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Microscopic calculation of thermally induced spin-transfer torques

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Spin-transfer torques, both reactive and dissipative, induced by temperature gradients in conducting ferromagnets are calculated microscopically for smooth magnetization textures. Temperature gradients are treated *à la* Luttinger by introducing a fictitious gravitational field that couples to the energy density. The thermal torque coefficients obtained by the Kubo formula contain unphysical terms that diverge towards zero temperature. Such terms are caused by equilibrium components and should be subtracted before applying the Einstein-Luttinger relation. Only by following this procedure a familiar Mott-like formula is obtained for the dissipative spin-transfer torque. The result indicates that a fictitious field that couples to the entropy rather than energy would solve the issue from the outset.

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I. INTRODUCTION

A spin current is a flow of angular momentum, which can be transferred to other degrees of freedom and thereby exerts a torque on them. In ferromagnetic conductors, an ordinary (Ohmic) electric current, induced by an applied electric field, is accompanied by a spin current, and this can be utilized to control magnetization dynamics [1,2].

Spin currents can also be induced by a temperature gradient in ferromagnets, which may be used to control magnetization without the need to apply an electric field [3–5]. For permalloy, a temperature gradient of 2 K/nm has been estimated to induce a torque equivalent to that of the electric current density of 10^8 A/cm² necessary to move magnetic domain walls in permalloy [6,7]. Such a large temperature gradient can be realized in magnetic nanostructures by focused pulsed laser heating. Evidence for thermal torques affecting the magnetization dynamics has been obtained in spin valves [8] and magnetic tunnel junctions [9]. Domain wall motion under a temperature gradient has been observed in magnetic insulators in which spin currents are carried by magnons [10].

In this paper, we calculate spin torques induced by a temperature gradient in a conducting ferromagnet focusing on mobile conduction electrons (not magnons). We consider a general but smooth magnetization texture as described by the Landau-Lifshitz-Gilbert (LLG) equation. We follow Luttinger [11] by treating thermal perturbations in terms of a (fictitious) gravitational field that couples to the energy (or heat) density of the system and exploit the Einstein relation [12]. Thermally induced torques can then be computed by linear response theory in close analogy with the well-studied electrically induced torques, as is shown in the first half of this paper. However, a straightforward calculation leads to a physically wrong contribution which diverges towards zero temperature. The resolution of this difficulty is the main subject of this paper.

A similar problem exists in thermoelectric transport in strong magnetic fields [13–15]. In this case, the problem was resolved by separating the transport current from the

magnetization current and applying the Einstein relation to the former. In calculating spin torques, we need to generalize this idea and propose to separate the nonequilibrium and equilibrium components, applying the Einstein relation to the former. The same feature exists in the ‘spin-orbit torques’ due to Rashba-type spin-orbit coupling [16,17].

This paper is organized as follows. After a brief description of spin torques in Sec. II, we define a model in Sec. III. Based on the formulation outlined in Sec. IV, we evaluate explicitly the thermal torque in Sec. V and observe that the result contains an unphysical contribution. The resolution of this problem is described in Sec. VI, and the correct result is given in Sec. VII. A consequence of our results is illustrated in Sec. VIII for thermal torques in the absence of applied electric fields. In Sec. IX, we discuss our procedure in a more general context. The results are summarized in Sec. X. Technical details of the calculations are deferred to the Appendices. Mathematical notations are summarized in the Supplemental Material [18].

II. GENERAL DESCRIPTION OF SPIN TORQUES

The LLG-Slonczewski (LLGS) equation, in which the effects of spin currents are included, reads

$$\dot{\mathbf{n}} = \gamma_0 \mathbf{H}_{\text{eff}} \times \mathbf{n} + \alpha_0 \dot{\mathbf{n}} \times \mathbf{n} + \tilde{\mathbf{t}}, \quad (1)$$

where $\mathbf{n} = \mathbf{n}(x)$ is a unit-vector field representing the spin direction of magnetization, $x = (\mathbf{r}, t)$ denotes the space-time coordinate, and the dot represents the time derivative. The first two terms on the right-hand side are the precessional torque (\mathbf{H}_{eff} : effective field, γ_0 : gyromagnetic constant) and the Gilbert damping (α_0 : damping constant). Current-induced spin torques are collected in the third term $\tilde{\mathbf{t}}$.

For a smooth magnetization texture \mathbf{n} , the torques due to an electrically-induced spin current density $\mathbf{j}_s \equiv \mathbf{j}_\uparrow - \mathbf{j}_\downarrow = \sigma_s \mathbf{E}$, where σ_s is the ‘spin conductivity’ [see Eq. (63) below] and \mathbf{E} is the electric field, have the form,

$$\tilde{\mathbf{t}}_{\text{el}} = -(\mathbf{v}_s \cdot \nabla) \mathbf{n} - \beta \mathbf{n} \times (\mathbf{v}_s \cdot \nabla) \mathbf{n}. \quad (2)$$

The first term is the celebrated spin-transfer torque [19] with the (renormalized) “spin-transfer velocity”

$$\mathbf{v}_s = -\frac{\hbar}{2e s_{\text{tot}}} \mathbf{j}_s, \quad (3)$$

where s_{tot} is the angular-momentum density of total magnetization (including conduction electrons, see Ref. [20]). The electron charge is denoted as $-e$ so that $e > 0$. The second term is caused by spin-relaxation processes in the conduction electron system, which is often referred to as ‘ β term’ [21,22]. Although the dimensionless constant β is expected to be small (~ 0.01), it importantly affects the dynamics of a domain wall [21–24]. These two terms can be viewed as reactive and dissipative parts, respectively, of the spin-transfer torque.

Torques induced by a temperature gradient ∇T take the same form

$$\tilde{\mathbf{t}}_{\text{th}} = -(\mathbf{v}_T \cdot \nabla) \mathbf{n} - \beta_T \mathbf{n} \times (\mathbf{v}_T \cdot \nabla) \mathbf{n}, \quad (4)$$

with the coefficient vector \mathbf{v}_T being proportional to ∇T . Any spin-relaxation process is expected to produce the second term, with β_T being a dimensionless parameter. By scattering theory Hals *et al.* [25] demonstrated that $\beta_T \neq \beta$. A formulation by linear response theory that would fit the diagrammatic perturbation theory is still lacking, however. In this paper, we develop a microscopic linear response theory and calculate the coefficients \mathbf{v}_T and β_T for a simple model. The results presented in Sec. VII agree with published ones.

III. MODEL

The microscopic origin of spin torques is the s - d exchange interaction $H_{sd} = \int d^3x h_{sd}(x)$,

$$h_{sd}(x) = -M \mathbf{n}(x) \cdot \hat{\boldsymbol{\sigma}}(x), \quad (5)$$

between the spin $\hat{\boldsymbol{\sigma}}(x) \equiv c^\dagger \boldsymbol{\sigma} c$ of conduction electrons and magnetization unit vector $\mathbf{n}(x)$, where $c = c(x) = \begin{pmatrix} c_\uparrow(x) \\ c_\downarrow(x) \end{pmatrix}$ is a spinor of electron annihilation operators, $\boldsymbol{\sigma}$ is a vector of Pauli spin matrices, and M is a coupling constant. For example, if an electron moves through a magnetization texture $\mathbf{n}(x)$, its spin experiences a time-dependent ‘field’ $M\mathbf{n}$. The electron, in turn, exerts a reaction (spin) torque [26–28]

$$\mathbf{t}_{sd} = M \mathbf{n}(x) \times (\hat{\boldsymbol{\sigma}}(x)) \quad (6)$$

on the magnetization since the effective field seen by \mathbf{n} is given by $\delta H_{sd} / \delta \mathbf{n} = -M (\hat{\boldsymbol{\sigma}}(x))$, where the brackets $\langle \cdots \rangle$ indicate a quantum statistical average. The calculation of the torque is thus reduced to calculating the electron spin density in the current-carrying nonequilibrium state.

To be specific, let us consider a free electron system subject to impurity scattering. The Hamiltonian is given by $H = \int d^3x h(x)$,

$$h(x) = \frac{\hbar^2}{2m} (\nabla c^\dagger)(\nabla c) + c^\dagger V_{\text{imp}}(\mathbf{r}) c + h_{sd}, \quad (7)$$

where m is the electron mass and

$$V_{\text{imp}}(\mathbf{r}) = u_i \sum_j \delta(\mathbf{r} - \mathbf{R}_j) + u_s \sum_\ell (S_\ell \cdot \boldsymbol{\sigma}) \delta(\mathbf{r} - \mathbf{R}'_\ell) \quad (8)$$

is the impurity potential. In Eq. (8) the summation is carried out over normal and magnetic impurities with scattering strengths

u_i and u_s , respectively. We assume a uniform and isotropic distribution of impurity positions (\mathbf{R}_j and \mathbf{R}'_ℓ) and impurity-spin direction (S_ℓ), respectively, and take a quenched average as

$$\overline{V_{\text{imp}}(\mathbf{r}) V_{\text{imp}}(\mathbf{r}')} = (n_i u_i^2 + \frac{1}{3} n_s u_s^2 S_{\text{imp}}^2 \boldsymbol{\sigma} \otimes \boldsymbol{\sigma}) \delta(\mathbf{r} - \mathbf{r}'), \quad (9)$$

where n_i (n_s) is the concentration of normal (magnetic) impurities and S_{imp} is the magnitude of the impurity spin. Equation (9) is a tensor in spinor space.

We consider a small transverse deviation field \mathbf{u} on top of a static and uniform magnetization pointing in the z direction:

$$\mathbf{n}(\mathbf{r}) = \hat{z} + \mathbf{u}(\mathbf{r}) = \hat{z} + \mathbf{u}_q e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (10)$$

where $\mathbf{u} \perp \hat{z}$, $|\mathbf{u}| \ll 1$. We may then focus on a single Fourier component with wave vector \mathbf{q} and amplitude \mathbf{u}_q and calculate the induced spin density to first order in \mathbf{u}_q and \mathbf{q} . This is sufficient to determine the coefficients \mathbf{v}_s , β , \mathbf{v}_T , and β_T in Eqs. (2) and (4) [29–31]. The impurity potential V_{imp} is treated in the Born approximation for the self-energy combined with ladder-type vertex corrections. The renormalized Green function (for $\mathbf{u} = \mathbf{0}$) is given by

$$G_{k\sigma}(z) = [z + \mu - \hbar^2 k^2 / 2m + M\sigma + i\gamma_\sigma \text{sgn}(\text{Im}z)]^{-1}, \quad (11)$$

with complex frequency z , chemical potential μ , wave vector \mathbf{k} , spin projection $\sigma = \pm 1$, and broadening (damping)

$$\gamma_\sigma = \frac{\hbar}{2\tau_\sigma} = \pi n_i u_i^2 v_\sigma + \frac{\pi}{3} n_s u_s^2 S_{\text{imp}}^2 (v_\sigma + 2v_{\bar{\sigma}}), \quad (12)$$

where τ_σ is the spin-dependent scattering lifetime, and v_σ is the density of states of spin- σ electrons at the Fermi energy. At low enough temperatures, μ equals the Fermi energy ε_F . We also define a (kinetic) Fermi energy for each spin, $\sigma = \pm 1$, by $\varepsilon_{F\sigma} = \varepsilon_F + M\sigma$. As in Ref. [30], we assume a good ferromagnetic metal characterized by the small $\gamma_\sigma / (\mu + \sigma M)$ and γ_σ / M (collectively denoted by γ) and retain only terms to the lowest nontrivial order in γ , viz. $\mathcal{O}(\gamma^{-1})$ for the spin-transfer torque and $\mathcal{O}(\gamma^0)$ for the dissipative correction (β term).

IV. FORMULATION

Thermal torques induced by a temperature gradient ∇T can be calculated analogous to ordinary current-induced torques due to an electric field \mathbf{E} as outlined in the following. Let us consider the general case in which conduction electrons in a ferromagnet are subject to an applied electric field (\mathbf{E}), chemical-potential gradient ($\nabla \mu$), temperature gradient (∇T), and applied gravitational field ($-\nabla \psi$). The gravitational potential ψ was introduced by Luttinger [11] as a field which couples to the local energy density $h(x)$, thus driving an energy-current density \mathbf{j}_E . For convenience, we prefer to work with the field that couples to $h(x) - \mu n(x)$, where $n(x)$ is the (local) number density, that drives the heat-current density, $\mathbf{j}_Q = \mathbf{j}_E - \mu \mathbf{j}$. Then the *nonequilibrium part* of the transverse spin polarization, which is responsible for (nonequilibrium) spin torques, can be written as

$$\langle \hat{\sigma}_\perp^a(\mathbf{q}) \rangle_{\text{ne}} = \chi_i^\alpha \left(E_i + \frac{1}{e} \nabla_i \mu \right) + \chi_{Q,i}^\alpha \left(-\frac{\nabla_i T}{T} - \nabla_i \psi \right), \quad (13)$$

where χ_i^α and $\chi_{Q,i}^\alpha$ are linear-response coefficients with α and i being spin and spatial indices, respectively. [In Eq. (13), sum over $i = x, y, z$ is assumed.] We use the same coefficient for E_i and $\nabla_i \mu/e$, as well as for $\nabla_i T/T$ and $\nabla_i \psi$. This can be justified by an argument *à la* Einstein [11,12]: under static, finite wavelength, and longitudinal perturbation, the system is in an equilibrium state, implying that *nonequilibrium* torques should not arise.

Thus we consider the Hamiltonian

$$H_{\phi,\psi} = \int d^3x \{h(x) - (\mu + e\phi(x))n(x)\} \{1 + \psi(x)\}, \quad (14)$$

where ϕ is the electromagnetic scalar potential, ψ is the gravitational potential, and $h(x)$ is given by Eq. (7). The linear-response coefficients, χ_i^α and $\chi_{Q,i}^\alpha$, to the mechanical perturbations, $E_i = -\nabla_i \phi$ and $-\nabla_i \psi$, are given by the standard Kubo formula [11,32]

$$\chi_i^\alpha = \lim_{\omega \rightarrow 0} \frac{K_i^\alpha(\mathbf{q}, \omega + i0) - K_i^\alpha(\mathbf{q}, 0)}{i\omega}, \quad (15)$$

$$\chi_{Q,i}^\alpha = \lim_{\omega \rightarrow 0} \frac{K_{Q,i}^\alpha(\mathbf{q}, \omega + i0) - K_{Q,i}^\alpha(\mathbf{q}, 0)}{i\omega}, \quad (16)$$

where the response functions for real frequencies ω are obtained from those defined in the imaginary time $\tau = it$ or the corresponding Matsubara frequencies $\omega_\lambda = 2\pi\lambda k_B T_0$ (λ : integer) by analytic continuation $i\omega_\lambda \rightarrow \hbar\omega + i0$ in the complex plane [33],

$$K_i^\alpha(\mathbf{q}, i\omega_\lambda) = -e \int_0^{\beta_0} d\tau e^{i\omega_\lambda \tau} \langle T_\tau \hat{\sigma}_\perp^\alpha(\mathbf{q}, \tau) J_i \rangle, \quad (17)$$

$$K_{Q,i}^\alpha(\mathbf{q}, i\omega_\lambda) = \int_0^{\beta_0} d\tau e^{i\omega_\lambda \tau} \langle T_\tau \hat{\sigma}_\perp^\alpha(\mathbf{q}, \tau) J_{Q,i} \rangle, \quad (18)$$

cf. Appendix A. The linear-response coefficients are computed for a uniform background temperature T_0 and $\beta_0 = (k_B T_0)^{-1}$ that is perturbed by a small ∇T . For simplicity, we use the notation T_0 only here but use T instead of T_0 in the remaining sections including the Appendices. On the other hand, we keep the notation β_0 throughout the paper in order to distinguish it from the β term in the LLGS equation. In Eqs. (17) and (18), \mathbf{J} is the total charge current (in units of $-e$) and \mathbf{J}_Q is the total heat current; they are given by the volume integral of the corresponding current densities (see Appendix B);

$$\mathbf{j}(\tilde{x}) = \frac{\hbar}{2mi} \lim_{\tilde{x}' \rightarrow \tilde{x}} (\nabla' - \nabla) c^\dagger(\tilde{x}) c(\tilde{x}'), \quad (19)$$

$$\begin{aligned} \mathbf{j}_Q(\tilde{x}) &= \frac{i\hbar}{4m} \lim_{\tilde{x}' \rightarrow \tilde{x}} (\nabla' - \nabla) (\partial_{\tau'} - \partial_\tau) c^\dagger(\tilde{x}) c(\tilde{x}') \\ &\quad - \frac{i\hbar^2}{4m} \nabla \partial_\tau [c^\dagger(\tilde{x}) c(\tilde{x})], \end{aligned} \quad (20)$$

where $\tilde{x} = (\mathbf{r}, \tau)$ and $\tilde{x}' = (\mathbf{r}', \tau')$. Note that the expression (20) is written in the imaginary-time representation [33]. Note also that the last term in Eq. (20) drops out for the total heat current \mathbf{J}_Q .

The response functions, K_i^α and $K_{Q,i}^\alpha$, are nonzero in the presence of magnetization textures, Eq. (10), and we extract u^β and q_j from K_i^α and $K_{Q,i}^\alpha$. In the next section, we derive

the forms [34]

$$K_i^\alpha(\mathbf{q}, i\omega_\lambda) = -e M^{-1} (\tilde{b} \delta^{\alpha\beta} + \tilde{a} \varepsilon^{\alpha\beta}) \omega q_i u_q^\beta, \quad (21)$$

$$K_{Q,i}^\alpha(\mathbf{q}, i\omega_\lambda) = M^{-1} (\tilde{b}_T \delta^{\alpha\beta} + \tilde{a}_T \varepsilon^{\alpha\beta}) \omega q_i u_q^\beta, \quad (22)$$

where $\delta^{\alpha\beta}$ is the Kronecker's delta and $\varepsilon^{\alpha\beta}$ is the antisymmetric tensor (with $\varepsilon^{xy} = 1$) in two dimensions, while $\tilde{a}, \tilde{b}, \tilde{a}_T$, and \tilde{b}_T are yet unspecified coefficients. These expressions indeed lead to the torques given by Eqs. (2) and (4), with

$$\mathbf{v}_s = -\frac{\tilde{a}}{s_{\text{tot}}} (e\mathbf{E} + \nabla\mu), \quad \beta = \tilde{b}/\tilde{a}, \quad (23)$$

$$\mathbf{v}_T = -\frac{\tilde{a}_T}{s_{\text{tot}}} \left(\frac{\nabla T}{T} + \nabla\psi \right), \quad \beta_T = \tilde{b}_T/\tilde{a}_T. \quad (24)$$

The calculation of the coefficients $\tilde{a}, \tilde{b}, \tilde{a}_T$, and \tilde{b}_T in Eqs. (21) and (22) is the subject of the next two sections.

Before proceeding, we show that the two cases (electrical and thermal) can actually be calculated simultaneously. In Eqs. (17) and (18), the (imaginary-)time evolution and thermal average are determined by H . Since this is a one-body Hamiltonian, $\dot{c} = [c, H]/i\hbar$ is also a one-body operator. We therefore can use Wick's theorem to obtain

$$K_i^\alpha(\mathbf{q}, i\omega_\lambda) = eT_0 \sum_n \sum_{\mathbf{k}, \mathbf{k}'} v_{\mathbf{k}, i} \text{tr}[\sigma^\alpha \mathcal{G}_{\mathbf{k}'+\mathbf{q}, \mathbf{k}}^+ \mathcal{G}_{\mathbf{k}, \mathbf{k}'}], \quad (25)$$

and

$$\begin{aligned} K_{Q,i}^\alpha(\mathbf{q}, i\omega_\lambda) &= -T_0 \sum_n (i\varepsilon_n + i\omega_\lambda/2) \sum_{\mathbf{k}, \mathbf{k}'} v_{\mathbf{k}, i} \text{tr}[\sigma^\alpha \mathcal{G}_{\mathbf{k}'+\mathbf{q}, \mathbf{k}}^+ \mathcal{G}_{\mathbf{k}, \mathbf{k}'}] \\ &\quad + \frac{1}{2} T_0 \sum_n \sum_{\mathbf{k}} \text{tr}[\sigma^\alpha (\mathcal{G}^+ \hat{v}_i + \hat{v}_i \mathcal{G})_{\mathbf{k}+\mathbf{q}, \mathbf{k}}]. \end{aligned} \quad (26)$$

Here, $\varepsilon_n = (2n+1)\pi k_B T_0$, $\mathcal{G}_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} \equiv \mathcal{G}_{\mathbf{k}\sigma, \mathbf{k}'\sigma'}(i\varepsilon_n) \equiv -\int_0^{\beta_0} d\tau e^{i\varepsilon_n \tau} \langle T_\tau c_{\mathbf{k}\sigma}^\dagger(\tau) c_{\mathbf{k}'\sigma'} \rangle$ is the exact Green function of H (before the impurity average is taken), \mathcal{G}^+ is the one with frequency $i\varepsilon_n + i\omega_\lambda$, $\mathbf{v}_{\mathbf{k}} = \hbar\mathbf{k}/m$ is the electron velocity, and “tr” means trace in spin space. (Since H includes $\mathbf{u}(\mathbf{r})$ and V_{imp} , \mathcal{G} has off-diagonal components in both spin and wave vector.) In deriving Eq. (26), we used the relation

$$\langle T_\tau c(\tau) \dot{c}^\dagger \rangle = -\langle T_\tau \dot{c}(\tau) c^\dagger \rangle = \frac{d}{d\tau} \mathcal{G}(\tau) + \delta(\tau). \quad (27)$$

The last term of Eq. (26) is invariant with respect to the translation $\varepsilon_n + \omega_\lambda \rightarrow \varepsilon_n$ and after summing over ε_n does not depend on ω_λ . Such terms not depending on ω (hence ω_λ) cancel in Eq. (16), and can be dropped beforehand. Thus we are left only with the first term of Eq. (26), showing that the heat-current vertex is simply governed by the factor $(i\varepsilon_n + i\omega_\lambda/2) \mathbf{v}_{\mathbf{k}}$. We confirmed this statement starting from an explicit expression for the heat current (without using the time derivative) in Appendix C. (For many-body Hamiltonians, see Ref. [35].)

V. EXPLICIT CALCULATION

We calculate the torque coefficients, $K_{ij}^{\alpha\beta}$ and $K_{Q,ij}^{\alpha\beta}$ [Eqs. (21) and (22)] by first extracting q_j and u_q^β from K_i^α

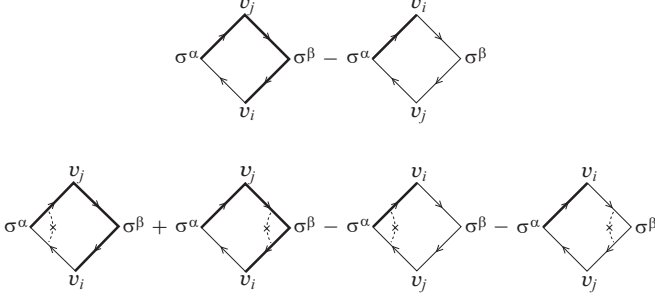


FIG. 1. Diagrammatic expressions for the coefficient $K_{ij}^{\alpha\beta}$ and $K_{Q,ij}^{\alpha\beta}$ that govern the transverse spin polarization, $\langle \hat{\sigma}_\perp^\alpha(\mathbf{q}) \rangle_{\text{ne}}$, which is linear in E_i (or $-\nabla_i T/T$), q_j and u^β , in the presence of currents, induced by either electric field E_i or temperature gradient $\nabla_i T$, and the magnetization texture $(q_j u^\beta)$. The velocity vertices v_i and v_j are associated with E_i and q_j , respectively. In the thermally induced torque ($K_{Q,ij}^{\alpha\beta}$), the vertex v_i is multiplied by $i(\varepsilon_n + \omega_\lambda/2)$. The thick (thin) solid lines represent electrons with Matsubara frequency $i\varepsilon_n + i\omega_\lambda$ ($i\varepsilon_n$). The dotted line with a cross represents scattering by nonmagnetic or magnetic impurities.

and $K_{Q,i}^\alpha$ as

$$K_i^\alpha(\mathbf{q}, i\omega_\lambda) = -eMK_{ij}^{\alpha\beta}(i\omega_\lambda)q_j u_q^\beta, \quad (28)$$

$$K_{Q,i}^\alpha(\mathbf{q}, i\omega_\lambda) = MK_{Q,ij}^{\alpha\beta}(i\omega_\lambda)q_j u_q^\beta, \quad (29)$$

where summing over $j = x, y, z$ and $\beta = x, y$ is implied. Up to the second-leading order in γ , they are expressed diagrammatically in Fig. 1. These “four-point diagrams” are obtained from the “two-point bubble diagrams” that express the correlation functions of spin and current, Eqs. (17) and (18) or Eqs. (25) and (26), by extracting u_q^β and q_j . They read

$$K_{ij}^{\alpha\beta}(i\omega_\lambda) = T \sum_n \varphi_{ij}^{\alpha\beta}(i\varepsilon_n + i\omega_\lambda, i\varepsilon_n), \quad (30)$$

$$K_{Q,ij}^{\alpha\beta}(i\omega_\lambda) = T \sum_n (i\varepsilon_n + i\omega_\lambda/2) \varphi_{ij}^{\alpha\beta}(i\varepsilon_n + i\omega_\lambda, i\varepsilon_n), \quad (31)$$

where [36]

$$\begin{aligned} \varphi_{ij}^{\alpha\beta}(i\varepsilon_n + i\omega_\lambda, i\varepsilon_n) &= \sum_k v_i v_j \{ \text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta G^+ G] - \text{tr}[\sigma^\alpha G^+ G \sigma^\beta G G] \} \\ &+ \tilde{\Gamma}_0 \sum_{k,k'} v_i v_j \{ \text{tr}[(G' \sigma^\alpha G^{+'}) G^+ G^+ \sigma^\beta G^+ G] \\ &- \text{tr}[(G' \sigma^\alpha G^{+'}) G^+ G \sigma^\beta G G] \\ &+ \text{tr}[\sigma^\alpha G^+ G^+ (G^{+'} \sigma^\beta G^{+'}) G^+ G] \\ &- \text{tr}[\sigma^\alpha G^+ G (G^{+'} \sigma^\beta G^{+'}) G G] \}. \end{aligned} \quad (32)$$

Here, the following notation has been used: $G^+ = G_k(i\varepsilon_n + i\omega_\lambda)$, $G = G_k(i\varepsilon_n)$, $G^{+'} = G_{k'}(i\varepsilon_n + i\omega_\lambda)$, $G' = G_{k'}(i\varepsilon_n)$, $v_i = \hbar k_i/m$, and $\tilde{\Gamma}_0 = n_i u_i^2 - n_s u_s^2 S_{\text{imp}}^2/3$. The electrically-induced torques, Eqs. (30) and (32), have been studied in Ref. [30]. New in this paper is the introduction and treatment of Eq. (31). As stated in the previous section, we will not distinguish T_0 and T as in Eqs. (30) and (31).

After the analytic continuation, $i\omega_\lambda \rightarrow \hbar\omega + i0$, we expand $K_{ij}^{\alpha\beta}$ and $K_{Q,ij}^{\alpha\beta}$ with respect to ω as

$$\begin{aligned} K(\omega + i0) - K(0) &= \frac{i\hbar\omega}{2\pi} \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \{ \text{Re}[\varphi^{(1)}(\varepsilon, \varepsilon)] - \varphi^{(2)}(\varepsilon, \varepsilon) \} \\ &- \frac{\hbar\omega}{2\pi} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) (\partial_\varepsilon - \partial_{\varepsilon'}) \text{Im}[\varphi^{(1)}(\varepsilon, \varepsilon')] |_{\varepsilon'=\varepsilon} \\ &+ \mathcal{O}(\omega^2), \end{aligned} \quad (33)$$

where $f(\varepsilon)$ is the Fermi-Dirac distribution function, and $\partial_\varepsilon = \partial/\partial\varepsilon$, $\partial_{\varepsilon'} = \partial/\partial\varepsilon'$. In Eq. (33), $\varphi = \varphi_{ij}^{\alpha\beta}(\varepsilon, \varepsilon')$ for $K = K_{ij}^{\alpha\beta}$, and $\varphi = [(\varepsilon + \varepsilon')/2] \varphi_{ij}^{\alpha\beta}(\varepsilon, \varepsilon')$ for $K = K_{Q,ij}^{\alpha\beta}$; the superscripts on $\varphi^{(i)}$ specify the analytic continuations, $\varphi^{(1)}(\varepsilon, \varepsilon') = \varphi(\varepsilon + i0, \varepsilon' + i0)$, $\varphi^{(2)}(\varepsilon, \varepsilon') = \varphi(\varepsilon + i0, \varepsilon' - i0)$, and $\varphi^{(3)}(\varepsilon, \varepsilon') = \varphi(\varepsilon - i0, \varepsilon' - i0)$.

After some manipulations, the coefficients can be cast into the form,

$$\tilde{a} = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) A(\varepsilon), \quad (34)$$

$$\tilde{b} = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) B(\varepsilon) - \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \partial_\varepsilon C(\varepsilon), \quad (35)$$

for electrically-induced torques, and

$$\tilde{a}_T = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \varepsilon A(\varepsilon), \quad (36)$$

$$\tilde{b}_T = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \varepsilon B(\varepsilon) - \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \varepsilon \partial_\varepsilon C(\varepsilon), \quad (37)$$

for thermally induced torques. The terms containing $-\partial f/\partial\varepsilon$ are called “Fermi-surface terms,” and those with $f(\varepsilon)$ as “Fermi-sea terms” [37]. This separation is not unique in a strict sense, but convenient in practice (at least in the present context) if defined symmetrically ($\varepsilon \pm \omega/2$) as in Eq. (33). The functions A, B , and C are given by

$$A(\varepsilon) = \frac{M^2}{\pi} \sum_\sigma \sigma \text{Re} L_\sigma(\varepsilon), \quad (38)$$

$$B(\varepsilon) = \frac{M^2}{\pi} \sum_\sigma \text{Im} L_\sigma(\varepsilon), \quad (39)$$

$$C(\varepsilon) = \frac{M^2}{\pi} \text{Im} \sum_k v_i v_j (G_{k\uparrow}^R G_{k\downarrow}^R)^2, \quad (40)$$

with $G_{k\sigma}^R = G_{k\sigma}^R(\varepsilon) \equiv G_{k\sigma}(\varepsilon + i0)$ and $G_{k\sigma}^A = G_{k\sigma}^A(\varepsilon) \equiv G_{k\sigma}(\varepsilon - i0)$ being retarded (R) and advanced (A) Green functions, respectively, and

$$\begin{aligned} L_\sigma(\varepsilon) &= \sum_k v_i v_j G_{k\sigma}^R (G_{k\sigma}^R)^2 G_{k\sigma}^A \\ &\times \left\{ 1 + \tilde{\Gamma}_0 \sum_{k'} G_{k'\sigma}^R (G_{k'\sigma}^R + G_{k'\sigma}^A) \right\}. \end{aligned} \quad (41)$$

In Eqs. (40) and (41), all Green functions share the frequency argument ε . Equations (34)–(37) can be rewritten as

$$\tilde{a} = A_0, \quad \tilde{b} = B_0 - C_0, \quad (42)$$

$$\tilde{a}_T = A_1, \quad \tilde{b}_T = B_1 - C_1 + c, \quad (43)$$

where

$$A_n = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \varepsilon^n A(\varepsilon), \quad (44)$$

and similarly for B_n and C_n , with

$$c = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) C(\varepsilon). \quad (45)$$

Using Eq. (6), the torques are obtained as

$$\mathbf{t}_{\text{el}} = [A_0 \partial_i \mathbf{n} + (B_0 - C_0)(\mathbf{n} \times \partial_i \mathbf{n})] e E_i, \quad (46)$$

$$\mathbf{t}^{(\psi)} = [A_1 \partial_i \mathbf{n} + (B_1 - C_1 + c)(\mathbf{n} \times \partial_i \mathbf{n})] \partial_i \psi. \quad (47)$$

Note that as $T \rightarrow 0$, A_1, B_1 , and C_1 vanish, but c remains finite.

The c term in Eq. (47),

$$\Delta \mathbf{t}^{(\psi)} \equiv c (\mathbf{n} \times \partial_i \mathbf{n}) \partial_i \psi, \quad (48)$$

is problematic because the Einstein-Luttinger relation (13) leads to a thermally induced torque

$$\Delta \mathbf{t}_{\text{th}} = c (\mathbf{n} \times \partial_i \mathbf{n}) \partial_i T / T, \quad (49)$$

that diverges as $T \rightarrow 0$ (since c is finite as $T \rightarrow 0$). This contradicts the thermodynamic law (Nernst theorem) that thermally induced effects should vanish with temperature. Also, the predicted finite β_T even in the absence of spin relaxation violates the spin conservation. Therefore, the contribution (48) must be carefully reconsidered.

VI. SUBTRACTION OF EQUILIBRIUM COMPONENTS

To settle the problem encountered in the last section, we note that the combination $-\nabla \psi - \nabla T / T$ in Eq. (13) should be applied only to *nonequilibrium* components that must be identified beforehand. Even at equilibrium, i.e., without external fields $E_i = 0$ and $\psi = 0$, a finite spin density $\langle \hat{\sigma} \rangle_{\text{eq}} = (c/M) \nabla^2 \mathbf{n}$ exists, which corresponds to the exchange-stiffness torque

$$\mathbf{t}_{\text{eq}} = c (\mathbf{n} \times \nabla^2 \mathbf{n}). \quad (50)$$

The coefficient c is the same as in Eq. (45), and represents the contribution of the conduction electrons to the exchange-stiffness constant; see Appendix D for the calculation.

This equilibrium torque is affected by ψ in two ways. First, the torque formula, Eq. (6), acquires an additional factor

$$\mathbf{t}_{sd}^{(\psi)} = M \mathbf{n}(x) \times \langle \hat{\sigma}(x) \rangle (1 + \psi) \quad (51)$$

because the s - d coupling h_{sd} [Eq. (5)] is multiplied by $(1 + \psi)$ [see Eq. (14)] and so are the effective field, $\sim \delta H_{sd} / \delta \mathbf{n}$, and the s - d exchange torque, $\sim (\delta H_{sd} / \delta \mathbf{n}) \times \mathbf{n}$ [cf. Eq. (6)] [28]. Secondly, it seems that the spin density $\langle \hat{\sigma} \rangle$ may be modified by ψ (on top of a term proportional to $\partial_i \psi$). It turns out, however, that this is not the case; see Eq. (E8) for an explicit expression

and Appendix A for a formal derivation. From a general point of view, this reflects the adiabatic nature of the Kubo formula and the conserved nature of the perturbed quantity (energy), as shown in Appendix F. Therefore, the equilibrium spin density $\langle \hat{\sigma} \rangle_{\text{eq}}$ in the previous paragraph (for $\psi = 0$) is not affected by a uniform ψ (namely, in the zeroth-order gradient of ψ). Therefore, using Eq. (50) in Eq. (51), we obtain

$$\mathbf{t}_{\text{eq}}^{(\psi)} = c (\mathbf{n} \times \nabla^2 \mathbf{n}) (1 + \psi). \quad (52)$$

(The suffix eq' means that this does not exhaust the equilibrium torque in the presence of ψ .) The total torque is the sum of Eq. (52) and Eq. (47); the former contains all torques proportional to ψ , and the latter those proportional to $\partial_i \psi$. Focussing on terms containing c

$$\mathbf{t}_{\text{eq}}^{(\psi)} + \Delta \mathbf{t}^{(\psi)} = -\partial_i \mathbf{j}_{s,i}^{(\psi)}, \quad (53)$$

where

$$\mathbf{j}_{s,i}^{(\psi)} = -c (\mathbf{n} \times \partial_i \mathbf{n}) (1 + \psi) \quad (54)$$

is the spin-current density carried by the \mathbf{n} field in the presence of ψ . The right-hand side of Eq. (53) represents the (generalized) exchange-stiffness torque in the presence of ψ , which we identify as the total equilibrium torque. By subtracting this equilibrium component, we identify the nonequilibrium component to be Eq. (47) without the offensive c term. The replacement, $\partial_i \psi \rightarrow \partial_i T / T$, should be enforced only in this nonequilibrium component such that

$$\mathbf{t}_{\text{th}} = [A_1 \partial_i \mathbf{n} + (B_1 - C_1)(\mathbf{n} \times \partial_i \mathbf{n})] \partial_i T / T, \quad (55)$$

behaves regularly (namely, vanishes) as $T \rightarrow 0$.

The above procedure, Eqs. (52)–(55), may be better understood by subjecting an *insulating* ferromagnet (without mobile s electrons) to ψ . Its Lagrangian is given by

$$L = \int d^3x \left\{ \hbar S \dot{\varphi} \cos \theta - \frac{J}{2} (\nabla \mathbf{n})^2 (1 + \psi) \right\}, \quad (56)$$

where (θ, φ) represents the direction of \mathbf{n} . Note that ψ couples only to the energy density $J(\nabla \mathbf{n})^2/2$ (anisotropy, damping, etc. are neglected for simplicity), and not to the kinetic term (first term). The variational principle leads to the equation of motion [28]

$$\hbar S \dot{\mathbf{n}} = J \partial_i [(\mathbf{n} \times \partial_i \mathbf{n}) (1 + \psi)], \quad (57)$$

whose right-hand side precisely corresponds to Eq. (53). This supports the identification of the equilibrium torque in the preceding paragraph. The subtraction procedure becomes necessary because the equilibrium component $J(\mathbf{n} \times \partial_i \mathbf{n})(\partial_i \psi)$ contained in Eq. (57) creeps into the Kubo-formula result.

This kind of difficulty has been noted for thermal transport in magnetic fields. To resolve it, the authors of Refs. [13–15] proposed to extract the transport current by subtracting the magnetization current, and then to apply the substitution $\partial_i \psi \rightarrow \partial_i T / T$ to the transport current. In this procedure, it is essential that the expressions for electric and heat currents are modified by ψ [as in Eq. (51)]. As we have seen in this section, precisely the same features exist in the calculation of (ordinary) spin torques.

VII. RESULT

We thus arrive at expressions for the nonequilibrium torque $\mathbf{t}_{\text{tot}} = \mathbf{t}_{\text{el}} + \mathbf{t}_{\text{th}}$,

$$\mathbf{t}_{\text{el}} = [A_0 \partial_i \mathbf{n} + (B_0 - C_0)(\mathbf{n} \times \partial_i \mathbf{n})] e E_i, \quad (58)$$

$$\mathbf{t}_{\text{th}} = [A_1 \partial_i \mathbf{n} + (B_1 - C_1)(\mathbf{n} \times \partial_i \mathbf{n})] \partial_i T / T, \quad (59)$$

where the coefficients are given by (44) with [30]

$$A(\varepsilon) = \frac{\hbar}{2e} \sigma_s(\varepsilon), \quad B(\varepsilon) - C(\varepsilon) = \frac{\hbar}{2e} \beta(\varepsilon) \sigma_s(\varepsilon), \quad (60)$$

and thus

$$\mathbf{t}_{\text{el}} = \frac{\hbar}{2} E_i \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \sigma_s(\varepsilon) [\partial_i \mathbf{n} + \beta(\varepsilon)(\mathbf{n} \times \partial_i \mathbf{n})], \quad (61)$$

$$\mathbf{t}_{\text{th}} = \frac{\hbar}{2e} \frac{\nabla_i T}{T} \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \varepsilon \sigma_s(\varepsilon) [\partial_i \mathbf{n} + \beta(\varepsilon)(\mathbf{n} \times \partial_i \mathbf{n})]. \quad (62)$$

Here, $\sigma_s(\varepsilon)$ is the “spin conductivity” and $\beta(\varepsilon)$ is dissipative correction,

$$\sigma_s = \frac{e^2}{m} (n_{\uparrow} \tau_{\uparrow} - n_{\downarrow} \tau_{\downarrow}), \quad (63)$$

$$\beta = \frac{2\pi}{3} n_s u_s^2 S_{\text{imp}}^2 \frac{v_{\uparrow} + v_{\downarrow}}{M}, \quad (64)$$

evaluated at energy $\mu + \varepsilon$ (or $\varepsilon_F + \varepsilon$ at low enough temperatures), with n_{σ} being the density of spin- σ electrons. The relation between \mathbf{t}_{th} and \mathbf{t}_{el} may be symbolically written as

$$\mathbf{t}_{\text{th}} = \int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \varepsilon \mathbf{t}_{\text{el}}(\varepsilon) \Big|_{e\mathbf{E} \rightarrow \nabla T / T}, \quad (65)$$

where the electric field \mathbf{E} in \mathbf{t}_{el} is replaced by the temperature gradient ∇T in \mathbf{t}_{th} . [$\mathbf{t}_{\text{el}}(\varepsilon)$ is defined by the total integrand of Eq. (61) including the prefactor.]

For sufficiently low temperatures, the Sommerfeld expansion

$$\int_{-\infty}^{\infty} d\varepsilon F(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) = F(0) + \frac{\pi^2}{6} F''(0) (k_B T)^2 + \dots \quad (66)$$

can be used to evaluate as $A_0 = A(0)$, $A_1 = (\pi^2/3) A'(0) (k_B T)^2$, etc. Here, the prime originally refers to the ε derivative, but it can be redefined to be the ε_F derivative, since ε and ε_F appear only as $\varepsilon + \varepsilon_F$ in the unperturbed Green function, Eq. (11), and the factor ε in Eqs. (36) and (37) does not appear in $F''(0)$. Hence

$$\tilde{a}_T = \frac{\pi^2}{3} \frac{d\tilde{a}}{d\varepsilon_F} (k_B T)^2, \quad \tilde{b}_T = \frac{\pi^2}{3} \frac{d\tilde{b}}{d\varepsilon_F} (k_B T)^2, \quad (67)$$

or

$$\mathbf{t}_{\text{th}} = \frac{\pi^2}{3} (k_B T)^2 \frac{d}{d\varepsilon_F} \mathbf{t}_{\text{el}} \Big|_{e\mathbf{E} \rightarrow \nabla T / T}. \quad (68)$$

These are ‘Mott formulas’ for the thermally induced spin-transfer torques in terms of the ε_F derivative of the electrical counterpart.

Explicitly, the total torque is written as

$$\tilde{\mathbf{t}}_{\text{tot}} = \frac{\hbar}{2eS_{\text{tot}}} \{ (\mathbf{j}_s^{\text{tot}} \cdot \nabla) \mathbf{n} + \beta \mathbf{n} \times (\mathbf{j}_s^{\text{tot}} \cdot \nabla) \mathbf{n} + \beta' \mathbf{n} \times (\mathbf{j}_{Q,s} \cdot \nabla) \mathbf{n} \}, \quad (69)$$

where

$$\mathbf{j}_s^{\text{tot}} = \sigma_s (\mathbf{E} + \mathcal{S}_s \nabla T), \quad \mathcal{S}_s = \frac{\pi^2 k_B^2}{3e} \frac{\sigma'_s}{\sigma_s} T, \quad (70)$$

with \mathcal{S}_s reflecting the spin dependence of the Seebeck coefficient, and

$$\mathbf{j}_{Q,s} = \frac{\pi^2 k_B^2}{3e} \sigma_s T \nabla T \quad (= \mathbf{j}_{Q\uparrow} - \mathbf{j}_{Q\downarrow}) \quad (71)$$

is the ‘spin-heat’ current density, i.e., spin-polarized part of the heat-current density (multiplied by $-e$). The second and the third terms in the brackets of Eq. (69) follow from $(\beta \sigma_s)' = \beta \sigma'_s + \beta' \sigma_s$. While the first and the second terms are the ordinary spin-transfer torque and the β term due to thermoelectric spin current, the third term (with β') is the spin torque directly driven by the heat current.

Although the present calculation is based on a specific model (as to the band structure and the spin-relaxation process), the principal result, Eq. (65), relating the thermal torques to the electrical ones, will hold quite generally. The same relation has also been derived for the so-called “spin-orbit torque” [16,17].

Hals *et al.* [25] derived β_T by scattering theory and evaluated it numerically for finite-length wires of magnetic semiconductors. They did not encounter unphysical divergences because their formalism focuses on the dissipation into contacts to the magnet, which automatically excludes any equilibrium components.

VIII. APPLICATIONS

To illustrate the implications of the microscopic result, we consider now a temperature gradient without external electric field, $\mathbf{E}_{\text{ext}} = \mathbf{0}$. The spin torque depends on the type of the circuit (closed or open) because of the internal field \mathbf{E}_{int} , where $\mathbf{E} = \mathbf{E}_{\text{ext}} + \mathbf{E}_{\text{int}}$ [6,38]. The total spin torque (69) may then be rewritten as

$$\tilde{\mathbf{t}}_{\text{tot}}(\mathbf{E}_{\text{ext}} = \mathbf{0}) = \frac{\hbar}{2eS_{\text{tot}}} (1 + \beta_T^{\text{eff}} \mathbf{n} \times) (\mathbf{j}_s^T \cdot \nabla) \mathbf{n}, \quad (72)$$

where \mathbf{j}_s^T is proportional to ∇T and β_T^{eff} is an effective beta parameter. For a closed circuit, $\mathbf{E} = \mathbf{0}$, the thermal spin-transfer torque is governed by the thermoelectric spin current $\mathbf{j}_s^{T,\text{closed}} = \sigma_s \mathcal{S}_s \nabla T$, and the thermal β term by

$$\beta_T^{\text{closed}} \mathbf{j}_s^{T,\text{closed}} = \frac{\pi^2 k_B^2}{3e} \beta \sigma_s \left(\frac{\sigma'_s}{\sigma_s} + \frac{\beta'}{\beta} \right) T \nabla T, \quad (73)$$

where

$$\beta_T^{\text{closed}} = \beta + \beta' \frac{\sigma_s}{\sigma'_s}. \quad (74)$$

For open circuits $\mathbf{j}_c = \sigma_c (\mathbf{E} + \mathcal{S}_c \nabla T) = \mathbf{0}$ with $\sigma_c = (e^2/m) (n_{\uparrow} \tau_{\uparrow} + n_{\downarrow} \tau_{\downarrow})$ and $\mathcal{S}_c = (\pi^2 k_B^2 / 3e) (\sigma'_c / \sigma_c) T$, the thermal spin-transfer torque is governed by $\mathbf{j}_s^{T,\text{open}} = \sigma_s (\mathcal{S}_s - \mathcal{S}_c) \nabla T$.

The thermal β term then reads

$$\beta_T^{\text{open}} \mathbf{j}_s^{T,\text{open}} = \frac{\pi^2 k_B^2}{3e} \beta \sigma_s \left(-\frac{\sigma'_c}{\sigma_c} + \frac{\sigma'_s}{\sigma_s} + \frac{\beta'}{\beta} \right) T \nabla T, \quad (75)$$

where

$$\beta_T^{\text{open}} = \beta + \beta' \left(\frac{\sigma'_s}{\sigma_s} - \frac{\sigma'_c}{\sigma_c} \right)^{-1}. \quad (76)$$

Thus, the thermal β_T differs from the electrical one (β) when $\beta' \neq 0$.

In the present model (7) with parabolic electron dispersion and high electron densities, σ_s depends on ε_F only weakly [39] and the thermoelectric spin current ($\propto \sigma'_s$) is vanishingly small, whereas $\sigma'_c/\sigma_c \sim 1/\varepsilon_F$ and $\beta'/\beta = (v'_\uparrow + v'_\downarrow)/(v_\uparrow + v_\downarrow) \sim 1/2\varepsilon_F$ (if $\varepsilon_F \pm M$ are not too small compared to ε_F). Therefore, in closed circuits, the thermal spin-transfer torque is dominated by the thermal β term $\propto \beta' \sigma_s T \nabla T$ driven by the spin-heat current, Eq. (71). By opening the circuits, both torques change sign by the effect of \mathbf{E}_{int} ($\propto -\sigma'_c/\sigma_c$). A domain wall can therefore be driven into opposite directions in closed and open circuits. In real materials, such features of course depend on the details of spin-relaxation mechanism and band structure, but the driving by spin-heat currents dominates when the energy dependence (at the Fermi level) of the spin conductivity is weak (such that thermoelectric spin currents are suppressed) while that of β is strong.

IX. GENERAL ASPECTS

In this section, we draw some general conclusion out of the analysis in the previous sections. For this purpose, it is convenient to shift the (off-shell) energy variable ε as $\varepsilon \rightarrow \varepsilon - \mu$, so that the Fermi-Dirac distribution function is explicitly μ dependent but the Green functions are not. Without introducing new functions, we redefine $f(\varepsilon) = (e^{\beta_0(\varepsilon-\mu)} + 1)^{-1}$ instead of $f(\varepsilon) = (e^{\beta_0\varepsilon} + 1)^{-1}$, and $G(\varepsilon) = (\varepsilon - \varepsilon_k + \dots)^{-1}$ instead of $G(\varepsilon) = (\varepsilon + \mu - \varepsilon_k + \dots)^{-1}$, and similarly for $B(\varepsilon)$ and $C(\varepsilon)$. (We focus on \tilde{b} and \tilde{b}_T .)

Following Luttinger's prescription, we considered the linear response to a field ψ which couples to the energy (or heat) density. Thermal response functions have been obtained from the electrical response functions by simply introducing an $(\varepsilon - \mu)$ factor inside the ε integral. This “ $(\varepsilon - \mu)$ -factor prescription” works well for the Fermi-surface term,

$$\chi_{\text{el}}^{\text{surface}} = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) B(\varepsilon), \quad (77)$$

$$\chi_{\text{th}}^{\text{surface}} = \int_{-\infty}^{\infty} d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu) B(\varepsilon). \quad (78)$$

On the other hand, for the Fermi-sea terms, it leads to an unphysical contribution that can be repaired by subtracting the equilibrium components, leading to

$$\chi_{\text{el}}^{\text{sea}} = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) D(\varepsilon), \quad (79)$$

$$\chi_{\text{th}}^{\text{sea}} = \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) (\varepsilon - \mu) D(\varepsilon) - \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) C(\varepsilon), \quad (80)$$

where $D(\varepsilon) \equiv -\partial_\varepsilon C(\varepsilon)$. The first term in $\chi_{\text{th}}^{\text{sea}}$ includes the $(\varepsilon - \mu)$ factor for the heat (or heat-current) vertex, while

the second term subtracts the equilibrium component. By integration by parts,

$$\chi_{\text{th}}^{\text{sea}} = \int_{-\infty}^{\infty} d\varepsilon \{(\varepsilon - \mu) f(\varepsilon) - \Omega(\varepsilon)\} D(\varepsilon), \quad (81)$$

where

$$\Omega(\varepsilon) = - \int_{\varepsilon}^{\infty} d\varepsilon' f(\varepsilon') = -T \ln(1 + e^{-\beta_0(\varepsilon-\mu)}), \quad (82)$$

assuming that $\varepsilon C(\varepsilon) \rightarrow 0$ as $\varepsilon \rightarrow -\infty$. We note that $\Omega(\varepsilon)$ is nothing but the grand-canonical free energy for fermions at energy ε [40]. Since the first term in the brackets of Eq. (81) represents the (average) energy, $E(\varepsilon) = \varepsilon f(\varepsilon)$, the terms in the brackets can be regarded as $E(\varepsilon) - \mu f(\varepsilon) - \Omega(\varepsilon) = E(\varepsilon) - F(\varepsilon) = TS(\varepsilon)$, where $F(\varepsilon) \equiv \Omega(\varepsilon) + \mu f(\varepsilon)$ is the corresponding Helmholtz free energy, and

$$S(\varepsilon) = \frac{\varepsilon - \mu}{T} f(\varepsilon) + \ln(1 + e^{-\beta_0(\varepsilon-\mu)}) \quad (83)$$

is the entropy. Thus we obtain the suggestive expression,

$$\chi_{\text{th}}^{\text{sea}} = T \int_{-\infty}^{\infty} d\varepsilon S(\varepsilon) D(\varepsilon). \quad (84)$$

Since the entropy behaves regularly and vanishes in the limit $T \rightarrow 0$, so does $\chi_{\text{th}}^{\text{sea}}/T$ [41]. The unphysical divergence has thus been removed.

If we define

$$\Phi(T, \mu) = \int_{-\infty}^{\infty} d\varepsilon \Omega(\varepsilon) D(\varepsilon), \quad (85)$$

and note the relations, $f(\varepsilon) = -\partial \Omega(\varepsilon)/\partial \mu$ and $S(\varepsilon) = -\partial \Omega(\varepsilon)/\partial T$,

$$\chi_{\text{el}}^{\text{sea}} = -\frac{\partial}{\partial \mu} \Phi(T, \mu), \quad (86)$$

$$\chi_{\text{th}}^{\text{sea}} = -T \frac{\partial}{\partial T} \Phi(T, \mu), \quad (87)$$

which look very much like thermodynamic formulas. Similar expressions are possible for the Fermi-surface terms as well [42]. A formula similar to Eq. (86) has been derived by Středa for the Fermi-sea term of the Hall conductivity [43].

The above considerations suggest the following prescription for the calculation of thermal response functions. Given the electrical response functions, Eqs. (77) and (79), the thermal response functions, Eqs. (78) and (84), are obtained by the replacement,

$$f(\varepsilon) \rightarrow TS(\varepsilon). \quad (88)$$

This prescription works for the Fermi-surface term as well, since $(-\partial f/\partial \varepsilon)$ is replaced by

$$T \left(-\frac{\partial S}{\partial \varepsilon} \right) = (\varepsilon - \mu) \left(-\frac{\partial f}{\partial \varepsilon} \right), \quad (89)$$

which is identical with the $(\varepsilon - \mu)$ -factor prescription for the Fermi-surface term, leading to Eq. (78). Although we did not derive this procedure from first principles, it suggests that a (fictitious) field that couples to the *entropy density* (times temperature), rather than to the energy (or heat) density, has more direct relevance for the problem.

X. SUMMARY

We presented a microscopic model calculation of spin torques induced by a temperature gradient in a conducting ferromagnet. Based on the observation that Luttinger's prescription leads to an unphysical result, we recognized that the Einstein relation should be applied only to the nonequilibrium contributions; the equilibrium component from the Kubo formula should therefore be removed before applying the Einstein relation.

In the subtraction procedure, we noted (i) the modification of the torque formula by ψ [Eq. (51)], but (ii) the absence of a linear response to ψ (not $\nabla\psi$); the latter reflects the adiabatic nature of the Kubo formula and the conservation of energy (to which the field ψ couples). We note that a field that couples to the entropy density appears to directly lead to the desired results, but a formal proof is still necessary.

A general thermoelectric relation between thermal and electrical torques Eq. (65) leads to a generalized Mott formula Eq. (68) for sufficiently low temperatures. When the dissipative correction (β term) depends on energy, an additional “ β_T term” beyond the simple thermoelectric effect (due to spin currents induced by temperature gradients) arises that can be important when the energy dependence of the spin conductivity is weak and/or that of the density of states is strong.

Note added. Recently, a paper appeared [44] in which thermal transport phenomena are studied by introducing a thermal vector potential. The terms which lead to the unphysical divergence at zero temperature presumably automatically cancel by the diamagnetic current associated with this thermal vector potential. However, at the end of the day Tataru calculates an equivalent of our Eqs. (A5)–(A8), and both his and our treatment (before the subtraction procedure) should give the same results. Tataru demonstrates that the weak-field thermal Hall effect vanishes for zero temperature, but only to leading order in the electron scattering rate. However, this does not resolve the divergence we address here, which originates from the higher-order scattering terms. The thermal vector potential is therefore not a substitute for the subtraction technique proposed here. Tataru mentions in passing that the thermal spin torque is well behaved at zero temperature. However, this is because the divergence has already been removed in the starting expression of his Ref. [20] rather than by the thermal vector potential.

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APPENDIX A: LINEAR RESPONSE TO GRAVITATIONAL FIELD

Here we summarize some formulas of the linear response to a “gravitational potential” ψ , which couples to the energy density of the system, as considered by Luttinger [11]. To be specific, let us take $\psi(\mathbf{r}, t) = \psi_{\mathbf{q}} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)}$. Then the

perturbation is described by

$$H' = \psi_{\mathbf{q}} h(-\mathbf{q}) e^{-i\omega t}, \quad (\text{A1})$$

where $h(\mathbf{q})$ is the Fourier component of the energy density $h(x)$. (In this paper, h actually means $h - \mu n$, as stated just above Eq. (13).) To first order in ψ , the response of a physical quantity \hat{A} is expressed as

$$\langle \hat{A} \rangle_{\psi} = -K_0(\mathbf{q}, \omega + i0) \psi_{\mathbf{q}} e^{-i\omega t}. \quad (\text{A2})$$

The response function $K_0(\mathbf{q}, \omega + i0)$ is obtained from

$$K_0(\mathbf{q}, i\omega_{\lambda}) = \int_0^{\beta_0} d\tau e^{i\omega_{\lambda}\tau} \langle T_{\tau} \hat{A}(\tau) h(-\mathbf{q}) \rangle \quad (\text{A3})$$

by analytic continuation, $i\omega_{\lambda} \rightarrow \hbar\omega + i0$. Let us introduce the heat-current operator \mathbf{j}_Q by the continuity equation for the energy (measured from the chemical potential),

$$\frac{\partial}{\partial t} h(x) + \nabla \cdot \mathbf{j}_Q = 0. \quad (\text{A4})$$

In the Fourier (\mathbf{q}) and imaginary-time (τ) representation, $\partial_{\tau} h(-\mathbf{q}) = \hbar \mathbf{q} \cdot \mathbf{j}_Q(-\mathbf{q})$. Using this in Eq. (A3) after integration by parts,

$$K_0(\mathbf{q}, i\omega_{\lambda}) = \frac{\hbar q_i}{i\omega_{\lambda}} [K_i(\mathbf{q}, i\omega_{\lambda}) - K_i(\mathbf{q}, 0)], \quad (\text{A5})$$

where

$$K_i(\mathbf{q}, i\omega_{\lambda}) = \int_0^{\beta_0} d\tau e^{i\omega_{\lambda}\tau} \langle T_{\tau} \hat{A}(\tau) j_{Q,i}(-\mathbf{q}) \rangle. \quad (\text{A6})$$

The factor $i q_i$ in Eq. (A5) is combined with $\psi_{\mathbf{q}}$ in Eq. (A2) to yield $\nabla\psi$. When $\nabla\psi$ is uniform and static, we can take the limit $\mathbf{q} \rightarrow \mathbf{0}$ and $\omega \rightarrow 0$ in the coefficient [Eq. (A6)] and obtain

$$\langle \hat{A} \rangle_{\psi} = \lim_{\omega \rightarrow 0} \frac{K_i(\omega + i0) - K_i(0)}{i\omega} (-\nabla_i \psi), \quad (\text{A7})$$

$$K_i(i\omega_{\lambda}) = \int_0^{\beta_0} d\tau e^{i\omega_{\lambda}\tau} \langle T_{\tau} \hat{A}(\tau) J_{Q,i} \rangle, \quad (\text{A8})$$

where $\mathbf{J}_Q \equiv \mathbf{j}_Q(\mathbf{q} = \mathbf{0})$ is the total heat current. An explicit form of \mathbf{j}_Q is studied in Appendix B and given in Eq. (20).

APPENDIX B: EXPRESSIONS OF HEAT-CURRENT DENSITY

Here, we derive the expression for the heat-current density, \mathbf{j}_Q , using Eq. (A4). Let us consider the following two forms of Hamiltonian density,

$$\hat{h}^{(1)}(x) = \frac{\hbar^2}{2m} (\nabla c^{\dagger})(\nabla c) + c^{\dagger} V c, \quad (\text{B1})$$

$$\hat{h}^{(2)}(x) = -\frac{\hbar^2}{4m} \{c^{\dagger} (\nabla^2 c) + (\nabla^2 c^{\dagger}) c\} + c^{\dagger} V c, \quad (\text{B2})$$

where

$$V(\mathbf{r}) = -M\mathbf{n} \cdot \boldsymbol{\sigma} - \mu + V_{\text{imp}}(\mathbf{r}). \quad (\text{B3})$$

They differ from each other by a total divergence,

$$\hat{h}^{(1)}(x) - \hat{h}^{(2)}(x) = \frac{\hbar^2}{4m} \nabla^2 \rho, \quad (\text{B4})$$

where $\rho = c^\dagger c$ is the (number) density. Using the field equation,

$$i\hbar\dot{c}(x) = -\frac{\hbar^2}{2m}\nabla^2 c + V c, \quad (\text{B5})$$

and its conjugate, we can rewrite the above as follows;

$$\hat{h}^{(1)}(x) = \frac{i\hbar}{2}(c^\dagger\dot{c} - \dot{c}^\dagger c) + \frac{\hbar^2}{4m}\nabla^2 \rho, \quad (\text{B6})$$

$$\hat{h}^{(2)}(x) = \frac{i\hbar}{2}(c^\dagger\dot{c} - \dot{c}^\dagger c). \quad (\text{B7})$$

To derive the expression for \mathbf{j}_Q , we use Eq. (A4) and first take a time derivative of Eqs. (B1) and (B2), and then use Eq. (B5). The results are

$$\mathbf{j}_Q^{(1)}(x) = -\frac{\hbar^2}{2m}\{\dot{c}^\dagger(\nabla c) + (\nabla c^\dagger)\dot{c}\}, \quad (\text{B8})$$

$$\begin{aligned} \mathbf{j}_Q^{(2)}(x) &= -\frac{\hbar^2}{2m}\{\dot{c}^\dagger(\nabla c) + (\nabla c^\dagger)\dot{c}\} + \frac{\hbar^2}{4m}\nabla\dot{\rho} \\ &= \frac{\hbar^2}{4m}\lim_{x'\rightarrow x}(\nabla - \nabla')(\partial_t - \partial_{t'})c^\dagger(x)c^\dagger(x'), \end{aligned} \quad (\text{B9})$$

where $x = (\mathbf{r}, t)$, $x' = (\mathbf{r}', t')$. In Fourier components ($\mathbf{r} \rightarrow \mathbf{q}$), they read

$$\hat{h}^{(1)}(\mathbf{q}) = \frac{i\hbar}{2}\sum_k(c_{k-}^\dagger\dot{c}_{k+} - \dot{c}_{k-}^\dagger c_{k+}) - \frac{\hbar^2}{4m}q^2\rho_q, \quad (\text{B10})$$

$$\mathbf{j}_Q^{(1)}(\mathbf{q}) = \frac{i\hbar}{2}\sum_k \mathbf{v}_k(c_{k-}^\dagger\dot{c}_{k+} - \dot{c}_{k-}^\dagger c_{k+}) - \frac{\hbar^2}{4m}i\mathbf{q}\dot{\rho}_q, \quad (\text{B11})$$

$$\hat{h}^{(2)}(\mathbf{q}) = \frac{i\hbar}{2}\sum_k(c_{k-}^\dagger\dot{c}_{k+} - \dot{c}_{k-}^\dagger c_{k+}), \quad (\text{B12})$$

$$\mathbf{j}_Q^{(2)}(\mathbf{q}) = \frac{i\hbar}{2}\sum_k \mathbf{v}_k(c_{k-}^\dagger\dot{c}_{k+} - \dot{c}_{k-}^\dagger c_{k+}), \quad (\text{B13})$$

where $\mathbf{k}\pm \equiv \mathbf{k} \pm \mathbf{q}/2$, $\mathbf{v}_k = \hbar\mathbf{k}/m$, and

$$\rho_q = \sum_k c_{k-}^\dagger c_{k+}. \quad (\text{B14})$$

Both choices, $(\hat{h}^{(1)}, \mathbf{j}_Q^{(1)})$ and $(\hat{h}^{(2)}, \mathbf{j}_Q^{(2)})$, coincide in the limit, $\mathbf{q} \rightarrow \mathbf{0}$, but they are not equal in general. We use $(\hat{h}^{(1)}, \mathbf{j}_Q^{(1)})$ in the main text.

APPENDIX C: CANCELLATION IN THE INTERACTION PICTURE

At the end of Sec. IV, we showed that in the ‘Heisenberg’ picture (defined for the full Hamiltonian, H) the heat-current vertex differs from the charge current vertex only by the factor $i(\varepsilon_n + \omega_\lambda/2)$. Here we confirm this statement by a calculation based on the following explicit formula [Eq. (C1)] for the heat current. As seen below, due to many cancellations we are indeed left only with the first term of Eq. (26).

The explicit form of the total heat current operator [without invoking a time derivative as in Eq. (20)] is given by

$$\begin{aligned} J_Q &= \sum_k \mathbf{v}_k c_k^\dagger \hat{\xi}_k c_k - M \sum_k \mathbf{v}_k c_{k+}^\dagger (\mathbf{u}_q \cdot \boldsymbol{\sigma}) c_{k-} \\ &\quad + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{v}_k + \mathbf{v}_{k'}) c_k^\dagger V_{\text{imp}}(\mathbf{k} - \mathbf{k}') c_{k'}, \end{aligned} \quad (\text{C1})$$

where $c_k = \langle c_{k\uparrow} \rangle$ is the spatial Fourier transform of $c(x)$, $\mathbf{v}_k = \hbar\mathbf{k}/m$, $\mathbf{k}\pm \equiv \mathbf{k} \pm \mathbf{q}/2$,

$$\hat{\xi}_k = \frac{\hbar^2 \mathbf{k}^2}{2m} - M\sigma^z - \mu, \quad (\text{C2})$$

and $V_{\text{imp}}(\mathbf{k} - \mathbf{k}')$ is the Fourier transform of Eq. (8).

Let us examine each contribution to $K_{ij}^{\alpha\beta}$;

$$K_{ij}^{\alpha\beta} = T \sum_n \sum_k v_i v_j (\varphi_1 + \varphi_2 + \varphi_3 + \varphi'_2 + \varphi'_3). \quad (\text{C3})$$

The contribution from the first term of Eq. (C1) is obtained by replacing the v_i vertex in $\varphi_{ij}^{\alpha\beta}$ [Eq. (32)] as $G^+ v_i G \rightarrow G^+ v_i \hat{\xi}_k G$. Using the identity, $G^{-1} = i\varepsilon_n - \hat{\xi}_k - \Sigma$, or

$$\hat{\xi}_k = i\left(\varepsilon_n + \frac{\omega_\lambda}{2}\right) - \frac{(G^+)^{-1} + G^{-1}}{2} - \frac{\Sigma^+ + \Sigma}{2}, \quad (\text{C4})$$

where Σ is the self-energy, we have

$$\begin{aligned} \varphi_1 &= i(\varepsilon_n + \omega_\lambda/2)\{\text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta G^+ G] \\ &\quad - \text{tr}[\sigma^\alpha G^+ G \sigma^\beta G G]\}, \end{aligned} \quad (\text{C5})$$

$$\begin{aligned} \varphi_2 &= -\frac{1}{2}\{\text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta (G^+ + G)] \\ &\quad - \text{tr}[\sigma^\alpha (G^+ + G) \sigma^\beta G G]\}, \end{aligned} \quad (\text{C6})$$

$$\begin{aligned} \varphi_3 &= -\frac{1}{2}\{\text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta G^+ (\Sigma^+ + \Sigma)G] \\ &\quad - \text{tr}[\sigma^\alpha G^+ (\Sigma^+ + \Sigma)G \sigma^\beta G G]\}. \end{aligned} \quad (\text{C7})$$

In order to evaluate the contribution by the second term in Eq. (C1), we start from

$$K_i^\alpha(i\omega_\lambda) = M u_q^\beta T \sum_n \sum_k v_i \text{tr}[\sigma^\alpha G_{k+q/2}^+ \sigma^\beta G_{k-q/2}], \quad (\text{C8})$$

and expand it with respect to q_j . We obtain [Fig. 2(a)]

$$\varphi'_2 = \frac{1}{2}\{\text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta G] - \text{tr}[\sigma^\alpha G^+ \sigma^\beta G G]\}, \quad (\text{C9})$$

which partly cancels φ_2 ; the remaining terms

$$\varphi_2 + \varphi'_2 = \frac{1}{2}\{\text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta G^+] - \text{tr}[\sigma^\alpha G \sigma^\beta G G]\} \quad (\text{C10})$$

do not depend on ω_λ after summing over ε_n and can be dropped. This corresponds to the second term of Eq. (26).

The contribution from the third term of Eq. (C1) is shown diagrammatically in Figs. 2(b) and 2(c). The diagrams of Fig. 2(b) give

$$\begin{aligned} \varphi'_3 &= \frac{1}{2}\{\text{tr}[\sigma^\alpha G^+ G^+ \sigma^\beta G^+ (\Sigma^+ + \Sigma)G] \\ &\quad - \text{tr}[\sigma^\alpha G^+ (\Sigma^+ + \Sigma)G \sigma^\beta G G]\}, \end{aligned} \quad (\text{C11})$$

which cancels with φ_3 . The contribution of Fig. 2(c) is $\sim \mathcal{O}(\gamma)$ and is disregarded.

For the diagrams including vertex corrections in Fig. 1, similar arguments hold. As a result, we need to take into

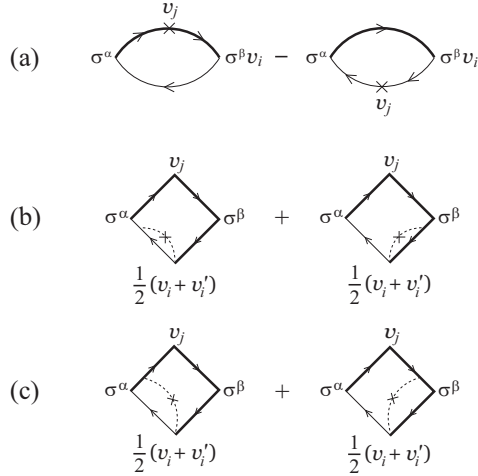


FIG. 2. Diagrammatic expressions for $K_{Q,ij}^{\alpha\beta}$ calculated with the second term (a) and the third term (b),(c) of the heat-current operator, Eq. (C1).

account only φ_1 (including vertex corrections), in accordance with the observation made around Eq. (26).

APPENDIX D: EQUILIBRIUM EXCHANGE TORQUE

Here we calculate the equilibrium exchange torque, Eq. (50), to show that it indeed has the same coefficient c [Eq. (45)] as the problematic term, Eq. (48). In the presence of a static magnetization texture, Eq. (10), the equilibrium spin density to the first order in \mathbf{u}_q reads

$$\langle \hat{\sigma}_\perp(\mathbf{q}) \rangle_{\text{eq}} = M J^{\alpha\beta}(\mathbf{q}) u_q^\beta, \quad (\text{D1})$$

where

$$\begin{aligned} J^{\alpha\beta}(\mathbf{q}) &= -T \sum_n \sum_k \text{tr}[\sigma^\alpha G_{k+q}(i\varepsilon_n) \sigma^\beta G_k(i\varepsilon_n)] \\ &= J^{\alpha\beta}(\mathbf{0}) + J_{ij}^{\alpha\beta} q_i q_j + \mathcal{O}(q^4). \end{aligned} \quad (\text{D2})$$

In the second line, we expanded $J^{\alpha\beta}(\mathbf{q})$ with respect to \mathbf{q} with coefficients $J^{\alpha\beta}(\mathbf{0}) = (\rho_s/M) \delta^{\alpha\beta}$, where $\rho_s = n_\uparrow - n_\downarrow$ is the conduction electron spin polarization for uniform \mathbf{n} , and

$$\begin{aligned} J_{ij}^{\alpha\beta} &= \frac{1}{2} T \sum_n \sum_k v_i v_j \text{tr}[\sigma^\alpha G G \sigma^\beta G G] \\ &= \delta^{\alpha\beta} T \sum_n \sum_k v_i v_j (G_\uparrow G_\downarrow)^2 \end{aligned} \quad (\text{D3})$$

with $G \equiv G_k(i\varepsilon_n)$ and $G_\sigma \equiv G_{k\sigma}(i\varepsilon_n)$. Standard procedure leads to

$$\begin{aligned} J_{ij}^{\alpha\beta} &= -\frac{1}{\pi} \delta^{\alpha\beta} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \sum_k v_i v_j \text{Im}[G_\uparrow^R(\varepsilon) G_\downarrow^R(\varepsilon)]^2 \\ &= -\delta^{\alpha\beta} \frac{1}{M^2} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) C(\varepsilon) \\ &= -\frac{c}{M^2} \delta^{\alpha\beta}, \end{aligned} \quad (\text{D4})$$

where we used Eqs. (40) and (45). This gives the spin density, $\langle \hat{\sigma} \rangle_{\text{eq}} = \rho_s \hat{z} + \langle \hat{\sigma}_\perp(\mathbf{q}) \rangle_{\text{eq}} = \rho_s (\hat{z} + \mathbf{u}) + (c/M) \nabla^2 \mathbf{u} = \rho_s \mathbf{n} + (c/M) \nabla^2 \mathbf{n}$, and the torque, Eq. (50).

APPENDIX E: RESPONSE TO SCALAR POTENTIALS

Here we directly calculate the linear response to the scalar potentials of electric (ϕ) and gravitational (ψ) fields. This confirms our assertion that no terms proportional to ψ arise (next to those with $\partial_i \psi$), which is crucial for the procedure proposed in Sec. VI. It also serves as a check of Eqs. (A7) and (A8).

The linear response of the s -electron spin density to ϕ or ψ may be expressed as

$$\langle \hat{\sigma}_\perp \rangle_\phi = -e (A_\phi - i\omega B_\phi)/M, \quad (\text{E1})$$

$$\langle \hat{\sigma}_\perp \rangle_\psi = (A_\psi - i\omega B_\psi)/M, \quad (\text{E2})$$

respectively, retaining the terms up to first order in ω , i.e., the frequency of ϕ or ψ . The coefficients are

$$A_\phi = -C_0 \partial_i [(\partial_i \mathbf{n}) \phi], \quad (\text{E3})$$

$$B_\phi = \frac{C_0 (\nabla^2 \mathbf{n}) \phi + [B_0 \partial_i \mathbf{n} - A_0 (\mathbf{n} \times \partial_i \mathbf{n})] \partial_i \phi}{-i\omega}, \quad (\text{E4})$$

$$A_\psi = (c - C_1) \partial_i [(\partial_i \mathbf{n}) \psi] - c (\nabla^2 \mathbf{n}) \psi, \quad (\text{E5})$$

$$B_\psi = \frac{C_1 (\nabla^2 \mathbf{n}) \psi + [B_1 \partial_i \mathbf{n} - A_1 (\mathbf{n} \times \partial_i \mathbf{n})] \partial_i \psi}{-i\omega}, \quad (\text{E6})$$

where A_n, B_n, C_n , and c are given by Eqs. (44) and (45). The second term in Eq. (E5) is a correction similar to the second term in Eq. (26) treating the heat vertex by the factor $i(\varepsilon_n + \omega_\lambda/2)$. Each factor $(-i\omega)^{-1}$ in Eqs. (E4) and (E6) reflects conservation of electron number and energy, respectively, and comes from ladder-type vertex correction [45,46]. Therefore, even in the static limit, $\omega \rightarrow 0$, the B_ϕ and B_ψ terms survive in Eqs. (E1) and (E2) and lead to

$$M \langle \hat{\sigma}_\perp \rangle_\phi = -e [(B_0 - C_0) \partial_i \mathbf{n} - A_0 (\mathbf{n} \times \partial_i \mathbf{n})] \partial_i \phi, \quad (\text{E7})$$

$$M \langle \hat{\sigma}_\perp \rangle_\psi = [(B_1 - C_1 + c) \partial_i \mathbf{n} - A_1 (\mathbf{n} \times \partial_i \mathbf{n})] \partial_i \psi. \quad (\text{E8})$$

Note that the terms proportional to ϕ or ψ (but not $\partial_i \phi$ or $\partial_i \psi$) cancel exactly, which reflects the adiabatic nature of the Kubo formula (see Appendix F) and is crucial for the procedure described in Sec. VI. Torques obtained from Eqs. (E7) and (E8) agree with Eqs. (46) and (47), confirming the validity of Eqs. (A7) and (A8).

APPENDIX F: RESPONSE TO STATIC AND UNIFORM SCALAR POTENTIALS

In this Appendix, we consider ϕ and ψ that are static and uniform. The response to such potentials can be compared with equilibrium theory.

The perturbation is described by the Hamiltonian

$$H' = -eN\phi + K\psi, \quad (\text{F1})$$

where $K = H - \mu N$, N is the total number of electrons, and H is the Hamiltonian of the (unperturbed) system. (We neglect the nonlinear perturbation proportional to $\phi\psi$.) Let us consider the adiabatic and isothermal response of a physical quantity \hat{A} ,

$$\delta\langle\hat{A}\rangle^{\text{ad}} = e\chi_N^{\text{R}}(0)\phi - \chi_K^{\text{R}}(0)\psi, \quad (\text{F2})$$

$$\delta\langle\hat{A}\rangle^T = e\chi_N^T(0)\phi - \chi_K^T(0)\psi, \quad (\text{F3})$$

respectively. The response functions are given by the static limit of

$$\chi_B^{\text{R}}(\omega) = \frac{i}{\hbar} \int_0^\infty dt e^{i(\omega+i0)t} \langle[\hat{A}(t), \hat{B}]\rangle, \quad (\text{F4})$$

$$\chi_B^T(i\omega_\lambda) = \int_0^{\beta_0} d\tau e^{i\omega_\lambda\tau} \langle T_\tau \hat{A}(\tau) \Delta\hat{B} \rangle, \quad (\text{F5})$$

where $\Delta\hat{B} = \hat{B} - \langle\hat{B}\rangle$, with $\hat{B} = N$ or K [47]. Since \hat{B} commutes with K , we have

$$\chi_B^{\text{R}}(\omega) = 0, \quad (\text{F6})$$

$$\chi_B^T(i\omega_\lambda) = \beta_0 \langle \Delta\hat{A} \Delta\hat{B} \rangle \delta_{\lambda,0}, \quad (\text{F7})$$

where $\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$. Therefore, the adiabatic response vanishes,

$$\delta\langle\hat{A}\rangle^{\text{ad}} = 0. \quad (\text{F8})$$

The Kubo formula corresponds to this case [47]. The isothermal response (F7) can be expressed by the thermodynamic

formula,

$$\chi_N^T(0) = \frac{\partial}{\partial\mu} \langle\hat{A}\rangle, \quad (\text{F9})$$

$$\chi_K^T(0) = -\beta_0 \frac{\partial}{\partial\beta_0} \langle\hat{A}\rangle = T \frac{\partial}{\partial T} \langle\hat{A}\rangle, \quad (\text{F10})$$

for $\hat{B} = N$ and K , respectively, leading to

$$\delta\langle\hat{A}\rangle^T = e\phi \frac{\partial}{\partial\mu} \langle\hat{A}\rangle - \psi T \frac{\partial}{\partial T} \langle\hat{A}\rangle. \quad (\text{F11})$$

This is natural since $e^{-\beta_0(K+H')} = e^{-\beta_0[(1+\psi)K - e\phi N]}$ is nothing but $e^{-\beta_0 K} = e^{-\beta_0(H-\mu N)}$ with β_0 and μ modified by $\delta\beta_0 = \beta_0\psi$ and $\delta\mu = e\phi$, respectively.

Here we are interested in $\hat{A} = \hat{\sigma}_\perp^\alpha$ with equilibrium value (see Appendix D)

$$\langle\hat{\sigma}_\perp\rangle = c \nabla^2 \mathbf{n} / M, \quad (\text{F12})$$

where c is given by Eq. (45). Since $\partial c / \partial\mu = C_0$ and $T(\partial c / \partial T) = C_1$, the isothermal response is given by

$$\delta\langle\hat{\sigma}_\perp\rangle^T = (e\phi C_0 - \psi C_1) \nabla^2 \mathbf{n} / M. \quad (\text{F13})$$

The susceptibilities read $\chi_N^T = C_0 \nabla^2 \mathbf{n} / M$ and $\chi_K^T = C_1 \nabla^2 \mathbf{n} / M$. The adiabatic susceptibilities, χ_N^{ad} and χ_K^{ad} , are obtained by subtracting the corrections due to changes in T and μ [47], giving $\chi_N^{\text{ad}} = \chi_K^{\text{ad}} = 0$, consistent with Eq. (F8). We recognize these isothermal components (F13) in Eqs. (E3) and (E5), which are eventually canceled by the corresponding terms in Eqs. (E4) and (E6), resulting in a vanishing adiabatic response to static and uniform ϕ and ψ .

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- [34] The letter β is used for the coefficient of the β term as well as for the spin index (such as $\varepsilon^{\alpha\beta}$ and u_q^β), but we hope no confusion will arise; the latter appears only as indices while the former never appears as indices.
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- [36] In Eq. (32), σ^β can be moved to the position adjacent to σ^α by reversing the spin, $\sigma^z \rightarrow -\sigma^z$, in G , which allows making use of $\sigma^\alpha \sigma^\beta = \delta^{\alpha\beta} + i\sigma^z \varepsilon^{\alpha\beta}$. This dependence on α and β was exploited in Eqs. (21) and (22).
- [37] Since $f(\varepsilon)$ is multiplied by a total derivative $\partial_\varepsilon C(\varepsilon)$ in the Fermi-sea term in \tilde{b} [second term in Eq. (35)], this term can be transformed into a Fermi-surface term by partial integration. However, this is specific to the present case; in general such a total-derivative form does not appear at the formal Green function level, see Ref. [17].
- [38] We define a closed circuit in terms of an electrical short, i.e., a situation in which the two ends of the sample have different temperatures but identical electrochemical potential (as in Ref. [6]). In other words, the circuit is closed by either an ideal ammeter (closed circuit) or voltmeter (open circuit).
- [39] If we neglect magnetic impurities, $\tau_\sigma^{-1} \propto \nu_\sigma$ [Eq. (12)] and thus $\sigma_s \propto \sum_\sigma \sigma n_\sigma \tau_\sigma \propto \sum_\sigma \sigma \varepsilon_{F\sigma} = 2M$ does not depend on ε_F . Magnetic impurities give rise to ε_F -dependent terms in σ_s with a relative magnitude $\sim (n_s u_s^2 S_{\text{imp}}^2 / n_i u_i^2)^3$.
- [40] Note that ε is the off-shell energy and does not need to correspond to real energy levels of the system.
- [41] If $D(\varepsilon)$ were a (single-particle) density of states, $\chi_{\text{el}}^{\text{sea}}$, $\chi_{\text{th}}^{\text{sea}}/T$, and Φ [defined in Eq. (85)] would represent the number, entropy, and the grand-canonical free energy, respectively. The ‘unsubtracted’ $\chi_{\text{th}}^{\text{sea}}$ [first term of $\chi_{\text{th}}^{\text{sea}}$ in Eq. (80)] then corresponds to an energy, which does not vanish at zero temperature because of Fermi degeneracy.
- [42] With $\Psi \equiv \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) B(\varepsilon)$, we have $\chi_{\text{el}}^{\text{surface}} = \partial\Psi/\partial\mu$ and $\chi_{\text{th}}^{\text{surface}} = T(\partial\Psi/\partial T)$.
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