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. Namely we will reproduce the figure 2 shown in Physical Review Letters 92, 037204 (2004) "First Principles Calculation of Anomalous Hall Conductivity in Ferromagnetic bcc Fe". In that paper, the anomalous Hall conductivity is calculated by integrating the Berry curvature in the Brillouin zone, but here we just calculate the integrand, or the Berry curvature, 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 is difficult to calculate with the original definition but is a one 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.

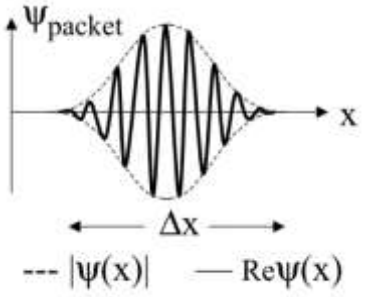
First Principles Calculation of Anomalous Hall Conductivity in Ferromagnetic bcc Fe

The target of the study is to describe AHC of bcc Fe numerically. AHC is the Hall conductivity 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

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

but the BZ integration was too expensive to perform. To overcome the difficulty, the integrand was related to the Berry curvature $\Omega^z(\boldsymbol{k})$ and was obtained using the Wannier function method. We will follow this study. In the rest of this memo, I will show how the integrand of the original formulation cab be related to Berry curvature.

Effective mass theory



Suppose you make a wave packet using Bloch states at and around the wave vector $\boldsymbol{k}$. The group velocity of the packet is given by

$$\boldsymbol{v} = \frac{dE}{d\boldsymbol{p}} = \frac{1}{\hbar}\frac{dE}{d\boldsymbol{k}},$$

where E is the band dispersion, or the eigenvalue of the Kohn-Sham orbital $E_n(\boldsymbol{k})$. When the system is applied with static electromagnetic field,

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

To make the equation gauge invariant, we replace the kinetic energy as

$$-\mathrm{i}\hbar\boldsymbol{\nabla} \rightarrow -\mathrm{i}\hbar\boldsymbol{\nabla} + e\boldsymbol{A},$$

so that the group velocity is modified as

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

Suppose also that the wave packet is expanded in terms of the Wannier functions as

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

Then the equation of motion followed by the smooth envelope function is

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

The effective mass Hamiltonian is thus

$$\widehat{H} = E\big(-\mathrm{i}\hbar\boldsymbol{\nabla} + e\boldsymbol{A}(\boldsymbol{x}, t)\big) - e\phi(\boldsymbol{x}, t).$$

This is the conventional effective mass theory.

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

One should be careful about the non-commutable nature of $\boldsymbol{x}$ **and** $\boldsymbol{p}$. To show this, let us expanded the effective mass Hamiltonian around a position $\boldsymbol{x}_c$ like

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

where β is a function determined by the vector and scalar potentials. Then we can define the Bloch states from

$$\widehat{H}_c(\boldsymbol{x}_c,t)\big|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c,t)\big\rangle = E(\boldsymbol{x}_c,\boldsymbol{q},t)\big|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c,t)\big\rangle,$$

which can be written as a phase factor and a periodic function as

$$\big|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c,t)\big\rangle = e^{\mathrm{i}\boldsymbol{q}\cdot\hat{\boldsymbol{x}}}|u(\boldsymbol{q},t)\rangle \equiv e^{\mathrm{i}\boldsymbol{q}\cdot\hat{\boldsymbol{x}}}|u\rangle.$$

Using the Bloch states, let us expand the wave packet as

$$|\Psi\rangle = \int d^3q\, a(\boldsymbol{q},t)\big|\psi_{\boldsymbol{q}}(\boldsymbol{x}_c,t)\big\rangle$$

with the amplitude, $a(\boldsymbol{q},t) \equiv |a(\boldsymbol{q},t)|\exp[-\mathrm{i}\gamma(\boldsymbol{q},t)]$, normalized as

$$\int d^3q\, |a(\boldsymbol{q},t)|^2 = 1.$$

It is easy to show (from the identity $\langle\psi_{\boldsymbol{q}}|\hat{\boldsymbol{x}}|\psi_{\boldsymbol{q}'}\rangle = \left(\mathrm{i}\frac{\partial}{\partial\boldsymbol{q}} + \left\langle u_{\boldsymbol{q}}\middle|\mathrm{i}\frac{\partial}{\partial\boldsymbol{q}'}\middle|u_{\boldsymbol{q}'}\right\rangle\right)\delta(\boldsymbol{q}-\boldsymbol{q}')$) that the center of the wave packet is given by

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

where (with the unit cell volume v_c)

$$\langle u|v\rangle \equiv \frac{(2\pi)^3}{v_c}\int_{\text{cell}} d^3r\, u(\boldsymbol{r})v(\boldsymbol{r}).$$

Then, when the wave packet is narrow and is centered around at a point

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

one can show that

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

This is a semiclassical description that the time-evolution of the WP center is given by the phase and the Berry curvature of the band.

The equation of motion

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

can be explicitly written for the center can be derived from the time-dependent Schrödinger equation as (derivation is skipped)

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

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

where Ω's are known as Berry curvature defined by

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

and

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

This equation can be further simplified using the orbital magnetic moment

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

where $E_0(\boldsymbol{k})$ is the band energy and $\hat{H}_0(\boldsymbol{k})$ is the Hamiltonian of the unperturbed crystal (derivation skipped).

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

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

where

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

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

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

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

This means that the energy $E_0(\boldsymbol{k}_c)$ is modified by the magnetic moment of Bloch orbital $\boldsymbol{M}$ and that the velocity $\frac{\partial E_M}{d\boldsymbol{q}_c}$ is modified by the Hall velocity term $-\dot{\boldsymbol{k}}_c \times \boldsymbol{\Omega}$. The latter is related to the Chern's theory.

Electrons (wave packet) in the n-th band follows

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

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

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

This result can be used to show, in the absence of magnetic field, that the electric current is given by

$$-\boldsymbol{E} \times \int d^3k \sum_n f_n(\boldsymbol{k})\boldsymbol{\Omega}_{\boldsymbol{n}}(\boldsymbol{k}) - \int d^3k \sum_n \delta f_n(\boldsymbol{k}) \frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}},$$

where f is the occupation number and δf is the change in the occupation number yielded by the electric field and by the relaxation time. The anharmonic Hall conductance is then given by the BZ integration over the Berry phase as

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

In the paper, the anomalous Hall conductivity was calculated as

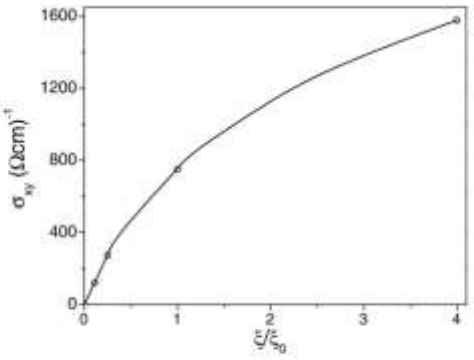


FIG. 4. Calculated anomalous Hall conductivity (open circles) vs the effective spin-orbit coupling strength relative to its value for iron. The line is a guide to the eye.

In the calculation, over the BZ the Berry curvature was integrated, which was shown to behave along paths connecting symmetric points as

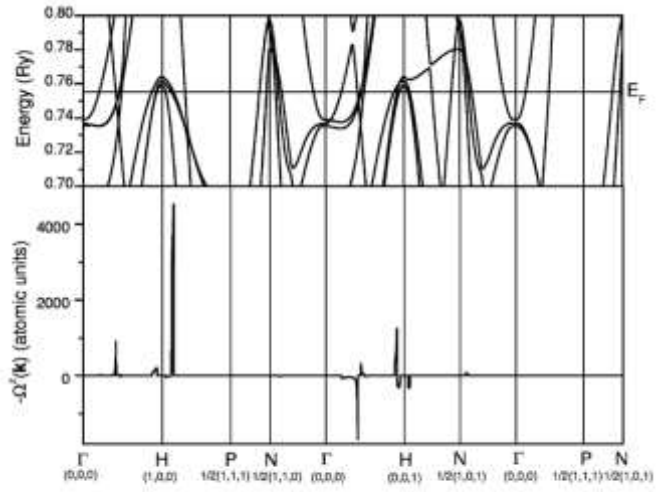


FIG. 2. Band structure near Fermi energy (upper panel) and Berry curvature $\Omega^z(\mathbf{k})$ (lower panel) along symmetry lines.

Let us reproduce the figure using QE and Wannier90. Note that, because of the spiky nature of the integrand, it is not so easy to accurately integrate it over the BZ. But, it is rather easy to reproduce Fig. 2.