Magnetic interactions



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Outline



- Introduction
- Interactions
- Models
- STONER model
- HEISENBERG model

Introduction

Quantum mechanical description of solids







$$\hat{H} = \hat{T}_{I} + \hat{T}_{e} + V_{II} + V_{ee} + + V_{eI}$$

Adiabatic approximation

Electrons: $\hat{H}(\mathbf{R}) = \hat{T}_e(\mathbf{R}) + V_{ee}(\mathbf{R}) + +V_{eI}(\mathbf{R})$

lons:

$$\hat{H} = \hat{T}_I + V_{II} + E(\mathbf{R})$$

 $\mathbf{R} = \{\mathbf{R_1}, \mathbf{R_2}, \mathbf{R_3}, \ldots\}$



$$\hat{H}(\mathbf{R}) = \hat{T}_e(\mathbf{R}) + V_{ee}(\mathbf{R}) + +V_{eI}(\mathbf{R})$$

Many-electron Schrödinger equation:

$$\hat{H}(\mathbf{R})\Phi(\mathbf{r},\mathbf{R}) = E(\mathbf{R})\Phi(\mathbf{r},\mathbf{R})$$

Electron coordinates:

$$\mathbf{r} = \{\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3}, ...\}$$

Fixed ion coordinates:

$$\mathbf{R} = \{\mathbf{R_1}, \mathbf{R_2}, \mathbf{R_3}, \ldots\}$$



Many-electron Schrödinger equation:

$\hat{H}(\mathbf{R})\Phi(\mathbf{r},\mathbf{R}) = E(\mathbf{R})\Phi(\mathbf{r},\mathbf{R})$

- Free electrons
- Hartree approximation
- Hartree-Fock approximation
- Density functional theory

One-electron Schrödinger equation:

$$\hat{H}\varphi(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}^2} + V(\mathbf{r})\right)\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r})$$

Magnetic interactions

Interactions

There is no elementary magnetic interaction!

Dipol-dipol interaction between magnetic moments:

$$E_{DD}(\mathbf{R}) = \frac{1}{R^3} (\mathbf{M_1} \cdot \mathbf{M_2} - 3(\mathbf{M_1} \cdot \hat{\mathbf{R}})(\mathbf{M_2} \cdot \hat{\mathbf{R}}))$$

$$E_{DD} \sim 10^{-5} eV$$

$$M \sim 1\mu_B$$

$$\mu_B = \frac{e\hbar}{2mc}$$

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Exchange interaction caused by Pauli principle:

Ansatz for the wave function:

$$\Phi_{HF}(\mathbf{r}_1...\mathbf{r}_i...\mathbf{r}_N) = \frac{1}{\sqrt{N!}} \det |\varphi_{\alpha_i}(\mathbf{r}_i)|$$

Hartee-Fock energy:

$$E_{HF}[\varphi_{\alpha}] = \sum_{i}^{N} \int d^{3}r \varphi_{\alpha_{i}}^{*}(\mathbf{r}) \hat{H}(\mathbf{r}) \varphi_{\alpha_{i}}(\mathbf{r})$$
$$+ \frac{1}{2} \sum_{i \neq j} \int d^{3}r d^{3}r' \frac{\epsilon^{2}}{|\mathbf{r} - \mathbf{r}'|} [\varphi_{\alpha_{i}}^{*}(\mathbf{r}) \varphi_{\alpha_{i}}(\mathbf{r}) \varphi_{\alpha_{j}}^{*}(\mathbf{r}') \varphi_{\alpha_{j}}(\mathbf{r}')$$
$$- \varphi_{\alpha_{j}}^{*}(\mathbf{r}) \varphi_{\alpha_{i}}(\mathbf{r}) \varphi_{\alpha_{i}}^{*}(\mathbf{r}') \varphi_{\alpha_{j}}(\mathbf{r}')]$$

Exchange of two electrons!



Electrons in isolated atoms:

Mostly magnetic, Hund's rule

Electrons in an ideal Fermi gas:

Mostly non-magnetic





Localisation of the electrons



Atomic orbitals:

localised



delocalised





s

р_у

dyz

pz

 $d_{x^{2}-y^{2}}$

p_x

 d_{xz}

d_{xy}



d _z 2



Degree of electron localisation causes magnetism or not!

- Simple metals and semiconductors: non-magnetic
- Rare earth atoms: atomic magnetic moments
- Transition metals and actinide: weakly localised electrons

Interatomic exchange



Direct exchange:



Indirect exchange:



Superexchange:



Itinerant exchange: magnetism of delocalised electrons





 $\begin{aligned} & \text{Mean field approximation} \\ & < \hat{A}\hat{B} >= \hat{A} < \hat{B} > + < \hat{A} > \hat{B} - < \hat{A} > < \hat{B} > \\ & \text{WEISS} & \text{STONER} \end{aligned}$





One-electron Schrödinger equation for spin-dependent potential:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}^2} + V^{\pm}(\mathbf{r})\right)\varphi_m^{\pm}(\mathbf{r}) = \varepsilon_m^{\pm}\varphi_m^{\pm}(\mathbf{r})$$

Charge density:

$$n(\mathbf{r}) = n^{+}(\mathbf{r}) + n^{-}(\mathbf{r}) = \sum_{m} |\varphi_{m}^{+}(\mathbf{r})|^{2} + \sum_{m} |\varphi_{m}^{-}(\mathbf{r})|^{2}$$

Magnetization density:

$$m(\mathbf{r}) = n^{+}(\mathbf{r}) - n^{-}(\mathbf{r}) = \sum_{m} |\varphi_{m}^{+}(\mathbf{r})|^{2} - \sum_{m} |\varphi_{m}^{-}(\mathbf{r})|^{2}$$

Magnetization density and magnetization



$$m(\mathbf{r}) = n^{+}(\mathbf{r}) - n^{-}(\mathbf{r}) = \sum_{m} |\varphi_{m}^{+}(\mathbf{r})|^{2} - \sum_{m} |\varphi_{m}^{-}(\mathbf{r})|^{2}$$



Local magnetic moment per unit cell **M**

$$M = \int_{V_Z} d^3 r \ m(\mathbf{r})$$



One-electron Schrödinger equation for spin-dependent potential:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\mathbf{r}^2} + V^{\pm}(\mathbf{r})\right)\varphi_m^{\pm}(\mathbf{r}) = \varepsilon_m^{\pm}\varphi_m^{\pm}(\mathbf{r})$$

Spin-dependent potential:

$$V^{\pm}(\mathbf{r}) = V(\mathbf{r}) \mp \frac{1}{2}IM$$

$$M = \int_{V_Z} d^3 r \ m(\mathbf{r})$$



Wave function unchanged by spin polarization, constant potential:

$$\varphi_m^{\pm}(\mathbf{r}) = \varphi_m(\mathbf{r})$$

Splitting of the eigenvalues:





Spin-polarized density of states





Number of electrons:

$$N = \int^{E_F} dE \{ D_0(E + IM/2) + D_0(E - IM/2) \}$$

Magnetic moment:

$$M = \int^{E_F} dE \{ D_0(E + IM/2) - D_0(E - IM/2) \}$$

Fixed: $N, D_0(E)$ To be determined: E_F, M

$$F(M) = \int^{E_F(M)} dE \{ D_0(E + IM/2) - D_0(E - IM/2) \}$$

Self-consistent solution





Properties of F(M):

•
$$F(0) = 0$$

•
$$F(-M) = -F(M)$$
 bzw. $E_F(-M) = E_F(M)$

- $F(\pm\infty) = \pm M_{\infty}$ and $-M_{\infty} \le F(M) \le M_{\infty}$
- $F'(M) \ge 1$ monotonically increasing





$$F(M) = \int^{E_F(M)} dE \{ D_0(E + IM/2) - D_0(E - IM/2) \}$$

$$\frac{dF}{dM} = \int^{E_F(M)} dE \left[\frac{d}{dM} \{ D_0(E + IM/2) - D_0(E - IM/2) \} + \{ D_0(E + IM/2) - D_0(E - IM/2) \} \frac{dE_F}{dM} \right]$$

$$F'(M) = \int^{E_F(M)} dE[\{D_0(E + IM/2) + D_0(E - IM/2)\} + \{D_0(E + IM/2) - D_0(E - IM/2)\} \frac{dE_F}{dM}]$$



Calculation of
$$\frac{dE_F}{dM}$$
 from $dN = 0$

$$dN = \frac{dN}{dE_F}dE_F + \frac{dN}{dM}dM = 0$$

$$N = \int^{E_F} dE \{ D_0(E + IM/2) + D_0(E - IM/2) \}$$

$$0 = (D_0^+ + D_0^-)dE_F + \frac{I}{2}(D_0^+ - D_0^-)dM \qquad \frac{dE_F}{dM} = \frac{I}{2}\frac{(D_0^+ - D_0^-)}{(D_0^+ + D_0^-)}$$







$$F'(M) = \int^{E_F(M)} dE[\{D_0(E + IM/2) + D_0(E - IM/2)\} + \{D_0(E + IM/2) - D_0(E - IM/2)\} \frac{dE_F}{dM}]$$

$$\frac{dE_F}{dM} = \frac{I}{2} \frac{(D_0^+ - D_0^-)}{(D_0^+ + D_0^-)}$$

$$F'(M) = \frac{I}{2}(D_0^+ + D_0^-)\{1 - \frac{(D_0^+ - D_0^-)^2}{(D_0^+ + D_0^-)^2}\} \ge 0$$



Paramagnetic solution:

trivial solution M=0









Ferromagnetic solution:

- trivial solution M=0
- two solutions with spontaneous magnetization ${}_+M_{S}$



STONER criterion: $F'(0) = ID_0(E_F) > 1$



STONER criterion: $F'(0) = ID_0(E_F) > 1$

	$D_0(E_F) \left[eV^{-1} \right]$	$I \; [eV]$	$ID_0(E_F)$	$M \; [\mu_B/atom]$
Na	0.23	1.82	0.41	
Al	0.21	1.22	0.25	
Cr	0.35	0.76	0.27	
Mn	0.77	0.82	0.63	
Fe	1.54	0.93	1.434	2.22
Со	1.72	0.99	1.70	1.71
Ni	2.02	1.01	2.04	0.61
Cu	0.14	0.73	0.11	
Pd	1.14	0.68	0.78	
Pt	0.79	0.63	0.5	

Density of states for bulk ferromagnets





13.10.2017

Cargèse

HEISENBERG model

Magnons and second quantization





Dispersion relation of spin waves in ferromagnets:

 $arepsilon(m{k})=2Js\left(1-\cos(ka)
ight)$ (only one basis atom)

 $n\,$ basis atoms lead to $n\,$ magnon branches $arepsilon_i(m{k})\,$.



Magnons in second quantization



Hamiltonian:
$$H = -J \sum_{\langle ij \rangle} s_i \cdot s_j = -J \sum_{\langle ij \rangle} \left[s_i^z s_j^z + \frac{1}{2} \left(s_i^- s_j^+ + s_i^+ s_j^- \right) \right]$$

 $s_i^{\pm} = s_i^x \pm i s_i^y$
 $[s_i^z, s_j^{\pm}] = \pm s_i^{\pm} \delta_{i,j}, \quad [s_i^+, s_j^-] = 2s_i^z \delta_{i,j}$ lowers z component raises z component

Bosonization: $|0\rangle$ is the ground state (magnon vacuum); analyze **small** fluctuations



Magnons in second quantization





Topological states and magnetism



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Outline



- Introduction
- Topological electron states
- The quantum Hall effects
- The topological Hall effect
- Summary

What is a Berry phase?



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Schrödinger equation and adiabatic evolution

$H(\mathbf{R})|\varphi_n(\mathbf{R})\rangle = E_n(\mathbf{R})|\varphi_n(\mathbf{R})\rangle$

$|\varphi_n(\mathbf{R_0})\rangle = \exp(i\gamma_n(C))|\varphi_n(\mathbf{R_0})\rangle$

M. V. Berry, Proc. R. Soc. A 392, 1802 (1984)

 $\mathbf{R}_{\mathbf{0}}$

Cargèse

What is a Berry curvature?



Berry phase:

$$\gamma_n(C) = i \oint_c dR \langle \varphi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \varphi_n(\mathbf{R}) \rangle$$

Berry connection:

$$\mathbf{A}_n(\mathbf{R}) = i \langle \varphi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \varphi_n(\mathbf{R}) \rangle$$

Berry curvature:

$$egin{aligned} oldsymbol{\Omega}_n(\mathbf{R}) &=
abla imes \mathbf{A}_n(\mathbf{R}) \ &= i \langle
abla_{\mathbf{R}} arphi_n(\mathbf{R}) | imes |
abla_{\mathbf{R}} arphi_n(\mathbf{R}) | \end{aligned}$$

M. V. Berry, Proc. R. Soc. A 392, 1802 (1984)

Berry curvature of Bloch states







Change of momentum:

$$\begin{split} \hbar \dot{\mathbf{k}} &= -e\mathbf{E} \qquad -e\dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r}) \\ \text{Change of position:} & \text{Lorentz force} \\ \dot{\mathbf{r}} &= \frac{\partial E_n(\mathbf{k})}{\hbar \partial \mathbf{k}} \underbrace{-\dot{\mathbf{k}} \times \mathbf{\Omega}_n(\mathbf{k})}_{\text{Anomalous velocity}} \end{split}$$

M.-C. Chang and Q. Niu, Phys. Rev. B 53, 7010 (1996)

Transversal transport coefficients

Ohm's law and conductivity tensor





Cargèse



The Hall trio





Lorentz force

Berry curvature $\mathbf{\Omega}_n(\mathbf{k})$

spin-orbit interaction:

 $\mathbf{s} \cdot \mathbf{L}$

Nagaosa, Sinova et al., Rev. Mod. Phys. 82, 1539 (2010)



$$\sigma_{xy}^{\pm} = \frac{e^2}{\hbar (2\pi)^3} \sum_n \int_{BZ} d^3k f_n(\mathbf{k}) \Omega_z^n(\mathbf{k})$$

$$\sigma_{xy}^{\pm} = \frac{e^2}{\hbar (2\pi)^3} \sum_n \int^{E_F} dE \Omega_z^n(E)$$

Anomalous Hall effect:

 $\sigma_{xy} = \sigma_{xy}^+ + \sigma_{xy}^-$

Spin Hall effect:

$$\sigma_{xy}^s = \sigma_{xy}^+ - \sigma_{xy}^-$$

Intrinsic spin Hall conductivity





Guo et al., PRL 100, 096401 (2008); J. Appl. Phys. 105, 07C701 (2009)

Diabolic points

Band crossing and diabolic points







Point charge field:

$$\mathbf{E}_{\pm}(\mathbf{r}) = \pm Q \frac{\mathbf{r} - \mathbf{r_0}}{|\mathbf{r} - \mathbf{r_0}|^3}$$



Magnetic monopole:

$$\mathbf{B}_{\pm}(\mathbf{r}) = \pm g \frac{\mathbf{r} - \mathbf{r_0}}{|\mathbf{r} - \mathbf{r_0}|^3}$$

Berry curvature monopole:

$$\mathbf{\Omega}_{\pm}(\mathbf{k}) = \pm g \frac{\mathbf{k} - \mathbf{k_0}}{|\mathbf{k} - \mathbf{k_0}|^3}$$

P.A.M. Dirac, Phys. Rev. 1948

Dirac quantization



Monopole field: $\mathbf{B}_{\pm}(\mathbf{r}) = \pm g \frac{\mathbf{r} - \mathbf{r_0}}{|\mathbf{r} - \mathbf{r_0}|^3}$



Dirac's quantization of the monopole field:

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r}) + \sum_{j} g_{j} \frac{\mathbf{r} - \mathbf{r}_{j}}{|\mathbf{r} - \mathbf{r}_{j}|^{3}} \qquad g_{j} = \pm \frac{1}{2}$$

$$\frac{1}{2\pi} \int_{V} d\mathbf{r} \, \nabla \cdot \mathbf{B}(\mathbf{r}) \; = \; \frac{1}{2\pi} \int_{\partial V} d\sigma \, \mathbf{n} \cdot \mathbf{B}(\mathbf{r}) \; = \; C \quad C \in \mathbf{Z}$$

P.A.M. Dirac, Phys. Rev. 1948

Berry curvature monopoles



Monopole field: $\Omega_{\pm}({\bf k})=\pm\frac{1}{2}\frac{{\bf k}-{\bf k_0}}{|{\bf k}-{\bf k_0}|^3}$

Dirac's quantization of the monopole field:

$$\mathbf{\Omega}(\mathbf{k}) = \nabla \times \mathbf{A}(\mathbf{k}) + \sum_{j} g_{j} \frac{\mathbf{k} - \mathbf{k}_{j}}{|\mathbf{k} - \mathbf{k}_{j}|^{3}} \qquad g_{j} = \pm \frac{1}{2}$$

$$\frac{1}{2\pi} \int_{V} d\mathbf{k} \, \nabla \cdot \mathbf{\Omega}(\mathbf{k}) = \frac{1}{2\pi} \int_{\partial V} d\sigma \, \mathbf{n} \cdot \mathbf{\Omega}(\mathbf{k}) = C \quad C \in \mathbf{Z}$$

P.A.M. Dirac, Phys. Rev. 1948



Topological states

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Tomáš Rauch

Alexander Mook

Jürgen Henk

Intrinsic spin Hall conductivity





Spin Hall effect of an insulator and Chern number





Chern number





Band inversion without TRS







Band inversion with TRS





Z2 TI:

gap in 2d and 3d Kramers degeneracy

DIRAC semimetal: no gap in 3d + crystal symmetry

Cargèse

Topological surface state of a Z2 TI



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B. A. Bernevig, T. L. Hughes, S. C. Zhang, Science 314, 1757 (2006)

Topological surface state in Bi_2Te_3



The quantum Hall trio





The conductance is quantized!

S Oh Science 2013;340:153-154

Topological Hall effect

B. Göbel, A. Mook, J. Henk, and I. M., Phys. Rev. B **95**, 094413 (2017) B. Göbel, A. Mook, J. Henk, and I. M., New Journ. Phys., accepted (2017)

Experiment to measure the THE





Skyrmions





M. Nagao et al., Experimental observation of multiple-q states for the magnetic skyrmion lattice and skyrmion excitations under a zero magnetic field. Phys. Rev. B 92, 140415 (2015)



Skyrmion lattice





B. Göbel, A. Mook, J. Henk, and I.M., Phys. Rev. B 95, 094413 (2017)

Skyrmion – background spin texture





Electron bandstructure in background spin texture







14.10.2017

Electrons in the skyrmion field and THE





14.10.2017

THE from Berry curvature of the electrons



$$\sigma_{xy}^{\pm} = \frac{e^2}{h} \frac{1}{2\pi} \sum_{n} \int_{BZ} d^2 k f_n(\mathbf{k}) \Omega_z^n(\mathbf{k})$$



Börge Göbel, Alexander Mook, Jürgen Henk and Ingrid Mertig, Phys. Rev. B 95, 094413 (2017)

From THE to QHE

Spin texture, skyrmion number and emergent field



Börge Göbel, Alexander Mook, Jürgen Henk and Ingrid Mertig, Phys. Rev. B **95**, 094413 (2017) Keita Hamamoto, Motohiko Ezawa, and Naoto Nagaosa, Phys. Rev. B **92**, 115417 (2015)
Free electrons in a triangular lattice





Börge Göbel, Alexander Mook, Jürgen Henk and Ingrid Mertig, Phys. Rev. B 95, 094413 (2017)

Comparison of THE and QHE



Cargèse







The conductance is quantized!

S. Oh, Science **340**,153-154 (2013)

Summary



- Chern number topological invariant
- Berry curvature acts like a magnetic field and causes anomalous veolcity!
- Anomalous velocity is the origin of the transversal transport coefficients: spin and anomalous Hall effect and quantum spin and anomalous Hall effect, as well as the topological Hall and quantum topological Hall effect!