced by the spin-flip scattering from the static disorder at the interface [37]. For zero strain-induced SOC ($u_\perp = u_\parallel = 0$), we recover the spin-loss conductance G_r^l and G_s^l, with the latter being $G_r^l \simeq 1.5\times10^{13}\ \Omega^{-1}\,\mathrm{m}^{-2}$ in BiO_x/Cu [43]. Moreover, we also find new interfacial spin-orbit magnetic fields [Ω_-^{ac} terms in Eq. (35)]

$$G_i^l = e^2\nu_F\Omega_{-,1}^{xy}, \tag{49}$$

$$G_j^l = e^2\nu_F\Omega_{-,1}^{yz}, \tag{50}$$

with

$$\Omega_{-,1}^{xy} = \frac{\ell_F^{\perp}Dm^2}{\hbar^2}\big[(\beta^2 - (\alpha - u_\parallel\lambda)^2)\theta_C^{z0} + (\alpha - \beta - u_\parallel\lambda) \times u_\perp\lambda\theta_C^{y0} - (\alpha - \beta - u_\parallel\lambda)u_\perp\lambda\theta_C^{x0}\big], \tag{51}$$

$$\Omega_{-,1}^{yz} = \frac{\ell_F^{\parallel}Dm^2}{\hbar^2}\big[-(\beta - \alpha + u_\parallel\lambda)u_\perp\lambda\theta_C^{z0} - u_\perp^2\lambda^2\theta_C^{y0} - u_\perp^2\lambda^2\theta_C^{x0}\big]. \tag{52}$$

Linear to the ordinary Hall angle, $G_{i,j}^l$ should be an order of magnitude smaller than G_r^l. Taking $\tilde{\mathbf{m}} = \hat{\mathbf{z}}$ as an example. The spin-loss conductance G_s^l ($G_r^l + iG_i^l$) competes with the spin-sink conductance G_s^m (spin-mixing conductance $G_r^m + iG_i^m$). But the spin loss of the former can not be transferred into the local moments [Fig. 3(c)]. The G_j^l interfacial magnetic field [Fig. 3(d)] couples μ^3 with $\mu^{1,2}$ that is further transferred into the local moments by the damping-like torque (G_r^m) or induces the spin precession of the local moments via the field-like torque (G_i^m).

Interestingly, the interplay of the interfacial SOC, as shown in Eq. (36), results in a brand new interfacial spin-orbit magnetic field [Ω_+^{ac} terms in Eq. (35)]

$$e\boldsymbol{J}^S \simeq G_\perp^n\|\hat{\mathbf{x}}\times\boldsymbol{\mu}\| + G_\perp^n\|\hat{\mathbf{y}}\times\boldsymbol{\mu}\| + G_\parallel^n\|\hat{\mathbf{z}}\times\boldsymbol{\mu}\|, \tag{53}$$

which is described by a *symmetric* tensor ($|\epsilon^{abc}|$), i.e., $\|\boldsymbol{n}\times\boldsymbol{\mu}\|^a \equiv |\epsilon^{abc}|n^b\mu^c$. The spin-loss conductance $G_\parallel^n$ and $G_\perp^n$ arise from the interaction among the Rashba, Dresselhaus and strain-induced SOC,

$$G_\parallel^n \simeq -e^2\nu_F\Omega_{+,0}^{xy}, \tag{54}$$

$$G_\perp^n \simeq -e^2\nu_F\Omega_{+,0}^{yz}, \tag{55}$$

where

$$\Omega_{+,0}^{xy} = \frac{\ell_F^{\perp}Dm^2}{\hbar^2}[2\beta(\alpha - u_\parallel\lambda) + u_\perp^2\lambda^2], \tag{56}$$

$$\Omega_{+,0}^{yz} = -\frac{\ell_F^{\parallel}Dm^2}{\hbar^2}u_\perp\lambda(\alpha - \beta - u_\parallel). \tag{57}$$

The spin-loss conductance $G_{\perp,\parallel}^n$ and $G_{s,r}^l$ are quadratic (linear) in the interfacial SOC for SEC (SOC)-dominated ℓ_F^a (see Appendix D). Thus, we expect that $G_{\perp,\parallel}^n$ should be the same order as $G_{s,r}^l$. So far, all spin conductance are linear in ℓ_F.

Finally, we show the interfacial SOC itself (A^{ib}) or its interplay with the ordinary Hall effect (θ_C^0) produces new in-plane interfacial spin-orbit magnetic fields [Γ_-^{ac} terms in Eq. (35)]

$$e\boldsymbol{J}^A \simeq G_\lambda^a\hat{\mathbf{x}}\times\boldsymbol{\mu} - G_\lambda^a\hat{\mathbf{y}}\times\boldsymbol{\mu} + G_\alpha^a\boldsymbol{n}^\alpha\times\boldsymbol{\mu} + G_\beta^a\boldsymbol{n}^\beta\times\boldsymbol{\mu}, \tag{58}$$

with

$$G_\lambda^a = e^2\nu_F\frac{2Dm}{\hbar}u_\perp\lambda, \tag{59}$$

$$G_\alpha^a = e^2\nu_F\frac{2Dm}{\hbar}\theta_C^0\alpha, \tag{60}$$

$$G_\beta^a = e^2\nu_F\frac{2Dm}{\hbar}\theta_C^0\beta, \tag{61}$$

where $\boldsymbol{n}^\alpha = [-\theta_C^{x0}, -\theta_C^{y0}, 0]/\theta_C^0$, $\boldsymbol{n}^\beta = [\theta_C^{y0}, \theta_C^{x0}, 0]/\theta_C^0$, and we have used the fact $\Gamma_+^{aa} \simeq 0$ ($\Gamma_+^{ac} \simeq 0$) due to $\Gamma^{aa} \simeq 0$ ($\Gamma^{ac} \simeq -\Gamma^{ca}$) [see Eqs. (37) and (38)]. The corresponding spin-loss conductance, linear to the interfacial SOC and independent of ℓ_F^a, are responsible for the spin precession of the interfacial spin density. The spin-orbit lengths in general are much larger than the spin-diffusion length in the ferromagnet, i.e., $\hbar/(mu_\perp\lambda), \hbar/(m\alpha), \hbar/(m\beta) \gg \ell_F^a$. Hence, G_λ^a is much larger than $G_{s,r}^l$, while $G_{\alpha,\beta}^a$, linear to θ_C^0, is the same order as $G_{s,r}^l$. The in-plane interfacial spin-orbit magnetic fields (58) couple μ^3 with $\mu^{1,2}$ that again can be further transferred into the local moments of the ferromagnet via the damping-like torque (G_r^m).

IV. CONCLUSIONS

We have developed a SU(2) theory to describe the spin transport across the HM|FI interface. It was shown that the interfacial SOC causes the spin relaxation and precession of the interfacial spin density that exerts damping- and field-like torques on the local moments of ferromagnet and controls the spin-orbit torque and spin memory loss. We derived the spin-mixing (-loss) conductance in terms of the microscopic parameters of the interface. Our theory demonstrates both the noncollinear SEC that tunes the damping- and field-like torques via rotating $\mathbf{m} \propto \langle\mathbf{S}\rangle$ into $\tilde{\mathbf{m}} \propto \langle\tilde{\mathbf{S}}\rangle$ and the spin-transfer efficiency suppression after considering the interfacial spin-loss conductance. We envision bright experiments in vdW ferromagnets and their heterostructures to test our predictions. The generalization of our theory to ferrimagnet, antiferromagnet, and/or altermagnet is an appealing issue for future study.

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APPENDIX A: DERIVATION OF GAUGE FIELDS (8)

In this Appendix, we study the interplay of the Rashba-and- Dresselhaus-type spin-orbit coupling (SOC) as well as the strain-induced SOC.

We start by considering the Pauli Hamiltonian, acting on two-component spinors

$$\mathcal{H} = \frac{\boldsymbol{P}^2}{2m} + \hbar\omega_H \hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{s}} + e\phi + \mathcal{V}_\mathrm{R} + \mathcal{V}_\mathrm{D} + \mathcal{V}_\mathrm{S}, \tag{A1}$$

with

$$\mathcal{V}_\mathrm{R} = 2\alpha(\boldsymbol{P}\times\hat{z})\cdot\boldsymbol{s}, \tag{A2}$$

$$\mathcal{V}_\mathrm{D} = 2\beta(P^x s^x + P^y s^y), \tag{A3}$$

$$\begin{aligned}\mathcal{V}_\mathrm{S} = 2\lambda[&s^1(u_{zx}P_z - u_{xy}P_y) + s^2(u_{xy}P_x - u_{yz}P_z)\\ &+ s^3(u_{yz}P_y - u_{zx}P_x)],\end{aligned} \tag{A4}$$

where α, β, and λ are the constants of Rashba, Dresselhaus, and strain-induced SOC, respectively, and $e<0$ is the charge of electron. u_{ij} are elements of the strain tensor [63]. $\boldsymbol{P} = -i\hbar\nabla_{\boldsymbol{r}} - e\boldsymbol{A}(\boldsymbol{r})$ is canonical momentum with a minimal coupling to the electromagnetic field, which is described by the Abelian gauge field $A^\nu(\boldsymbol{r}) = [\phi(\boldsymbol{r})/c, \boldsymbol{A}(\boldsymbol{r})]$. Next we rewrite the kinetic energy plus SOC as

$$\frac{1}{2m}[\boldsymbol{p} - e\hat{\mathbf{A}}(\boldsymbol{r})]^2 - m\big[(\alpha^2+\beta^2) + \lambda^2\big(u_{xy}^2 + u_{yz}^2 + u_{zx}^2\big)\big]. \tag{A5}$$

Thus, the non-Abelian gauge field reads

$$\hat{A}_\mu(x_n) = \left[\frac{1}{c}\Phi(x_n) + \frac{1}{c}\Phi^a(x_n)\hat{s}^a, -\boldsymbol{A}(x_n) - \boldsymbol{A}^a(x_n)\hat{s}^a\right]. \tag{A6}$$

The spatial components of gauge field read

$$\hat{A}^x = A^x + \frac{2m}{e}[-\beta\hat{s}^1 + (\alpha - u_{xy}\lambda)\hat{s}^2 + u_{zx}\lambda\hat{s}^3], \tag{A7}$$

$$\hat{A}^y = A^y + \frac{2m}{e}[+(-\alpha + u_{xy}\lambda)\hat{s}^1 + \beta\hat{s}^2 - u_{yz}\lambda\hat{s}^3], \tag{A8}$$

$$\hat{A}^z = A^z + \frac{2m}{e}[-u_{zx}\lambda\hat{s}^1 + u_{yz}\lambda\hat{s}^2]. \tag{A9}$$

The temporal components of the gauge field read

$$e\Phi(x) = e\phi(\boldsymbol{r}) - m\big[(\alpha^2+\beta^2) + \lambda^2\big(u_{xy}^2 + u_{yz}^2 + u_{zx}^2\big)\big], \tag{A10}$$

$$e\Phi^a(x) = \mathrm{g}\mu_B B^{0a} - (n_m K_s/2)\langle\tilde{S}^a\rangle. \tag{A11}$$

The Zeeman interaction is written as the time component of the non-Abelian gauge field $\hat{A}_0(x)$. The Hamiltonian has $\mathrm{U}(1)\otimes\mathrm{SU}(2)$ form [51–57]

$$\hat{\mathcal{H}}(x_n) = ce\hat{A}_0(x_n) + \frac{\hbar^2}{2m}\hat{D}_j(x_n)\hat{D}_j(x_n) \tag{A12}$$

with

$$\hat{D}_\mu(x_n) = \frac{\partial}{\partial x_n^\mu} + \frac{ie}{\hbar}\hat{A}_\mu(x_n). \tag{A13}$$

The gauge field reads

$$\hat{A}_\mu(x_n) = \left[\frac{1}{c}\Phi^0(x_n) + \frac{1}{c}\Phi^a(x_n)\hat{s}^a, -\boldsymbol{A}^0(x_n) - \boldsymbol{A}^a(x_n)\hat{s}^a\right]. \tag{A14}$$

$\hat{s}^a$ are the generators of SU(2) with algebra $[\hat{s}^a, \hat{s}^b] = i\epsilon^{abc}\hat{s}^c$ and $\mathrm{tr}\{\hat{s}^a, \hat{s}^b\} = \delta_{ab}$. The scalar $[\Phi^0(x_n)]$ and vector $[\boldsymbol{A}^0(x_n)]$ potentials correspond to the temporal and spatial components of the Abelian U(1) Maxwell gauge fields, while the Zeeman $[\Phi^a(x_n)]$ and spin-orbit $[\boldsymbol{A}^a(x_n)]$ interactions correspond to the temporal and spatial components of the non-Abelian SU(2) Yang–Mills gauge fields. The Zeeman magnetic field reads $e\Phi^a(x) = \mathrm{g}\mu_B B^{a0}$, where μ_B is the Bohr magneton, g is the g factor, and $\boldsymbol{B}^0$ is the external magnetic field in the direction $\boldsymbol{n} = \boldsymbol{B}^0/B^0$.

The spin electric and magnetic fields, respectively, are derived from the gauge fields (A14)

$$E^{ja} = -\partial_j\Phi^a - \partial_0 cA_j^a - \frac{e}{\hbar}\epsilon^{abc}A_j^b\Phi^c, \tag{A15}$$

and

$$B^{ia} = -\frac{1}{2}\epsilon^{ijk}\big[\partial_j A_k^a - \partial_k A_j^a - \frac{e}{\hbar}\epsilon^{abc}A_j^b A_k^c\big]. \tag{A16}$$

We first show the detailed expressions of the spin electric fields (A15) as follows:

$$\begin{aligned}\boldsymbol{E}^1 &= 2m\omega_H\lambda[-u_{xy}n^3 - u_{zx}n^2, +u_{yz}n^2, +u_{yz}n^3]\\ &\quad + 2m\omega_H[\alpha n^3, \beta n^3, 0],\end{aligned} \tag{A17}$$

$$\begin{aligned}\boldsymbol{E}^2 &= 2m\omega_H\lambda[+u_{zx}n^1, -u_{xy}n^3 - u_{yz}n^1, u_{zx}n^3]\\ &\quad + 2m\omega_H[\beta n^3, \alpha n^3, 0],\end{aligned} \tag{A18}$$

$$\begin{aligned}\boldsymbol{E}^3 &= 2m\omega_H\lambda[u_{xy}n^1, u_{xy}n^2, -u_{yz}n^1 - u_{zx}n^2]\\ &\quad + 2m\omega_H[-\alpha n^1 - \beta n^2, -\alpha n^2 - \beta n^1, 0].\end{aligned} \tag{A19}$$

Next, we also give the detailed expressions of the spin magnetic fields (A16) as follows:

$$\begin{aligned}\boldsymbol{B}^1 &= \boldsymbol{\mathcal{B}}^1 + \frac{4m^2}{e\hbar}\lambda^2 u_{yz}[u_{yz}, u_{zx}, u_{xy}]\\ &\quad + \frac{4m^2}{e\hbar}\lambda[0, 0, -u_{yz}\alpha - u_{zx}\beta],\end{aligned} \tag{A20}$$

$$\begin{aligned}\boldsymbol{B}^2 &= \boldsymbol{\mathcal{B}}^2 + \frac{4m^2}{e\hbar}\lambda^2 u_{zx}[u_{yz}, u_{zx}, u_{xy}]\\ &\quad + \frac{4m^2}{e\hbar}\lambda[0, 0, -u_{zx}\alpha - u_{yz}\beta],\end{aligned} \tag{A21}$$

$$\boldsymbol{B}^3 = \boldsymbol{\mathcal{B}}^3 + \frac{4m^2}{e\hbar}\lambda^2 u_{xy}[u_{yz}, u_{zx}, u_{xy}] + \frac{4m^2}{e\hbar}[\lambda u_{yz}(u_{xy}\lambda - \alpha), \lambda u_{zx}(u_{xy}\lambda - \alpha), (\alpha - u_{xy}\lambda)^2] + \frac{4m^2}{e\hbar}\lambda[-u_{yz}\alpha + u_{zx}\beta, -u_{zx}\alpha + u_{yz}\beta, -2u_{xy}\lambda\alpha] + \frac{4m^2}{e\hbar}[0, 0, \alpha^2 - \beta^2], \tag{A22}$$

where $\mathcal{B}^{ia} = -\frac{1}{2}\epsilon^{ijk}(\partial_j A_k^a - \partial_k A_j^a)$ arises from the the spatial derivatives of the spatial components of gauge field. The spin magnetic fields (A20), (A21), and (A22) will induce a conversion from charge current to spin Hall currents polarized in spin $\hat{s}^1$, $\hat{s}^2$, and $\hat{s}^3$, respectively, whose conversion efficiencies are respectively described by spin Hall angles

$$\boldsymbol{\theta}_C^1 = \frac{el_F \boldsymbol{B}^1}{\hbar k_F}, \tag{A23}$$

$$\boldsymbol{\theta}_C^2 = \frac{el_F \boldsymbol{B}^2}{\hbar k_F}, \tag{A24}$$

$$\boldsymbol{\theta}_C^3 = \frac{el_F \boldsymbol{B}^3}{\hbar k_F}. \tag{A25}$$

APPENDIX B: DERIVATIONS OF EQ. (16)

In this Appendix, we give the detailed derivations of the gauge-invariant quantum kinetic equation (13) in the main text.

1. SU(2) gauge transformation

In this section, we introduce the SU(2) gauge transformation. Now let us consider the gauge transformation

$$\hat{\psi}_g(x) = \hat{R}(x)\hat{\psi}(x), \quad \hat{\psi}_g^\dagger(x) = \hat{\psi}^\dagger(x)\hat{R}^{-1}(x). \tag{B1}$$

The original Wigner transform depends on the "center-of-mass" and "relative" coordinates, defined as

$$X = \frac{x_1 + x_2}{2}, \quad x = x_1 - x_2. \tag{B2}$$

It is the Fourier transform of GF with respect to the relative coordinates x,

$$\hat{\varrho}(p, X) = \int dx e^{+ip\cdot x}\hat{\varrho}\Big(X + \frac{x}{2}, X - \frac{x}{2}\Big), \tag{B3}$$

with $p \cdot x = p_\mu x^\mu = p_0 x^0 - p^i x^i$. One can rewrite it as

$$\varrho_{s_1 s_2}^{ab}(p, X) = -i\int dx e^{+ip\cdot x}\big[e^{+\frac{1}{2}x^\mu\partial_\mu}\psi_{s_1}(X)\big] \times \big[e^{-\frac{1}{2}x^\mu\partial_\mu}\psi_{s_2}^\dagger(X)\big], \tag{B4}$$

with

$$e^{+x^\mu\partial_\mu}\psi_s(X) = \psi_s(X + x). \tag{B5}$$

However, the definition above Wigner transformation (B3) breaks the gauge invariance. This may be understood by noting that the gauge transformation (B4) depends on both $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ instead of $\boldsymbol{r}$, so that the simple Fourier transform with respect to $\boldsymbol{r}$ necessarily breaks the gauge invariance.

To remove this difficulty, a gauge-invariant Wigner transformation would be simply deduced from Eq. (B4) by the substitution of the usual derivatives with covariant ones, $\hat{D}_{\mu,\pm}$ [82],

$$\hat{\varrho}(p, X) = -i\int dx e^{+ip\cdot x}\big[e^{+\frac{1}{2}x^\mu\hat{D}_{\mu,+}}\hat{\psi}(X)\big] \times \big[\hat{\psi}^\dagger(X)e^{-\frac{1}{2}x^\mu\hat{D}_{\mu,-}}\big], \tag{B6}$$

where $e^{\pm x^\mu\hat{D}_{\mu,\pm}}$ is the covariant translation operator. $\hat{D}_{\mu,\pm}(x_n) = \frac{\partial}{\partial x_n^\mu} \pm \frac{ie}{\hbar}\hat{A}_\mu(x_n)$ is the covariant derivatives, where m is the mass of electron and c is the velocity of light. Its action on fermion operator is given by [83]

$$e^{y^\mu\hat{D}_{\mu,+}}\hat{\Psi}_1(X) = \hat{W}(X, X + y)\hat{\Psi}_1(X + y), \tag{B7}$$

$$\hat{\Psi}_2(X)e^{y^\mu\hat{D}_\mu^-} = \hat{\Psi}_2(X + y)\hat{W}(X + y, X). \tag{B8}$$

Wilson line $\hat{W}(X, Z)$ reads (see its derivation and properties in Appendix B 2)

$$\hat{W}(X, Z) = \mathrm{P}e^{-\frac{ie}{\hbar}\int_Z^X d\zeta^\kappa\hat{A}_\kappa(\zeta)}, \tag{B9}$$

where P means the path of integration is the straight line from $\zeta = Z$ to $\zeta = X$. Substituting Eqs. (B7) and (B8) into Eq. (B6), one obtains

$$\hat{\varrho}(p, X) = \int dx e^{+ip\cdot x}\hat{W}\Big(X, X + \frac{x}{2}\Big) \times \hat{\varrho}\Big(X + \frac{x}{2}, X - \frac{x}{2}\Big)\hat{W}\Big(X - \frac{x}{2}, X\Big), \tag{B10}$$

$$\hat{\varrho}(x_1, x_2) = \frac{1}{V}\sum_p e^{-ip\cdot x}\hat{W}\Big(X + \frac{x}{2}, X\Big) \times \hat{\varrho}(p, X)\hat{W}\Big(X, X - \frac{x}{2}\Big). \tag{B11}$$

2. Wilson line in Keldysh-spin space

In this subsection, we introduce the definition and properties of Wilson line in Keldysh-spin (KS) space. The corresponding gauge-invariant Wigner transformation reads

$$\widehat{G}(p, X) = \int dx e^{+ip\cdot x}\widehat{W}\Big(X, X + \frac{x}{2}\Big)\widehat{G}\Big(X + \frac{x}{2}, X - \frac{x}{2}\Big) \times \widehat{W}\Big(X - \frac{x}{2}, X\Big), \tag{B12}$$

$$\widehat{G}(x_1, x_2) = \frac{1}{V}\sum_p e^{-ip\cdot x}\widehat{W}\Big(X + \frac{x}{2}, X\Big) \times \widehat{G}(p, X)\widehat{W}\Big(X, X - \frac{x}{2}\Big), \tag{B13}$$

where Wilson line in KS space is given by

$$\widehat{W}(X, Z) = \begin{bmatrix} \hat{W}(X, Z) & 0 \\ 0 & \hat{W}(X, Z) \end{bmatrix}. \tag{B14}$$

Then, let us find the expression of Wilson line in spin space (B14). It appears, when we undergo a gauge-invariant Wigner transformation of Green's function

$$\hat{\mathcal{G}}^{ab}(p,X) = -i\int dx e^{+ip\cdot x}\langle \hat{T}_K\{[e^{+\frac{1}{2}x^\mu \hat{D}_{\mu,+}}\hat{\Psi}_1(X)] \times [\hat{\Psi}_2(X)e^{-\frac{1}{2}x^\mu \hat{D}_{\mu,-}}]\}\rangle, \tag{B15}$$

with

$$\hat{D}_{\mu,+}(X) = \partial_\mu + \frac{ie}{\hbar}\hat{A}_\mu(X), \tag{B16}$$

$$\hat{D}_{\mu,-}(X) = \partial_\mu - \frac{ie}{\hbar}\hat{A}_\mu(X). \tag{B17}$$

Thus, one inevitably encounters the calculation

$$e^{+y^\mu \hat{D}_{\mu,+}(X)} = \lim_{n\to\infty}[1+\Delta y^\mu \hat{D}_{\mu,+}(X)]^n = \lim_{n\to\infty}\left[1+\Delta y^\mu\partial_\mu + \Delta y^\mu\frac{ie}{\hbar}\hat{A}_\mu(X)\right]^n, \tag{B18}$$

with $\Delta y^\mu = y_\mu/n$. To realize the shift of X, we are required to obtain a translation operator $e^{+\Delta y^\mu\partial_\mu}$. Thus, Eq. (B18) becomes

$$\begin{aligned} e^{+y^\mu \hat{D}_{\mu,+}(X)} &= \lim_{n\to\infty}\left\{\left[1+\Delta y^\mu\frac{ie}{\hbar}\hat{A}_\mu(X)\right]e^{+\Delta y^\mu\partial_\mu} \times [1+\mathcal{O}((\Delta y^\mu)^2)]\right\}^n \\ &= \lim_{n\to\infty}\left[1+\Delta y^\mu\frac{ie}{\hbar}\hat{A}_\mu(X)\right]\dots \times\left[1+\Delta y^\mu\frac{ie}{\hbar}\hat{A}_\mu(X+(n-1)\Delta y^\mu)\right]e^{+y^\mu\partial_\mu}, \end{aligned} \tag{B19}$$

which can be written into integral form

$$e^{+y^\mu \hat{D}_{\mu,+}(X)} = \mathrm{P}e^{-\frac{ie}{\hbar}\int_{X+y}^{X}dz\hat{A}_\mu(z)}e^{\pm y^\mu\partial_\mu}. \tag{B20}$$

Hence, we reach

$$e^{y^\mu \hat{D}_{\mu,+}}\hat{\Psi}_1(X) = \hat{W}'(X,X+y)\hat{\Psi}_1(X+y), \tag{B21}$$

$$\hat{\Psi}_2(X)e^{y^\mu \hat{D}_{\mu,-}} = \hat{\Psi}_2(X+y)\hat{W}(X+y,X), \tag{B22}$$

where the Wilson line reads

$$\hat{W}(X,Z) = \mathrm{P}_i e^{-\frac{ie}{\hbar}\int_Z^X d\zeta^\kappa \hat{A}_\kappa(\zeta)}. \tag{B23}$$

It has important properties

$$\hat{W}(X,Z)\hat{W}(Z,Y) = \hat{W}'(X,Y), \widehat{W}(X,Z)\check{W}(Z,Y) = \widehat{W}(X,Y), \tag{B24}$$

$$\hat{W}_+(X,Z) = \hat{W}(Z,X), \widehat{W}_+(X,Z) = \widehat{W}(Z,X). \tag{B25}$$

It is easy to check Wilson line $\hat{W}(X,Z)$, can be transformed gauge invariantly as

$$\hat{R}(X)\hat{W}(X,Z)\hat{R}^{-1}(Z) = \hat{W}_g(X,Z), \tag{B26}$$

which lead into the gauge-invariant transform of Wilson line in Nambu and spin space

$$\check{R}(X)\check{W}(X,Z)\check{R}^{-1}(Z) = \check{W}_g(X,Z). \tag{B27}$$

Next, let us calculate the derivative of Wilson line

$$\frac{\partial}{\partial x^\mu}\hat{W}(X,Z) = \frac{\partial X^\nu}{\partial x^\mu}\frac{\partial}{\partial X^\nu}\hat{W}(X,Z) + \frac{\partial Z^\nu}{\partial x^\mu}\frac{\partial}{\partial Z^\nu}\hat{W}(X,Z). \tag{B28}$$

Here we follow the way of Ref. [84] to calculate the derivatives of Wilson lines. Defining

$$\hat{W}(X,\zeta(\lambda)) = \mathrm{P}\exp\left\{-\frac{ie}{\hbar}\int_\lambda^1 \hat{A}_\kappa(\zeta)\frac{d\zeta^\kappa}{d\lambda'}d\lambda'\right\}, \tag{B29}$$

$$\hat{W}(\zeta(\lambda),Z) = \mathrm{P}\exp\left\{-\frac{ie}{\hbar}\int_0^\lambda \hat{A}_\kappa(\zeta)\frac{d\zeta^\kappa}{d\lambda'}d\lambda'\right\}, \tag{B30}$$

we find

$$\begin{aligned} \frac{\partial}{\partial X^\nu}\hat{W}(X,Z) &= \hat{W}(X,Z)\left\{-\frac{ie}{\hbar}\int_0^1\left(\frac{\partial}{\partial X^\nu}\hat{A}_\kappa(\zeta)\frac{d\zeta^\kappa}{d\lambda}\right)d\lambda\right\} \\ &= -\frac{ie}{\hbar}\int_0^1 \hat{W}(X,\zeta)\left(\frac{\partial}{\partial X^\nu}\hat{A}_\kappa(\zeta)\frac{d\zeta^\kappa}{d\lambda}\right) \times \hat{W}(\zeta,Z)d\lambda \\ &= -\frac{ie}{\hbar}\int_0^1 \hat{W}(X,\zeta)\left(\frac{\partial\hat{A}_\kappa(\zeta)}{\partial\zeta^\mu}\frac{\partial\zeta^\mu}{\partial X^\nu}\frac{d\zeta^\kappa}{d\lambda} + \hat{A}_\kappa(\zeta)\frac{d}{d\lambda}\frac{\partial\zeta^\kappa}{\partial X^\nu}\right)\hat{W}(\zeta,Z)d\lambda \end{aligned} \tag{B31}$$

where the integral path is given by

$$\zeta(\lambda) = Z + (X-Z)\lambda, (0\leqslant\lambda\leqslant 1). \tag{B32}$$

Integrating by parts, one reaches

$$\begin{aligned} \int_0^1 \hat{W}(X,\zeta)\left(\hat{A}_\kappa(\zeta)\frac{d}{d\lambda}\frac{\partial\zeta^\kappa}{\partial X^\nu}\right)\hat{W}(\zeta,Z)d\lambda &= \hat{W}(X,\zeta)\left(\hat{A}_\kappa(\zeta)\frac{\partial\zeta^\kappa}{\partial X^\nu}\right)\hat{W}(\zeta,Z)\Big|_0^1 \\ &- \int_0^1 \hat{W}(X,\zeta)\left\{\frac{\partial\hat{A}_\kappa(\zeta)}{\partial\zeta^\mu} + \frac{ie}{\hbar}[\hat{A}_\mu(\zeta),\hat{A}_\kappa(\zeta)]\right\}\frac{d\zeta^\mu}{d\lambda}\frac{\partial\zeta^\kappa}{\partial X^\nu}\hat{W}(\zeta,Z)d\lambda, \end{aligned} \tag{B33}$$

where we have used the relations

$$\frac{d}{d\lambda}\hat{W}(X,\zeta) = \hat{W}(X,\zeta)\left\{+\frac{ie}{\hbar}\hat{A}^\iota_\mu(\zeta)\frac{d\zeta^\mu}{d\lambda}\right\}, \tag{B34}$$

$$\frac{d}{d\lambda}\hat{W}(\zeta,Z)=\left\{-\frac{ie}{\hbar}\hat{A}_\mu(\zeta)\frac{d\zeta^\mu}{d\lambda}\right\}\hat{W}(\zeta,Z). \tag{B35}$$

Equation (B33) can be simplified by using the relation

$$\frac{\partial\zeta^\kappa(\lambda)}{\partial X^\nu}=\lambda\frac{\partial X^\kappa}{\partial X^\nu}=\lambda\delta^\kappa_\nu. \tag{B36}$$

Hence, we reach

$$\begin{aligned}\int_0^1\hat{W}(X,\zeta)\left(\hat{A}_\kappa(\zeta)\frac{d}{d\lambda}\frac{\partial\zeta^\kappa}{\partial X^\nu}\right)\hat{W}(\zeta,Z)d\lambda&=\hat{A}_\nu(X)\hat{W}(X,Z)\\&-\int_0^1\hat{W}(X,\zeta)\left\{\frac{\partial\hat{A}_\nu(\zeta)}{\partial\zeta^\mu}+\frac{ie}{\hbar}[\hat{A}_\mu(\zeta),\hat{A}_\nu(\zeta)]\right\}(X^\mu-Z^\mu)\hat{W}(\zeta,Z)\lambda d\lambda.\end{aligned} \tag{B37}$$

Substituting Eq. (B37) into Eq. (B31), we reach

$$\frac{\partial}{\partial X^\nu}\hat{W}(X,Z)=-\frac{ie}{\hbar}\left[\hat{A}_\nu(X)\hat{W}(X,Z)-(X^\mu-Z^\mu)\int_0^1\hat{W}(X,\zeta)\hat{F}_{\mu\nu}(\zeta)\hat{W}(\zeta,Z)\lambda d\lambda\right], \tag{B38}$$

with

$$\hat{F}_{\mu\nu}(\zeta)=\frac{\partial\hat{A}_\nu(\zeta)}{\partial\zeta^\mu}-\frac{\partial\hat{A}_\mu(\zeta)}{\partial\zeta^\nu}+\frac{ie}{\hbar}[\hat{A}_\mu(\zeta),\hat{A}_\nu(\zeta)]. \tag{B39}$$

Following the same way, one can obtain

$$\frac{\partial}{\partial Z^\nu}\hat{W}(X,Z)=\frac{ie}{\hbar}\left[\hat{W}(X,Z)\hat{A}_\nu(Z)-(X^\mu-Z^\mu)\int_0^1\hat{W}(X,\zeta)\hat{F}_{\mu\nu}(\zeta)\hat{W}(\zeta,Z)(\lambda-1)d\lambda\right], \tag{B40}$$

where we have used the relations

$$\frac{\partial\zeta^\kappa(\lambda)}{\partial Z^\nu}=(1-\lambda)\frac{\partial Z^\kappa}{\partial Z^\nu}=(1-\lambda)\delta^\kappa_\nu. \tag{B41}$$

Substituting Eqs. (B38) and (B40) into Eq. (B28), we find the important property of Wilson line [82,85]

$$\begin{aligned}\frac{\partial}{\partial x^\sigma}\hat{W}(X,Z)=-\frac{ie}{\hbar}\bigg\{&\frac{\partial X^\nu}{\partial x^\sigma}\left[\hat{A}_\nu(X)\hat{W}(X,Z)+(X^\mu-Z^\mu)\int_0^1d\lambda(0-\lambda)\hat{W}(X,\zeta)\hat{F}_{\mu\nu}(\zeta)\hat{W}(\zeta,Z)\right]\\&-\frac{\partial Z^\nu}{\partial x^\sigma}\left[\hat{W}(X,Z)\hat{A}_\nu(Z)+(X^\mu-Z^\mu)\int_0^1d\lambda(1-\lambda)\hat{W}(X,\zeta)\hat{F}_{\mu\nu}(\zeta)\hat{W}(\zeta,Z)\right]\bigg\}.\end{aligned} \tag{B42}$$

3. Gauge-invariant Wigner transformation in Keldysh-spin space

In this subsection, we make a gauge-invariant Wigner transformation of Gorkov equation in Keldysh-Spin space

$$\widehat{\mathcal{G}}_+^{-1}(x_1)\widehat{\mathcal{G}}(x_1,x_2)=\hbar c\delta(x_1-x_2)\widehat{1}, \tag{B43}$$

$$\widehat{\mathcal{G}}(x_1,x_2)\widehat{\mathcal{G}}_-^{-1}(x_2)=\hbar c\delta(x_1-x_2)\widehat{1}, \tag{B44}$$

with

$$\widehat{\mathcal{G}}_\pm^{-1}(x)=\begin{bmatrix}\hat{\mathcal{G}}_\pm^{-1}(x)&0\\0&\hat{\mathcal{G}}_\pm^{-1}(x)\end{bmatrix}. \tag{B45}$$

The propagators in (B45) read

$$\hat{\mathcal{G}}_\pm^{-1}(x)=\pm i\hbar c\hat{D}_{0,\pm}(x)+\frac{\hbar^2}{2m}\hat{D}_{i,\pm}(x)\hat{D}_{i,\pm}(x)+\mu, \tag{B46}$$

where the covariant derivatives read

$$\hat{D}_{\mu,\pm}(x)=\frac{\partial}{\partial x^\mu}\pm\frac{ie}{\hbar}\hat{A}_\mu. \tag{B47}$$

Obviously, propagator $\widehat{\mathcal{G}}_-^{-1}(x)$ are Hermitian conjugates of propagator $\widehat{\mathcal{G}}_+^{-1}(x)$.

To make a gauge-invariant transformation, one is required to calculate the derivative of Wilson line. For the sake of simplicity, we rewrite Eq. (B42) into

$$\frac{\partial}{\partial x^\sigma}\hat{W}(X,Z) = -\frac{ie}{\hbar}\left\{\left[\frac{\partial X^\nu}{\partial x^\sigma}\hat{A}_\nu(X)\hat{W}(X,Z) - \frac{\partial Z^\nu}{\partial x^\sigma}\hat{W}(X,Z)\hat{A}_\nu(Z)\right] - (X^\mu - Z^\mu)\int_0^1 d\lambda\left[\lambda\frac{\partial X^\nu}{\partial x^\sigma} - (\lambda-1)\frac{\partial Z^\nu}{\partial x^\sigma}\right]\hat{W}(X,\zeta)\hat{F}_{\mu\nu}(\zeta)\hat{W}(\zeta,Z)\right\}, \tag{B48}$$

where $\zeta(\lambda) = Z + (X-Z)\lambda$. Thus, the derivative of Wilson line with coordinate x_1^μ reads

$$\frac{\partial}{\partial x_1^\mu}\hat{W}(x_1,X) = -\frac{ie}{\hbar}\left[\hat{A}_\mu(x_1)\hat{W}(x_1,X) - \frac{1}{2}\hat{W}(x_1,X)\hat{A}_\mu(X)\right] + \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda;x_1,X), \tag{B49}$$

$$\frac{\partial}{\partial x_1^\mu}\hat{W}(X,x_2) = -\frac{ie}{\hbar}\left[\frac{1}{2}\hat{A}_\mu(X)\hat{W}(X,x_2) - 0\right] + \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda-1;X,x_2), \tag{B50}$$

$$\frac{\partial}{\partial x_1^\mu}\hat{W}(X,x_1) = -\frac{ie}{\hbar}\left[\frac{1}{2}\hat{A}_\mu(X)\hat{W}(X,x_1) - \hat{W}(X,x_1)\hat{A}_\mu(x_1)\right] - \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda;X,x_1), \tag{B51}$$

$$\frac{\partial}{\partial x_1^\mu}\hat{W}(x_2,X) = -\frac{ie}{\hbar}\left[0 - \frac{1}{2}\hat{W}(x_2,X)\hat{A}_\mu(X)\right] - \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda-1;x_2,X), \tag{B52}$$

with

$$\hat{\mathcal{F}}^{\lambda}_{\mu\nu;+}(Y_1,Y_2) = \int_0^1 d\lambda(1+\lambda)\hat{W}\left(Y_1, X+\frac{x}{2}\lambda\right)\hat{F}_{\mu\nu}\left(X+\frac{x}{2}\lambda\right)\hat{W}\left(X+\frac{x}{2}\lambda, Y_2\right). \tag{B53}$$

We have changed integral variables $\lambda \to 1-\lambda$ in Eqs. (B51) and (B52).

Next, we calculate the gauge-invariant Wigner transformation of Eq. (B43). Let us calculate the first-order covariant derivatives of GF,

$$\hat{I}^{ab}_{1;\mu,+}(x) = \hat{W}(X,x_1)[\hat{D}_{\mu,+}(x_1)\hat{\mathcal{G}}^{ab}(x_1,x_2)]\hat{W}(x_2,X). \tag{B54}$$

By substitution of Eq. (B13), Eq. (B54) becomes

$$\hat{I}^{ab}_{1;\mu,+}(x) = \frac{1}{V}\sum_p \hat{W}(X,x_1)[\hat{D}_{\mu,+}(x_1)\hat{W}(x_1,X)e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p,X)\hat{W}(X,x_2)]\hat{W}(x_2,X). \tag{B55}$$

By substitution of Eq. (B16), Eq. (B55) becomes

$$\hat{I}^{ab}_{1;\mu,+}(x) = \frac{1}{V}\sum_p \hat{W}(X,x_1)\left[+\frac{ie}{\hbar}\hat{A}_\mu(x_1)\right]\hat{W}(x_1,X)e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p,X) + \frac{1}{V}\sum_p\left\{\hat{W}(X,x_1)\left[\frac{\partial}{\partial x_1^\mu}\hat{W}(x_1,X)\right]e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p,X) + \left[\frac{\partial}{\partial x_1^\mu}e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p,X)\right] + e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p,X)\left[\frac{\partial}{\partial x_1^\mu}\hat{W}(X,x_2)\right]\hat{W}(x_2,X)\right\}. \tag{B56}$$

By means of Eqs. (B49) and (B50), we reach

$$\hat{W}(X,x_1)\left[\frac{\partial}{\partial x_1^\mu}\hat{W}(x_1,X)\right] = \frac{ie}{2\hbar}\hat{A}_\mu(X) + \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{W}(X,x_1)\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda;x_1,X) + \hat{W}(X,x_1)\left[-\frac{ie}{\hbar}\hat{A}_\mu(x_1)\right]\hat{W}(x_1,X), \tag{B57}$$

$$\left[\frac{\partial}{\partial x_1^\mu}\hat{W}(X,x_2)\right]\hat{W}(x_2,X) = -\frac{ie}{2\hbar}\hat{A}_\mu(X) + \frac{ie}{\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda-1;X,x_2)\hat{W}(x_2,X). \tag{B58}$$

By substitution of Eqs. (B57) and (B58), Eq. (B56) becomes

$$\hat{I}^{ab}_{1;\mu,+}(x) = \frac{1}{V}\sum_p\left\{\frac{ie}{2\hbar}\left[+\hat{A}_\mu + \frac{x^\nu}{2}\hat{W}(X,x_1)\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda;x_1,X)\right]e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p) + \frac{ie}{2\hbar}e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p)\left[-\hat{A}_\mu + \frac{x^\nu}{2}\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda-1;X,x_2)\hat{W}(x_2,X)\right] + \frac{\partial}{\partial x_1^\mu}e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p)\right\}. \tag{B59}$$

The first term of the right-hand side of Eq. (B56) have canceled with the last term of the right-hand side of Eq. (B57). Hereafter, we have omitted the argument (X) without loss of ambiguity. Defining the hat derivative as

$$\frac{\hat{\partial}}{\partial X^\mu}\hat{\mathcal{G}}^{ab} = \frac{\partial}{\partial X^\mu}\hat{\mathcal{G}}^{ab} + \frac{ie}{\hbar}[\hat{A}_\mu, \hat{\mathcal{G}}^{ab}], \tag{B60}$$

Equation (B59) can be written as

$$\hat{I}^{ab}_{1;\mu,+}(x) = \frac{1}{V}\sum_p e^{-ip\cdot x}\{\hat{P}_{\mu,+}(p) + \hat{F}_{1;\mu,+}(p)\}\hat{\mathcal{G}}^{ab}(p), \tag{B61}$$

with

$$\hat{P}_{\mu,+}(p) = \left(\frac{1}{2}\frac{\hat{\partial}}{\partial X^\mu} - ip_\mu\right), \tag{B62}$$

$$\hat{F}_{1;\mu,+}(p)\hat{\mathcal{G}}^{ab}(p) = +\frac{e}{4\hbar}\{\hat{W}(X,x_1)\hat{\mathcal{F}}^+_{\nu\mu}(\lambda;x_1,X)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)] + [\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\hat{\mathcal{F}}^+_{\nu\mu}(\lambda-1;X,x_2)\hat{W}(x_2,X)\}, \tag{B63}$$

where we have used relations

$$\frac{\partial}{\partial x_1^\mu} = \frac{1}{2}\frac{\partial}{\partial X^\mu} + \frac{\partial}{\partial x^\mu}, \tag{B64}$$

$$x^\nu\hat{\mathcal{G}}(p,X) = x^\nu\int dx e^{+ip\cdot x}\hat{\mathcal{G}}(x_1,x_2) = -i\frac{\partial}{\partial p_\nu}\hat{\mathcal{G}}(p,X). \tag{B65}$$

Making the gauge-invariant Wigner transformation, Eq. (B61) becomes

$$\hat{I}^{ab}_{1;\mu,+}(k) = \int dx e^{+ik\cdot x}\hat{I}^{ab}_{1,\mu+}(x) = \{\hat{P}_{\mu,+}(k) + \hat{F}_{1;\mu,+}(k)\}\hat{\mathcal{G}}^{ab}(k). \tag{B66}$$

Then, let us work on the second-order covariant derivatives of GF. A convenient method is to rewrite it as

$$\hat{I}^{ab}_{2;\mu,+}(x) = \hat{W}\left[\frac{ie}{\hbar}\hat{A}_\mu\right](\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})\hat{W} + \partial_\mu[\hat{W}(\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})\hat{W}] - (\partial_\mu\hat{W})(\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})\hat{W} - \hat{W}(\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})(\partial_\mu\hat{W}). \tag{B67}$$

Next, one can calculate term by term. Using the relations (B51), one obtains

$$\hat{W}\left[\frac{ie}{\hbar}\hat{A}_\mu\right](\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})\hat{W} - (\partial_\mu\hat{W})(\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})\hat{W} = \frac{ie}{2\hbar}\left[\hat{A}_\mu + \frac{x^\nu}{2}\hat{\mathcal{F}}^+_{\nu\mu}(\lambda;X,x_1)\hat{W}(x_1,X)\right]\hat{I}^{ab}_{1,\mu+}(x), \tag{B68}$$

where the second term of the right-hand side of Eq. (B51) cancels with the first term of the left-hand side of Eq. (B68). By substitution of relation (B52), the last term of the right-hand side of Eq. (B67) becomes

$$-\hat{W}(\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})(\partial_\mu\hat{W}) = \frac{ie}{2\hbar}\hat{I}^{ab}_{1,\mu+}(x)\left[-\hat{A}_\mu + \frac{x^\nu}{2}\hat{W}(X,x_2)\hat{\mathcal{F}}^+_{\nu\mu}(\lambda-1;x_2,X)\right]. \tag{B69}$$

Using the relation (B61), the second term of the right-hand side of Eq. (B67) reads

$$\partial_\mu[\hat{W}(\hat{D}_{\mu,+}\hat{\mathcal{G}}^{ab})\hat{W}] = \left(\frac{1}{2}\frac{\partial}{\partial X^\mu} - ip_\mu\right)\hat{I}^{ab}_{1,\mu+}(x). \tag{B70}$$

By substitution of Eqs. (B68), (B69), and (B70), Eq. (B67) becomes

$$\hat{I}^{ab}_{2;\mu,+}(x) = \frac{1}{V}\sum_p e^{-ip\cdot x}\big\{\hat{P}^2_{\mu,+}(p) + \hat{F}_{2;\mu,+}(p) + \hat{K}_{2,\mu+}(p)\big\}\hat{\mathcal{G}}^{ab}(p), \tag{B71}$$

with

$$\begin{aligned}\hat{F}_{2;\mu,+}(p)\hat{\mathcal{G}}^{ab}(p) = \frac{e}{4\hbar}\big\{&\hat{P}_{\mu,+}(p)\hat{W}(X,x_1)\hat{\mathcal{F}}^+_{\nu\mu}(\lambda;x_1,X)\big[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)\big]\\ &+ \hat{P}_{\mu,+}(p)\big[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)\big]\hat{\mathcal{F}}^+_{\nu\mu}(\lambda-1;X,x_2)\hat{W}(x_2,X)\\ &+ \hat{\mathcal{F}}^+_{\nu\mu}(\lambda;X,x_1)\hat{W}(x_1,X)\hat{P}_{\mu,+}(p)\big[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)\big]\\ &+ \hat{P}_{\mu,+}(p)\big[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)\big]\hat{W}(X,x_2)\hat{\mathcal{F}}^+_{\nu\mu}(\lambda-1;x_2,X)\big\},\end{aligned} \tag{B72}$$

$$\hat{K}_{2;\mu+}(p)\hat{\mathcal{G}}^{ab}(p) = \frac{e}{4\hbar}\{\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda; X, x_1)\hat{W}(x_1, X)\hat{F}_{1;\mu,+}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)] + \hat{F}_{1;\mu,+}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\hat{W}(X, x_2)\hat{\mathcal{F}}^{+}_{\nu\mu}(\lambda-1; x_2, X)\}. \tag{B73}$$

Here the x^ν in Eqs. (B68) and (B69) is replace by a $-i\partial_{p_\nu}$ acting on GF, as shown in Eq. (B65). Then, we make a Fourier transformation of Eq. (B71), and reach

$$\hat{I}^{ab}_{2;\mu,+}(k) = \int dx e^{+ik\cdot x}\hat{I}^{ab}_{2,\mu+}(x) = \{\hat{P}^2_{\mu,+}(k) + \hat{F}_{2;\mu,+}(k) + \hat{K}_{2;\mu,+}(k)\}\hat{\mathcal{G}}^{ab}(k). \tag{B74}$$

Hence, the gauge-covariance Wigner transformation of the left-hand side of Eq. (B43) reads

$$\hat{I}^{ab}_{+}(k) = \int dx e^{+ik\cdot x}\hat{W}\{[\hat{\mathcal{G}}^{-1}_{+}]\hat{\mathcal{G}}^{ab}\}\hat{W} = \left\{i\hbar c\hat{I}^{ab}_{1;0,+}(k) + \frac{\hbar^2}{2m}\hat{I}^{ab}_{2;j,+}(k) + \mu\hat{\mathcal{G}}^{ab}(k)\right\}$$
$$= \left\{i\hbar c[\hat{P}_{0,+}(k) + \hat{F}_{1;0,+}(k)] + \frac{\hbar^2}{2m}[\hat{P}^2_{j,+}(k) + \hat{F}_{2;j,+}(k) + \hat{K}_{2;j,+}(k)] + \mu\right\}\hat{\mathcal{G}}^{ab}(k). \tag{B75}$$

Next, we are required to calculate the following four products:

$$\hat{W}(X, x_1)\hat{\mathcal{F}}^{\lambda}_{\nu\mu;+}(x_1, X) = \int_0^1 d\lambda(1+\lambda)\hat{W}\left(X, X + \frac{x}{2}\lambda\right)\hat{F}_{\mu\nu}\left(X + \frac{x}{2}\lambda\right)\hat{W}\left(X + \frac{x}{2}\lambda, X\right), \tag{B76}$$

$$\hat{\mathcal{F}}^{\lambda-1}_{\nu\mu;+}(X, x_2)\hat{W}(x_2, X) = \int_0^1 d\lambda\lambda\hat{W}\left(X, X + \frac{x}{2}(\lambda-1)\right)\hat{F}_{\mu\nu}\left(X + \frac{x}{2}(\lambda-1)\right)\hat{W}\left(X + \frac{x}{2}(\lambda-1), X\right), \tag{B77}$$

$$\hat{\mathcal{F}}^{\lambda}_{\nu\mu;+}(X, x_1)\hat{W}(x_1, X) = \int_0^1 d\lambda(1+\lambda)\hat{W}\left(X, X + \frac{x}{2}\lambda\right)\hat{F}_{\mu\nu}\left(X + \frac{x}{2}\lambda\right)\hat{W}\left(X + \frac{x}{2}\lambda, X\right), \tag{B78}$$

$$\hat{W}(X, x_2)\hat{\mathcal{F}}^{\lambda-1}_{\nu\mu;+}(x_2, X) = \int_0^1 d\lambda\lambda\hat{W}\left(X, X + \frac{x}{2}(\lambda-1)\right)\hat{F}_{\mu\nu}\left(X + \frac{x}{2}(\lambda-1)\right)\hat{W}\left(X + \frac{x}{2}(\lambda-1), X\right). \tag{B79}$$

with

$$\hat{\mathcal{F}}^{\lambda}_{\mu\nu;+}(Y_1, Y_2) = \int_0^1 d\lambda(1+\lambda)\hat{W}\left(Y_1, X + \frac{x}{2}\lambda\right)\hat{F}_{\mu\nu}\left(X + \frac{x}{2}\lambda\right)\hat{W}\left(X + \frac{x}{2}\lambda, Y_2\right). \tag{B80}$$

Considering the complexity of Eq. (B75), we here make some approximations. First, we expand $\hat{F}_{\mu\nu}(\zeta)$ in Eq. (B80) around X and only keeping zero-order term, which leads into

$$\hat{W}(X, x_1)\hat{\mathcal{F}}^{+}_{\nu\mu;\lambda}(x_1, X) \simeq -\hat{F}_{\nu\mu}(X), \tag{B81}$$

$$\hat{\mathcal{F}}^{+}_{\nu\mu;\lambda-1}(X, x_2)\hat{W}(x_2, X) \simeq -\hat{F}_{\nu\mu}(X), \tag{B82}$$

$$\hat{\mathcal{F}}^{+}_{\nu\mu;\lambda}(X, x_1)\hat{W}(x_1, X) \simeq +\hat{F}_{\nu\mu}(X), \tag{B83}$$

$$\hat{W}(X, x_2)\hat{\mathcal{F}}^{+}_{\nu\mu;\lambda-1}(x_2, X) \simeq +\hat{F}_{\nu\mu}(X). \tag{B84}$$

Hence, Eqs. (B63), (B72), and (B73) reduce to

$$\hat{F}_{1;\mu,+}(p)\hat{\mathcal{G}}^{ab}(p) \simeq \frac{e}{4\hbar}\{\hat{F}_{\nu\mu}(X), [\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}, \tag{B85}$$

$$\hat{F}_{2;\mu,+}(p)\hat{\mathcal{G}}^{ab}(p) \simeq \frac{e}{4\hbar}[\hat{P}_{\mu,+}(p)\{\hat{F}_{\nu\mu}(X), [\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\} + \{\hat{F}_{\nu\mu}(X), \hat{P}_{\mu,+}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}], \tag{B86}$$

$$\hat{K}_{2;\mu+}(p)\hat{\mathcal{G}}^{ab}(p) \simeq \left(\frac{e}{4\hbar}\right)^2\{\hat{F}_{\nu\mu}(X), \{\hat{F}_{\nu\mu}(X), [\partial^2_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}\}. \tag{B87}$$

Furthermore, we remove the higher-order terms $(\partial_{k_\alpha}\partial_{k_\beta}\hat{\mathcal{G}})$, $(\partial_{X^\mu}\partial_{X^\mu}\hat{\mathcal{G}})$, and $(\partial_{X^\mu}\partial_{k_\beta}\hat{\mathcal{G}})$. Thus, Eq. (B86) reduces to

$$\hat{F}_{2;\mu,+}(p)\hat{\mathcal{G}}^{ab}(p) = -ip_\mu\frac{e}{2\hbar}\{\hat{F}_{\nu\mu}(X), [\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}. \tag{B88}$$

And Eq. (B75) becomes

$$\hat{I}^{ab}_{+}(k) = \left[+\frac{i}{2}\hbar v^\nu_k\frac{\hat{\partial}}{\partial X^\nu} + \frac{i}{2}\frac{ev^\mu_k}{2}\{\hat{F}_{\nu\mu}, (\partial_{k_\nu}\cdot)\} + \mu - \epsilon(k)\right]\hat{\mathcal{G}}^{ab}(k), \tag{B89}$$

with

$$v_k^\nu = \left(c, \frac{\hbar k^j}{m}\right), \tag{B90}$$

$$\epsilon(k) = \frac{\hbar^2}{2m}k_j^2 - \hbar c k_0. \tag{B91}$$

Then, we follow the same way to obtain the gauge-covariance Wigner transformation of Eq. (B44). The derivative of Wilson line with coordinate x_2^μ reads

$$\frac{\partial}{\partial x_2^\mu}\hat{W}(x_1, X) = -\frac{ie}{\hbar}\left[0 - \frac{1}{2}\hat{W}(x_1, X)\hat{A}_\mu(X)\right] + \frac{ie}{\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^-_{\nu\mu}(\lambda; x_1, X), \tag{B92}$$

$$\frac{\partial}{\partial x_2^\mu}\hat{W}(X, x_2) = -\frac{ie}{\hbar}\left[\frac{1}{2}\hat{A}_\mu(X)\hat{W}(X, x_2) - \hat{W}(X, x_2)\hat{A}_\mu(x_2)\right] + \frac{ie}{\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^-_{\nu\mu}(\lambda - 1; X, x_2), \tag{B93}$$

$$\frac{\partial}{\partial x_2^\mu}\hat{W}(X, x_1) = -\frac{ie}{\hbar}\left[\frac{1}{2}\hat{A}_\mu(X)\hat{W}(X, x_1) - 0\right] - \frac{ie}{\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^-_{\nu\mu}(\lambda; X, x_1), \tag{B94}$$

$$\frac{\partial}{\partial x_2^\mu}\hat{W}(x_2, X) = -\frac{ie}{\hbar}\left[\hat{A}_\mu(x_2)\hat{W}(x_2, X) - \frac{1}{2}\hat{W}(x_2, X)\hat{A}_\mu(X)\right] - \frac{ie}{\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}^-_{\nu\mu}(\lambda - 1; x_2, X), \tag{B95}$$

with

$$\hat{\mathcal{F}}^-_{\mu\nu}(\lambda; X, Z) = \int_0^1 d\lambda \frac{1-\lambda}{2}\hat{W}\left(X, X + \frac{x}{2}\lambda\right)\hat{F}_{\mu\nu}\left(X + \frac{x}{2}\lambda\right)\hat{W}\left(X + \frac{x}{2}\lambda, Z\right). \tag{B96}$$

The first-order covariant derivatives of GF reads

$$\hat{I}^{ab}_{1;\mu,-}(x) = \hat{W}(X, x_1)[\hat{\mathcal{G}}^{ab}(x_1, x_2)\hat{D}_{\mu,-}(x_2)]\hat{W}(x_2, X). \tag{B97}$$

By substitution of Eq. (B13), Eq. (B97) becomes

$$\hat{I}^{ab}_{1;\mu,-}(x) = \sum_p \hat{W}(X, x_1)[\hat{W}(x_1, X)e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p, X)\hat{W}(X, x_2)\hat{D}_{\mu,-}(x_2)]\hat{W}(x_2, X). \tag{B98}$$

Note that the derivatives of $\hat{D}^J_{\mu,-}$ act on GF from the left-hand side. Hence,

$$\begin{aligned}\hat{I}^{ab}_{1;\mu,-}(x) = {}& \frac{1}{V}\sum_p e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p, X)\hat{W}(X, x_2)\left[-\frac{ie}{\hbar}\hat{A}_\mu(x_2)\right]\hat{W}(x_2, X) + \frac{1}{V}\sum_p \left\{\hat{W}(X, x_1)\left[\frac{\partial}{\partial x_2^\mu}\hat{W}(x_1, X)\right]e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p, X)\right. \\ &\left. + \left[\frac{\partial}{\partial x_2^\mu}e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p, X)\right] + e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p, X)\left[\frac{\partial}{\partial x_2^\mu}\hat{W}(X, x_2)\right]\hat{W}(x_2, X)\right\}.\end{aligned} \tag{B99}$$

Using Eqs. (B92) and (B93), one reaches

$$\hat{W}(X, x_1)\left[\frac{\partial}{\partial x_2^\mu}\hat{W}(x_1, X)\right] = +\frac{ie}{2\hbar}\hat{A}_\mu(X) + \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{W}(X, x_1)\hat{\mathcal{F}}_{\nu\mu}(1; x_1, X), \tag{B100}$$

$$\left[\frac{\partial}{\partial x_2^\mu}\hat{W}(X, x_2)\right]\hat{W}(x_2, X) = -\frac{ie}{2\hbar}\hat{A}_\mu(X) + \frac{ie}{2\hbar}\frac{x^\nu}{2}\hat{\mathcal{F}}_{\nu\mu}(2; X, x_2)\hat{W}(x_2, X) + \hat{W}(X, x_2)\left[+\frac{ie}{\hbar}\hat{A}_\mu(x_2)\right]\hat{W}(x_2, X). \tag{B101}$$

Substituting Eqs. (B100) and (B101) into Eq. (B99), we reach

$$\begin{aligned}\hat{I}^{ab}_{1;\mu,-}(x) = \frac{1}{V}\sum_p &\left\{\frac{ie}{2\hbar}\left[\hat{A}_\mu + \frac{x^\nu}{2}\hat{W}(X, x_1)\hat{\mathcal{F}}_{\nu\mu}(1; x_1, X)\right]e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p)\right. \\ &\left. + \frac{ie}{2\hbar}e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p)\left[-\hat{A}_\mu + \frac{x^\nu}{2}\hat{\mathcal{F}}_{\nu\mu}(2; X, x_2)\hat{W}(x_2, X)\right] + \frac{\partial}{\partial x_2^\mu}e^{-ip\cdot x}\hat{\mathcal{G}}^{ab}(p)\right\}.\end{aligned} \tag{B102}$$

The first term of the right-hand side of Eq. (B99) have canceled with the last term of the right-hand side of Eq. (B101). Hereafter, we have omitted the argument (X) without loss of ambiguity. By dint of Eq. (B60), Eq. (B102) can be written in compact form

$$\hat{I}^{ab}_{1;\mu,-}(x) = \frac{1}{V}\sum_p e^{-ip\cdot x}\{\hat{P}_{\mu,-}(p) + \hat{F}_{1;\mu,-}(p)\}\hat{\mathcal{G}}^{ab}(p), \tag{B103}$$

with

$$\hat{P}_{\mu,-}(p) = \left(\frac{1}{2}\frac{\hat{\partial}}{\partial X^\mu} + ip_\mu\right), \tag{B104}$$

$$\hat{F}_{1;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p) = \frac{e}{4\hbar}\{\hat{W}(X,x_1)\hat{\mathcal{F}}_{\nu\mu}(1;x_1,X)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)] + [\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\hat{\mathcal{F}}_{\nu\mu}(2;X,x_2)\hat{W}(x_2,X)\}, \tag{B105}$$

where we have used the relation

$$\frac{\partial}{\partial x_2^\mu} = \frac{1}{2}\frac{\partial}{\partial X^\mu} - \frac{\partial}{\partial x^\mu}. \tag{B106}$$

Making the gauge-invariant Wigner transformation of Eq. (B103) results into

$$\hat{I}^{ab}_{1;\mu,-}(k) = \int dx e^{+ik\cdot x}\hat{I}^{ab}_{1;\mu,-}(x) = \{\hat{P}_{\mu,-}(k) + \hat{F}_{1;\mu,-}(k)\}\hat{\mathcal{G}}^{ab}(k). \tag{B107}$$

Then, we work on the second-order covariant derivatives of GF,

$$\hat{I}^{ab}_{2;\mu,-}(x) = \hat{W}(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})\left[-\frac{ie}{\hbar}\hat{A}_\mu\right]\hat{W} + \partial_\mu[\hat{W}(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})\hat{W}] - (\partial_\mu\hat{W})(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})\hat{W} - \hat{W}(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})(\partial_\mu\hat{W}). \tag{B108}$$

Next, one can calculate term by term. Using the relations (B95), one obtains

$$\hat{W}(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})\left[-\frac{ie}{\hbar}\hat{A}_\mu\right]\hat{W} - \hat{W}(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})(\partial_\mu\hat{W}) = \hat{I}^{ab}_{1;\mu,-}(x)\frac{ie}{2\hbar}\left[-\hat{A}_\mu - \frac{x^\nu}{2}\hat{W}(X,x_2)\hat{\mathcal{F}}_{\nu\mu}(-1;x_2,X)\right], \tag{B109}$$

where the second term of the right-hand side of Eq. (B95) cancels with the first term of the left-hand side of Eq. (B110). By substitution of relation (B94), the third term of the right-hand side of Eq. (B108) becomes

$$-(\partial_\mu\hat{W})(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})\hat{W} = \frac{ie}{2\hbar}\left[\hat{A}'_\mu(X) - \frac{x^\nu}{2}\hat{\mathcal{F}}_{\nu\mu}(0;X,x_1)\hat{W}(x_1,X)\right]\hat{I}^{ab}_{1;\mu,-}(x). \tag{B110}$$

Using the relation (B103), the second term of the right-hand side of Eq. (B108) reads

$$\partial_\mu[\hat{W}(\hat{\mathcal{G}}^{ab}\hat{D}_{\mu,-})\hat{W}] = \left(\frac{1}{2}\frac{\partial}{\partial X^\mu} + ip_\mu\right)\hat{I}^{ab}_{1;\mu,-}(x). \tag{B111}$$

By substitution of Eqs. (B109), (B110), and (B111), Eq. (B108) becomes

$$\hat{I}^{ab}_{2;\mu,-}(x) = \frac{1}{V}\sum_p e^{-ip\cdot x}\{\hat{P}^2_{\mu,-}(p) + \hat{F}_{2;\mu,-}(p) + \hat{K}_{2;\mu,-}(p)\}\hat{\mathcal{G}}^{ab}(p), \tag{B112}$$

with

$$\begin{aligned}\hat{F}_{2;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p) = \frac{e}{4\hbar}\{&\hat{P}_{\mu,-}(p)\hat{W}(X,x_1)\hat{\mathcal{F}}_{\nu\mu}(1;x_1,X)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)] + \hat{P}_{\mu,-}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\hat{\mathcal{F}}_{\nu\mu}(2;X,x_2)\hat{W}(x_2,X)\\ &- \hat{\mathcal{F}}_{\nu\mu}(0;X,x_1)\hat{W}(x_1,X)\hat{P}_{\mu,-}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)] - \hat{P}_{\mu,-}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\hat{W}(X,x_2)\hat{\mathcal{F}}_{\nu\mu}(-1;x_2,X)\},\end{aligned} \tag{B113}$$

$$\begin{aligned}&\hat{K}_{2;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p)\\ &= -\frac{e}{4\hbar}\{\hat{\mathcal{F}}_{\nu\mu}(0;X,x_1)\hat{W}(x_1,X)\hat{F}_{1;\mu,-}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\\ &\quad + \hat{F}_{1;\mu,-}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\hat{W}(X,x_2)\hat{\mathcal{F}}_{\nu\mu}(-1;x_2,X)\}.\end{aligned} \tag{B114}$$

Then, we make a Fourier transformation of Eq. (B112), and reach

$$\begin{aligned}\hat{I}^{ab}_{2;\mu,-}(k) &= \int dx e^{+ik\cdot x}\hat{I}^{ab}_{2;\mu,-}(x)\\ &= \{\hat{P}^2_{\mu,-}(k) + \hat{F}_{2;\mu,-}(k) + \hat{K}_{2;\mu,-}(k)\}\hat{\mathcal{G}}^{ab}(k).\end{aligned} \tag{B115}$$

Hence, the gauge-covariance Wigner transformation of the left hand side of Eq. (B44) reads

$$\begin{aligned}\hat{I}^{ab}_{-}(k) &= \int dx e^{+ik\cdot x}\hat{W}\{\hat{\mathcal{G}}^{ab}[\mathcal{G}^{-1}_{-}]\}\hat{W}\\ &= \left\{-i\hbar c\hat{I}^{ab}_{1;0,-}(k) + \frac{\hbar^2}{2m}\hat{I}^{ab}_{2;j,-}(k) + \mu\hat{\mathcal{G}}^{ab}(k)\right\}\\ &= \bigg\{-i\hbar c[\hat{P}_{0,-}(k) + \hat{F}_{1;0,-}(k)] + \frac{\hbar^2}{2m}[\hat{P}^2_{j,-}(k)\\ &\quad + \hat{F}_{2;j,-}(k) + \hat{K}_{2;j,-}(k)] + \mu\bigg\}\hat{\mathcal{G}}^{ab}(k).\end{aligned} \tag{B116}$$

Considering the complexity of Eq. (B116), we here make some approximations. First, we expand $\hat{F}_{\mu\nu}(\zeta)$ in

Eq. (B96) around X and only keeping zero-order term, which leads to

$$\hat{W}(X,x_1)\hat{\mathcal{F}}_{\nu\mu}(1;x_1,X)\simeq +\hat{F}_{\nu\mu}(X), \tag{B117}$$

$$\hat{\mathcal{F}}_{\nu\mu}(2;X,x_2)\hat{W}(x_2,X)\simeq +\hat{F}_{\nu\mu}(X), \tag{B118}$$

$$\hat{\mathcal{F}}_{\nu\mu}(0;X,x_1)\hat{W}(x_1,X)\simeq -\hat{F}_{\nu\mu}(X), \tag{B119}$$

$$\hat{W}(X,x_2)\hat{\mathcal{F}}_{\nu\mu}(-1;x_2,X)\simeq -\hat{F}_{\nu\mu}(X). \tag{B120}$$

Hence, Eqs. (B105), (B113), and (B114) reduce to

$$\hat{F}_{1;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p)=\frac{e}{4\hbar}\{\hat{F}_{\nu\mu},[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}, \tag{B121}$$

$$\hat{F}_{2;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p)=\frac{e}{4\hbar}[\hat{P}_{\mu,-}(p)\{\hat{F}_{\nu\mu},[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\} + \{\hat{F}_{\nu\mu},\hat{P}_{\mu,-}(p)[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}], \tag{B122}$$

$$\hat{K}_{2;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p)=\left(\frac{e}{4\hbar}\right)^2\{\hat{F}_{\nu\mu},\{\hat{F}_{\nu\mu},[\partial^2_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}\}. \tag{B123}$$

Furthermore, we remove the higher-order terms $(\partial_{k_\alpha}\partial_{k_\beta}\hat{\mathcal{G}})$, $(\partial_{X^\mu}\partial_{X^\mu}\hat{\mathcal{G}})$, and $(\partial_{X^\mu}\partial_{k_\beta}\hat{\mathcal{G}})$. Thus, Eq. (B122) reduces to

$$\hat{F}_{2;\mu,-}(p)\hat{\mathcal{G}}^{ab}(p)=+ip_\mu\frac{e}{2\hbar}\{\hat{F}_{\nu\mu},[\partial_{p_\nu}\hat{\mathcal{G}}^{ab}(p)]\}. \tag{B124}$$

By substitution of Eqs. (B121) and (B124), Eq. (B116) becomes

$$\hat{I}^{ab}_{-}(k)=\left[-\frac{i}{2}\hbar v^\nu_k\frac{\hat{\partial}}{\partial X^\nu}-\frac{i}{2}\frac{ev^\mu_k}{2}\{\hat{F}_{\nu\mu},(\partial_{k_\nu}\cdot)\} + \mu-\epsilon(k)\right]\hat{\mathcal{G}}^{ab}(k). \tag{B125}$$

By substitution of Eqs. (B89) and (B125), we reach the gauge-invariant Wigner transformation of Gorkov equations (B43) and (B44) [56,57]

$$+\frac{i}{2}\widehat{\mathcal{G}}_0^{-1}(k,X)\widehat{\mathcal{G}}(k,X)+[\mu-\epsilon(k)]\widehat{\mathcal{G}}(k,X)=+\hbar c\check{1}, \tag{B126}$$

$$-\frac{i}{2}\widehat{\mathcal{G}}_0^{-1}(k,X)\widehat{\mathcal{G}}(k,X)+[\mu-\epsilon(k)]\widehat{\mathcal{G}}(k,X)=+\hbar c\check{1}, \tag{B127}$$

with

$$\widehat{\mathcal{G}}_0^{-1}(k,X)=\begin{bmatrix}\hat{\mathcal{G}}_0^{-1}(k,X) & 0\\ 0 & \hat{\mathcal{G}}_0^{-1}(k,X)\end{bmatrix}, \tag{B128}$$

where

$$\hat{\mathcal{G}}_0^{-1}(k,X)=\hbar v^\nu_k\frac{\hat{\partial}}{\partial X^\nu}+\frac{ev^\mu_k}{2}\{\hat{F}_{\nu\mu},(\partial_{k_\nu}\cdot)\}. \tag{B129}$$

Finally, we obtain the gauge-invariant quantum kinetic equation

$$\widehat{\mathcal{G}}_0^{-1}(k,X)\widehat{\mathcal{G}}(k,X)=0. \tag{B130}$$

Integrating Eq. (B130) over k^0, we reach

$$\hat{\mathcal{G}}_{\boldsymbol{k}}(X)\hat{\varrho}_{\boldsymbol{k}}(X)=0, \tag{B131}$$

with

$$\hat{\varrho}_{\boldsymbol{k}}(X)=\int\frac{dk^0}{2\pi}\hat{\varrho}_k(X), \tag{B132}$$

$$\hat{\mathcal{G}}_{\boldsymbol{k}}(X)=v^\nu_k\frac{\hat{\partial}}{\partial X^\nu}+\frac{ev^\mu_k}{2\hbar}\{\hat{F}_{j\mu},(\partial_{k_j}\cdot)\}, \tag{B133}$$

where we have assumed

$$\hat{\varrho}_k(X)|_{k^0=+\infty}-\hat{\varrho}_k(X)|_{k^0=-\infty}=0, \tag{B134}$$

to remove the $\hat{F}_{0\mu}$ term. Notably, the SU(2) technology does not require the translation invariance, and hence $\boldsymbol{k}$, as the gauge-invariant Fourier transformation of $\boldsymbol{r}=\boldsymbol{r}_1-\boldsymbol{r}_2$, is not a good quantum number.

APPENDIX C: DERIVATION OF NONCOLLINEAR SPIN EXCHANGE (3)

In this Appendix, we derive the noncollinear spin exchange, Eq. (10) in the main text.

The detailed derivations of the noncollinear spin exchange [Eq. (4) of main text], in principle, can be conducted by following Refs. [49,50], where the SOC introduces a rotation of the spin operator of magnetic moments {Eq. (9) of Ref. [49]}. This is because the itinerant electron spin rotates along the spin-orbit magnetic field during the exchange {Eq. (2) of Ref. [86]}

$$t_{ij}\to t_{ij}\exp\left(\frac{ie}{\hbar c}\int_{\mathbf{r}_i}^{\mathbf{r}_j}d\mathbf{r}'\cdot\hat{\mathbf{A}}(\mathbf{r}')\right). \tag{C1}$$

This is the so-called Peierls substitution in the presence of SOC, i.e., SU(2) gauge fields $\hat{\mathbf{A}}(\mathbf{r}')$. Note that the imperfection of the ferromagnetic interface causes the complicated SOC, i.e., SU(2) gauge fields [Eqs. (9)–(11) in main text]. In spite of this complicity, we can always include the effect of the SOC with a rotation of the spin operator of local moments, which is treated as a phenomenological parameter for simplicity

$$\mathcal{R}^{-1}=e^{+i\boldsymbol{A}_{\rm so}\cdot\boldsymbol{s}/2}\leftarrow\exp\left(\frac{ie}{\hbar c}\int_{\mathbf{r}_i}^{\mathbf{r}_j}d\mathbf{r}'\cdot\hat{\mathbf{A}}(\mathbf{r}')\right). \tag{C2}$$

Thus, the hybrid itinerant electron and local moments system can be described by the following Hamiltonian:

$$H=H_0+H_1, \tag{C3}$$

with

$$H_0=\sum_{\boldsymbol{k},s}\epsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}s}c_{\boldsymbol{k}s}+\epsilon_D\sum_{ns}d^\dagger_{ns}d_{ns}+U\sum_n d^\dagger_{n\uparrow}d_{n\uparrow}d^\dagger_{n\downarrow}d_{n\downarrow}, \tag{C4}$$

$$H_1=\sum_{\boldsymbol{k}ss'}tc^\dagger_{\boldsymbol{k}s}\mathcal{R}^{-1}_{ss'}d_{ns'}+\text{H.c.} \tag{C5}$$

Here, we have $t_{ij}=t$ is assumed to be independent of $\boldsymbol{k}$ for simplicity. $c_{\boldsymbol{k}s}$ is the annihilation operator of the itinerant electron with momentum $\boldsymbol{k}$, spin s, and energy spectrum $\epsilon_{\boldsymbol{k}}$, while $d_{ns'}$ is annihilation operator of the local moment in site n with energy level ϵ_D.

Following the standard way of the Schrieffer-Wolff transformation [87], we attain the Kondo coupling in the absence

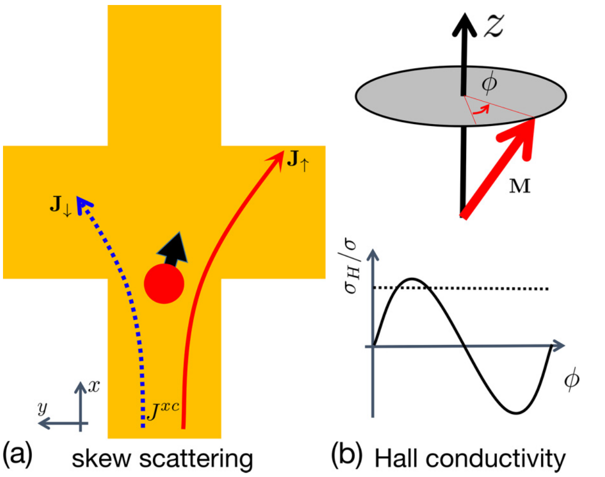

FIG. 4. Detection of the noncollinear spin exchange via the anomalous Hall effect. (a) The sketches of skew scattering from the spin-orbit magnetic field that is responsible for anomalous Hall effect. (b) The angular dependence of Hall conductivity. The solid and dash lines correspond to collinear and noncollinear spin exchanges between itinerant electrons and local moments, respectively.

of the spin rotation from the spin-orbit coupling ($\boldsymbol{A}_{\rm so} = \mathbf{0}$),

$$V = -\sum_j K_s \mathbf{S}_j \cdot \mathbf{s}\delta(\boldsymbol{r} - \boldsymbol{r}_j), \tag{C6}$$

with

$$K_s \simeq 2t^2\left(\frac{1}{\epsilon_D} - \frac{1}{\epsilon_D + U}\right). \tag{C7}$$

The effect of spin-orbit coupling can be simply captured by a spin rotation of the spin basis of the local moments (taking $S = 1/2$ as an example)

$$\begin{bmatrix}\tilde{d}_{n\uparrow}\\ \tilde{d}_{n\downarrow}\end{bmatrix} = \mathcal{R}^{-1}\begin{bmatrix}d_{n\uparrow}\\ d_{n\downarrow}\end{bmatrix}. \tag{C8}$$

Following the same procedure as the case of $\boldsymbol{A}_{\rm so} = \mathbf{0}$, we obtain [49,50]

$$V = -\sum_j K_s \tilde{\mathbf{S}}_j \cdot \mathbf{s}\delta(\boldsymbol{r} - \boldsymbol{r}_j) = -\sum_j K_s \mathbf{S}_j \cdot \tilde{\mathbf{s}}\delta(\boldsymbol{r} - \boldsymbol{r}_j). \tag{C9}$$

The tilde spin operator of itinerant electrons $\tilde{s}^a = R_{ab}s^b$, where 3×3 spin-rotation matrix R_{ab} in read space can be calculated from a 2×2 spin rotation matrix in spin space $\mathcal{R} = e^{-i\boldsymbol{A}_{\rm so}\cdot \boldsymbol{s}/2}$. The interfacial SOC rotates $\mathbf{m} = \langle \mathbf{S}\rangle/\langle \hat{S}_\parallel\rangle$ [Fig. 2(b) in the main text] into $\tilde{\mathbf{m}} = \langle \tilde{\mathbf{S}}\rangle/\langle \hat{S}_\parallel\rangle$ [Fig. 2(c) in the main text]. The relative tilde magnetization $\delta\tilde{\mathbf{m}} = \tilde{\mathbf{m}} - \mathbf{m}$ quantifies the noncollinear effect and can be modified by the interfacial SOC in a linear manner, i.e., $\delta\tilde{\mathbf{m}} \propto A^i_{\rm so}$.

The noncollinear spin exchange in principle can be detected by the anomalous Hall effect [1]—the conversion of a charge current into a transverse polarized charge current in a ferromagnet [Figs. 4(a) and 4(b)]. The effective Zeeman magnetic field contains a correction from the noncollinear spin exchange $e\Phi^a = g\mu_B B^{0a} - (n_m K_s/2)\langle \tilde{S}^a\rangle$ with $\langle \tilde{S}^a\rangle = R^{-1}_{ab}\langle S^b\rangle$ [14]. The external electric field drives a longitudinal spin drift current $\boldsymbol{J}^a = \sigma\kappa_a \boldsymbol{E}_{\rm ex}$ due to the different density of state for $s^a = +1/2$ and $s^a = -1/2$ electrons. The drift charge-to-spin conversion efficiency $\kappa_a \simeq -[\ln \nu(\mu_F)]'(n_m K_s/2)\langle \tilde{S}^a\rangle$ is approximately proportional to the magnetization of the ferromagnet $\langle \tilde{S}^a\rangle$ when $B^a \to 0$ T. Then, the longitudinal spin drift current is converted into a transverse charge current via the inverse spin Hall effect, $\boldsymbol{J}^0 \simeq -\theta^3_C \hat{z}\times \boldsymbol{J}^3$ as depicted by the skew scattering in Fig. 4(a), where we consider the spin Hall angles from the Rashba SOC $\boldsymbol{\theta}^a_C = \delta_{a3}\theta^3_C\hat{z}$ due to the inversion asymmetry at the interface or surface [60]. Thus, the anomalous Hall conductivity becomes $\sigma_H/\sigma \simeq [\ln \nu(\mu_F)]'(n_m K_s/2)\theta_C R^{-1}_{3b}\langle S^b\rangle$. The magnetization of the local moments follows the magnetic field direction and hence σ_H can oscillate for the magnetic field rotating along z direction for the noncollinear spin exchange, while becomes constant for collinear spin exchange with $R^{-1}_{3b} = \delta_{3b}$ as shown by Fig. 4(b). We can obtain the tilde direction $\langle \tilde{S}^3\rangle = R^{-1}_{3b}\langle S^b\rangle$ corresponding to angular-independent Hall conductivity.

APPENDIX D: INTERFACIAL SOC DEPENDENCE OF THE SPIN-DEPENDENT CONDUCTANCE

In this Appendix, we show the interfacial SOC dependence of the spin-dependent conductance for spin-orbit torque.

For simplicity, let us consider out-of-plane magnetic field as and omit the noncollinear effect of the spin-exchange coupling. Thus, the longitudinal (∥) and transverse (⊥) spin components are out-of-plane and in-plane directions, respectively. Note that the total spin relaxation time in the spin-orbit-coupled ferromagnet includes two contributions, i.e.,

$$\frac{1}{\tau^F_{\parallel,\perp}} = \frac{1}{\tau^{\rm SEC}_{\parallel,\perp}} + \frac{1}{\tau^{\rm SOC}_{\parallel,\perp}}. \tag{D1}$$

Here, $1/\tau^{\rm SEC}_{\parallel,\perp}$ comes from the SEC [Eqs. (4) and (5)]

$$\frac{1}{\tau^{\rm SEC}_{\parallel}} = \frac{2\pi}{\hbar}n_m\nu_F K_s^2\beta\epsilon_L n_B(\epsilon_L)[1 + n_B(\epsilon_L)]|\langle S^\parallel\rangle|, \tag{D2}$$

$$\frac{1}{\tau^{\rm SEC}_{\perp}} = \frac{1}{2\tau^m_\parallel} + \frac{\pi}{\hbar}n_m\nu_F K_s^2\langle S^\parallel S^\parallel\rangle, \tag{D3}$$

and $1/\tau^{\rm SOC}_{\parallel,\perp}$ arises from the interfacial SOC [Eqs. (47) and (48)]

$$\frac{1}{\tau^{\rm SOC}_{\parallel}} = \frac{2Dm^2}{\hbar^2}[(\alpha - u_\parallel\lambda)^2 + \beta^2 + u_\perp^2\lambda^2], \tag{D4}$$

$$\frac{1}{\tau^{\rm SOC}_{\perp}} = \frac{Dm^2}{\hbar^2}[(\alpha - u_\parallel\lambda)^2 + \beta^2 + 3u_\perp^2\lambda^2]. \tag{D5}$$

The latter is quadratic in the interfacial SOC.

For SEC-dominated regime ($\tau^{\rm SEC}_{\parallel,\perp}/\tau^{\rm SOC}_{\parallel,\perp} \ll 1$), we have $\tau^F_{\parallel,\perp} \simeq \tau^{\rm SEC}_{\parallel,\perp}$ and hence spin diffusion length in the ferromagnet $\ell^F_{\parallel,\perp} = \sqrt{D\tau^F_{\parallel,\perp}}$ is almost independent of the interfacial SOC. The spin-dependent conductance G^m_x is linear in $\ell^F_{\parallel,\perp}$ and hence is independent of the interfacial SOC. For SOC-dominated regime ($\tau^{\rm SEC}_{\parallel,\perp}/\tau^{\rm SOC}_{\parallel,\perp} \gg 1$), we have $\tau^F_{\parallel,\perp} \simeq \tau^{\rm SOC}_{\parallel,\perp}$ and hence $\ell^F_{\parallel,\perp}$ is inversely proportional to the interfacial SOC. Then, the spin-dependent conductance ($G^m_x \propto \ell_F$) is inversely proportional to the interfacial SOC.

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