Gradient expansion formalism for generic spin torques

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Atsuo Shitade, arXiv:1708.03424.

Outline

1. Spintronics
    a. Magnetoresistance and spin torques
    b. Two microscopic formalisms for spin torques
2. Gradient expansion
    a. Wilson line
    b. Moyal product
3. Application to spin torques
    a. 1st. order → spin renormalization and Gilbert damping
    b. 2nd. order → spin transfer torque and β-term

Magnetic systems → nonvolatile memories

- Reading = magnetization measurement
  - Giant MagnetoResistance

    Baibich *et al*., PRL **61**, 2472 (1988).

    Binasch *et al*., PRB **38**, 4828 (1989).
  - Tunnel MagnetoResistance

    Julliere, Phys. Lett. **54A**, 225 (1975).

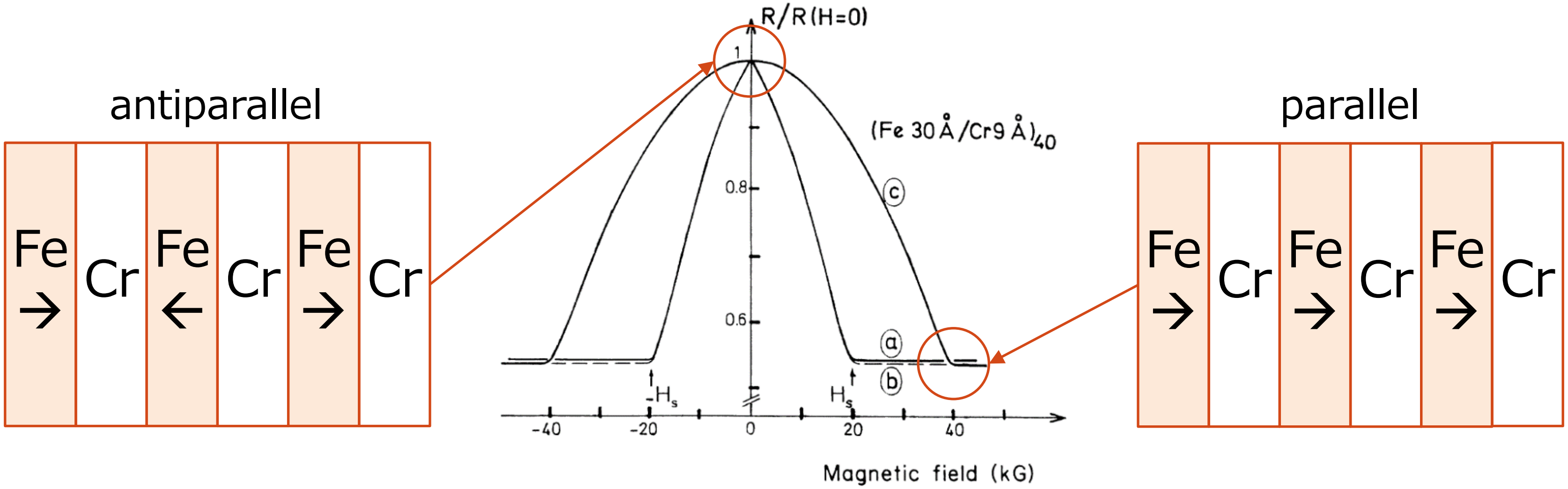
    Miyazaki and Tezuka, J. Magn. Magn. Mater. **139**, L231 (1995).

    Moodera *et al*., PRL **74**, 3273 (1995).

Fert

Grünberg

Nobel Prize 2007



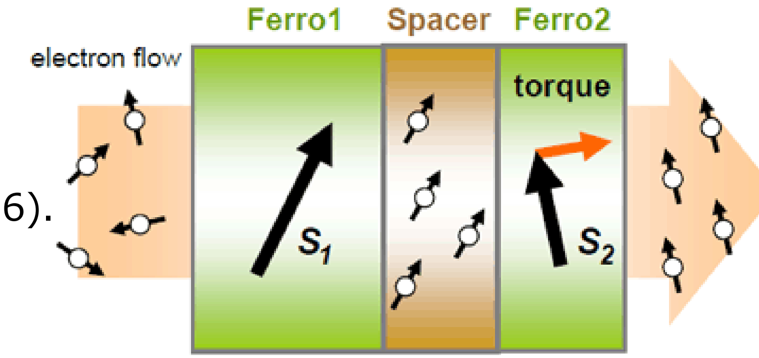
Magnetic systems → nonvolatile memories

- Writing = magnetization reversal
  - Magnetic field → Magnetoresistive Random Access Memory
  - Spin Transfer Torque → STT-MRAM

    Berger, J. Appl. Phys. **55**, 1954 (1984).

    Berger, PRB **54**, 9353 (1996).

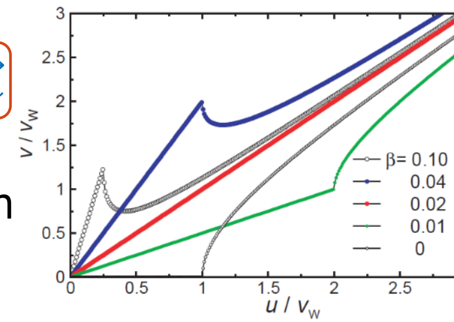
    Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996).



$$\hbar\dot{\vec{n}} = \vec{n} \times \left(-\frac{\partial H_{\rm sp}}{\partial \vec{n}}\right) + \vec{\tau}$$

$$\vec{\tau} = -\hbar s \dot{\vec{n}} - \hbar\alpha\vec{n} \times \dot{\vec{n}} - (\vec{j}_s \cdot \vec{\partial})\vec{n} - \beta\vec{n} \times (\vec{j}_s \cdot \vec{\partial})\vec{n}$$

Spin renormalization | Gilbert damping | STT | β-term



- β-term
  - Due to spin relaxation Zhang and Li, PRL **93**, 127204 (2004).
  - $\beta = 0$, $\beta \neq \alpha$, or $\beta = \alpha$ Thiaville *et al*., Europhys. Lett. **69**, 990 (2005).

Real materials are more complicated

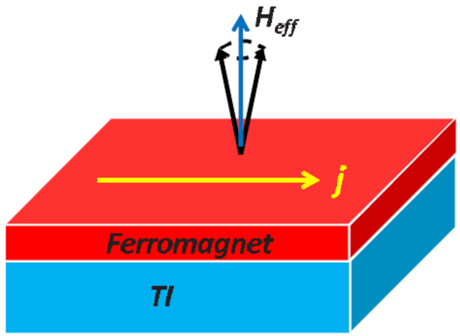
- Textured ferromagnets w/o Spin-Orbit Interactions
  - STT and β-term $\vec{\tau} = -(\vec{j}_s \cdot \vec{\partial})\vec{n} - \beta\vec{n} \times (\vec{j}_s \cdot \vec{\partial})\vec{n}$
- Uniform ferromagnets w/ SOIs
  - Spin-Orbit Torque $\vec{\tau} = (2m\alpha/\hbar)\vec{z}(\vec{j}_s \cdot \vec{n})$ for Rashba SOI

    Manchon and Zhang, PRB **78**, 212405 (2008); PRB **79**, 094422 (2009).
- Textured ferromagnets w/ SOIs
  - Topological insulator surface

    Yokoyama *et al*., PRB **81**, 241410 (2010);

    Sakai and Kohno, PRB **89**, 165307 (2014).
    - different forms of STT, β-term, and SOT
  - Noncentrosymmetric Weyl ferromagnet

    Kurebayashi and Nomura, arXiv:1702.04918.
    - SOT only, no STT or β-term



$\vec{n}$ is assumed to have small fluctuations from $\vec{z}$.
→ small-amplitude formalism

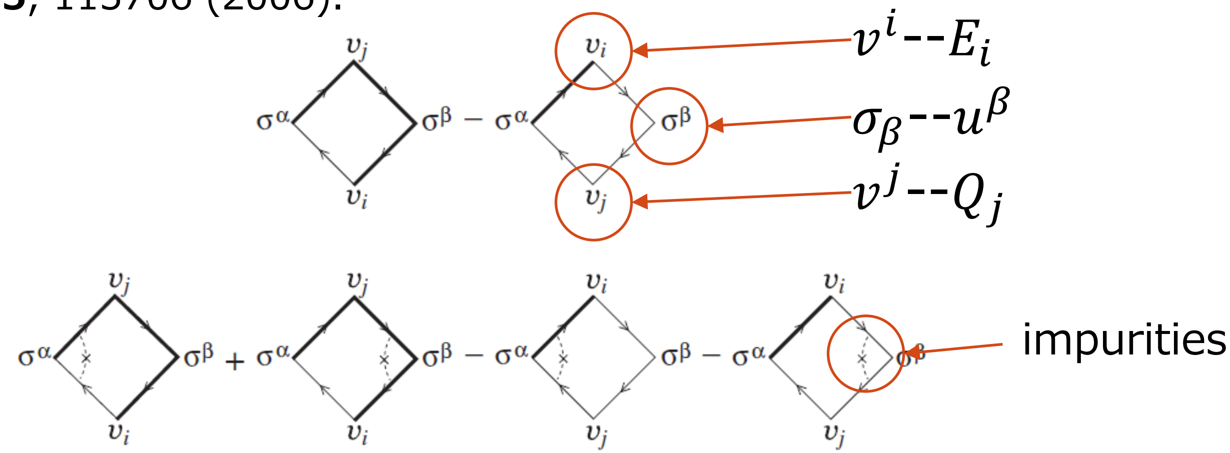
Small-amplitude formalism

- Assume small transverse fluctuations around a uniform state

$$\vec{n} = \vec{z} + \vec{u}, \vec{u}(X) = \vec{u}(Q)e^{iQ_\mu X^\mu} = (u^x, u^y, 0), \vec{u}^2 \ll 1$$

- Pick up the first order w.r.t. $\vec{Q}, \vec{u}, \vec{E}$ → four-point vertices

Kohno *et al*., JPSJ **75**, 113706 (2006).



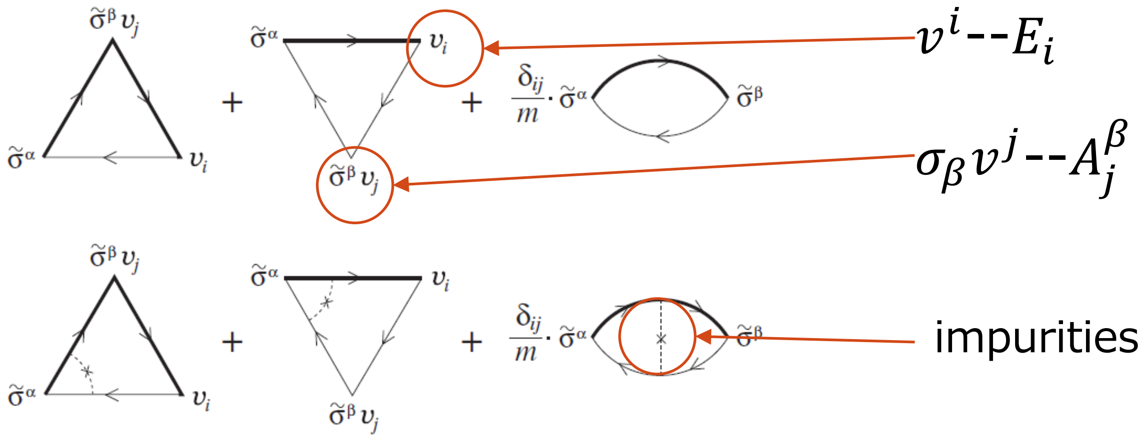
✓ Cannot extrapolate the small-amplitude dynamics to the finite-amplitude one except for some simple cases

Gauge transformation formalism

- Apply a gauge transformation $\psi(X) \to U(X)\psi(X), \vec{n}(X) \cdot \vec{\sigma} \to \sigma_z$
- Magnetization texture is described by an emergent gauge field

  $A_\mu(X) \equiv -iU^\dagger(X)\partial_{X^\mu}U(X) = \vec{u}(X) \times \partial_{X^\mu}\vec{u}(X) \cdot \vec{\sigma}$.
- Pick up the first order w.r.t. A_μ, E_i

  Kohno and Shibata, JPSJ **76**, 063710 (2007).



✓ Quenched magnetic impurities are transformed to dynamical ones, which yield an additional A_μ.

Motivations

- $\vec{n}$ can be controlled by $\vec{E}$.
- In real materials, we have (non)magnetic impurities, SOIs, sublattice degree of freedom (in antiferromagnets), etc.
- Small-amplitude formalism
  - Cannot be applied to the finite-amplitude dynamics.
- Gauge transformation formalism
  - Needs careful calculation not to miss A_μ.
  - Particularly in the presence of magnetic impurities; otherwise $\alpha = 0$.
- Can we derive a first-principles formula (into which we only have to input our Hamiltonian)?

  → Gradient expansion

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Gradient expansion

- Green's function $\hat{G}(x_1, x_2)$ which satisfies the Dyson equation,

$$\mathcal{L}(x_1)\hat{G}(x_1, x_2) - \hat{\Sigma} * \hat{G}(x_1, x_2) = \delta(x_1 - x_2)$$

- Wigner representation to deal with convolution,

$$\tilde{G}(X_{12}, p_{12}) = \int d^D x_{12}\, e^{-ip_{12\mu}x_{12}^{\mu}/\hbar}\tilde{G}(x_1, x_2)$$

- Gauge covariance → Wilson line
  - $\hat{G}(x_1, x_2)$ transforms as $\hat{G}'(x_1, x_2) = V(x_1)\hat{G}(x_1, x_2)V^{\dagger}(x_2)$.
  - $\tilde{G}(x_1, x_2)$ should transform as $\tilde{G}'(x_1, x_2) = V(X_{12})\tilde{G}(x_1, x_2)V^{\dagger}(X_{12})$.
- Wigner representation of convolution → Moyal product

  Levanda and Fleurov, J. Phys.:Condens. Matter **6**, 7889 (1994); Ann. Phys. **292**, 199 (2001).
  - Ordinary product if translationally invariant, but not in general.

Wilson line

- Gauge covariance → Wilson line
  - $\hat{G}(x_1, x_2)$ transforms as $\hat{G}'(x_1, x_2) = V(x_1)\hat{G}(x_1, x_2)V^\dagger(x_2)$.
  - $\tilde{G}(x_1, x_2)$ should transform as $\tilde{G}'(x_1, x_2) = V(X_{12})\tilde{G}(x_1, x_2)V^\dagger(X_{12})$.
- Wilson line which satisfies $\widehat{W}'(x_1, x_2) = V(x_1)\widehat{W}(x_1, x_2)V^\dagger(x_2)$,

$$\widehat{W}(x_1, x_2) \equiv P \exp\left[\frac{i}{\hbar}\int_{x_2}^{x_1} dy^\mu\, \mathcal{A}_\mu(y)\right]$$

- Locally gauge-covariant Green's function

$$\tilde{G}(x_1, x_2) \equiv \widehat{W}(X_{12}, x_1)\hat{G}(x_1, x_2)\widehat{W}(x_2, X_{12})$$

$$\tilde{G}(X_{12}, p_{12}) = \int d^D x_{12}\, e^{-ip_{12\mu}x_{12}^\mu/\hbar}\tilde{G}(x_1, x_2)$$

Moyal product

- Wigner representation of convolution → Moyal product
  - Ordinary product if translationally invariant, but not in general.
- Moyal product

Locally gauge-covariant

convolution

$$\tilde{A}(X_{12},p_{12}) \star \tilde{B}(X_{12},p_{12}) \equiv \int d^D x_{12}\, e^{-ip_{12\mu}x_{12}^{\mu}/\hbar} \widehat{W}(X_{12},x_1) \int d^D x_3\, \hat{A}(x_1,x_3)\hat{B}(x_3,x_2) \widehat{W}(x_2,X_{12})$$

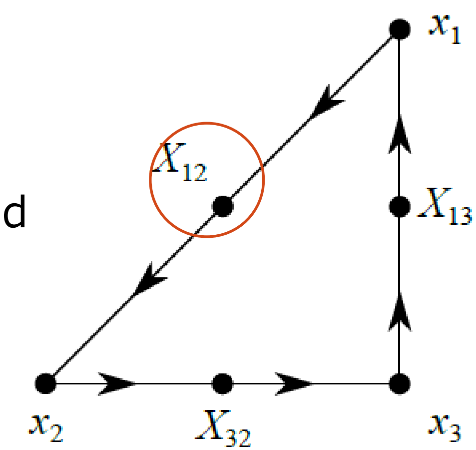
$$= \int d^D x_{12} \int d^D x_3\, e^{-ip_{12\mu}x_{12}^{\mu}/\hbar} e^{ip_{13\mu}x_{13}^{\mu}/\hbar} e^{ip_{32\mu}x_{32}^{\mu}/\hbar}$$

$$\times \widehat{W}(X_{12},x_1)[\widehat{W}(x_1,X_{13})\tilde{A}(X_{13},p_{13})\widehat{W}(X_{13},x_3)][\widehat{W}(x_3,X_{32})\tilde{B}(X_{32},p_{32})\widehat{W}(X_{32},x_2)]\widehat{W}(x_2,X_{12})$$

  - Integrand is expanded w.r.t. x_{13}, x_{32} around X_{12}.
  - Wilson loop is evaluated by the Stokes theorem.
    - Nonabelian Stokes theorem for a nonabelian gauge field

      Aref'eva, Theor. Math. Phys. **43**, 353 (1980);

      Bralić, PRD **22**, 3090 (1980).



- Dyson equation $(\tilde{\mathcal{L}} - \tilde{\Sigma}) \star \tilde{G} = 1$

Moyal product

- Minimum for calculating spin torques

$$\tilde{A} \star \tilde{B} = \tilde{A}\tilde{B} + (i\hbar/2)\mathcal{P}_D\left(\tilde{A},\tilde{B}\right) + (i\hbar/2)\mathcal{P}_\mathcal{F}\left(\tilde{A},\tilde{B}\right) + (i\hbar/2)^2\mathcal{P}_{D*\mathcal{F}}\left(\tilde{A},\tilde{B}\right)$$

$$\mathcal{P}_D\left(\tilde{A},\tilde{B}\right) = \partial_{X^\lambda}\tilde{A}\partial_{p_\lambda}\tilde{B} - \partial_{p_\lambda}\tilde{A}\partial_{X^\lambda}\tilde{B}$$

U(1) field strength

$$\mathcal{P}_\mathcal{F}\left(\tilde{A},\tilde{B}\right) = \mathcal{F}_{\mu\nu}\partial_{p_\mu}\tilde{A}\partial_{p_\nu}\tilde{B}$$

$$\mathcal{P}_{D*\mathcal{F}}\left(\tilde{A},\tilde{B}\right) = \mathcal{F}_{\mu\nu}\left(\partial_{X^\lambda}\partial_{p_\mu}\tilde{A}\partial_{p_\lambda}\partial_{p_\nu}\tilde{B} - \partial_{p_\lambda}\partial_{p_\mu}\tilde{A}\partial_{X^\lambda}\partial_{p_\nu}\tilde{B}\right)$$

- More for something

$$\tilde{A} \star \tilde{B} = \cdots + (1/2!)(i\hbar/2)^2\mathcal{P}_{D^2}\left(\tilde{A},\tilde{B}\right) + (1/2!)(i\hbar/2)^2\mathcal{P}_{\mathcal{F}^2}\left(\tilde{A},\tilde{B}\right)$$

$$\mathcal{P}_{D^2}\left(\tilde{A},\tilde{B}\right) = \partial_{X^\lambda}\partial_{X^\kappa}\tilde{A}\partial_{p_\lambda}\partial_{p_\kappa}\tilde{B} - 2\partial_{X^\lambda}\partial_{p_\kappa}\tilde{A}\partial_{p_\lambda}\partial_{X^\kappa}\tilde{B} + \partial_{p_\lambda}\partial_{p_\kappa}\tilde{A}\partial_{X^\lambda}\partial_{X^\kappa}\tilde{B}$$

$$\mathcal{P}_{\mathcal{F}^2}\left(\tilde{A},\tilde{B}\right) = \mathcal{F}_{\mu\nu}\mathcal{F}_{\rho\sigma}\partial_{p_\mu}\partial_{p_\rho}\tilde{A}\partial_{p_\nu}\partial_{p_\sigma}\tilde{B}$$

more terms up to 4th. order w.r.t. x_{13}, x_{32} for a nonabelian field strength

Perturbation theory of Green's function

- Dyson equation $\left(\tilde{\mathcal{L}} - \tilde{\Sigma}\right) \star \tilde{G} = 1$

$$\tilde{A} \star \tilde{B} = \tilde{A}\tilde{B} + (i\hbar/2)\mathcal{P}_D\left(\tilde{A}, \tilde{B}\right) + (i\hbar/2)\mathcal{P}_{\mathcal{F}}\left(\tilde{A}, \tilde{B}\right) + (i\hbar/2)^2\mathcal{P}_{D*\mathcal{F}}\left(\tilde{A}, \tilde{B}\right)$$

$$\tilde{G} = \tilde{G}_0 + (\hbar/2)\tilde{G}_D + (\hbar/2)\tilde{G}_{\mathcal{F}} + (\hbar/2)^2\tilde{G}_{D*\mathcal{F}}$$

$$\tilde{\Sigma} = \tilde{\Sigma}_0 + (\hbar/2)\tilde{\Sigma}_D + (\hbar/2)\tilde{\Sigma}_{\mathcal{F}} + (\hbar/2)^2\tilde{\Sigma}_{D*\mathcal{F}}$$

STT and β-term

SOT

Spin renormalization
Gilbert damping

- First-principles formula $(P = D, \mathcal{F})$

$$\tilde{G}_0^{-1}\tilde{G}_P = \tilde{\Sigma}_P\tilde{G}_0 - i\mathcal{P}_P\left(\tilde{G}_0^{-1}, \tilde{G}_0\right)$$

$$\tilde{G}_0^{-1}\tilde{G}_{P*Q} = \tilde{\Sigma}_{P*Q}\tilde{G}_0 + \left[\tilde{\Sigma}_Q\tilde{G}_P + i\mathcal{P}_P\left(\tilde{\Sigma}_Q, \tilde{G}_0\right) - i\mathcal{P}_P\left(\tilde{G}_0^{-1}, \tilde{G}_Q\right) + (P \leftrightarrow Q)\right] - i^2\mathcal{P}_{P*Q}\left(\tilde{G}_0^{-1}, \tilde{G}_0\right)$$

- Advantages
  - Deals with spacetime gradient and field strength on an equal footing
  - Guarantees gauge covariance
  - Contains retarded, advanced and lesser Green's functions

    → Spin expectation value is available from the above formula.

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Benchmark: textured ferromagnet w/o SOIs

- Hamiltonian $\mathcal{H}(X,\vec{p}) = \vec{p}^2/2m - J\,\vec{n}(X)\cdot\vec{\sigma}$
- Impurities by the self-consistent Born approximation
  - Nonmagnetic $v_\mathrm{i}\delta(\vec{X}-\vec{X}_{\mathrm{i}j})$
  - Magnetic $v_\mathrm{s}\vec{m}_j\cdot\vec{\sigma}\delta(\vec{X}-\vec{X}_{\mathrm{s}j})$; otherwise $\alpha=\beta=0$.
- What we calculate
  - Spin torques $\vec{\tau}=\vec{n}\times J\langle\vec{\sigma}\rangle$
  - Spin expectation value

$$\langle\vec{\sigma}\rangle(X) = \pm i\hbar\int\frac{d\xi}{2\pi\hbar}\boxed{\int\frac{d^3p}{(2\pi\hbar)^3}\mathrm{tr}}[\vec{\sigma}G^<(X,\xi,\vec{p})]$$

    - Momentum integral and spin trace are carried out during the self-consistent calculation of the self-energy.

Spin renormalization and Gilbert damping

- 1st. order w.r.t. time gradient ∂_{X^0}

$$\mathcal{P}_P^{IJ}\left(\tilde{A},\tilde{B}\right) \equiv \eta_P^{IJ}\partial_I\tilde{A}\partial_J\tilde{B}$$
$$\eta_D^{X^\mu p_\nu} = -\eta_D^{p_\nu X^\mu} = \delta_\nu^\mu$$
$$\eta_{\mathcal{F}}^{p_\mu p_\nu} = \mathcal{F}_{\mu\nu}$$

$$\tilde{G}_0^{-1}\tilde{G}_P = \tilde{\Sigma}_P\tilde{G}_0 - i\eta_P^{IJ}\partial_I\tilde{G}_0^{-1}\partial_J\tilde{G}_0$$

- Lesser Green's function

$$G_P^< = \pm\left[\left(G_P^{\mathrm{R}} - G_P^{\mathrm{A}}\right)f(-p_0) + G_P^{<(1)}f'(-p_0)\right]$$

$$\left(G_0^{\mathrm{R}}\right)^{-1}G_P^{\mathrm{R}} = \Sigma_P^{\mathrm{R}}G_0^{\mathrm{R}} - i\eta_P^{IJ}\partial_I\left(G_0^{\mathrm{R}}\right)^{-1}\partial_J G_0^{\mathrm{R}}$$

Fermi-surface terms only for ∂_{X^0} or $\mathcal{F}_{j0}$

$$\left(G_0^{\mathrm{R}}\right)^{-1}G_P^{<(1)} = \Sigma_P^{<(1)}G_0^{\mathrm{A}} + i\eta_P^{Ip_0}\left\{\partial_I\left(G_0^{\mathrm{R}}\right)^{-1}\left(G_0^{\mathrm{R}} - G_0^{\mathrm{A}}\right) - \left[\left(G_0^{\mathrm{R}}\right)^{-1} - \left(G_0^{\mathrm{A}}\right)^{-1}\right]\partial_I G_0^{\mathrm{A}}\right\}$$

- Example of calculation

Momentum integral

$$g_D^{\mathrm{R}}(X,\xi) = g_{D2}^{\mathrm{R}}(\xi)\vec{n}(X)\times\dot{\vec{n}}(X)\cdot\vec{\sigma}$$

Contribution to spin renormalization

$$g_{D2}^{\mathrm{R}}(\xi) = A(\xi)\Sigma_{D2}^{\mathrm{R}}(\xi) + B(\xi)$$

$$\Sigma_{D2}^{\mathrm{R}}(\xi) = (\gamma_{\mathrm{i}} - \gamma_{\mathrm{s}}/3)g_{D2}^{\mathrm{R}}(\xi)$$

$\gamma_{\mathrm{i}} \propto n_{\mathrm{i}}v_{\mathrm{i}}^2, \gamma_{\mathrm{s}} \propto n_{\mathrm{s}}v_s^2$

STT and β-term

- 2nd. order w.r.t. space gradient ∂_{X^i} and electric field $\mathcal{F}_{j0}$
- Lesser Green's function

$$G^{<}_{P*Q} = \pm\left[\left(G^{\mathrm{R}}_{P*Q} - G^{\mathrm{A}}_{P*Q}\right)f(-p_0) + G^{<(1)}_{P*Q} f'(-p_0) + G^{<(2)}_{P*Q} f''(-p_0)\right]$$

$$\left(G^{\mathrm{R}}_0\right)^{-1} G^{\mathrm{R}}_{P*Q} = \Sigma^{\mathrm{R}}_{P*Q} G^{R}_0 + \left[\Sigma^{\mathrm{R}}_Q G^{\mathrm{R}}_P + i\eta^{IJ}_P \partial_I \Sigma^{\mathrm{R}}_Q \partial_J G^{\mathrm{R}}_0 - i\eta^{IJ}_P \partial_I \left(G^{\mathrm{R}}_0\right)^{-1} \partial_J G^{\mathrm{R}}_Q + (P \leftrightarrow Q)\right] + \eta^{IJ}_P \eta^{KL}_Q \partial_I \partial_K \left(G^{\mathrm{R}}_0\right)^{-1} \partial_J \partial_L G^{\mathrm{R}}_0$$

$$\left(G^{\mathrm{R}}_0\right)^{-1} G^{<(1)}_{P*Q} = \Sigma^{<(1)}_{P*Q} G^{\mathrm{A}}_0 + \Sigma^{\mathrm{R}}_Q G^{<(1)}_P + (\Sigma^{<(1)}_Q G^{\mathrm{A}}_P + i\eta^{IJ}_P \partial_I \Sigma^{<(1)}_Q \partial_J G^{\mathrm{A}}_0 - i\eta^{Ip_0}_P [\partial_I \Sigma^{\mathrm{R}}_Q (G^{\mathrm{R}}_0 - G^{\mathrm{A}}_0) - (\Sigma^{\mathrm{R}}_Q - \Sigma^{\mathrm{A}}_Q) \partial_I G^{\mathrm{A}}_0] - i\eta^{IJ}_P \partial_I \left(G^{\mathrm{R}}_0\right)^{-1} \partial_J G^{<(1)}_Q + i\eta^{Ip_0}_P \left\{\partial_I \left(G^{\mathrm{R}}_0\right)^{-1} \left(G^{\mathrm{R}}_Q - G^{\mathrm{A}}_Q\right) - \left[\left(G^{\mathrm{R}}_0\right)^{-1} - \left(G^{\mathrm{A}}_0\right)^{-1}\right] \partial_I G^{\mathrm{A}}_Q\right\} - \eta^{Ip_0}_P \eta^{KL}_Q \left\{\partial_I \partial_K \left(G^{\mathrm{R}}_0\right)^{-1} \partial_L \left(G^{\mathrm{R}}_0 - G^{\mathrm{A}}_0\right) + \partial_L \left[\left(G^{\mathrm{R}}_0\right)^{-1} - \left(G^{\mathrm{A}}_0\right)^{-1}\right] \partial_I \partial_K G^{\mathrm{A}}_0\right\} + (P \leftrightarrow Q))$$

Momentum integral

- Example of calculation

Contribution to β-term

$$g^{\mathrm{R}}_{D*\mathcal{F}}(\vec{X}, \xi) = g^{\mathrm{R}}_{D*\mathcal{F}1}(\xi) \mathcal{F}_{i0} \partial_{X^i} \vec{n}(\vec{X}) \cdot \vec{\sigma}/m$$

$$g^{\mathrm{R}}_{D*\mathcal{F}1}(\xi) = C(\xi) \Sigma^{\mathrm{R}}_{D*\mathcal{F}1}(\xi) + D(\xi)$$

$$\Sigma^{\mathrm{R}}_{D*\mathcal{F}1}(\xi) = (\gamma_{\mathrm{i}} - \gamma_{\mathrm{s}}/3) g^{\mathrm{R}}_{D*\mathcal{F}1}(\xi)$$

Chemical-potential dependence $\vec{\tau} = \vec{n} \times J\langle\vec{\sigma}\rangle$

$$\vec{\tau} = -\frac{\hbar}{4\pi^2}\left(\frac{2mJ}{\hbar^2}\right)^{3/2}[\tau_{\mathrm{ren}} + \tau_\alpha \vec{n}\times]\dot{\vec{n}} - \frac{1}{4\pi^2}\left(\frac{2mJ}{\hbar^2}\right)^{1/2}\mathcal{F}_{i0}[\tau_{\mathrm{STT}} + \tau_\beta \vec{n}\times]\partial_{X^i}\vec{n}$$

$$\tau_{ren} = J^{-1/2}\int d\xi \left\{ f(\xi)[-\Im g^R_{D2}(\xi)] - [-f'(\xi)]\left[i g^{<(1)}_{D2}/2 \right] \right\}$$

$$\tau_\alpha = J^{-1/2}\int d\xi [-f'(\xi)]\left[i g^{<(1)}_{D1}(\xi)/2 \right]$$

$$\tau_{\mathrm{STT}} = J^{1/2}\int d\xi [-f'(\xi)]\left[g^{<(1)}_{D*\mathcal{F}2}(\xi)/2i \right]$$

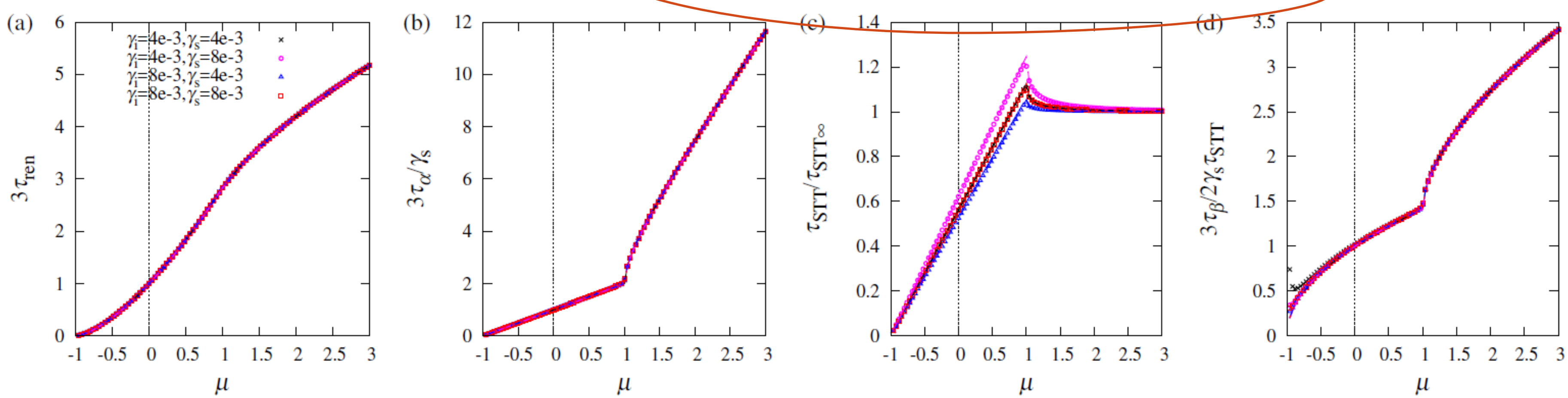
$$\tau_\beta = -J^{1/2}\int d\xi \left\{ f(\xi)[-\Im g^R_{D*\mathcal{F}1}(\xi)] + [-f'(\xi)]\left[g^{<(1)}_{D*\mathcal{F}1}/2i \right] \right\}$$

Fermi-sea term of $G^<_D$

Fermi-surface term of $G^<_D$

Fermi-surface term of $G^<_{D*\mathcal{F}}$

Fermi-sea term of $G^<_{D*\mathcal{F}}$



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Summary

- Gradient expansion: Wilson line → Wigner representation
  - Perturbation theory w.r.t. spacetime gradient and field strength
  - Explicit gauge covariance
- Application to spin torques
  - Spin renormalization and Gilbert damping

    ← 1st. order w.r.t time gradient
  - SOT ← 1st. order w.r.t. electric field
  - STT and β-term ← 2nd. order w.r.t. space gradient and electric field