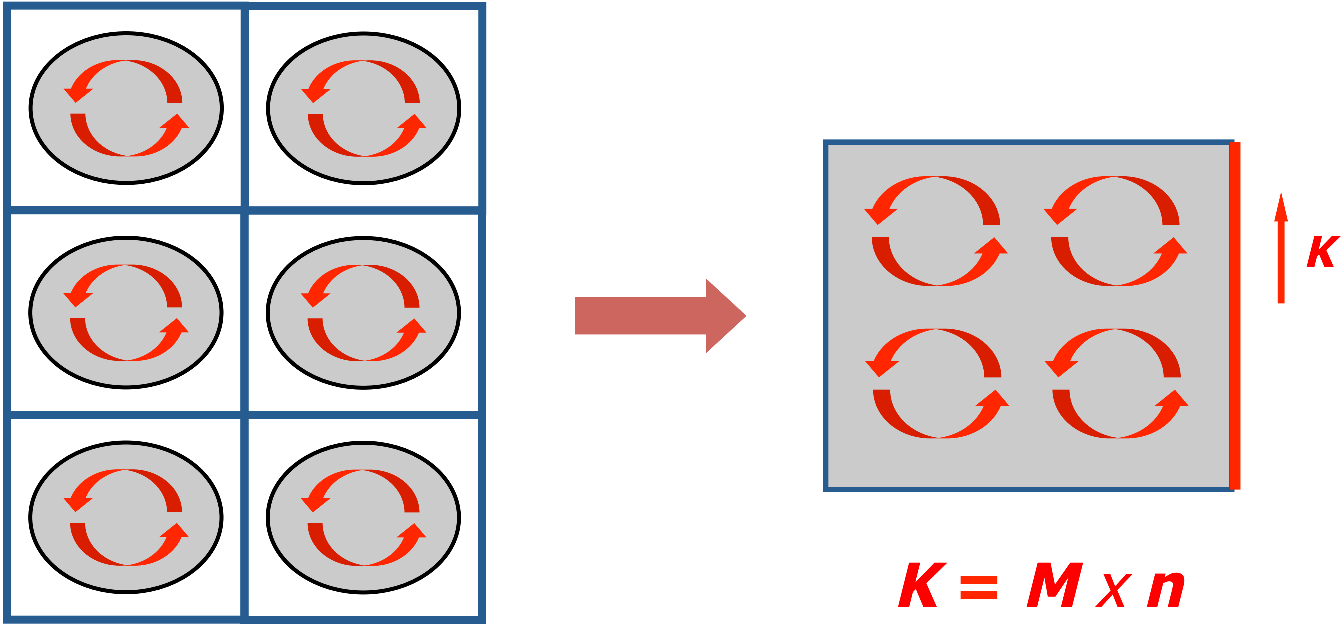
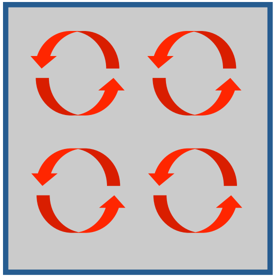
Orbital magnetization (2D)

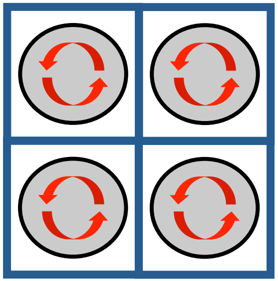


Interstitial regions are not empty

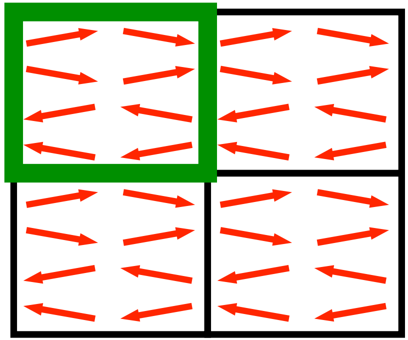
What if crystals look like

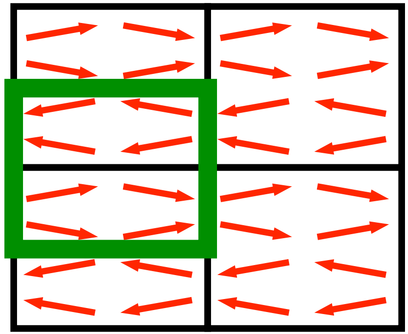


not like

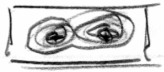


Problem:



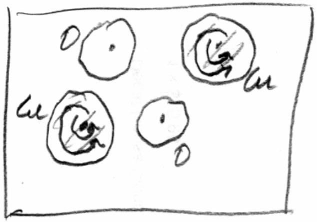


Usually not so bad in practice:

Polarization problem: $P \propto \langle \psi_{nk} | \mathbf{r} | \psi_{nk} \rangle$  $\int \mathbf{r}\,\rho(\mathbf{r})\,d\mathbf{r}$ ✗

Magnetization problem: $M \propto \langle \psi_{nk} | \mathbf{r} \times \mathbf{v} | \psi_{nk} \rangle$  $\int \mathbf{r} \times \mathbf{J}(\mathbf{r})\,d\mathbf{r}$ ✗

But standard approach:



In each open-shell d or f sphere,

$$\boldsymbol{\mu}_j \propto \int_{\substack{\text{atom}\\ \text{sphere}\\ j}} \mathbf{r} \times \mathbf{J}(\mathbf{r})\,d\mathbf{r}$$

$\mathbf{r}$ measured from center

$$\mathbf{M}_{orb} \propto \sum_j \boldsymbol{\mu}_j$$

"Atom Centered Approx"

Not a bad approx.

In addition, $|M_{orb}| \ll |M_{spin}|$ usually.

$|\mu_{spin}| \propto 1-5\,\mu_B$

$|\mu_{ORB}| \propto 0.1-0.2\,\mu_B$ Except strong SOC

E.g., Sr_2IrO_4 etc.

So in practice, problem is not as severe as for polarization.

But there is a problem in principle! [also, for topological systems...]

Measuring M_{orb}

Historical: Einsten – de Haas effect

The effect corresponds to the **mechanical rotation** that is induced in a **ferromagnetic material** (of cylindrical shape and originally at rest), suspended with the aid of a thin string inside a coil, on **driving an impulse of electric current through the coil**. To this mechanical rotation of the ferromagnetic material (say, iron) is associated a mechanical angular momentum, which, by the law of conservation of angular momentum, must be compensated by an equally large and oppositely directed angular momentum inside the ferromagnetic material.

g_e

$$M \propto (L + 2S)$$

$$J \propto (L + S)$$

http://www.ptb.de/en/publikationen/jahresberichte/jb2005/nachrdjahres/s23e.html

Modern methods: XMCD = X-ray magnetic circular dichroism

B. T. Thole, P. Carra, F. Sette, and G. van der Laan, Phys. Rev. Lett. **68**, 1943 (1992).

Modern Theory of Orbital Magnetization

Semiclassical derivation

D. Xiao, J. Shi, and Q. Niu, Phys. Rev. Lett. ***95****, 137204 (2005).*

Wannier representation derivation

T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett. ***95****, 137205 (2005).*

D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta, Phys. Rev. B ***74****, 024408 (2006).*

Long-wave derivation

J. Shi, G. Vignale, D. Xiao, and Q. Niu, Phys. Rev. Lett. ***99****, 197202 (2007).*

Calculations for Fe, Ni, Cu

D. Ceresoli, U. Gerstmann, A.P. Seitsonen, and F. Mauri, Phys. Rev. B 81, 060409(R) (2010).

Relation to magnetic circular dichroism

I. Souza and D. Vanderbilt, Phys. Rev. B ***77****, 054438 (2008).*

Magnetization of finite sample

Angular momentum : r x p term

$$M = \frac{q}{2Ac}\sum_j \langle\psi_j|xv_y - yv_x|\psi_j\rangle$$

$$= \frac{-iq}{2\hbar Ac}\sum_m \langle w_m|\, x[y,H] - y[x,H]\,|w_m\rangle$$

$$= \frac{-q}{\hbar Ac}\,\mathrm{Im}\sum_m \langle w_m|\, xHy\,|w_m\rangle$$

Magnetization in thermodynamic limit

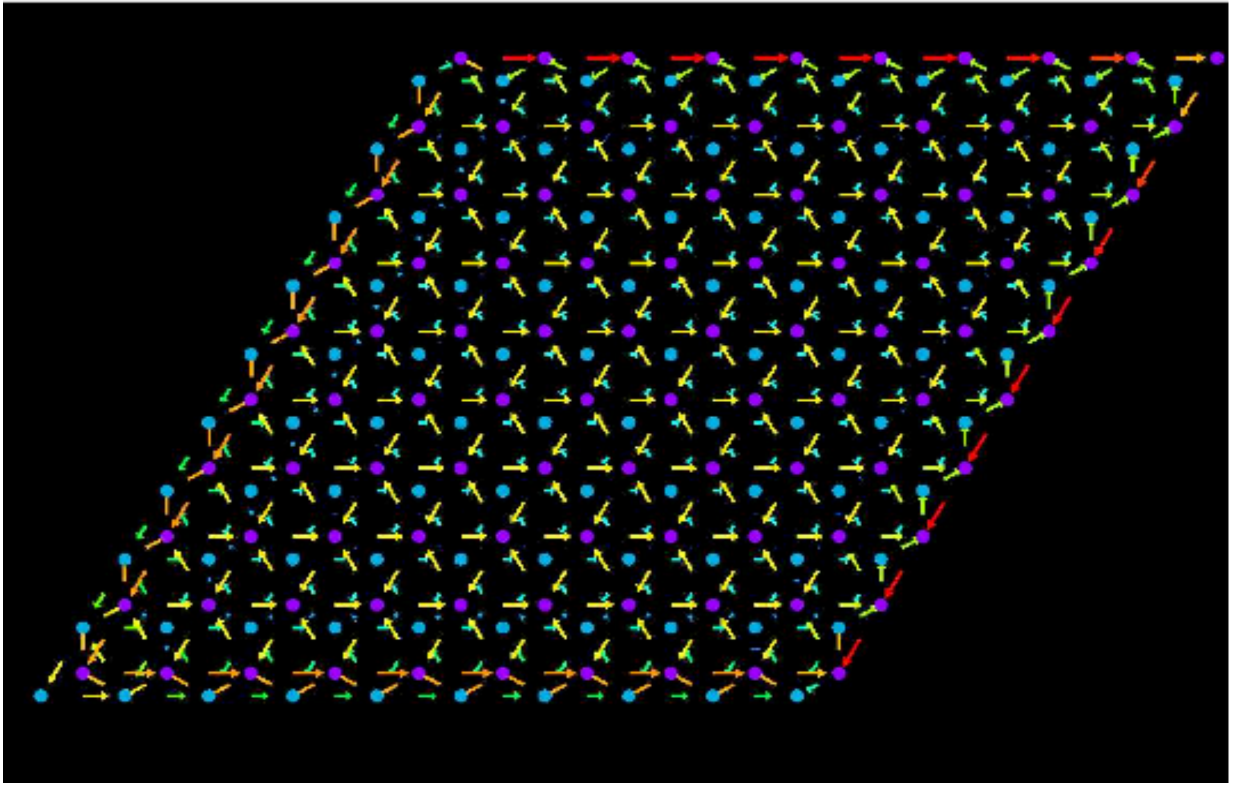
$$M_{\mathrm{LC}} = \frac{-q}{\hbar c A_0}\,\mathrm{Im}\,\langle\mathbf{0}|xHy|\mathbf{0}\rangle$$

Transform to k-space

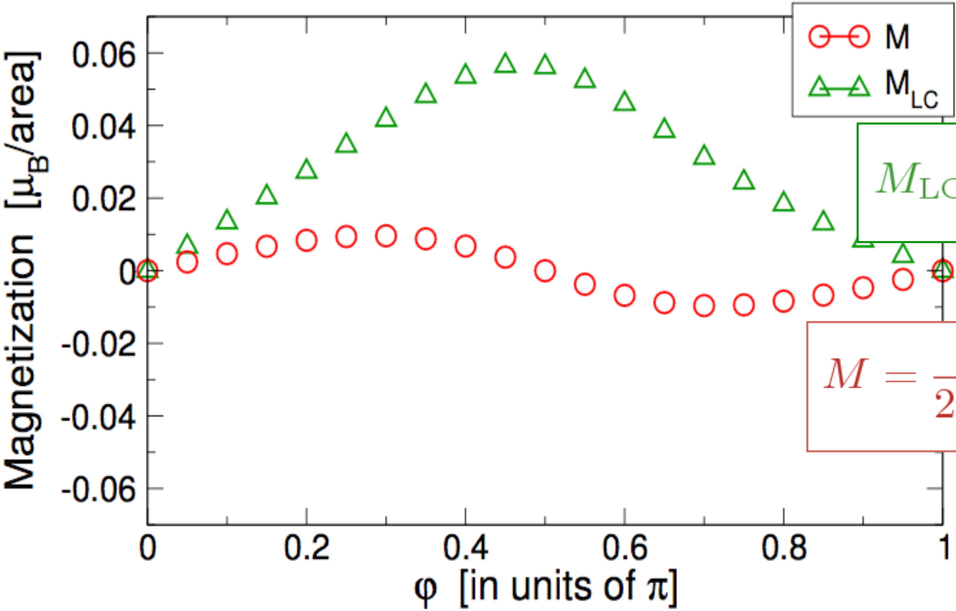
$$\boxed{M_{\mathrm{LC}} = \frac{-q}{\hbar c}\,\mathrm{Im}\int_{\mathrm{BZ}}\frac{d^2k}{(2\pi)^2}\,\langle\frac{\partial u_{\mathbf{k}}}{\partial k_x}|\,H_{\mathbf{k}}\,|\frac{\partial u_{\mathbf{k}}}{\partial k_y}\rangle}$$

?

Numerical Tests: Haldane model



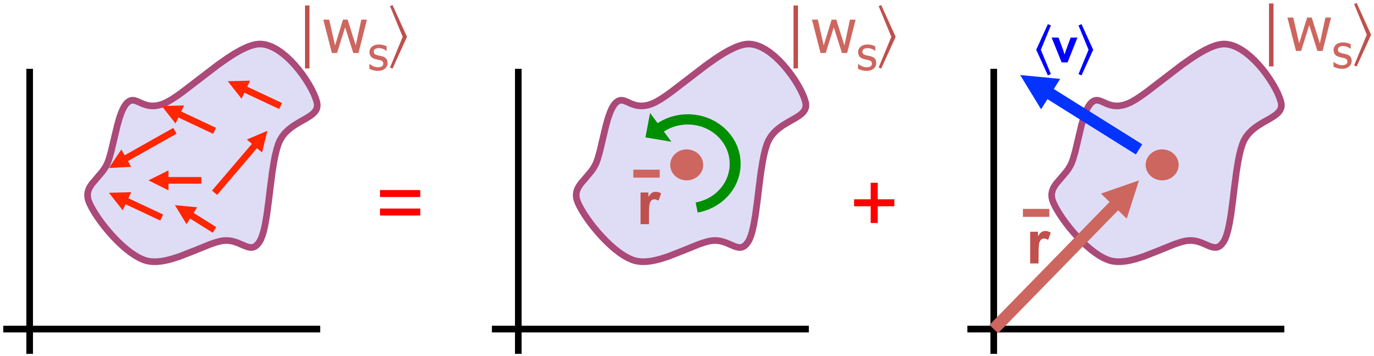
Numerical Tests: Haldane model



$$M_{\mathrm{LC}} = \frac{-q}{\hbar A_0 c} \, \mathrm{Im} \, \langle \mathbf{0} | x H y | \mathbf{0} \rangle$$

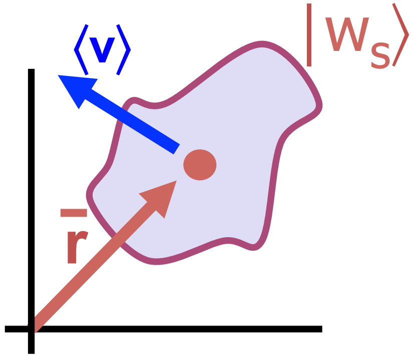
$$M = \frac{q}{2Ac} \sum_j \langle \psi_j | x v_y - y v_x | \psi_j \rangle$$

What is missing?



$$\langle w_s | \, \mathbf{r} \times \mathbf{v} \, | w_s \rangle \;=\; \underbrace{\langle w_s | \, (\mathbf{r} - \bar{\mathbf{r}}) \times \mathbf{v} \, | w_s \rangle}_{\text{Local Circulation (LC)}} \;+\; \underbrace{\bar{\mathbf{r}} \times \langle w_s | \mathbf{v} | w_s \rangle}_{\text{Itinerant Circulation (IC)}}$$

Itinerant Circulation

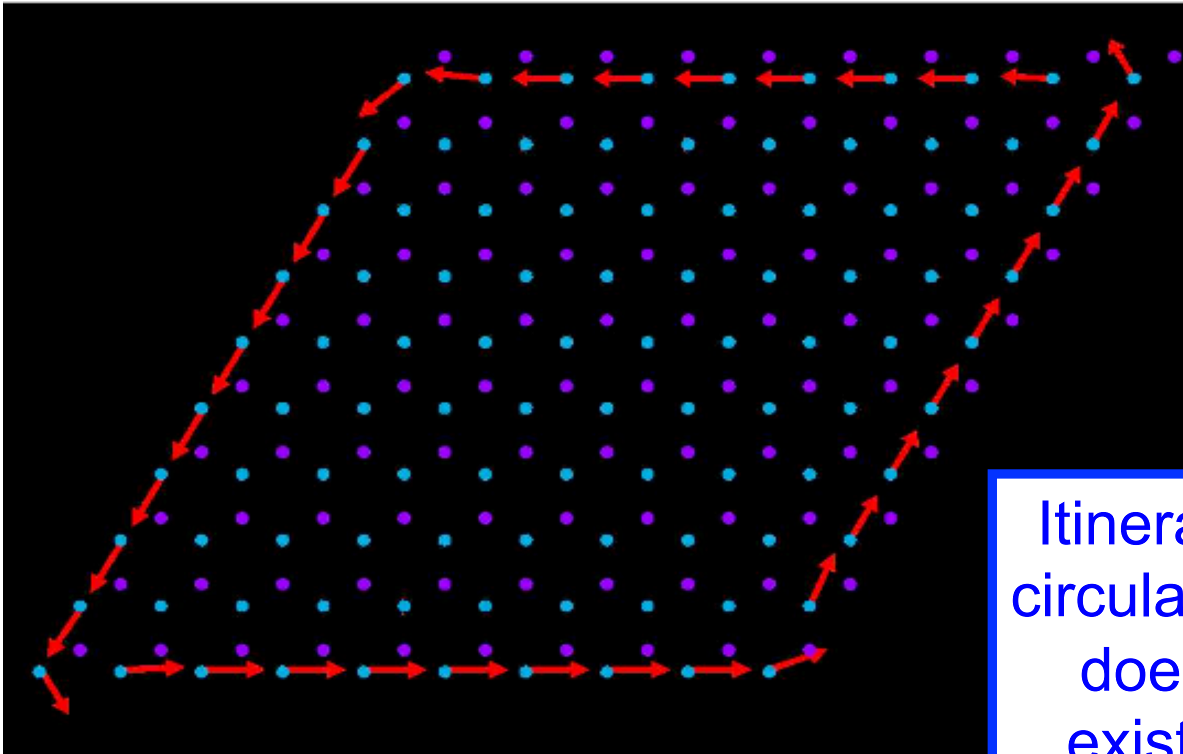


$$\bar{\mathbf{r}} \times \underbrace{\langle w_s | \mathbf{v} | w_s \rangle}_{}$$

Itinerant Circulation
(IC)

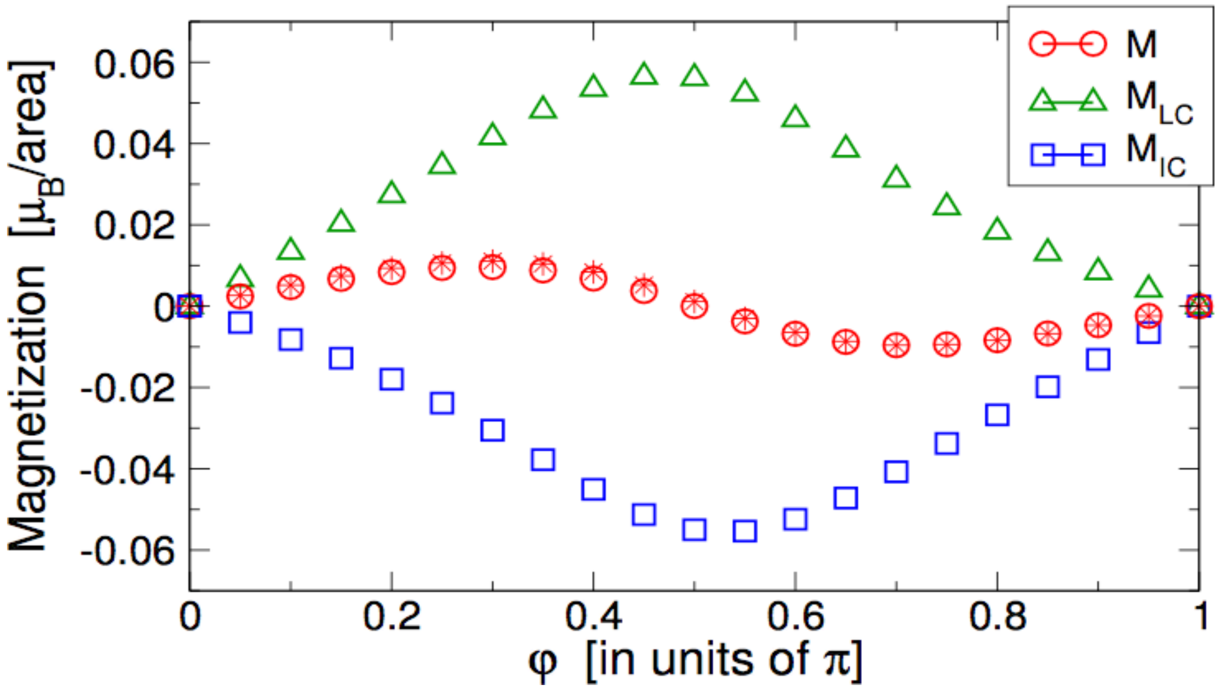
- Bulk WF:
  - Bulk band carries no net current
  - So $\langle \mathbf{v} \rangle = 0$
  - So $\bar{\mathbf{r}} \times \langle \mathbf{v} \rangle = 0$
- But what about a surface WF ?

Numerical Tests: Haldane model



Itinerant circulation does exist !

Numerical Tests: Haldane model



Itinerant Circulation

$$\boxed{M_{\mathrm{IC}} = \frac{-q}{2A_0\hbar c}\sum_{\mathbf{R}} \mathrm{Im}\ \left(R_x\, y_{\mathbf{0},\mathbf{R}}\, H_{\mathbf{R},\mathbf{0}} - R_y\, x_{\mathbf{0},\mathbf{R}}\, H_{\mathbf{R},\mathbf{0}} \right)}$$

M_{IC} can be written in terms of WFs !

$\therefore$ *M_{IC}* is a bulk quantity !

$$\boxed{M_{\mathrm{IC}} = \frac{q}{2\hbar c}\int \frac{d^2k}{(2\pi)^2}\ E(\mathbf{k})\,\Omega(\mathbf{k})}$$

Two Contributions to the Magnetization

$$M = M_{\rm LC} + M_{\rm IC}$$

$$\boxed{M_{\rm LC} = \frac{-q}{\hbar c}\,{\rm Im}\int_{\rm BZ}\frac{d^2k}{(2\pi)^2}\left\langle\frac{\partial u_{\bf k}}{\partial k_x}\right|H_{\bf k}\left|\frac{\partial u_{\bf k}}{\partial k_y}\right\rangle}$$

$$\boxed{M_{\rm IC} = \frac{q}{2\hbar c}\int\frac{d^2k}{(2\pi)^2}\;E({\bf k})\,\Omega({\bf k})}$$

$$\boxed{M = \frac{-q}{\hbar c}\,{\rm Im}\int_{\rm BZ}\frac{d^2k}{(2\pi)^2}\left\langle\frac{\partial u_{\bf k}}{\partial k_x}\right|H_{\bf k}+E_{\bf k}\left|\frac{\partial u_{\bf k}}{\partial k_y}\right\rangle}$$

Can also be applied to metallic ferromagnets and QAH insulators with:

$$\boldsymbol{M} = \frac{e}{2\hbar}\int^{\mu_0}\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\mathrm{i}\left\langle\frac{\partial u}{\partial \boldsymbol{k}}\right|\times\left[2\mu_0-\varepsilon_0(\boldsymbol{k})-\hat{H}_0\right]\left|\frac{\partial u}{\partial \boldsymbol{k}}\right\rangle$$

Semiclassical theory of D. Xiao, J. Shi, and Q. Niu, PRL **95**, 137205 (2005).

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **94**, 121114(R) (2016)

Role of Berry phase theory for describing orbital magnetism: From magnetic heterostructures to topological orbital ferromagnets

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(Received 25 March 2016; revised manuscript received 7 July 2016; published 15 September 2016)

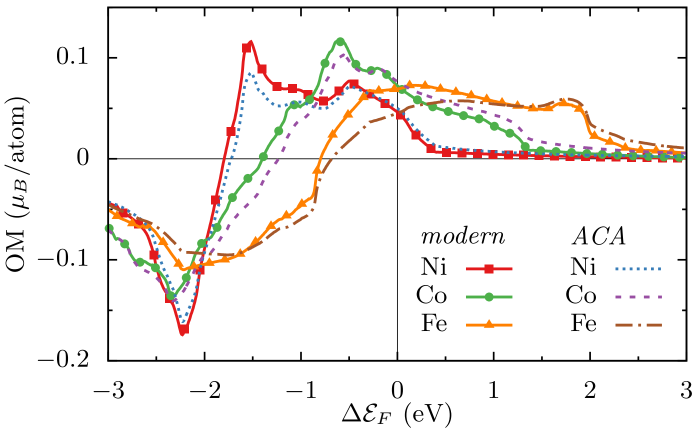


FIG. 1. Easy-axis orbital magnetization (OM) in the bulk ferromagnets fcc Ni, hcp Co, and bcc Fe, according to atom-centered approximation (ACA) and modern theory (per atom). The Fermi level is varied by $\Delta\mathcal{E}_F$ with respect to the true Fermi energy.

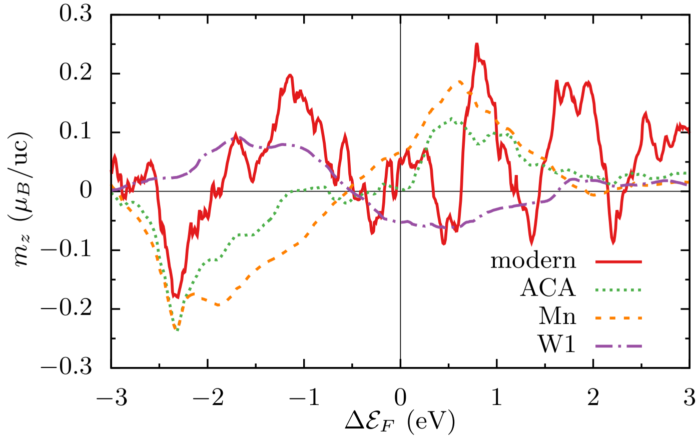
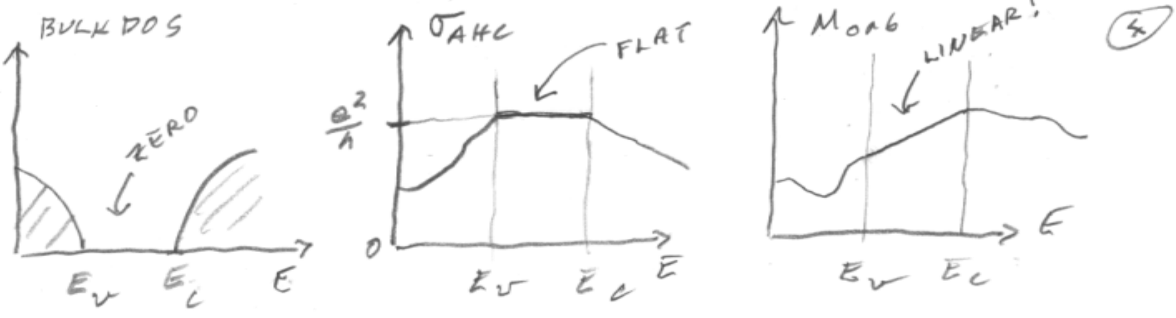


FIG. 2. Orbital magnetization m_z in Mn/W(001) according to ACA and modern theory (per two-dimensional unit cell, uc). Additionally, the local orbital moments in ACA of Mn and the first W (W1) layer are shown.

From April 1 lecture:



$$\boxed{\frac{dM}{d\phi} = \frac{1}{c}\sigma_{AHC} = \frac{1}{c}\frac{e^2}{h}C}$$ in gap of QAH insulator in 2D.

Now:

$$M = \frac{e}{2\hbar c}\frac{1}{(2\pi)^2}\sum_n \int_{BZ} d^2k \, \langle \partial_{\underline{k}} u_{n\underline{k}} | \times (H_{\underline{k}} + E_{n\underline{k}} - 2E_f) | \partial_{\underline{k}} u_{n\underline{k}} \rangle$$

$$\frac{dM}{dE_f} = \frac{e}{2\hbar c}\frac{1}{(2\pi)^2}\sum_n \int_{BZ} d^2k \, \langle \partial_{\underline{k}} u_{n\underline{k}} | \times | \partial_{\underline{k}} u_{n\underline{k}} \rangle \, (-2)$$

$$= \frac{-e}{hc}\left(-\sum_n C_n\right)$$

$$= \frac{1}{ec}\sigma_{AHC} \quad , \quad \sigma_{AHC} = \frac{e^2}{h}C \quad , \quad C = \sum_n C_n$$