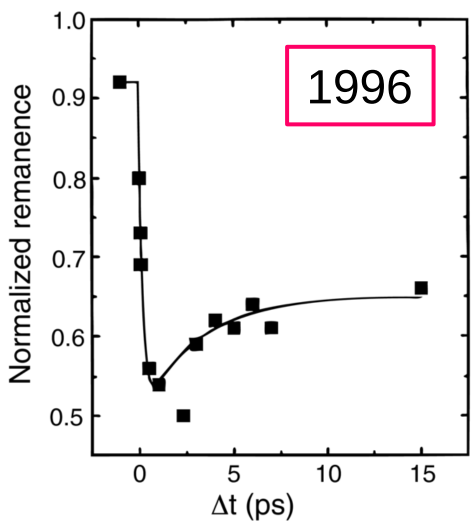
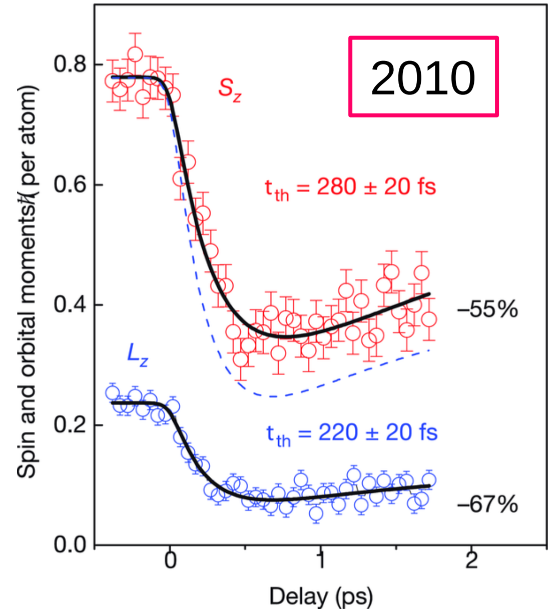
Spin dynamics

- Electrons possess not only an electric charge, but also a **spin**
- **Magnetic nanoparticles** and **films** have been studied for a couple of decades
- Early experiments revealed **ultrafast demagnetization** (≈ 100 fs) of magnetic nanoparticles excited with laser pulses
  - E. Beaurepaire et al. Phys. Rev. Lett. **76**, 4250 (1996).
- More recent results discriminate the **spin** and **orbital** parts of the angular momentum
  - C. Boeglin et al., Nature **465**, 458 (2010).





Spin and quantum mechanics

- The spin arises naturally in **relativistic quantum mechanics**
- **Dirac equation: 4-spinors**

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix} = \begin{pmatrix} \uparrow e^- \\ \downarrow e^- \\ \uparrow e^+ \\ \downarrow e^+ \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix}$$

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = H(t)\Psi(\mathbf{r}, t)$$
$$= \left(c\boldsymbol{\alpha}.\left(\mathbf{p} - e\mathbf{A}(\mathbf{r}, t)\right) + e\Phi(\mathbf{r}, t) + mc^2\beta\right)\Psi(\mathbf{r}, t)$$

- We want to separate the electron and positron components
  - **Foldy–Wouthuysen** transformation (expansion in 1/c) → Two-component spinor:

$$\Psi_\alpha(\boldsymbol{r}, t) = \begin{pmatrix} \psi_\alpha^\uparrow(\boldsymbol{r}, t) \\ \psi_\alpha^\downarrow(\boldsymbol{r}, t) \end{pmatrix}$$

- At lowest order in 1/c, we find the **Schrödinger-Pauli Hamiltonian**

$$H = \frac{(p - eA)^2}{2m} + e\phi + \underbrace{\frac{e\hbar}{2m}\,\sigma \cdot B}_{\text{Zeeman effect}}$$

Higher-order Hamiltonians

- **Second order**

$$\hat{H} = mc^2 + q\phi + \frac{(\hat{p} - qA)^2}{2m} - \overbrace{\frac{(\hat{p} - qA)^4}{8m^3c^2}}^{\text{Relativistic mass}} + \frac{q\hbar}{2m}\boldsymbol{\sigma}\cdot \boldsymbol{B}$$

$$+ \underbrace{\frac{q\hbar^2}{8m^2c^2}\nabla\cdot \boldsymbol{E}}_{\text{Darwin term}} + \underbrace{\frac{q\hbar}{8m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times(\hat{p} - qA) - (\hat{p} - qA)\times \boldsymbol{E})}_{\text{Spin-orbit coupling (SOC)}}$$

- At **third and higher orders**, many more terms couple the electro-magnetic fields with the spin. For instance, the third order term:

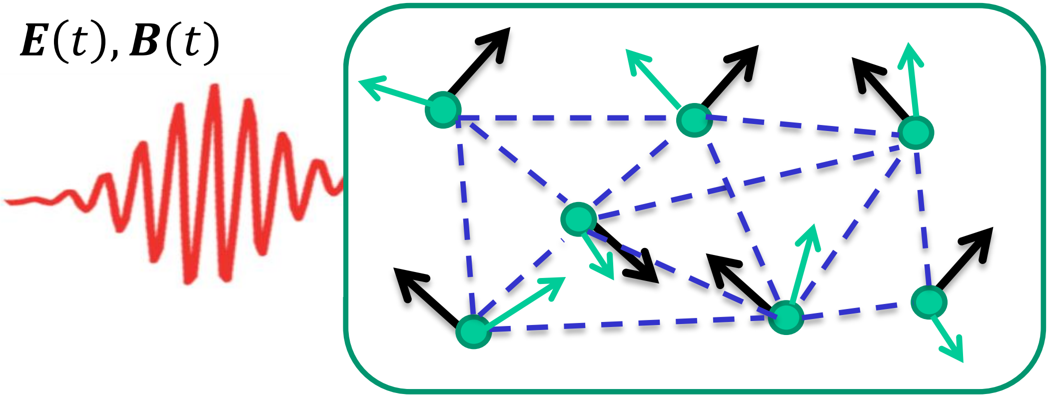
$$\frac{ie\hbar^2}{16m^3c^4}\underline{\boldsymbol{\sigma}\cdot\left(\frac{\partial}{\partial t}\mathbf{E}\wedge(\mathbf{p} - e\mathbf{A})\right.} + (\mathbf{p} - e\mathbf{A})\wedge\left.\frac{\partial}{\partial t}\mathbf{E}\right)$$

These additional terms may explain coherent laser-spin coupling observed in recent experiments.

Y. Hinschberger and P.-A. Hervieux, Phys. Lett. A **376**, 813 (2012)

Many-particle systems — Mean-field theory

- **Goal**: to develop a time-dependent semi-relativistic **mean-field** theory that is based on **two-component** wave functions.



Mean-field theory — Vlasov approach

- We focus on kinetic phase-space models (Vlasov and Wigner)
- The Wigner transform of a Pauli 2-spinor is a 2 X 2 matrix:

$$\mathcal{F}(\boldsymbol{r}, \boldsymbol{v}, t) = \begin{pmatrix} f^{\uparrow\uparrow} & f^{\uparrow\downarrow} \\ f^{\downarrow\uparrow} & f^{\downarrow\downarrow} \end{pmatrix}$$

- It is convenient to switch to the Pauli basis

$$\underbrace{f_0 = \mathrm{tr}(\mathcal{F}) = f^{\uparrow\uparrow} + f^{\downarrow\downarrow},}_{\text{Scalar, representing ordinary phase-space distribution}} \qquad \underbrace{\boldsymbol{f} = \frac{\hbar}{2}\mathrm{tr}\left(\mathcal{F}\boldsymbol{\sigma}\right)}_{\text{Vector, representing spin distribution}}$$

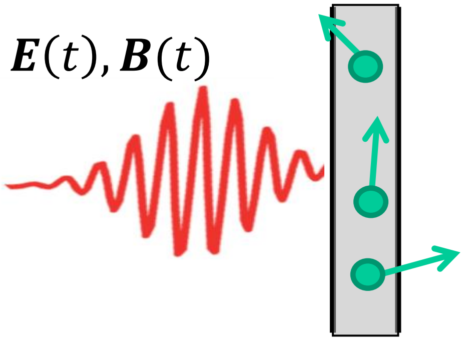
J. Hurst, O. Morandi, G. Manfredi, and P.-A. Hervieux, *Semiclassical Vlasov and fluid models for an electron gas with spin effects*, Eur. Phys. J. D **68**, 176 (2014).

Vlasov equations with spin

- The Wigner equations (at lowest order in 1/c) for the above functions are rather complicated
- In the classical limit, they tend to the **Vlasov equations**:

$$\boxed{\begin{aligned}&\frac{\partial f_0}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} f_0 - \frac{e}{m}(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B})\cdot\boldsymbol{\nabla}_{\boldsymbol{v}} f_0 - \frac{e}{m^2}\sum_i \boldsymbol{\nabla} B_i\cdot\boldsymbol{\nabla}_{\boldsymbol{v}} f_i = 0,\\ &\frac{\partial f_i}{\partial t} + \boldsymbol{v}\cdot\boldsymbol{\nabla} f_i - \frac{e}{m}\left[(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B})\cdot\boldsymbol{\nabla}_{\boldsymbol{v}} f_i - (\boldsymbol{f}\times\boldsymbol{B})_i\right] - \frac{\mu_B\hbar}{2m}\boldsymbol{\nabla} B_i\cdot\boldsymbol{\nabla}_{\boldsymbol{v}} f_0 = 0\end{aligned}} \qquad i = x, y, z$$

- **The dynamics is treated classically, while the spin is fully quantum.**
- The electric and magnetic fields can be either external or self-consistent.
- Extensions to higher orders in 1/c using the above Hamiltonians
- **Next application: electron dynamics in thin films including spin effects**



Including spin-orbit effects (order $1/c^2$)

$$\left\{\begin{aligned}
&\frac{\partial f_0}{\partial t} + \boldsymbol{v}\cdot\nabla f_0 - \frac{e}{m}(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B})\cdot\nabla_{\boldsymbol{v}} f_0 + \frac{\mu_B}{2mc^2}(\boldsymbol{E}\times\nabla)_i f_i \\
&- \frac{\mu_B}{m}\nabla\left[B_i - \left(\frac{\boldsymbol{v}\times\boldsymbol{E}}{2c^2}\right)_i\right]\cdot\nabla_{\boldsymbol{v}} f_i - \frac{\mu_B e}{2m^2c^2}[\boldsymbol{E}\times(\boldsymbol{B}\times\nabla_{\boldsymbol{v}})]_i f_i = 0 \\
&\frac{\partial f_i}{\partial t} + \boldsymbol{v}\cdot\nabla f_i - \frac{e}{m}(\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B})\cdot\nabla_{\boldsymbol{v}} f_i + \frac{\mu_B}{2mc^2}(\boldsymbol{E}\times\nabla)_i f_0 \\
&- \frac{\mu_B}{m}\nabla\left[B_i - \left(\frac{\boldsymbol{v}\times\boldsymbol{E}}{2c^2}\right)_i\right]\cdot\nabla_{\boldsymbol{v}} f_0 - \frac{\mu_B e}{2m^2c^2}[\boldsymbol{E}\times(\boldsymbol{B}\times\nabla_{\boldsymbol{v}})]_i f_0 \\
&- \frac{2\mu_B}{\hbar}\left\{\left[\boldsymbol{B} - \frac{1}{2c^2}(\boldsymbol{v}\times\boldsymbol{E})\right]\times\boldsymbol{f}\right\}_i = 0.
\end{aligned}\right.$$

$$\left\{\begin{aligned}
&\rho = -e\int f_0\, d\boldsymbol{v}, \qquad \boldsymbol{j} = -e\left[\int \boldsymbol{v} f_0\, d\boldsymbol{v} + \frac{\boldsymbol{E}\times\boldsymbol{M}}{2mc^2}\right] \\
&\boldsymbol{M} = -\mu_B\int \boldsymbol{f}\, d\boldsymbol{v}, \qquad \boldsymbol{P} = -\frac{\mu_B}{2c^2}\int \boldsymbol{v}\times\boldsymbol{f}\, d\boldsymbol{v}
\end{aligned}\right.$$

Relativistic corrections on the sources

J. Hurst, P.-A. Hervieux, G. Manfredi, Phil. Trans. R. Soc. A **375**(2092), 20160199 (2017).

A Dixit, Y. Hinschberger, J. Zamanian, G. Manfredi, et P.-A Hervieux, Phys. Rev. A 88, 032117 (2013).

Spin hydrodynamic model

- Compute **velocity moments** of the above Vlasov equations

$$n(\boldsymbol{r},t) = \sum_{\mu} \left|\Psi_{\mu}^{\dagger}(\boldsymbol{r},t)\right|^2 = \int f_0(\boldsymbol{r},\boldsymbol{v},t)d\boldsymbol{v},$$ Particle density

$$\boldsymbol{S}(\boldsymbol{r},t) = \frac{\hbar}{2}\sum_{\mu} \Psi_{\mu}^{\dagger}(\boldsymbol{r},t)\boldsymbol{\sigma}\Psi_{\mu}(\boldsymbol{r},t) = \int \boldsymbol{f}(\boldsymbol{r},\boldsymbol{v},t)d\boldsymbol{v}.$$ Spin density

$$\boldsymbol{u} = \frac{1}{n}\int \boldsymbol{v} f_0 d\boldsymbol{v},$$ Mean velocity

$$J_{i\alpha}^{S} = \int v_i f_\alpha d\boldsymbol{v},$$ Spin current (spin-velocity tensor)

$$P_{ij} = m\int w_i w_j f_0 d\boldsymbol{v},$$ Kinetic pressure

$$\Pi_{ij\alpha} = m\int v_i v_j f_\alpha d\boldsymbol{v},$$ Spin pressure (spin-pressure tensor)

$$Q_{ijk} = m\int w_i w_j w_k f_0 d\boldsymbol{v},$$ Energy flux tensor

Hydrodynamic equations with spin

- **Nonrelativistic three-moment closure** for a Fermi-Dirac distribution obtained using a maximum entropy principle

$$\boxed{\begin{aligned}
&\frac{\partial n}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot (\boldsymbol{u} n) = 0, \\
&\frac{\partial S_\alpha}{\partial t} + \partial_i \left(u_i S_\alpha\right) + \frac{e}{m} \left(\boldsymbol{S} \times \boldsymbol{B}\right)_\alpha = 0, \\
&\frac{\partial u_i}{\partial t} + u_j (\nabla_j u_i) + \frac{1}{nm} \nabla_j P_{ij} + \frac{e}{m} \left[E_i + (\boldsymbol{u} \times \boldsymbol{B})_i\right] \\
&\qquad\qquad\qquad + \frac{e}{nm^2} S_\alpha \left(\partial_i B_\alpha\right) = 0,
\end{aligned}}$$

Closure equations:

$$J^S_{i\alpha} = u_i S_\alpha.$$

$$P = \frac{\hbar^2}{5m} \frac{\left(6\pi^2\right)^{2/3}}{2^{5/3}} \left[\left(n - \frac{2}{\hbar} |\boldsymbol{S}| \right)^{5/3} + \left(n + \frac{2}{\hbar} |\boldsymbol{S}| \right)^{5/3} \right]$$

J. Hurst, O. Morandi, G. Manfredi, and P.-A. Hervieux, *Semiclassical Vlasov and fluid models for an electron gas with spin effects*, Eur. Phys. J. D **68**, 176 (2014).

QHD with spin-orbit coupling

$$\frac{\partial n}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot (n\bar{\boldsymbol{u}}) = 0,$$

$$\frac{\partial S_\alpha}{\partial t} + \partial_i(u_i S_\alpha) - \frac{\mu_\mathrm{B}}{2mc^2}(\boldsymbol{\nabla} \times n\boldsymbol{E})_\alpha + \frac{e}{m}\left[\boldsymbol{S} \times \left(\boldsymbol{B} - \frac{1}{2c^2}\boldsymbol{u} \times \boldsymbol{E}\right)\right]_\alpha = 0,$$

$$\frac{\partial u_i}{\partial t} + u_j(\nabla_j u_i) + \frac{1}{nm}\nabla_j P_{ij} + \frac{e}{m}[E_i + (\bar{\boldsymbol{u}} \times \boldsymbol{B})_i] + \frac{e}{nm^2}S_\alpha(\partial_i B_\alpha)$$
$$+ \frac{\mu_\mathrm{B}}{2mc^2 n}\epsilon_{jkl}[E_j(\partial_k u_i) - u_k(\partial_i E_j)]S_l = 0$$

With: $J^S_{i\alpha} = u_i S_\alpha \quad \text{and} \quad \Pi^S_{ij\alpha} = u_i J^S_{j\alpha}.$