1. Anomalous Hall Conductivity

VOLUME 92, NUMBER 3 PHYSICAL REVIEW LETTERS week ending 23 JANUARY 2004

First Principles Calculation of Anomalous Hall Conductivity in Ferromagnetic bcc Fe

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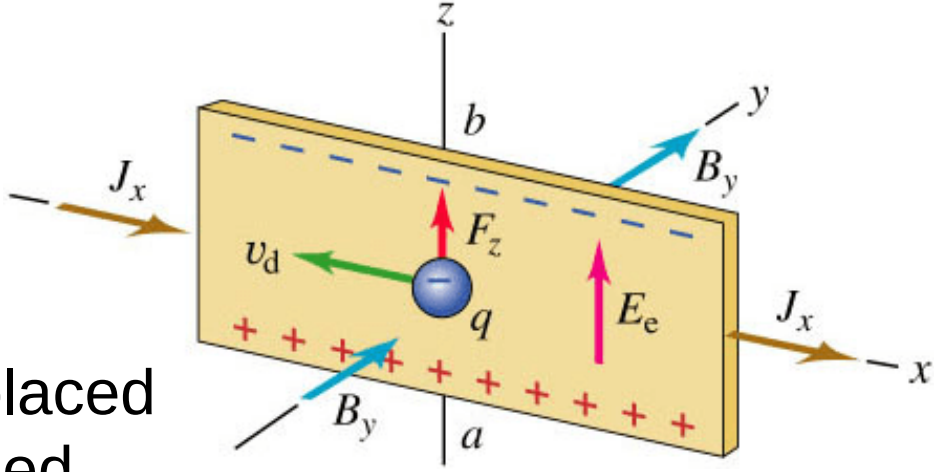
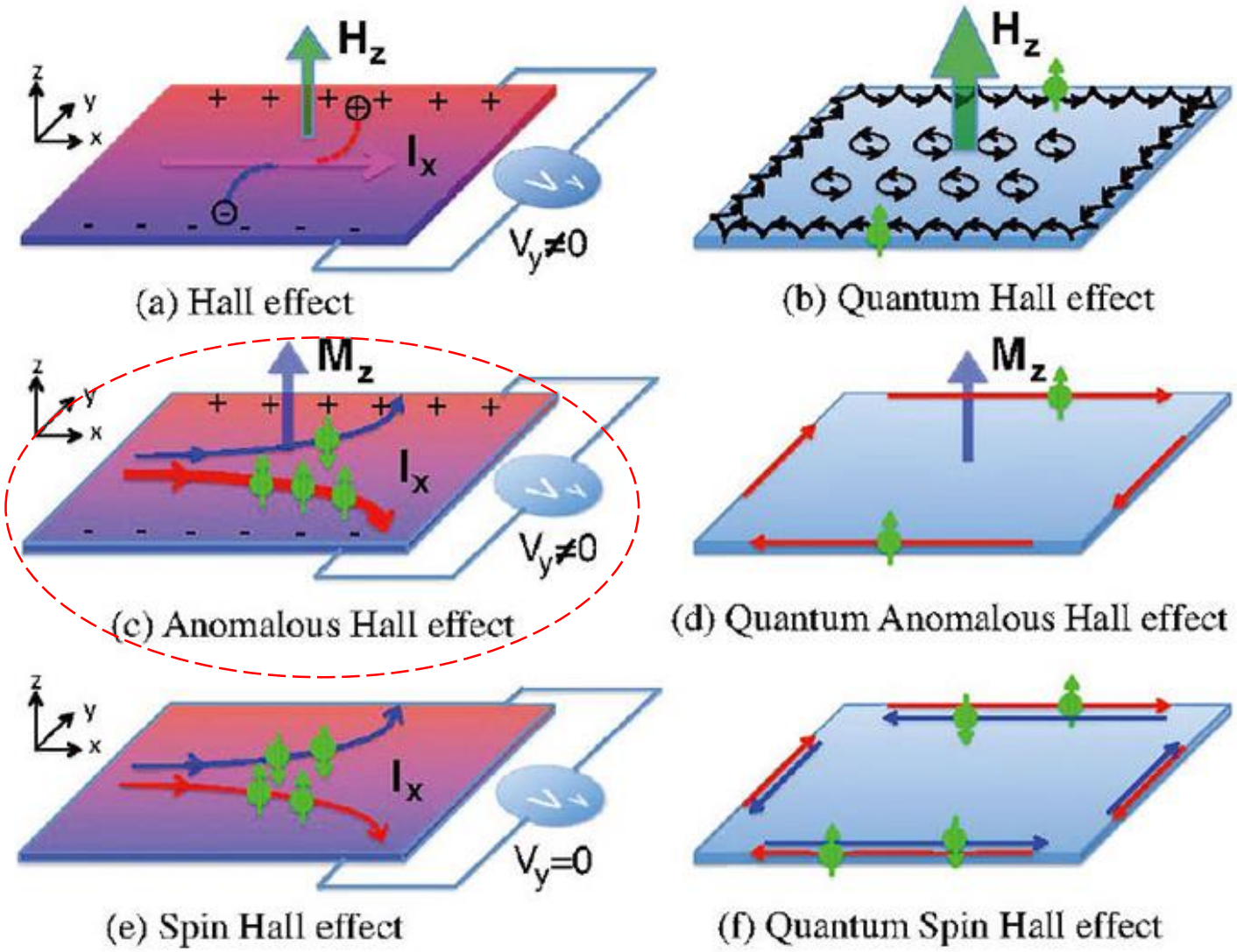
Hall effect



When a conductor carrying longitudinal current was placed in a vertical magnetic field, the carrier would be pressed against the transverse side of the conductor, which led to an observed transverse voltage. This is called the Hall effect (HE)

However, in ferromagnetic metals like Fe, Co, and Ni, the Hall effect is anomalous and controlled more by magnetization than by Lorentz forces.



HONGMING WENG, XI DAI, AND WHONG FANG

Anomalous Hall Conductivity (AHC)

- Hall conductivity is enhanced by the magnetization of the host material.
- This is due to the spin-dependent scattering of the charged carrier.
- This quantity can be described using the Kubo formula as

$$\sigma_{xy} = \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3} \sum_{n \neq n'} \frac{2\mathrm{Im}\langle \psi_{n\boldsymbol{k}} | v_x | \psi_{n'\boldsymbol{k}} \rangle \langle \psi_{n'\boldsymbol{k}} | v_y | \psi_{n\boldsymbol{k}} \rangle}{(\omega_{n'} - \omega_n)^2}$$

Kubo formula for Hall conductivity is given by the current-current correlation function

$$\sigma_{\alpha,\beta}(\omega) = \lim_{\delta\to 0}\frac{\hbar}{V}\sum_{nm}\frac{f_m - f_n}{\varepsilon_m - \varepsilon_n}\,\mathrm{Im}\,\frac{\langle n|J_\alpha|m\rangle\langle m|J_\beta|n\rangle}{\varepsilon_n - \varepsilon_m + \hbar(\omega+\delta)} \qquad J_\alpha = -qv_\alpha$$

For a system with Hamiltonian

$$H = H_0 + H_{\mathrm{SO}} \qquad H_{\mathrm{SO}} = \alpha_R\left(\sigma_x k_y - \sigma_y k_x\right)$$

in the static limit $\omega \to 0$,

$$\sigma_{\alpha,\beta} = \frac{q^2}{\hbar V}\sum_{\boldsymbol{k},m,n(\neq m)}\left(f_{\varepsilon_m(\boldsymbol{k})} - f_{\varepsilon_n(\boldsymbol{k})}\right)\mathrm{Im}\,\frac{\langle u_n(\boldsymbol{k})|\nabla_\alpha H(\boldsymbol{k})|u_m(\boldsymbol{k})\rangle\langle u_m(\boldsymbol{k})|\nabla_\beta H(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle}{\left(\varepsilon_n(\boldsymbol{k}) - \varepsilon_m(\boldsymbol{k})\right)^2}$$

Effective mass theory

Group velocity $\boldsymbol{v} = \frac{1}{\hbar}\frac{d}{d\boldsymbol{k}}E(-\mathrm{i}\hbar\nabla + e\boldsymbol{A})$

Envelope function $\Psi(\boldsymbol{x}, t) = \sum_l f_l(t) W(\boldsymbol{x} - \boldsymbol{R}_l)$

$$\mathrm{i}\hbar\frac{\partial f}{\partial t} = \left\{E\left(-\mathrm{i}\hbar\nabla + e\boldsymbol{A}(\boldsymbol{x}, t)\right) - e\phi(\boldsymbol{x}, t)\right\} f$$

Effective Hamiltonian $\widehat{H} = E\left(-\mathrm{i}\hbar\nabla + e\boldsymbol{A}(\boldsymbol{x}, t)\right) - e\phi(\boldsymbol{x}, t)$

Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and Berry-phase effects
by Sundaram and Niu PRB 59, 14915 (1999)

Expanded the effective mass Hamiltonian around a position $\boldsymbol{x}_c$

$$\simeq E\left(-\mathrm{i}\hbar\boldsymbol{\nabla} + e\boldsymbol{A}(\boldsymbol{x}_c, t)\right) - e\phi(\boldsymbol{x}_c, t) + (\boldsymbol{x} - \boldsymbol{x}_c)\cdot\boldsymbol{\nabla}_c\beta(\boldsymbol{x}_c, t)$$
$$\equiv \hat{H}_c + (\boldsymbol{x} - \boldsymbol{x}_c)\cdot\boldsymbol{\nabla}_c\beta(\boldsymbol{x}_c, t)$$

Define the Bloch state of $\hat{H}_c$

$$\hat{H}_c(\boldsymbol{x}_c, t)\left|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c, t)\right\rangle = E(\boldsymbol{x}_c, \boldsymbol{q}, t)\left|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c, t)\right\rangle$$

Expand a wave function as

$$|\Psi\rangle = \int d^3q\, a(\boldsymbol{q}, t)\left|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c, t)\right\rangle \qquad \begin{cases} a(\boldsymbol{q}, t) \equiv |a(\boldsymbol{q}, t)|\exp[-i\gamma(\boldsymbol{q}, t)] \\ \int d^3q\,|a(\boldsymbol{q}, t)|^2 = 1 \end{cases}$$

Then the center of WP is given by

$$\boldsymbol{x}_c = \langle \Psi | \hat{\boldsymbol{x}} | \Psi \rangle = \int d^3q \, |a(\boldsymbol{q}, t)|^2 \left[\frac{\partial \gamma}{\partial \boldsymbol{q}} + \left\langle u \middle| \mathrm{i} \frac{\partial}{\partial \boldsymbol{q}} \middle| u \right\rangle \right]$$

When the wave packet is narrow and is centered around at a point

$$\boldsymbol{q}_c = \int d^3q \, \boldsymbol{q} |a(\boldsymbol{q}, t)|^2,$$

The center is

$$\boldsymbol{x}_c \simeq \frac{\partial \gamma_c}{\partial \boldsymbol{q}} + \left\langle u \middle| \mathrm{i} \frac{\partial}{\partial \boldsymbol{q}} \middle| u \right\rangle \Bigg|_{\boldsymbol{q}=\boldsymbol{q}_c}$$

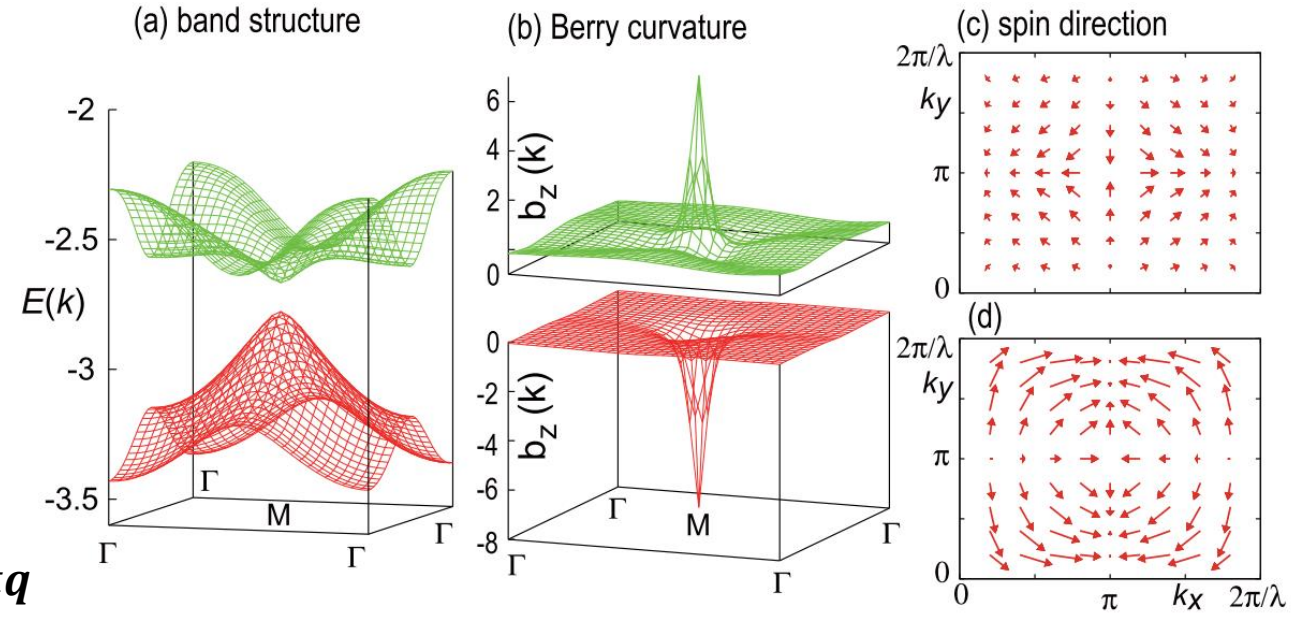
Now let us derive the equation of motion of the wave packet.

Using

$$\boldsymbol{v} = \frac{d}{d\boldsymbol{k}} E(-\mathrm{i}\nabla + e\boldsymbol{A})$$

One can show

$$\dot{\boldsymbol{x}}_c = \frac{\partial E}{d\boldsymbol{q}_c} - \left(\overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{qx}} \cdot \dot{\boldsymbol{x}}_c + \overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{qq}} \cdot \dot{\boldsymbol{q}}_c\right) + \boldsymbol{\Omega}_{tq}$$



With Berry curvature

$$\overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{qq}} = \mathrm{i}\left[\left\langle \frac{\partial u}{\partial q_{c\alpha}} \middle| \frac{\partial u}{\partial q_{c\beta}} \right\rangle - \left\langle \frac{\partial u}{\partial q_{c\beta}} \middle| \frac{\partial u}{\partial q_{c\alpha}} \right\rangle\right] \qquad \overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{tq}} = \mathrm{i}\left[\left\langle \frac{\partial u}{\partial t} \middle| \frac{\partial u}{\partial q_{c\alpha}} \right\rangle - \left\langle \frac{\partial u}{\partial q_{c\alpha}} \middle| \frac{\partial u}{\partial t} \right\rangle\right]$$

Likewise

$$\dot{\boldsymbol{q}}_c = -\frac{\partial E}{\partial \boldsymbol{x}_c} + \left(\overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{xx}} \cdot \dot{\boldsymbol{x}}_c + \overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{xq}} \cdot \dot{\boldsymbol{q}}_c\right) - \boldsymbol{\Omega}_{tx}$$

Further simplification

Defining

$$\boldsymbol{M} = e\mathrm{Im}\left\langle\frac{\partial u}{\partial \boldsymbol{k}}\right| \times (E_0(\boldsymbol{k}) - \hat{H}_0(\boldsymbol{k}) \left|\frac{\partial u}{\partial \boldsymbol{k}}\right\rangle\Bigg|_{\boldsymbol{k}=\boldsymbol{k}_c}$$

We derive intuitive equations

$$\dot{\boldsymbol{x}}_c = \frac{\partial E_M}{d\boldsymbol{q}_c} - \dot{\boldsymbol{k}}_c \times \boldsymbol{\Omega}$$

$$\dot{\boldsymbol{k}}_c = -e\boldsymbol{E} - e\dot{\boldsymbol{x}}_c \times \boldsymbol{B}$$

$$\mathbf{E} \equiv \boldsymbol{\nabla}_{\mathbf{x_c}}\phi(\boldsymbol{x}_c, t) - \frac{\partial \boldsymbol{A}(\boldsymbol{x}_c, t)}{\partial t}$$

$$\boldsymbol{B} \equiv \boldsymbol{\nabla}_{\mathbf{x_c}} \times \boldsymbol{A}(\boldsymbol{x}_c, \boldsymbol{t})$$

$$E_M \equiv E_0(\boldsymbol{k}_c) - \boldsymbol{M} \cdot \boldsymbol{B}$$

$$(\boldsymbol{\Omega})_\alpha \equiv \frac{1}{2}\epsilon_{\alpha\beta\gamma}\left(\overleftrightarrow{\boldsymbol{\Omega}}_{\boldsymbol{kk}}\right)_{\beta\gamma}$$

Current and conductance

With slightly simplified notation

$$\dot{\boldsymbol{x}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E} - e\dot{\boldsymbol{x}} \times \boldsymbol{B}$$

$$\boldsymbol{\Omega}_n(k) = -\mathrm{Im}\langle \boldsymbol{\nabla}_{\boldsymbol{k}} u_{n\boldsymbol{k}}| \times |\boldsymbol{\nabla}_{\boldsymbol{k}} u_{n\boldsymbol{k}}\rangle$$

Current is

$$\boldsymbol{J} = -\boldsymbol{E} \times \int d^3k \sum\nolimits_n f_n(\boldsymbol{k})\boldsymbol{\Omega}_{\boldsymbol{n}}(\boldsymbol{k}) - \int d^3k \sum\nolimits_n \delta f_n(\boldsymbol{k}) \frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}}$$

occupation number f_n

Conductance is

$$\sigma_{xy} = -\int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\,\Omega^z(\boldsymbol{k})$$

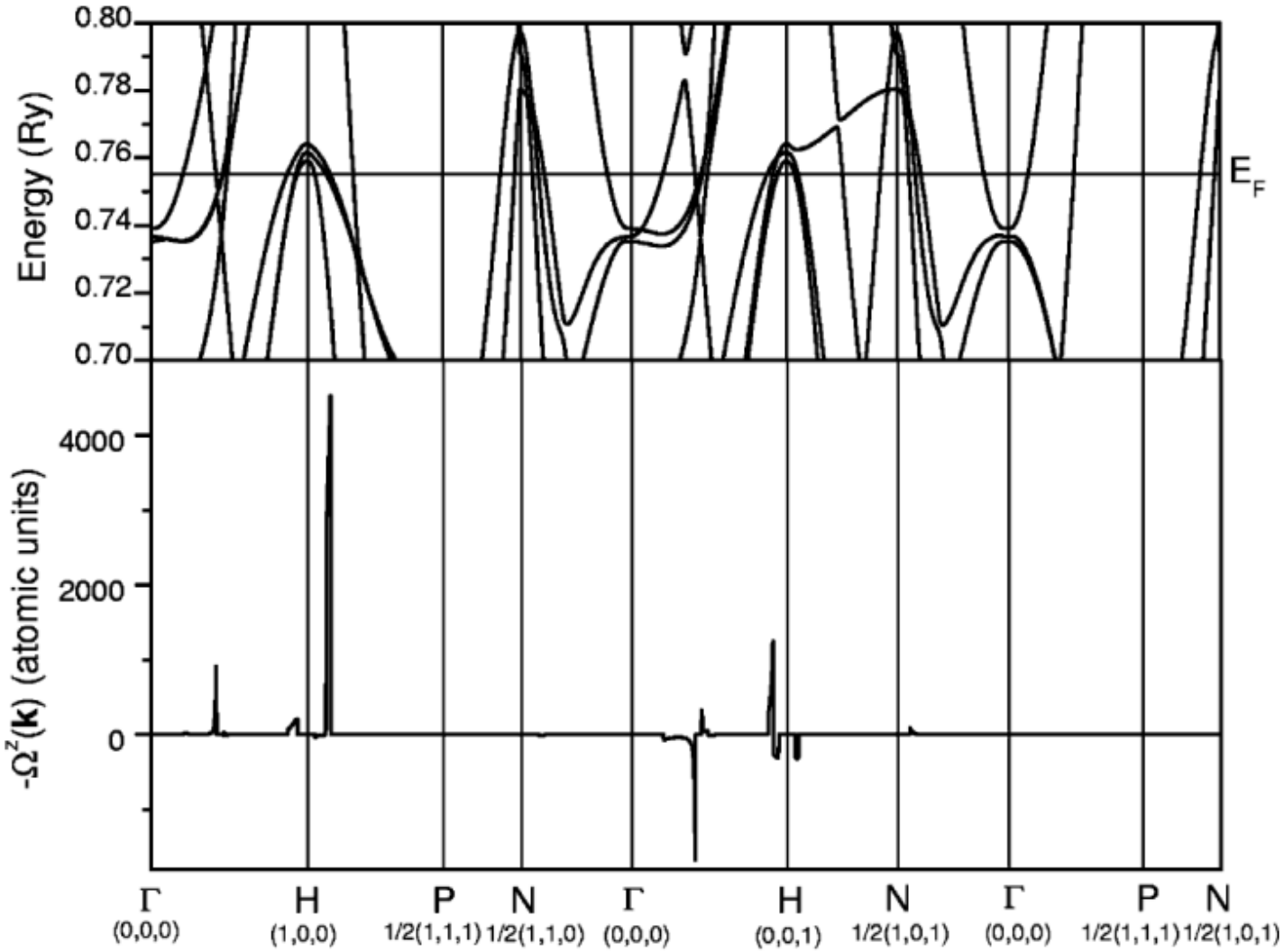


FIG. 2. Band structure near Fermi energy (upper panel) and Berry curvature $\Omega^z(\mathbf{k})$ (lower panel) along symmetry lines.

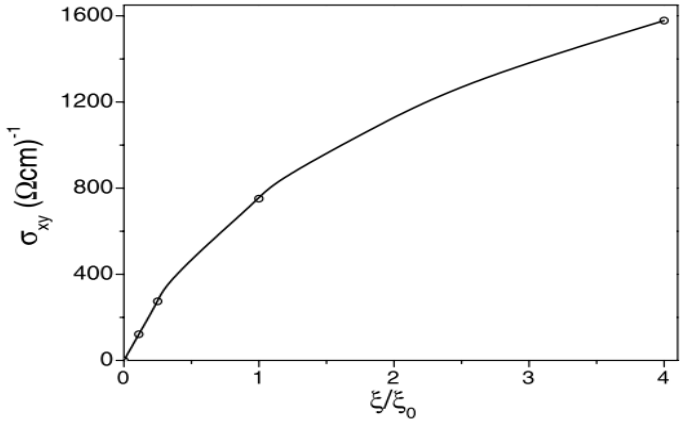


FIG. 4. Calculated anomalous Hall conductivity (open circles) vs the effective spin-orbit coupling strength relative to its value for iron. The line is a guide to the eye.

- The full-potential linearized augmented plane-wave (FLAPW) method was used.
- Generalized gradient approximation (GGA) for the exchange-correlation potential.
- Fully relativistic band calculations were performed using the program package WIEN2K.
- A converged ground state with magnetization in the 001 direction was obtained.
- 20 000 k points were used in the first Brillouin zone.

- After obtaining the self-consistent potential with 20 000 k points, we calculated the Berry curvature with several larger sets of k points in order to achieve the convergence.
- The Monkhorst-Park special-point method was used for the BZ integration.
- To go beyond 2x10^6 points, we adopted a method of adaptive mesh refinement; i.e., when $\Omega_{xy}^{z}(k)$ is large at a certain k point, we construct a finer mesh by adding 26 additional points around it. This procedure yields a converged value of $\sigma_{xy} = 751\ \mathrm{cm}^{-1}$ at zero temperature (using a step function for the Fermi-Dirac distribution) and a slightly smaller value of $\sigma_{xy} = 734\ \mathrm{cm}^{-1}$ at room temperature (300 K).
- Our result is in fair agreement with the value 1032 cm^{-1} extracted from Dheer's data on iron whiskers at room temperature.
- The slow convergence is caused by the appearance of large contributions of both signs to Ω^{z} which occur in very small regions of k space.
- Spin-orbit effects are small except when they mix states that are degenerate or nearly degenerate.
- A pair of mixed states contributes negligibly if both are occupied or are unoccupied.
- Therefore, only when the Fermi surface lies in a spin-orbit induced gap is

Let us study the electronic structure of bcc iron guided by the tutorial provided by the Wannier90 project.

As a first step, we calculate this material neglecting the spin-orbit coupling following the example 8. Explain which exchange-correlation potential and pseudo-potentials are used in this example.

Then, follow the tutorial to calculate (1) the solution (electron density) of the Kohn-Sham equation, (2) Kohn-Sham eigensystems on a uniform k-point mesh, and (3) change the basis from the plane wave to the maximally localize Wannier functions (MLWFs).

When using the Wannier interpolation scheme, we can speed up the calculation of the density of states (DOS). Note that the calculation is time consuming because we must use very fine mesh in the Brillouine zone (25×25×25) to be able to describe the rather spiky DOS. Even with that, the calculation will require a few hours; let us wait for the computer to finish the job. Draw the DOS and show how the measured magnetization can be reproduced by theory.

In the next step, let us consider the spin-orbit coupling following the example 17.

This is done by using the options “lspinorb” and “noncolin”. It is then become much more difficult to obtain the Kohn-Sham eigensystems, so that the option “cg” may not be so effective; if problematic, try to choose another solver called “david”.

Then, compare the band structure of the bcc iron with and without the spin-orbit coupling and discuss the difference.

In the final step, let us compute the Berry curvature following the example 18 and plot the result along a path connecting the symmetry lines. We will reproduce the fig. 2.

There, the anomalous Hall conductivity is calculated by integrating the Berry curvature in the BZ, but here we just calculate the integrand along symmetry lines to get insight into its spiky structure because of our limited computational power.

In this step, as well as in the previous steps, carefully read the document for the “Wannier90 Tutorial” so that you may not loose too much time with careless trials and errors; the individual calculation requires up to 2 hours and thus about 6-8 hours in total.

Input the calculated value of the Fermi energy into the Fe.win as required by instruction and don’t forget to switch on the flag “write_spn” in Fe.pw2wan. Recognize that the Berry curvature is a quantity that can be much more easily calculated with the MLWFs. Describe how the calculation (equation (2) of the PRL paper) is done in your QE+Wannier90 simulation; especially specify which band and k-point mesh are used. In your report, show the y-component of the Berry curvature together with the z-component.

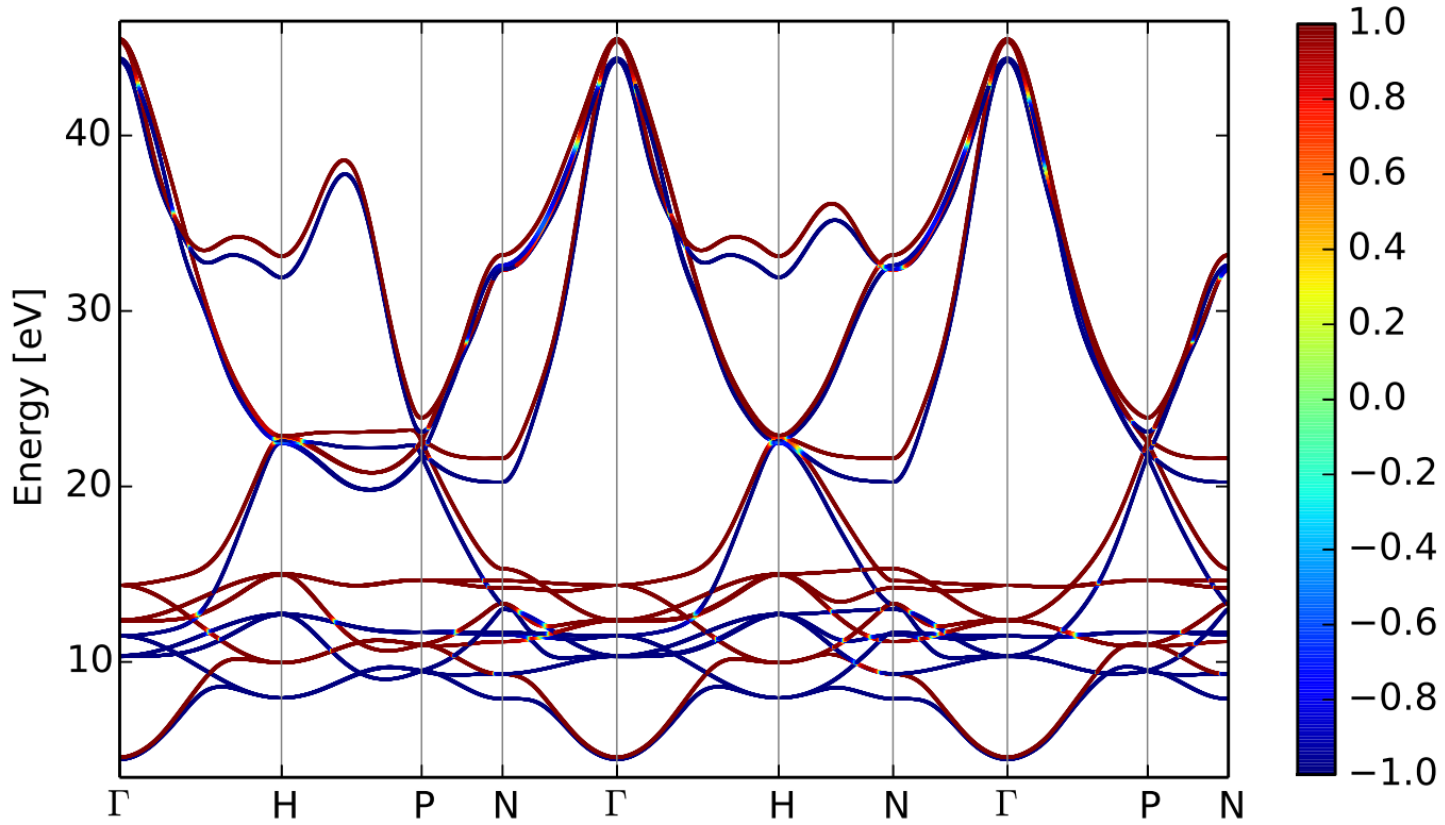


Figure 55: Wannier90 interpolated bands of Fe computed from a DFT calculation with spin-orbit interaction. Colorscheme shows the expectation value $\langle \hat{S}_z \rangle$ in units of $\hbar/2$.