SU(2) formulation of spin-resolved orbital magnetization

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We propose an approach concerning the derivation of the spin-resolved orbital magnetization in ferromagnets with spin-orbit interaction. An approach is presented in full detail based on non-Abelian Keldysh formalism. The self-consistency and reliability of results are examined through verifications of the equilibrium thermodynamic relation and nonequilibrium thermal transport. The study of equilibrium thermodynamic features reveals the non-transport spin-resolved properties. Meanwhile, the nonequilibrium spin thermal transport with the incorporation of SU(2) structures offers a route to explore the nature of correlations in the charge-spin response.

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I. INTRODUCTION

Appealing properties originating from spin-orbit interaction (SOI) have drawn huge attention for their intriguing physics and applications in spintronics. Through coupling the spin orientation of an electron with its orbital motion, various transport phenomena, such as the spin Hall effect [1–4], spin filters [5], spin accumulation [6], spin optics [7], and the quantum anomalous spin Hall effect [8], are led. Studies have been extended continuously to topological insulators and other novel quantum materials [9–11]. Due to the degree of freedom of the carrier's spin, there has been increasing interest in inspecting the spin-resolved rather than the spin-integrated contributions in the dynamics of spintronics. Since a finite SOI gives rise to additional features for an implementation of spin-selective effects, correlational spin-polarized motions are expected. Within the recent few years, a lot of effort has been given to understanding a novel spin-resolved effect in ferromagnetically spintronic materials using the semiclassical and quantum Boltzmann equation. As has been seen in ferromagnets with the Rashba SOI [12] or the Dresselhaus SOI [13], SOI segregates two polarized orientations of spins into two subbands and produces a spin imbalance. Such a spin imbalance creates a spin transport under the externally applied fields. Existing research has indicated that the interaction between the spin and momentum leads to emergent non-Abelian potentials. As a consequence, the spin emerges no longer as the internal degrees of freedom and behaves like a vector in the SU(2) space.

Regarding the SOIs in terms of the non-Abelian SU(2) gauge has been done for many years [14–21]. The mathematical formalism of the SU(2) gauge has been linked to phenomena in the many relevant areas of spintronics, optics, cold-atom physics [22–24], superconductors [9,25,26], and quantum computation [27]. Theoretically, the effective gauge potentials, arising from SOI, acting on the spin degrees of freedom of electrons have a non-Abelian structure [28]. The non-Abelian fields impose spin-dependent phases on the traveling electron [29], and their components need not commute [30]. As the typical examples, for the Rashba SOI [12] and the Dresselhaus SOI [13] in two-dimensional semiconductors, the non-Abelian gauge field gives rise to an effective magnetic field which is responsible for the rotation of the spins [18]. Except for studies of the spin transport and magnetization dynamics [20,21,31–38], non-Abelian field theories have been also used to study the nonrelativistic behavior of non-Abelian quantum fluids [39] to explain the electromagnetism of magnons [40]. Despite these advances, however, most previous theoretical investigations of spin-polarized electrons were limited to SU(2)⊗U(1) gauge models [18,34], in which the external electromagnetic field appears as a U(1) field and the SU(2) gauge fields account for the effect of SOIs. Since the external U(1) field affects the kinetic degrees of freedom of electrons, its influence is transmitted via SOI to the spin degrees of freedom. Such a treatment makes it hard to resolve the orbital and spin contributions clearly. An external SU(2) magnetic field has been proposed theoretically in explorations of spin-resolved phenomena for spintronics [16,41–43]. The diamagnetic response to the effective non-Abelian SO magnetic field has been studied [16].

The current-induced orbital magnetization (OM) has been studied by means of semiclassical wave-packet dynamics [44–46]. Expressions of the OM have been derived for Bloch electrons in crystalline solids [47–49]. Analogous to the orbital motion of electrons contributing to the OM [47,50–55], the spin-dependent motion is characterized by two types of variables: the spin, which relates to the spin orientation of the state, and the orbital variables, which concern the spatial evolution. The orbital-driven magnetization is associated with spin orientation due to spin-orbit coupling and produces a finite spin-resolved orbital magnetization (SROM). The current-induced nonequilibrium spin polarization of conduction electrons was recently studied with U(1) external fields [56]. Mott-like relations have been presented for electrically and thermally induced electric polarization [57,58]. The indispensable role of SROM has been demonstrated in the spin Nernst conductivity of the Rashba ferromagnet [59,60]. In particular, the OM is an orbital analog of a dipole moment of the current from the point of view of the orbital magnetic moment of the Bloch states [58]. It has been shown [58] in the strategy of the semiclassical theory [44–46] that the dipole density contains not only the statistical sum of the dipole moment but also a Berry phase correction. However, the extension of the semiclassical theory to the spin orientation phenomena is difficult [58]. Investigation of the consequences of quantum input (the spin Berry phase [61]) by altering subtly the classical canonical structure for the spin-resolved effects in spintronic systems is an interesting issue. Because the spin emerges as a degree of freedom in phase space and behaves like a vector in the SU(2) space, spin conservation breaking by the SOI makes an identification of the spin-resolved phase-space volume form with the non-Abelian gauge anomaly a challenge. This motivates us fundamentally to look for a theoretical approach which is capable of addressing the spin-resolved phenomena by treating the charge and spin degrees of freedom on an equal footing. The external SU(2) magnetic field might offer a route to explore the nature of spin-resolved properties. Therefore this paper aims to discuss how to adapt the external SU(2) magnetic field to dissect the emergence of spin-resolved effects in a SU(2) theoretical framework. We propose an approach concerning the derivation of spin-resolved magnetization. An approach to the spin-resolved orbital magnetization is presented in full detail based on non-Abelian Keldysh formalism. The role of correlations in the charge-spin response will be examined explicitly for the case of arbitrary spin polarization.

In the following, we first introduce the theoretical framework of a SU(2) representation of the SOI ferromagnetic systems and subsequently apply our formalism to derive an explicit analytical formula for the SROM arising from the ensemble average energy in the presence of a magnetic field. We demonstrate that the appropriate incorporation of SU(2) structure leads to a formula for the SROM by means of the states near the spin-resolved Fermi surfaces and the spin imbalance. The contributions from the spin imbalance are presented intrinsically in terms of the spin Berry phase representation. The calculation for a practical example of SROM is carried out in the Rashba ferromagnet. On the basis of the rationality, self-consistency, and reliability of the obtained results, we also verify the thermodynamical relation between the derivatives of SROM and electron density with respect to the chemical potential and magnetic field, respectively. To obey fundamental thermodynamics laws and require the Onsager relations [62,63], it is expected that the SROM should play an important role in the spin Nernst effect [64–66]. The physical origin of the spin Nernst effect [67–69] is very similar to that of the spin Hall effect, both of which are associated with different influences of the temperature gradient on the spin imbalance in the momentum space. Because the thermal spin current is a transport property while SROM is not, we obviously demonstrate that SROM can possibly explain the cancellation of those contributions arising from the diamagnetic currents in the thermal spin current [70,71].

This paper is structured as follows. We start by introducing the SROM from a SU(2) gauge representation of a ferromagnet with SOI in Sec. II A and provide a complete description of the SU(2) representation of the SOI ferromagnetic systems. The SU(2) formulation for the conduction electrons in an external magnetic field is developed in Sec. II B. The computational details are specified, relating the SU(2) formulation to the configurations that a physical system can attain. In Sec. III the formalism is applied to obtain a general formula of SROM. Application of the formalism to the Rashba ferromagnet is investigated. In Sec. IV, on analyticity with respect to the rationality and reliability, we examine the Maxwell's relation. By extending to the thermal transport property, we show in general how the orbital contribution is retracted in the charge Nernst effect. The results are discussed in Sec. V.

II. SU(2) GAUGE REPRESENTATION FOR THE CONDUCTION ELECTRONS IN AN EXTERNAL MAGNETIC FIELD

A. SU(2) gauge representation of a ferromagnet with SOI

Let us start our discussion with a Rashba ferromagnet Hamiltonian,

$$H_0 = \frac{\mathbf{p}^2}{2m_e}\mathbf{1}_2 + \alpha(p_y\sigma_x - p_x\sigma_y) - g\mathbf{M}\cdot\sigma, \tag{1}$$

where m_e is the effective electron mass, $\mathbf{p} = (p_x, p_y)$ are the electron momenta, α parametrizes the strength of the Rashba interaction, $\mathbf{1}_2$ is the unit matrix in spin space, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli spin matrices, $\mathbf{M}$ is the intrinsic magnetization, and g describes the strength of the s-d exchange interaction between the itinerant electron and intrinsic magnetization. We neglect electron-electron interactions and the disorder effect arising from the impurity scattering. Furthermore, we set $c = \hbar = k_B = 1$ throughout this paper.

Concerned with the SOI term in Eq. (1), we introduce the SU(2) vector potentials $\mathcal{A}_\mu = \sum_a A_\mu^{(a)}\tau^a$ [18,31,72], $A_y^{(x)} = 2m_e\alpha/e$, $A_x^{(y)} = -2m_e\alpha/e$, and $A_x^{(x)} = A_y^{(y)} = 0$. Similarly, we introduce the scalar potential for the exchange interaction, $A_0^{(a)} = -2gM_a$. In these SU(2) vector potentials, the upper indices $a, b, c \in \{x, y, z\}$ label spin projections, while the lower indices $\mu \in \{0, x, y\}$ label time and spatial directions. $\tau^a = \sigma^a/2$ are the generators of SU(2) (spin-1/2 operators) with the noncommutativity of the SU(2) spin algebra $[\tau^a, \tau^b] = i\sum_c \epsilon^{\text{abc}}\tau^c$, $\text{Tr}\{\tau^a, \tau^b\} = \delta^{ab}$, where ϵ^{abc} stands for the three-dimensional (3D) Levi-Civita tensor. According to $\mathcal{F}_{\mu\nu} = \partial_\mu\mathcal{A}_\nu - \partial_\nu\mathcal{A}_\mu - ie[\mathcal{A}_\nu, \mathcal{A}_\mu]$, the nonzero components of the field tensor are found as

$$F_{0i}^{(a)} = 2g\partial_i M_a - 4m_e\alpha g\sum_{j,b}\epsilon_{ij}\epsilon^{jab}M_b, \tag{2}$$

$$F_{xy}^{(x)} = F_{xy}^{(y)} = 0, \tag{3}$$

and

$$F_{xy}^{(z)} = 4m_e^2\alpha^2/e, \tag{4}$$

where ϵ_{ij} stands for the 2D Levi-Civita tensor running over two values $\epsilon_{xy} = -\epsilon_{yx} = 1$. A nonzero component $F_{xy}^{(z)}$ indicates that SOI can be interpreted as an effective magnetic field, normal to the xy plane, while the electric field $F_{0i}^{(a)}$ is generated by an interplay between the SOI and inhomogeneous magnetization of the ferromagnet. In terms of SU(2) gauge potentials, the Hamiltonian can be expressed generally (not confined to the Rashba SOI) as [21,36,73] $H_0 = \pi^2/(2m_e) - \mathcal{A}_0$, where $\pi = \mathbf{p} - |e|\mathcal{A}$ are kinetic momenta. The Hamiltonian is covariant with respect to the local non-Abelian gauge transformations [16,18] $A_\mu \to UA_\mu U^{-1} + i(\partial_\mu U)U^{-1}/e$, where $U = e^{i\theta^a(r,t)\tau^a}$ is an arbitrary SU(2) matrix.

B. SU(2) formulation for the conduction electrons in an external magnetic field

To resolve the spin features of electron motion with the microscopic linear response calculations, we introduce the non-Abelian potential $\mathcal{A}^{\text{ext}}_\mu$, $\mathcal{A}^{\text{ext}}_x = A^{(a)}_y\tau^a = -B^{(a)}y\tau^a$, $\mathcal{A}^{\text{ext}}_y = 0$, and $\mathcal{A}^{\text{ext}}_0 = 0$, for the external magnetic field [42], where $B^{(a)}$ is the external magnetic field in company with τ_a and perpendicular to the two-dimensional plane. The field strengths of the external field are $\mathcal{F}^{\text{ext}}_{i0} = 0$ and $\mathcal{F}^{\text{ext}}_{xy} = B^{(a)}\tau_a$. The planar motion of a spin-1/2 particle under the action of a non-Abelian magnetic field is described by the Hamiltonian

$$H = (\pi - |e|\mathcal{A}^{\text{ext}})^2/2m_e - \mathcal{A}_0. \tag{5}$$

To the first order in $\mathcal{A}^{\text{ext}}$, the perturbed Hamiltonian is approximated as $H = H_0 + H_{\text{ext}}$, where $H_{\text{ext}} = -(|e|/2)\{v_x, \mathcal{A}^{\text{ext}}_x\}$. The anticommutator is defined as $\{v_x, \mathcal{A}^{\text{ext}}_x\} = v_x\mathcal{A}^{\text{ext}}_x + \mathcal{A}^{\text{ext}}_x v_x$, and v_i is the velocity matrix given by $v_i = \partial_{p_i}H_0 = \pi_i/m_e$. H_{ext} has a form $H_{\text{ext}} = -B^{(a)}\mathcal{M}^{(a)}$, which is the SU(2) magnetic field coupling to a SROM,

$$\mathcal{M}^{(a)} = -(|e|/2)\{v_x, y\tau^a\}. \tag{6}$$

Due to the two-dimensional geometry, the current density lies in the xy plane, so the OM, which is spin orientation (a) dependent, is restricted to the z direction. Accordingly, the Hamiltonian of the ferromagnet with SOI in the external magnetic field is rewritten as $H = H_0 - B^{(a)}\mathcal{M}^a$. Since $[[\tau^a, v_x], y] = 0$, we can get an alternative form, $\mathcal{M}^{(a)} = -(|e|/2)\{j^a_x, y\}$, where $j^a_x = \{v_x, \tau^a\}/2$ is the spin current operator. This indicates that the SROM is actually a magnetic dipole moment [58] induced by the spin current.

The kinetic theory for the conduction electrons in spintronic systems can be formulated in terms of the matrix Green's function $\widehat{G}(1,2)$, which satisfies a SU(2) covariant Boltzmann equation [74,75]. In the Wigner representation the Green's function has a structure $\widehat{G}(1,2) = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}$ in the Keldysh space, where G^R, G^A, and G^K are the retarded, advanced, and Keldysh components, respectively, and 1,2 are generalized coordinates containing space and time coordinates as well as spin and other possible additional indices.

The Dyson equation in the presence of SU(2) external field $\mathcal{A}^{\text{ext}}$ is expressed as

$$\begin{aligned} 0 &= \widehat{G}_0^{-1}(\epsilon, \mathbf{p}, X)\widehat{G}[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)] \\ &\quad - \widehat{G}[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)]\widehat{G}_0^{-1}(\epsilon, \mathbf{p}, X). \end{aligned} \tag{7}$$

The solutions of Eq. (4) can be obtained using the gradient expansion approximation for $\mathcal{A}^{\text{ext}}(X)$. Working to the first order in gradient expansion, the solution is found as

$$G[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)] = G_0(\epsilon, \mathbf{p}, X) + \Delta G[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)], \tag{8}$$

where $\Delta G[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)]$ is found in the form

$$\Delta G[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)] = |e|B^{(a)}G_1^{(a)}(\epsilon, \mathbf{p}, X) \tag{9}$$

with a representation

$$\begin{aligned} &G_1^{(a)}(\epsilon, \mathbf{p}, X) \\ &\quad = -\frac{i}{2}G_0(\epsilon, \mathbf{p}, X)[j^a_x G_0(\epsilon, \mathbf{p}, X), v_y G_0(\epsilon, \mathbf{p}, X)]. \end{aligned} \tag{10}$$

The technical details of the derivation are given in Appendix.

III. SROM

A. Derivation of SROM based on non-Abelian Keldysh formalism

As shown in Eq. (9), the nonzero $G_1^{(a)<}$ is expected to induce an orbital response to the SU(2) external magnetic field. The expectation value of the energy in the presence of the external magnetic field is given by $K[B^{(a)}] = -i\int d\epsilon/(2\pi)\int[d\mathbf{p}]\,\text{Tr}\{(H_0 - \mu)G^<[\epsilon, \mathbf{p}, \mathcal{A}^{\text{ext}}(X)]\}$, where $[d\mathbf{p}] \equiv d^2\mathbf{p}/(2\pi)^2$. Correspondingly, the SROM should be obtained by the derivative of the energy $K[B^{(a)}] = \langle H\rangle$ with respect to $B^{(a)}$, $\mathcal{M}^{(a)} = -\beta^{-1}\int d\beta(\partial K/\partial B^{(a)})$ [48].

Using the fluctuation-dissipation theorem $G_i^<(\epsilon, \mathbf{p}) = [G_i^A(\epsilon, \mathbf{p}) - G_i^R(\epsilon, \mathbf{p})]f(\epsilon)$ ($i = 0, 1$), $G_1^{(a)<}$ is found as

$$G_1^{(a)<} = \frac{if(\epsilon)}{2}\left(G_0^R\left[j^a_x G_0^R, v_y G_0^R\right] - G_0^A\left[j^a_x G_0^A, v_y G_0^A\right]\right), \tag{11}$$

where $f(\epsilon) = [e^{\beta(\epsilon-\mu)} + 1]^{-1}$ is the Fermi-Dirac distribution function. To the first order of $B^{(a)}$, $K[B^{(a)}]$ can be written as $K[B^{(a)}] = K_0 - eB^{(a)}K_1^{(a)}$, where $K_i = -i\int d\epsilon/(2\pi)\int[d\mathbf{p}]\,\text{Tr}[(H_0 - \mu)G_i^<(\epsilon, \mathbf{p})]$. The trace is taken over the spin states of a conduction electron, or equivalently, the spectrum of $H_0(\mathbf{p})$. We introduce the complete set $\{|n, \mathbf{p}\rangle\}$ of eigenstates of the secular equation, $H_0(\mathbf{p})|n, \mathbf{p}\rangle = \epsilon_n(\mathbf{p})|n, \mathbf{p}\rangle$ [48,49,51], corresponding to the eigenvalues $\epsilon_n(\mathbf{p})$ (n is a generalized band index containing the energy and spin information). O_{nm} is defined as $\langle n, \mathbf{p}|O|m, \mathbf{p}\rangle$ for the operator $\widehat{O}$. K_0 and $K_1^{(a)}$ are found as $K_0 = \sum_n\int[d\mathbf{p}](\epsilon_n - \mu)f(\epsilon_n)$ and

$$K_1^{(a)} = -\sum_n\int[d\mathbf{p}]\left[f(\epsilon_n)L^{(\alpha)}_{n,xy} - \frac{1}{\beta}\ln[1 - f(\epsilon_n)]\Omega^{(n)}_{n,xy}\right], \tag{12}$$

where the Kubo expression $L^{(a)}_{n,xy} = i\sum_{m\neq n}[(j^a_x)_{nm}(v_y)_{mn} - (v_y)_{nm}(j^a_x)_{mn}]/\ [2(\epsilon_n - \epsilon_m)]$ corresponds to the orbital moment of state $|n, \mathbf{p}\rangle$ and $\Omega^{(a)}_{n,xy} = i\sum_{m\neq n}[(j^a_x)_{nm}(v_y)_{mn} - (v_y)_{nm}(j^a_x)_{mn}]/(\epsilon_n - \epsilon_m)^2$ is the quantum correction from a spin-resolved curvature [61]. Taking the derivative of the function $K[B^{(a)}]$ with respect to $B^{(a)}$, taking $B^{(a)} \to 0$ at the last step of the calculation, and integrating over β leads to the SROM

$$\mathcal{M}^{(a)}_{xy} = -|e|K_1^{(a)}.$$

$K_1^{(a)}$ indicates that the magnetic response for the magnetic modulated orbital motion in a magnetic field leads to a correction term for the energy, which is manifested by $\delta M^{(a)} = (1/\beta)\sum_n\ln(1 + e^{-\beta(\epsilon_n-\mu)})\Omega^{(a)}_{n,xy}$. At first glance, the form in

Eq. (12) closely resembles the expression of OM for the case of spin degree of freedom quenched [47,47–55]. However, it is worth emphasizing that the spin-resolved effect is retained in Eq. (12). Equation (12) shows that the SROM is not simply the sum of the orbital moments of all occupied spin correlative states: There is a spin-resolved curvature correction due to $\Omega^{(a)}_{n,xy}$ [49]. Because of the exchange spin with the non-Abelian field, it is explicit that the influence of the SU(2) external field on the spin-resolved motion would not be dissolved in the derivation of $K[B^{(a)}]$ with respect to $B^{(a)}$ even for $B^{(a)} \to 0$ at the last step of the calculation. In order to illustrate how the spin-resolved transitions between eigenstates induced by the operator j^a_x modify the thermal average of orbital motion, we express $L^{(a)}_{n,xy}$ and $\Omega^{(a)}_{n,xy}$ in the Berry phase representation

$$L^{(a)}_{n,xy} = -\frac{1}{2}\mathrm{Im}\sum_{m\neq n}\big[\big((\partial_{p_x}\langle n,\mathbf{p}|)\Pi^{(a)}_n + \langle n,\mathbf{p}|\Sigma^{(a)}_{x,nm}\big)(\epsilon_n - H_0)|m,\mathbf{p}\rangle\langle m,\mathbf{p}|\big(\partial_{p_y}|n,\mathbf{p}\rangle\big)\big] - \frac{1}{2}\mathrm{Im}\sum_{m\neq n}\big[\langle n,\mathbf{p}|\big(\partial_{p_y}|m,\mathbf{p}\rangle\big)(\partial_{p_x}\langle m,p|)\Pi^{(a)}_m(\epsilon_m - H_0)|n,\mathbf{p}\rangle\big] \tag{13}$$

and

$$\Omega^{(a)}_{n,xy} = -\mathrm{Im}\sum_{m\neq n}\big[\big((\partial_{p_x}\langle n,\mathbf{p}|)\Pi^{(a)}_n + \langle n,\mathbf{p}|\Sigma^{(a)}_{x,nm}\big)|m,\mathbf{p}\rangle\langle m,\mathbf{p}|\big(\partial_{p_y}|n,\mathbf{p}\rangle\big)\big] + \mathrm{Im}\sum_{m\neq n}\big[\langle n,\mathbf{p}|\big(\partial_{p_y}|m,\mathbf{p}\rangle\big)(\partial_{p_x}\langle m,\mathbf{p}|)\Pi^{(a)}_m|n,\mathbf{p}\rangle\big], \tag{14}$$

where we have defined $\Pi^{(a)}_n = (\epsilon_n - H_0)\tau^a(\epsilon_n - H_0)^{-1}$ and $\Sigma^{(a)}_{x,nm} = \partial_{p_x}(\epsilon_n + \epsilon_m)\tau^a(\epsilon_n - H_0)^{-1}$. These alternative expressions of curvature correction $\Omega^{(a)}_{n,xy}$ and orbital moment of states $L^{(a)}_{n,xy}$ embody the spin-resolved effect definitely. Conceptually, the direct evaluation of SROM from the Berry phase representation is very appealing and appears to be advantageous over the use of the corresponding Kubo expressions. It is instructive to note that when $\tau = \mathbf{1}_2$ and this is substituted into Eqs. (10) and (11), we get the usual expressions for the conventional OM [48].

B. SROM in the Rashba ferromagnet

We turn now to apply this formalism to the Rashba ferromagnet described by the Hamiltonian in Eq. (1). For simplicity, we ignore in-plane *s*-*d* exchange interaction $-gM_i \cdot \sigma_i$, $i \in (x, y)$ and confine our discussion to $\mathbf{M} = M\widehat{e_z}$. The eigenstates and eigenenergies of the Hamiltonian (1) are $\epsilon_\pm = p^2/(2m_e) \pm \sqrt{g^2M^2 + \alpha^2p^2}$, $|\psi_+\rangle = (e^{-i\phi}\cos(\theta/2), \sin(\theta/2))^T$ and $|\psi_-\rangle = (-\sin(\theta/2), e^{i\phi}\cos(\theta/2))^T$, respectively, where $\sin\theta = \alpha p/\sqrt{g^2M^2 + \alpha^2p^2}$, $\cos\theta = -gM/\sqrt{g^2M^2 + \alpha^2p^2}$, and $\tan\phi = -p_x/p_y$. The components of the orbital moment of states and quantum correction are found as

$$L^{(z)}_{+,xy} = L^{(z)}_{-,xy} = \frac{\alpha^2p^2\sin^2\phi}{4m_e(g^2M^2 + \alpha^2p^2)} \tag{15}$$

and

$$\Omega^{(z)}_{+,xy} = -\Omega^{(z)}_{-,xy} = \frac{\alpha^2p^2\sin^2\phi}{4m_e(g^2M^2 + \alpha^2p^2)^{3/2}}, \tag{16}$$

respectively. Substituting these into Eqs. (12) and (13) and integrating over the momentum, we can obtain $\mathcal{M}^{(z)}$. The results with various possible parameters are shown in Fig. 1.

Because

$$\frac{1}{\beta}\ln(1 + e^{-\beta(\epsilon_\pm - \mu)}) = -\Theta(\mu - \epsilon_\pm)(\epsilon_\pm - \mu) \tag{17}$$

at $\beta \to \infty$, the SROM at zero temperature can be written as $\mathcal{M}^{(z)}_{xy} = \sum_{n=\pm}\mathcal{M}^{(z)}_{xy,n}$, where

$$\mathcal{M}^{(z),0}_{xy,n} = \int [d\mathbf{p}]\Theta(\mu - \epsilon_n)\big[L^{(z)}_{n,xy}(\mathbf{p}) + (\mu - \epsilon_n)\Omega^{(z)}_{n,xy}(\mathbf{p})\big]. \tag{18}$$

Substituting $L^{(z)}_{\pm,xy}$ and $\Omega^{(z)}_{\pm,xy}$ into Eq. (18) and integrating over the momentum, we have

$$\mathcal{M}^{(z),0}_{xy,\pm} = \pm\int_0^{s_\pm} ds\frac{m\alpha^2 s(\mu - s)}{8\pi(M^2 + 2m\alpha^2 s)^{3/2}}, \tag{19}$$

where $s_\pm = m\alpha^2 + \mu \mp \sqrt{M^2 + m^2\alpha^4 + 2m\alpha^2\mu}$. We found $\mathcal{M}^{(z),0} = -em_e\alpha^2/(12\pi)$ for the case in which both bands are occupied ($\mu > gM$). The result is independent of the chemical potential μ and the strength of intrinsic magnetization M. This is in agreement with previous results [58,59]. Figure 1(a) shows that $M^{(z)}$ decreases as the temperature increases. $M^{(z)}$ approaches to $M^{(z),0}$ at low temperature [as shown in Figs. 1(a) and 1(b)] if $\mu \geqslant gM$. With the increase in temperature, $M^{(z)}$ tends to drop rapidly. Figure 1(b) shows that for a given k_BT, the interband transitions might happen only if it exceeds the energy gap. In addition, the SOI is expected to enhance the SROM. We also plot the classical components and quantum components at zero temperature independently in Fig. 1(d). We found that the spin-resolved effect is remarkable, i.e., the spin Berry curvatures of two spin subbands are opposite in sign: $L^{(z)}_{-,xy} > L^{(z)}_{+,xy}$, and $|\Omega^{(z)}_{-,xy}| > |\Omega^{(z)}_{+,xy}|$.

IV. RATIONALITY AND RELIABILITY

For the purpose of rationality, self-consistency, and reliability, the above results will be examined in the following two aspects: (1) *the role of* $L^{(a)}_{n,xy}$ *and* $\Omega^{(a)}_{n,xy}$ *in thermodynamic*

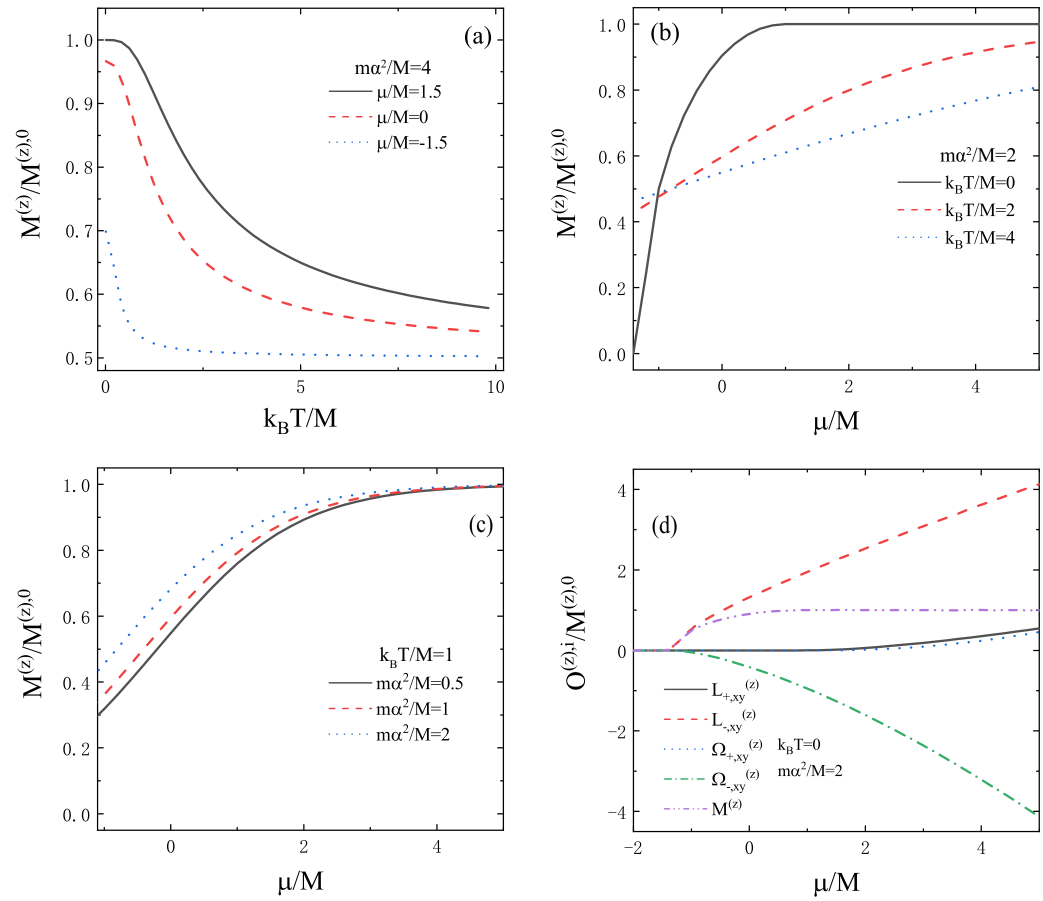

FIG. 1. SROM of a Rashba ferromagnet (a) as a function of the temperature for different chemical potentials, (b) as a function of the chemical potential at different temperatures, and (c) for different Rashba parameters. (d) $L_{s,xy}^{(z)}$, $\Omega_{s,xy}^{(z)}$ at zero temperature. $M^{(z),0}$ is the value at zero temperature. All parameters are nondimensionalized by M, and $g = 1$ is taken for simplicity.

quantities of systems and (2) *the role of SROM in the spin Nernst effect*, which will be discussed in Secs. IV A and IV B.

A. Maxwell's relation

We look at aspect (1) first. On analyticity with respect to the thermodynamic potential of the quasiequilibrium state, we examine the Maxwell's relation

$$(\partial\mathcal{M}^{(a)}/\partial\mu)_{B,T} = (\partial n/\partial B^{(a)})_{T,\mu}. \tag{20}$$

The density of electrons is defined by $n = -i\int(d\epsilon/2\pi)\int[d\mathbf{p}]\,\mathrm{Tr}[G^<]$. To the first order of $B^{(a)}$, n can be written as $n = n_0 - eB^{(a)}n_1^{(a)}$ using Eq. (8), where $n_i = -i\int d\epsilon/(2\pi)\int[d\mathbf{p}]\,\mathrm{Tr}[G_i^<(\epsilon,\mathbf{p})]$ $(i = 0,\ 1)$. Following the same steps as above, we find n_0 and $n_1^{(a)}$ as $n_0 = \sum_n\int[d\mathbf{p}]f(\epsilon_n)$ and

$$n_1^a = \sum_n\int[d\mathbf{p}]\big[\Omega_{n,xy}^{(a)}f(\epsilon_n) - L_{n,xy}^{(a)}f'(\epsilon_n)\big]. \tag{21}$$

The second term in the square brackets clearly stands for the renormalization of the energy dispersion. We can transcribe this correction into that of the arguments of $f(\epsilon_n)$. Generally, the density of electrons n can be expressed as

$$n = \sum_n\int[d\mathbf{p}]\big(1 + |e|B^{(a)}\Omega_{n,xy}^{(a)}\big)f\big(\epsilon_n - |e|B^{(a)}L_{n,xy}^{(a)}\big). \tag{22}$$

This shows that the application of an external magnetic field leads to additional responses of the system, besides the one due to these Berry curvature terms. Because the diamagnetic response results in the energy shift in terms of a magnetic moment, the states are occupied according to a nonequilibrium distribution function. $|e|B^{(a)}\Omega_{n,xy}^{(a)}$ manifests the expansion of phase-space volume in accordance with the density of states, while $-|e|B^{(a)}L_{n,xy}^{(a)}$ presents as the energy level shift due to the magnetic energy arising from the SROM. Calculating the derivatives of $\mathcal{M}^{(a)}$ with respect to the chemical potential μ and the density of electrons n with respect to $B^{(a)}$, respectively, the Maxwell's relation (12) is then proved definitely.

B. Role of SROM in the spin Nernst effect

For aspect (2), the SROM is an intrinsic characteristic of spintronic systems. As mentioned in the Introduction it is not a transport property, analog to retracting the orbital contribution in the charge Nernst effect [62,76,77]; it would be natural to inspect this through investigation of the interplay between the energy flow and SROM in the spin Nernst effect. The calculations inevitably require generalizations of linear response methods developed by Luttinger [78,79] to the generation of spin current from a temperature gradient. According to the Einstein relation, the gradient in the temperature has the same effects as the response to a gravitational field. We calculate the spin current driven by a "mechanical" inhomogeneous gravitational field ϕ_Q. The effect of the gravitational field can be replicated by introducing a perturbation, $F(\mathbf{r}') = [H(\mathbf{r}')\phi_Q(\mathbf{r}') + \phi_Q(\mathbf{r}')H(\mathbf{r}')]/2$, to the Hamiltonian, where $\mathbf{r}'$ is a single electron's coordinate. The total Hamiltonian is $H_T(\mathbf{r}') = H(\mathbf{r}') + F(\mathbf{r}')$. The nonequilibrium (induced by the gravitational field) density operator can be treated in a linear response to the perturbation as $\rho = \rho_0 + \rho_1$ [70]. The ensemble average of the spin current is then expressed as $\mathbf{j}^a = (1/V)\int d\mathbf{r}\,\mathrm{Tr}[\rho\widehat{\mathbf{j}}^a(\mathbf{r})] = \mathbf{j}^{a(0)} + \mathbf{j}^{a(1)}$, where $\mathbf{j}^{a(0)} = (1/V)\int d\mathbf{r}\,\mathrm{Tr}[\rho_1\mathbf{j}^{a(0)}(\mathbf{r})]$ and $\mathbf{j}^{a(1)} = (1/V)\int d\mathbf{r}\,\mathrm{Tr}[\rho_0\mathbf{j}^{a(1)}(\mathbf{r})]$. Here, the spin current operator is defined by $\widehat{\mathbf{j}}^a(\mathbf{r}) = -\{\tau_a, \widehat{\mathbf{j}}(\mathbf{r})\}/2$, where $\widehat{\mathbf{j}}(\mathbf{r})$ is the particle current operator and can be expressed as $\widehat{\mathbf{j}}(\mathbf{r}) = \widehat{\mathbf{j}}^{(0)}(\mathbf{r}) + \widehat{\mathbf{j}}^{(1)}(\mathbf{r})$ [70], with the free current operator $\widehat{\mathbf{j}}^{(0)}(\mathbf{r}) = \{\mathbf{v}', \delta(\mathbf{r} - \mathbf{r}')\}/2$ and the perturbed current operator $\widehat{\mathbf{j}}^{(1)}(\mathbf{r}) = \widehat{\mathbf{j}}^{(0)}(\mathbf{r})\phi_Q(\mathbf{r})$. Technically, $\mathbf{j}^{a(0)}$ is obtained by the standard linear response theory, and the component of $\mathbf{j}^{a(1)}$ is proportional to $\nabla\phi_Q$,

$$j_x^{a,(1)} = -\frac{1}{4V}\,\mathrm{Tr}\,[\rho_0\{\tau_a, \{y, v_x\}\}](-\partial_y\phi_Q), \tag{23}$$

where V is volume. Because $\{\tau_a, \{y, v_x\}\} = (2\tau_a y v_x + 2v_x\tau_a y + [[\tau_a, v_x], y])$ and $[[\tau_a, v_x], y] = 0$ for $H_0 = \pi^2/(2m_e) - \mathcal{A}_0$, we have $\{\tau_a, \{y, v_x\}\} = 2\{v_x, \tau_a y\}$. Substituting this into Eq. (23), the response of an operator $\widehat{\mathbf{j}}^{(1)}(\mathbf{r})$ to the temperature gradient reads $j_x^{a(1)} = (1/|e|)\mathcal{M}_{xy}^{(a)}(-\partial_y\phi_Q)$, where $\mathcal{M}_{xy}^{(a)} = -|e|/(2V)\,\mathrm{Tr}[\rho_0\{v_x, \tau_a y\}]$ is an equilibrium SROM previously given in Eqs. (6) and (13). Within the linear response regime, the spin Nernst current under thermal nonuniformity can be expressed in the form

$$j_x^a = \left(K_{xy}^{(a)Q} + |e|^{-1}\mathcal{M}_{xy}^{(a)}\right)(-\partial_y\phi_Q). \tag{24}$$

$K_{xy}^{(a)Q}$ is the thermal response coefficient, which can be obtained by considering the simplest bubble diagram via the calculation of $j_x^{a(0)}$ [71]. The response coefficient $K_{xy}^{(a)Q}$ is a sum of two contributions: $K_{xy}^{(a)Q} = K_{xy,\mathrm{I}}^{(a)Q} + K_{xy,\mathrm{II}}^{(a)Q}$, corresponding to the contributions from the Fermi surface $K_{xy,\mathrm{I}}^{(a)Q} = (1/4\pi V)\int d\epsilon[-f'(\epsilon)]Z_{xy,\mathrm{I}}^{(a)Q}$ and the distributions over all possible energies $K_{xy,\mathrm{II}}^{(a)Q} = (1/4\pi V)\int d\epsilon f(\epsilon)Z_{xy,\mathrm{II}}^{(a)Q}$, respectively. The strategy for calculating $K_{xy,\mathrm{I}}^{(a)Q}$ and $K_{xy,\mathrm{II}}^{(a)Q}$ consists of solving the kinetic equations (3)–(8) together with the expression for the heat current operator $j_y^Q = (1/2)\{H - \mu, v_y\}$. The thermal response coefficient is found to relate to the electric response coefficients at zero temperature [80]:

$$K_{xy}^{(a)Q}(T,\mu) = \frac{1}{|e|}\int_{-\infty}^{\infty} d\epsilon[-f'(\epsilon)](\epsilon-\mu)K_{xy}^{(a)E}(0,\epsilon) - \frac{1}{|e|}\int_{-\infty}^{\infty} d\epsilon f(\epsilon)K_{xy,\mathrm{II}}^{(a)E}(0,\epsilon), \tag{25}$$

where $K_{xy}^{(a)E} = K_{xy,\mathrm{I}}^{(a)E} + K_{xy,\mathrm{II}}^{(a)E}$ are electric response coefficients. $K_{xy,\mathrm{I}}^{(a)E}$ and $K_{xy,\mathrm{II}}^{(a)E}$ take the same form as $K_{xy,\mathrm{I}}^{(a)Q}$ and $K_{xy,\mathrm{II}}^{(a)Q}$ but replacing the heat current operator (j_y^Q) with a charge current operator ($j_y^E = -ev_y$). Compared with the contribution of the Fermi surface, the second term in Eq. (16) plays a special role. Because the term of SROM is found as $\mathcal{M}_{xy}^{(a)}(T,\mu) = \int_{-\infty}^{\infty} d\epsilon f(\epsilon)K_{xy,\mathrm{II}}^{(a)E}(0,\epsilon)$, we arrive at the conclusion that the Mott-like relation for the kinetic coefficients holds in the framework of a non-Abelian SU(2) gauge representation of a ferromagnet with SOI,

$$K_{xy}^{(a)Q}(T,\mu) - (1/e)\mathcal{M}^{(a)}(T,\mu) = -(1/e)\int_{-\infty}^{\infty} d\epsilon[-f'(\epsilon)](\epsilon-\mu)K_{xy}^{(a)E}(0,\epsilon), \tag{26}$$

as expected [80]. This relation clearly shows that $\mathcal{M}^{(a)}(T,\mu)$ is not a transport property and compensates the difference between the electric and the thermal Kubo contributions.

V. SUMMARY

To conclude, we have formulated the SROM in the framework of a non-Abelian SU(2) gauge representation of ferromagnets with SOI. An explicit expression for the SROM is derived from an extension of the Keldysh Green's function on which the SU(2) external field is based. Our comprehensive theoretical analysis reflects unequivocally the possibility of resolving spin correlative motion using a SU(2) external field. We have examined the self-consistency and reliability of results through the equilibrium thermodynamic relation and nonequilibrium thermal transport. Although we derive our formula analytically in the clean limit, this formalism allows for a straightforward inclusion of other effects, e.g., impurity scattering [81], and is easily transferable to nonequilibrium situations. In fact, the SU(2) Keldysh formalism should generally be suitable to compute the SROM in disordered systems [82]. Our study offers a fresh angle to understand the SROM in ferromagnets with SOI and provides an efficient formalism for calculating the novel spin-resolved phenomena which are covered up with U(1) gauge frameworks.

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APPENDIX: SU(2) FORMULATION FOR THE CONDUCTION ELECTRONS IN AN EXTERNAL MAGNETIC FIELD

In this Appendix we discuss the procedure to derive the Dyson equation in the presence of SU(2) external field $\mathcal{A}^{\mathrm{ext}}$. The kinetic theory for the conduction electrons in spintronic systems can be formulated in terms of the matrix Green's function $\widehat{G}(1,2)$, which satisfies a SU(2) covariant Boltzmann equation [74,75]. In the Wigner representation the Green's function has a structure $\widehat{G}(1,2) = \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix}$ in the Keldysh space, where G^R, G^A, and G^K are the retarded, advanced, Keldysh components, respectively, and 1,2 are generalized coordinates containing space and time coordinates as well as spin and other possible additional indices. Performing an orthogonal transformation $\Theta\widehat{G}(1,2)\Theta^{-1}$ with $\Theta = I + \sigma_+$ and $\sigma_+ = (\sigma_x + i\sigma_y)/2$, $\widehat{G}(1,2)$ can be rewritten in the same form but replacing G^K with $2G^<$ [83], where $G^<$ is the lesser Green's function. As the purpose is to reveal the essence of the procedure, we will limit ourselves to the clean limit [84,85].

$\widehat{G}$ satisfies the equations of motion $\widehat{G}^{-1}(1,1')\otimes\widehat{G}(1',2)=\delta_{1,2}$ for free electrons in a perfect lattice, where the symbol "$\otimes$" denotes convolution or matrix multiplication (in position, time, and spin). We introduce the center-of-mass coordinates $X=(T,\mathbf{R})$, $\mathbf{R}=(\mathbf{x}_1+\mathbf{x}_2)/2$, and $T=(t_1+t_2)/2$ and the relative time-space coordinates $x=(t,\mathbf{r})$, $\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$, and $t=t_1-t_2$. As long as a system is not so far from its equilibrium case, its dependencies on $\mathbf{R}$ and T are slowly varying in comparison with the lattice spacing and inverse of bandwidth, respectively. The length and time scale of relative time-space coordinates can be extracted by Fourier transformation, $F(X,p)=\int_{-\infty}^{\infty}d\mathbf{r}\int_{-\infty}^{\infty}dt e^{ipx}F(X+x/2,X-x/2)$, where $p=(\epsilon,\mathbf{p})$ and $px=-\epsilon t+\mathbf{p}\cdot\mathbf{r}$, where ϵ (energy) and $\mathbf{p}$ (momentum) are the conjugate variables of t and $\mathbf{r}$. The Dyson equation in the presence of SU(2) external field $\mathcal{A}^{\text{ext}}$ is expressed as

$$\widehat{G}_0^{-1}(\epsilon,\mathbf{p},X)\otimes\widehat{G}[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]=\mathbf{1}_2, \tag{A1}$$

where the subscript 0 labels the system without an external magnetic field, $\widehat{G}_0^{-1}(\epsilon,\mathbf{p},X)=\epsilon-\pi^2/2m_e+\mathcal{A}_0$ in the (X,p) representation. Together with its conjugate, Eq. (3) results in

$$\begin{aligned}0=&\,\widehat{G}_0^{-1}(\epsilon,\mathbf{p},X)\widehat{G}[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\\&-\widehat{G}[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\widehat{G}_0^{-1}(\epsilon,\mathbf{p},X).\end{aligned} \tag{A2}$$

As a stable system, all the quantities are time independent, and the derivative ∂_X is exerted only on $\mathcal{A}^{\text{ext}}(X)$. The solutions of Eq. (4) can be obtained using the gradient expansion approximation for $\mathcal{A}^{\text{ext}}(X)$. Working to the first order in gradient expansion, the convolution of two operators is taken approximately, $\widehat{A}\otimes\widehat{B}\simeq\widehat{A}\widehat{B}+(i/2)\sum_\mu(\widehat{A}\overleftarrow{\partial}_{X_\mu}\overrightarrow{\partial}_{p_\mu}\widehat{B}-\widehat{A}\overleftarrow{\partial}_{p_\mu}\overrightarrow{\partial}_{X_\mu}\widehat{B})$. Using the relation

$$\begin{aligned}&\partial_{X^\mu}G_0(\epsilon,\mathbf{p},X)\\&\quad=-G_0(\epsilon,\mathbf{p},X)\big[\partial_{X^\mu}G_0^{-1}(\epsilon,\pi,X)\big]G_0(\epsilon,\mathbf{p},X),\end{aligned} \tag{A3}$$

the solution is found as

$$G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]=G_0(\epsilon,\mathbf{p},X)+\Delta G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)], \tag{A4}$$

which indicates that $G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]$ deviates from the equilibrium Green's function $G_0(\epsilon,\mathbf{p},X)$ by an amount

$$\begin{aligned}&\Delta G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\\&\quad=-(i/2)\big\{G_0^{-1}(\epsilon,\mathbf{p},X),G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\big\}_{\text{PB}},\end{aligned} \tag{A5}$$

where the Poisson bracket is defined as $\{Q_1,Q_2\}_{\text{PB}}=\sum_\mu\partial_{X^\mu}Q_1\partial_{p_\mu}Q_2-\partial_{p_\mu}Q_1\partial_{X^\mu}Q_2$. Because $\mathcal{A}_i^{\text{ext}}=-B^{(a)}X_j\tau^a$, we have

$$\begin{aligned}&\partial_{X^\mu}G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\\&\quad=G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\partial_{X^\mu}HG[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]\\&\quad=-G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]|e|B^{(a)}j_x^a\delta_{\mu y}G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)],\end{aligned} \tag{A6}$$

where j_x^a is a spin current operator defined by $(1/2)\{\tau^a,v_x[\mathcal{A}^{\text{ext}}(X)]\}$ and $v_x(\mathcal{A}^{\text{ext}})=(\pi_x-|e|\mathcal{A}_x^{\text{ext}})/m_e$ is the velocity including the effect of the external SU(2) field. In addition, we have $\partial_{p_\mu}G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]=-v_\mu(\mathcal{A}^{\text{ext}})$. $\Delta G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]$ can then be written in the form

$$\Delta G[\epsilon,\mathbf{p},\mathcal{A}^{\text{ext}}(X)]=|e|B^{(a)}G_1^{(a)}(\epsilon,\mathbf{p},X), \tag{A7}$$

where

$$\begin{aligned}&G_1^{(a)}(\epsilon,\mathbf{p},X)\\&\quad=-\frac{i}{2}G_0(\epsilon,\mathbf{p},X)\big[j_x^aG_0(\epsilon,\mathbf{p},X),v_yG_0(\epsilon,\mathbf{p},X)\big].\end{aligned} \tag{A8}$$

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