Generalized Wannier functions for an ab initio description of the electronic structure of chiral magnets

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Outline

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3. Maximally localized Wannier functions
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   - Construction of GWFs
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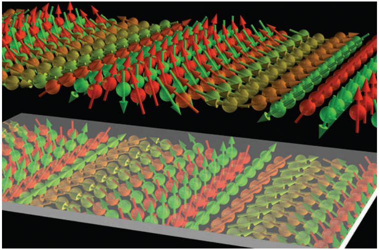
5. Conclusions

Motivation

- occurence of **nontrivial magnetic structures** in nature
- spin spirals (1D), skyrmions (2D) and others with fascinating properties



M. Bode et al., Nature 447, 7141 (2007)

- ultimate goal: **topological characterization** of complex magnetic structures in **real** and **momentum** space

Berry curvature in $\boldsymbol{\lambda}$-space

$$\Omega^n_{ij}(\boldsymbol{\lambda}) = -2\,\mathrm{Im}\sum_{m\neq n}\frac{\langle\boldsymbol{\lambda}n|\frac{\partial}{\partial\lambda_i}H(\boldsymbol{\lambda})|\boldsymbol{\lambda}m\rangle\langle\boldsymbol{\lambda}m|\frac{\partial}{\partial\lambda_j}H(\boldsymbol{\lambda})|\boldsymbol{\lambda}n\rangle}{(\epsilon_{\boldsymbol{\lambda}n}-\epsilon_{\boldsymbol{\lambda}m})^2}$$

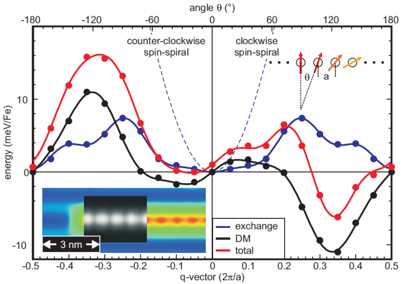
$\Rightarrow$ anomalous & topological Hall effect

Motivation

- **spin spiral vector q** as additional, tunable parameter
- topological characterization using **mixed Berry curvature**

mixed Berry curvature in (k, q)-space

$$\Omega^n_{kq} = -2\,\mathrm{Im} \sum_{m\neq n} \frac{\langle kqn|\frac{\partial}{\partial \mathbf{k}}\mathbf{H}(\mathbf{k},\mathbf{q})|kqm\rangle\langle kqm|\frac{\partial}{\partial \mathbf{q}}\mathbf{H}(\mathbf{k},\mathbf{q})|kqn\rangle}{(\epsilon_{kqn}-\epsilon_{kqm})^2}$$



- contributions to pumping ΔP and anomalous velocity
- **challenge**: poor convergence in ab initio calculation
- need **interpolation of $\mathbf{H}(\mathbf{k},\mathbf{q})$**

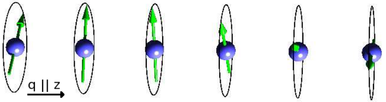
M. Menzel et al., PRL 108, 197204 (2012)

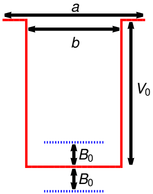
1D toy model

- chain of atoms + helical spin spiral

Hamiltonian

$$H = -\frac{\Delta}{2} + \sum_j \Theta_j(z)\,[V_0 + B_0\,\hat{n}\cdot\vec{\sigma}]$$
$$\hat{n} = (\,\cos(q\cdot ja)\,,\ \sin(q\cdot ja)\,,\ 0\,)^T$$



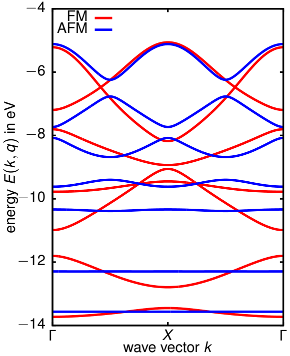


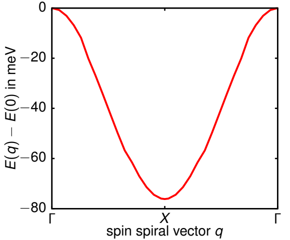
$V_0 = -12$ eV, $B_0 = 2$ eV, $a = 3$ Å, $b = 2.9$ Å

- antiferromagnetic groundstate

Generalized Bloch theorem

$$\Psi_{kqn}(z) = e^{ikz}\begin{pmatrix} e^{-i\frac{q}{2}z}u^{\uparrow}_{kqn}(z) \\ e^{i\frac{q}{2}z}u^{\downarrow}_{kqn}(z)\end{pmatrix}$$





Maximally localized Wannier functions

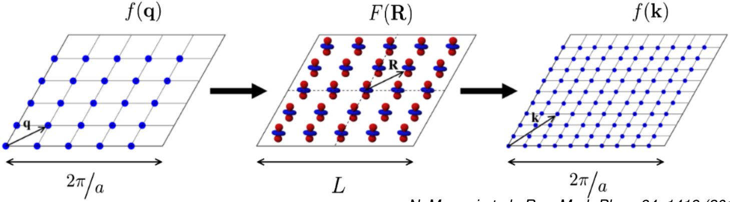
- exact tight-binding basis

Maximally localized Wannier functions (MLWF)

$$|W_R\rangle = \frac{1}{N_k}\sum_k \mathrm{e}^{-ikR}U(k)|\Psi_k\rangle = \mathcal{F}_k\left(U(k)|\Psi_k\rangle\right)$$

N. Marzari & D. Vanderbilt, PRB 56, 12847 (1997)

- $U(k)$ determined by **spread minimization** (e.g. wannier90)
  A. A. Mostofi et al., Comput. Phys. Commun. 178, 685 (2008)
- interpolating $H(k)$: main ingredient $\langle W_0|H|W_R\rangle$
- information on fine grid by inverse FT & **diagonalization**



N. Marzari et al., Rev. Mod. Phys. 84, 1419 (2012)

Generalized Wannier functions

Construction of GWFs

- include **additional parameter q**
- aim: obtain **useful** $|W_{RQn}\rangle$ via Fourier transformations

$$|W_{RQ}\rangle = \frac{1}{N_k N_q} \sum_{k,q} e^{-ikR} e^{-iqQ} U(k,q) |\Psi_{kq}\rangle$$

- **challenge**: unitary $U(k,q) \Leftrightarrow$ spread functional in q-space
- gauge choice $U(k,q) = U(k)V(q)$ and assume $V(q) = \mathbb{I}$

Generalized Wannier functions

1. $|W_R^q\rangle = \mathcal{F}_k\left(U(k)|\Psi_{kq}\rangle\right)$
2. $|W_{RQ}\rangle = \frac{1}{N_q}\sum_q e^{-iqQ}|W_R^q\rangle$

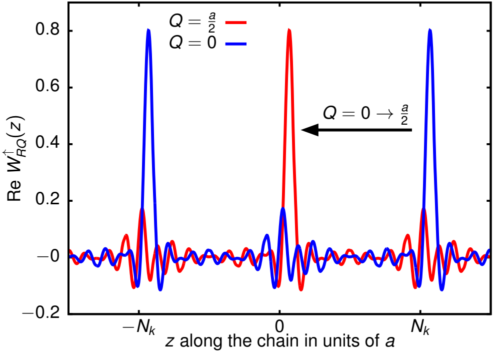
Generalized Wannier functions

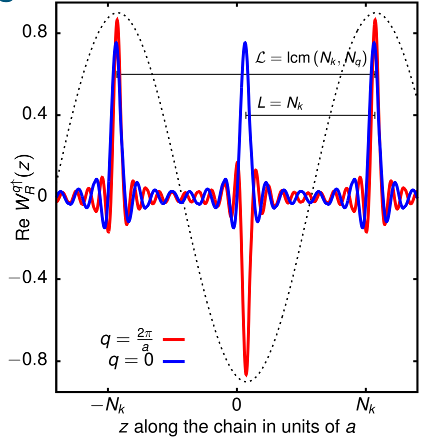
Construction of GWFs

1 $W_R^q(z) \sim \mathcal{F}_k\left(U(k)e^{ikz}e^{\mp i\frac{q}{2}z}u_{kq}\right)$

2 $W_{RQ}(z) \sim \sum_q e^{-iqQ}W_R^q(z)$

$\Rightarrow$ changes implied by q & Q ?





$\Rightarrow$ $q \sim$ **modulation**

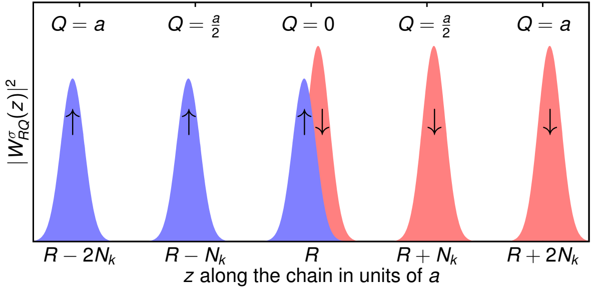
$\Rightarrow$ $Q \sim$ **shift**

Generalized Wannier functions

Interpretation of Q variable

- similar behaviour for $W^{\downarrow}_{RQ}(z)$ **but**...
- ... tuning Q introduces discrete **relative shift** between up- & down-component of GWFs (at least for certain choices of N_k, N_q)
- **center-of-mass** R and **relative** Q (unlike standard WFs)

Schematic plot



Generalized Wannier functions

Interpolation and Heisenberg model

Interpolation scheme

- **challenge**: overlap $\langle \Psi_{k'q'n} | \Psi_{kqm} \rangle \neq \delta_{kk'} \delta_{qq'} \delta_{nm}$
- scheme $H_\alpha = (1-\alpha) H_1 + \alpha H_2$ gauge invariant?
- proceed with $\langle W_{RQ} | H | W_{R'Q'} \rangle$ as main ingredient
- $\Rightarrow$ **generalized eigenvalue problem**

Heisenberg Hamiltonian $H = -J_{ij} S_i S_j$

- allows for interpretation of Q variable of GWFs

Exchange couplings

$$t_{QQ'} = -\frac{1}{2} M^2 \sin(\theta) \; J(Q' - Q)$$

Conclusions

- deal with additional parameters in Hamiltonian
- establish **interpolation** scheme for $H(k, q)$
- generalize formalism of Wannier functions

Challenges

- physical interpretation of shift by tuning Q
- cutoff Q_C for interpolation scheme
- implement within **ab initio** framework
- improve results by $V(q) \neq \mathbb{I}$
- evaluation of **exchange** J_{ij} and **Berry curvature**

Thank you for your attention