

# Quantum, kinetic and hydrodynamic descriptions on spin transfer torque

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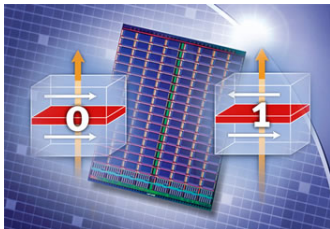
Joint work with  
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# Outline

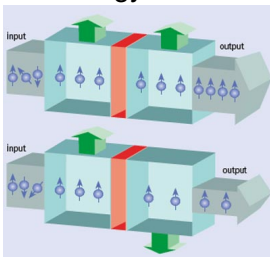
- 1 Motivation and introduction
- 2 STT model by moment system
- 3 Numerical comparison with Diffusion model
- 4 Formal connections between models at different level
- 5 Conclusion and future works

## ● Application<sup>1</sup>



- Magnetic recording devices: audio, video.
- Computer storage: floppy disks, hard disks.
- Magnetic Memory: Magnetoresistance Random Access Memory (MRAM).

## ● Methodology for detecting the orientation<sup>2</sup>



Julliere's model:

Constant tunneling matrix

$$\text{TMR} \equiv \frac{G_{\text{AP}} - G_{\text{P}}}{G_{\text{AP}}} = \frac{2P_{\text{L}}P_{\text{R}}}{1 - P_{\text{L}}P_{\text{R}}}$$

$$P_{\text{L}} = \frac{n_{\text{L}}^{\uparrow} - n_{\text{L}}^{\downarrow}}{n_{\text{L}}^{\uparrow} + n_{\text{L}}^{\downarrow}} \quad P_{\text{R}} = \frac{n_{\text{R}}^{\uparrow} - n_{\text{R}}^{\downarrow}}{n_{\text{R}}^{\uparrow} + n_{\text{R}}^{\downarrow}}$$

<sup>1</sup>Science@Berkeley Lab: The Current Spin on Spintronics

<sup>2</sup><http://ducthe.wordpress.com/category/spintronics/>

# The key is to control the relative orientation

- Spin transfer torque (STT) <sup>3</sup>



- Two layers of different thickness: different switching fields.
- The thin film is switched, and the resistance measured.

- Literature and references

- Proposed independently by Berger (1996) and Slonczewski (1996).
- Theoretical and experimental studies: Bazaliy et al., 1998; Tsoi et al., 1998; Myers et al., 1999; Sun, 2000; Waintal et al. 2000; Stiles and Zangwill, 2002; Zhang et al. 2002; Zutic et al. 2004 (Review); ...

<sup>3</sup>[http://www.wpi-aimr.tohoku.ac.jp/miyazaki\\_lab/spintorque.htm](http://www.wpi-aimr.tohoku.ac.jp/miyazaki_lab/spintorque.htm)



## Model equations – Magnetization

- Landau-Lifshitz-Gilbert (LLG) equation

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma \mathbf{M} \times (\mathbf{h}_e + \mathbf{cs}) + \alpha \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t},$$

where the first term is precession, and the second is Gilbert damping term.

- The effective field  $\mathbf{h}_e$  is defined as

$$\mathbf{h}_e = -\frac{2K_u}{M_s} (m_2 \mathbf{e}_2 + m_3 \mathbf{e}_3) + \frac{2C_{ex}}{M_s} \Delta \mathbf{M} + \mathbf{M} u_0 (\mathbf{h}_s + \mathbf{h}_0),$$

- The stray field,  $\mathbf{h}_s = -\nabla u$  is obtained by solving the magnetostatic equation:

$$\Delta u = \operatorname{div} \mathbf{M}, \quad \mathbf{x} \in \Omega, \quad \Delta u = 0, \quad \mathbf{x} \in \bar{\Omega}^c,$$

with jump boundary conditions

$$[u]_{\partial\Omega} = 0, \quad \left[ \frac{\partial u}{\partial \nu} \right]_{\partial\Omega} = -\mathbf{M} \cdot \nu.$$

## Model equations – Spin<sup>4</sup>

- Quantum (Schrödinger equation)

$$i\hbar \frac{\partial \psi}{\partial t} = \left( \left( -\frac{\hbar^2}{2m} \nabla_{\mathbf{x}}^2 + V(\mathbf{x}) \right) \hat{\mathbf{I}} + \frac{\mu_B}{2} \hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t) \right) \psi.$$

- Kinetic (Boltzmann equation)

$$\begin{aligned} \partial_t \mathbf{W}(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{W}(\mathbf{x}, \mathbf{v}, t) - \frac{e}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} \mathbf{W}(\mathbf{x}, \mathbf{v}, t) \\ + \frac{i}{2\hbar} [\mu_B \hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t), \mathbf{W}(\mathbf{x}, \mathbf{v}, t)] = -\frac{\mathbf{W} - \bar{\mathbf{W}}}{\tau} - \frac{2}{\tau_{sf}} (\bar{\mathbf{W}} - \frac{\hat{\mathbf{I}}}{2} \text{Tr} \bar{\mathbf{W}}) \end{aligned}$$

- Hydrodynamic (Diffusion equation)

$$\begin{aligned} \frac{\partial \mathbf{s}}{\partial t} &= -\text{div} \mathbf{J}_s - 2D_0(\mathbf{x}) \frac{\mathbf{s}}{\lambda_{sf}^2} - 2D_0(\mathbf{x}) \frac{\mathbf{s} \times \mathbf{M}}{\lambda_J^2}, \\ \mathbf{J}_s &= \frac{\beta \mu_B}{e} \mathbf{M} \otimes \mathbf{J}_e - 2D_0(\mathbf{x}) [\nabla \mathbf{s} - \beta \beta' \mathbf{M} \otimes (\nabla \mathbf{s} \cdot \mathbf{M})]. \end{aligned}$$

<sup>4</sup>Piechon and Thiaville, PRB 2007, Gaspari, PR 1966, Zhang, Levy and Fert, PRL 2002

# Ambitious goals

- Set up the connections of the models at different levels of physics.
- Develop new models based on moment system.
- Design efficient numerical algorithms that can capture physical details at different scales.

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## Spin-orbital decomposition

Define  $\boldsymbol{\sigma} = \sigma_x \hat{\mathbf{i}} + \sigma_y \hat{\mathbf{j}} + \sigma_z \hat{\mathbf{k}}$ , where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$$\mathbf{W} = w\mathbf{I} + \hat{\boldsymbol{\sigma}} \cdot \mathbf{w},$$

where  $w$  is the orbital part and  $\mathbf{w}$  is the spin part.

Macroscopic quantities

$$\text{charge density} \quad n(\mathbf{x}, t) = \int_{\mathbb{R}^3} \text{Tr} \mathbf{W} d\mathbf{v},$$

$$\text{charge current density} \quad \mathbf{j}_n(\mathbf{x}, t) = \int_{\mathbb{R}^3} \mathbf{v} \text{Tr}(\mathbf{W}) d\mathbf{v},$$

$$\text{spin density} \quad \mathbf{m}(\mathbf{x}, t) = \int_{\mathbb{R}^3} \text{Tr}(\hat{\boldsymbol{\sigma}} \mathbf{W}) d\mathbf{v},$$

$$\text{spin current density} \quad \mathbf{j}_m(\mathbf{x}, t) = \int_{\mathbb{R}^3} \mathbf{v} \otimes \text{Tr}(\hat{\boldsymbol{\sigma}} \mathbf{W}) d\mathbf{v}.$$

## Equations for $w$ and $\mathbf{w}$

$$\begin{aligned} \partial_t w + \mathbf{v} \cdot \nabla_{\mathbf{x}} w - \frac{e}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} w &= -\frac{w - \bar{w}}{\tau}, \\ \partial_t(\hat{\boldsymbol{\sigma}} \cdot \mathbf{w}) + \mathbf{v} \cdot \nabla_{\mathbf{x}}(\hat{\boldsymbol{\sigma}} \cdot \mathbf{w}) - \frac{e}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}}(\hat{\boldsymbol{\sigma}} \cdot \mathbf{w}) - \frac{\mu_B}{\hbar} \hat{\boldsymbol{\sigma}} \cdot (\mathbf{M} \times \mathbf{w}) \\ &= -\frac{(\hat{\boldsymbol{\sigma}} \cdot \mathbf{w}) - \overline{(\hat{\boldsymbol{\sigma}} \cdot \mathbf{w})}}{\tau} - \frac{2}{\tau_{\text{sf}}} \overline{(\hat{\boldsymbol{\sigma}} \cdot \mathbf{w})}, \end{aligned}$$

where we have used the fact

$$\frac{i}{2\hbar} [\mu_B \hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t), \mathbf{W}(\mathbf{x}, \mathbf{v}, t)] = -\frac{\mu_B}{\hbar} \hat{\boldsymbol{\sigma}} \cdot (\mathbf{M} \times \mathbf{w}).$$

Equations live in **6-dimension**, which creates numerical difficulties.

**Alternative: to develop and solve the moment system.**

# Hierarchical moment system

$$\partial_t n(\mathbf{x}, t) + \nabla \cdot \mathbf{j}_n(\mathbf{x}, t) = 0,$$

$$\partial_t \mathbf{j}_n(\mathbf{x}, t) + \int_{\mathbb{R}^3} (\mathbf{v} \otimes \mathbf{v}) \cdot \nabla w(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} + \frac{e}{m} \mathbf{E} n(\mathbf{x}, t) = -\frac{\mathbf{j}_n(\mathbf{x}, t)}{\tau},$$

$$\partial_t \mathbf{m}(\mathbf{x}, t) + \nabla \cdot \mathbf{j}_m(\mathbf{x}, t) - \frac{\mu_B}{\hbar} \mathbf{M} \times \mathbf{m} = -\frac{\mathbf{m}(\mathbf{x}, t)}{\tau_{\text{sf}}},$$

$$\begin{aligned} \partial_t \mathbf{j}_m(\mathbf{x}, t) + \int_{\mathbb{R}^3} (\mathbf{v} \otimes \mathbf{v}) \cdot \nabla w(\mathbf{x}, \mathbf{v}, t) d\mathbf{v} + \frac{e}{m} \mathbf{E} \otimes \mathbf{m}(\mathbf{x}, t) \\ - \frac{\mu_B}{\hbar} \varepsilon_{jkl} \mathbf{M}_k (\mathbf{j}_m)_{il}(\mathbf{x}, t) = -\frac{\mathbf{j}_m(\mathbf{x}, t)}{\tau}. \end{aligned}$$

**Unclosed!** Need equations of state for the second order moments.

## Closure assumption

- Assumption I.

$$w(\mathbf{x}, \mathbf{v}, t) \approx \beta_0 n(\mathbf{x}, t) + \beta'_0 \mathbf{M} \cdot \mathbf{m}(\mathbf{x}, t) + \beta_1 \cdot \mathbf{v} n_1(\mathbf{x}, t) + \beta'_1 \mathbf{v} \cdot \mathbf{m}_1(\mathbf{x}, t),$$

then the charge current equation becomes

$$\begin{aligned} \partial_t \mathbf{j}_n(\mathbf{x}, t) + \beta_0 \overline{v^2} \nabla_{\mathbf{x}} n(\mathbf{x}, t) + \beta'_0 \overline{v^2} \nabla_{\mathbf{x}} \mathbf{m}(\mathbf{x}, t) \mathbf{M} \\ + \frac{e}{m} \mathbf{E} n(\mathbf{x}, t) = -\frac{\mathbf{j}_n(\mathbf{x}, t)}{\tau}. \end{aligned}$$

- Assumption II.

$$w(\mathbf{x}, \mathbf{v}, t) \approx \beta \mathbf{M} n(\mathbf{x}, t) + \beta' \mathbf{m}(\mathbf{x}, t) + \beta_2 \mathbf{v} n_1(\mathbf{x}, t) + \beta'_2 \mathbf{v} (\mathbf{M} \cdot \mathbf{m}_1(\mathbf{x}, t)),$$

then the spin current equation becomes

$$\begin{aligned} \partial_t \mathbf{j}_m(\mathbf{x}, t) + \beta \overline{v^2} \nabla_{\mathbf{x}} n(\mathbf{x}, t) \otimes \mathbf{M} + \beta' \overline{v^2} \nabla_{\mathbf{x}} \mathbf{m}(\mathbf{x}, t) \\ + \frac{e}{m} \mathbf{E} \otimes \mathbf{m}(\mathbf{x}, t) - \frac{\mu_B}{\hbar} \varepsilon_{jkl} \mathbf{M}_k (\mathbf{j}_m)_{il}(\mathbf{x}, t) = -\frac{\mathbf{j}_m(\mathbf{x}, t)}{\tau}. \end{aligned}$$



## Motivation for the assumption

- Introduce the spin-orbital coupling in the moment system.
- Quasistatic approximation for the current equations yields

$$\mathbf{j}_n(\mathbf{x}, t) = -\frac{e}{m}\tau \mathbf{E} n(\mathbf{x}, t) - \beta_0 \overline{v^2} \tau \nabla_{\mathbf{x}} n(\mathbf{x}, t) - \beta'_0 \overline{v^2} \tau \nabla_{\mathbf{x}} \mathbf{m}(\mathbf{x}, t) \mathbf{M},$$

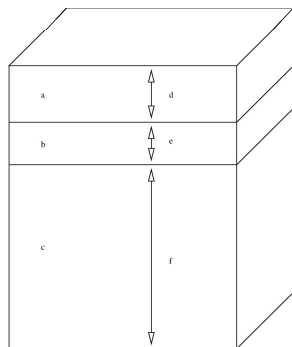
$$\mathbf{j}_m(\mathbf{x}, t) = -\frac{e}{m}\tau \mathbf{E} \otimes \mathbf{m}(\mathbf{x}, t) - \beta \overline{v^2} \tau \nabla_{\mathbf{x}} n(\mathbf{x}, t) \otimes \mathbf{M} + \frac{\mu_B}{\hbar} \varepsilon_{jkl} \mathbf{M}_k (\mathbf{j}_m)_{il}(\mathbf{x}, t) - \beta' \overline{v^2} \tau \nabla_{\mathbf{x}} \mathbf{m}(\mathbf{x}, t).$$

This is consistent with the linear response relation used in Zhang, Levy and Fert (PRL 2002) except the term in red.

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# Experiment setup



**Figure:** Device. From Bottom to Top: FM1 ( $128 \times 64 \times 200\text{nm}^3$ ); Spacer ( $128 \times 64 \times 20\text{nm}^3$ ); FM2 ( $128 \times 64 \times 60\text{nm}^3$ ).  $\mathbf{j}_n$  is applied from FM1 to FM2.

# Several locally stable states

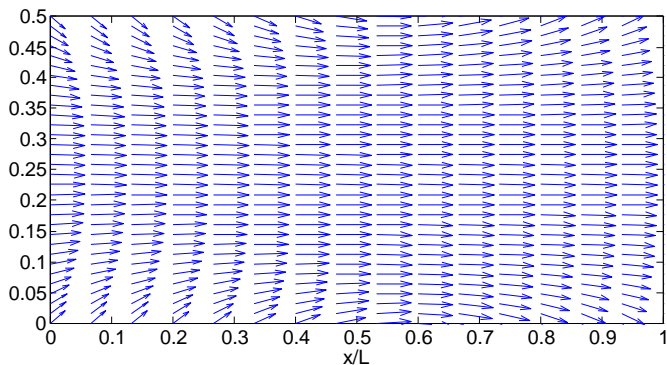


Figure: State 1

# Several locally stable states

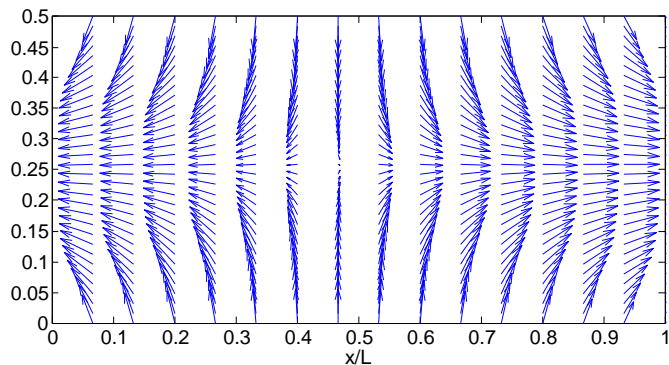


Figure: State 2

# Several locally stable states

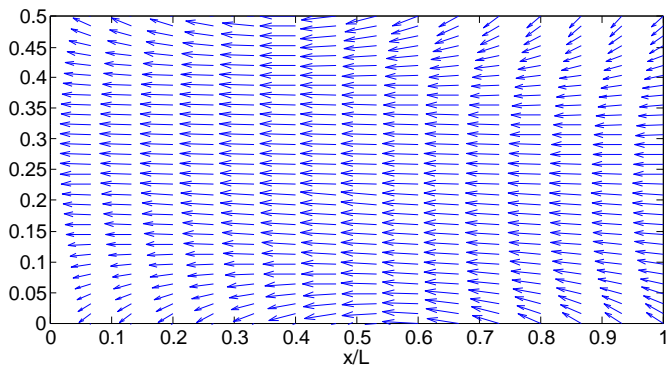


Figure: State 3

## Comparison results

$$\mathbf{j}_m = \frac{\beta\mu_B}{e} \mathbf{j}_n \otimes \mathbf{M} - 2D_0(\mathbf{x})[\nabla \mathbf{m} - \beta\beta'(\nabla \mathbf{m} \cdot \mathbf{M}) \otimes \mathbf{M}]$$

$$\mathbf{j}_m \mathbf{A}(\mathbf{M}) = \frac{\beta\mu_B}{e} \mathbf{j}_n \otimes \mathbf{M} - 2D_0(\mathbf{x})[\nabla \mathbf{m} - \beta\beta'(\nabla \mathbf{m} \cdot \mathbf{M}) \otimes \mathbf{M}]$$

where

$$\mathbf{A}(\mathbf{M}) = \begin{pmatrix} 1 & -M_3 & M_2 \\ M_3 & 1 & -M_1 \\ -M_2 & M_1 & 1 \end{pmatrix}$$

with eigenvalues  $1, 1 \pm i$ .

Initial states: random in FM1 and uniform in FM2

## Cont'd

Model	S1	S1→S2	S1→S3	S1→S2
Diffusion	$\leq 7.4$	$7.5 \sim 9.9$	<b>10.0</b>	$\geq 10.1$
Moment	$\leq 9.0$	$9.1 \sim 9.6$	<b>9.7 ~ 10.1</b>	$\geq 10.2$

**Table:** Critical applied current  $j_n$  for switching (unit:  $10^{10}$ As)

A larger admissible window for effective switching by moment model



## Cont'd

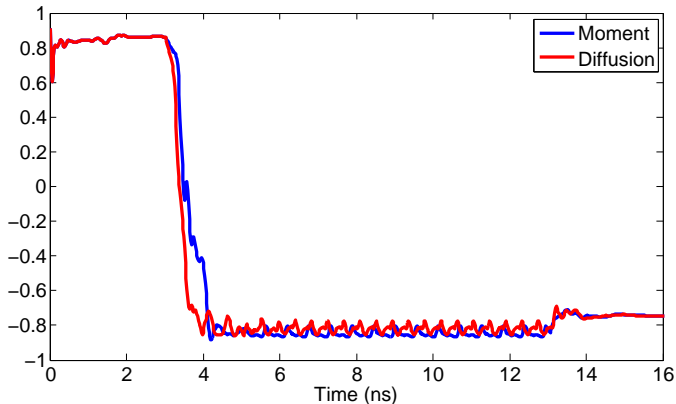


Figure:  $j_n = 10.0 \times 10^{10} \text{As}$

# Cont'd

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## Cont'd

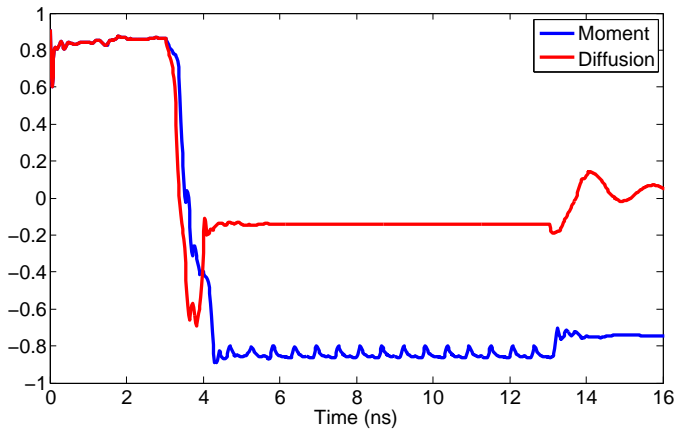


Figure:  $j_n = 9.8 \times 10^{10} \text{As}$

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## From moment system to diffusion<sup>5</sup>

- For a clearer illustration, forget the coupling term for the current moment, and rescale the moment system as follows,

$$\varepsilon \partial_t \mathbf{m}(x, t) + \partial_x \mathbf{j}_m(x, t) - \varepsilon \mathbf{M} \times \mathbf{m} = -\varepsilon \mathbf{m}(x, t),$$

$$\varepsilon \partial_t \mathbf{j}_m(x, t) + \overline{v^2} \partial_x \mathbf{m}(x, t) - E \mathbf{m}(x, t) - \frac{\mathbf{M} \times \mathbf{j}_m(x, t)}{\varepsilon} = -\frac{\mathbf{j}_m(x, t)}{\varepsilon}.$$

- Apply the following asymptotic expansion

$$\mathbf{m} = \mathbf{m}^0 + \varepsilon \mathbf{m}^1 + \varepsilon^2 \mathbf{m}^2 + \dots,$$

$$\mathbf{j}_m = \mathbf{j}_m^0 + \varepsilon \mathbf{j}_m^1 + \varepsilon^2 \mathbf{j}_m^2 + \dots.$$

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<sup>5</sup>A field with very rich literature: Bardos, Golse, Levermore, Degond, Ben Abdallah, Gamba, Jin, ...

To the leading order, we have the diffusion equation,

$$\begin{aligned}
 2\partial_t \mathbf{m} - (\mathbf{M} \cdot \partial_t \mathbf{m}) \mathbf{M} &= \overline{v^2} \partial_{x^2} \mathbf{m}(x, t) + \overline{v^2} \mathbf{M} \times \partial_{x^2} \mathbf{m}(x, t) \\
 &\quad - E \partial_x \mathbf{m}(x, t) - E \mathbf{M} \times \partial_x \mathbf{m}(x, t) \\
 &\quad + \mathbf{M} \times \mathbf{m} - \mathbf{m},
 \end{aligned}$$

Assuming  $M$  is uniform and only nonzero in  $z$ -direction,

$$\begin{aligned}
 \partial_t m^z(x, t) + \overline{v^2} \partial_{xx} m^z(x, t) \\
 \quad - E \partial_x m^z(x, t) - M m^z(x, t) &= -m^z(x, t), \\
 \partial_t m^\pm(x, t) - \frac{1}{1 \mp iM} \overline{v^2} \partial_{xx} m^\pm(x, t) \\
 \quad + \frac{1}{1 \mp iM} E \partial_x m^\pm(x, t) - M m^\pm(x, t) &= -m^\pm(x, t).
 \end{aligned}$$

This recovers the diffusion model in Zhang, Levy and Fert (PRL 2002) without the coupling term, which can be also included by a similar procedure on the coupling moment system.

# From Schrödinger to Liouville

In physical units,

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = \hat{\mathbf{H}}(\mathbf{x}, t) \psi(\mathbf{x}, t),$$

where

$$\hat{\mathbf{H}}(\mathbf{x}, t) = \left( -\frac{\hbar^2}{2m} \nabla_{\mathbf{x}}^2 + V(\mathbf{x}) \right) \hat{\mathbf{I}} + \frac{\mu_B}{2} \hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t).$$

What is the correct nondimensional regime?  $\hbar \rightarrow \varepsilon$ ?

Define the Wigner transformation of  $\psi$  as

$$\mathbf{W}(\mathbf{x}, \mathbf{v}, t) = \frac{m^{3/2}}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \psi(\mathbf{x} + \frac{\hbar}{2m}\mathbf{y}, t) \otimes \psi^*(\mathbf{x} - \frac{\hbar}{2m}\mathbf{y}, t) e^{i\mathbf{v}\cdot\mathbf{y}} d\mathbf{y}.$$

To the leading order,

$$\begin{aligned} \partial_t \mathbf{W}(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{W}(\mathbf{x}, \mathbf{v}, t) - \frac{e}{m} \mathbf{E} \cdot \nabla_{\mathbf{v}} \mathbf{W}(\mathbf{x}, \mathbf{v}, t) \\ + \frac{i}{2\hbar} [\mu_B \hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t) \cdot \mathbf{W}(\mathbf{x}, \mathbf{v}, t)] = 0. \end{aligned}$$

Compare the order of the last two terms in physical units<sup>6</sup>,

$$\begin{aligned} \frac{e}{m} \frac{|\mathbf{E}|}{|\bar{\mathbf{v}}|} &\approx \frac{10^{-19} \times 10^5}{10^{-30} \times 5 \times 10^5} \approx 10^{-12} \text{s}^{-1}, \\ \frac{\mu_B}{\hbar} |\mathbf{M}| &\approx \frac{10^{-23}}{10^{-34}} \times 0.1 = 10^{-12} \text{s}^{-1}. \end{aligned}$$

<sup>6</sup>Qi and Zhang, PRB 2003



## Semiclassical regime

Weak spinor term:

$$i\varepsilon \frac{\partial}{\partial t} \psi(\mathbf{x}, t) = \left( \left( -\frac{\varepsilon^2}{2} \nabla_{\mathbf{x}}^2 + V(\mathbf{x}) \right) \hat{\mathbf{I}} + \frac{\varepsilon}{2} \hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t) \right) \psi(\mathbf{x}, t).$$

The rescaled Wigner transform:

$$\mathbf{W}(\mathbf{x}, \mathbf{v}, t) = \frac{1}{(2\pi\varepsilon)^{3/2}} \int_{\mathbb{R}^3} \psi(\mathbf{x} + \frac{\varepsilon}{2} \mathbf{y}, t) \otimes \psi^*(\mathbf{x} - \frac{\varepsilon}{2} \mathbf{y}, t) e^{i\mathbf{v} \cdot \mathbf{y}} d\mathbf{y},$$

which leads to the Liouville equation in the leading order,

$$\begin{aligned} \partial_t \mathbf{W}(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{W}(\mathbf{x}, \mathbf{v}, t) - \mathbf{E} \cdot \nabla_{\mathbf{v}} \mathbf{W}(\mathbf{x}, \mathbf{v}, t) \\ + \frac{1}{2} [\hat{\boldsymbol{\sigma}} \cdot \mathbf{M}(\mathbf{x}, t), \mathbf{W}(\mathbf{x}, \mathbf{v}, t)] = 0. \end{aligned}$$

We still have the **collision term missing** in the picture.

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## ● Summary

- Develop STT model based on moment closure that introduces spin-orbital coupling.
- Numerically study the qualitative difference of moment system model from the diffusion model.
- Preliminary results on the connections of models at different scales.

## ● Future works

- Further understand the connections of different models, e.g. the origin of collision term, the modeling accuracy of moment system in the long time and large space regime.
- Develop multiscale numerical methods, e.g. Heterogeneous Multiscale Method (HMM), Asymptotic Preserving scheme (AP), and domain decomposition method (DD).
- Simulating STT of magnetic devices in experiments.