Lecture 2
New dynamics of Bloch electrons

Condensed matter theory
Particle view in crystals
Berry curvature in semiclassical dynamics
Anomalous Hall effect in magnets
Valley Hall effect in graphene

What is condensed matter physics?

- Definitions:
  - 1/3 of physics ---- according to Walter Kohn
  - solid & liquid --- traditional definition
  - hard & soft matter ---- according to deGennes
  - structure & transport: the old PRL division
  - basis of materials science and engineering
- The role of theory in this field:
  - To develop useful models for experimental systems
  - To reveal mechanisms for observed phenomena
  - To develop accurate methods to predict properties
  - To establish a systematic world view of condensed matter

Walter Kohn, Nobel prize (1999)

力学

$$\vec{F} = m\vec{a}$$

$$F = -\frac{Gm_1m_2}{r^2}$$

$$\delta\int_{t_a}^{t_b}\mathcal{L}(\vec{q},\dot{\vec{q}},t)\,\mathrm{dt} = 0$$

$$\dot{\vec{q}} = \frac{\partial H}{\partial\vec{p}}$$

$$\dot{\vec{p}} = -\frac{\partial H}{\partial\vec{q}}$$

电动

$$\nabla\cdot\vec{E} = \frac{\rho}{\epsilon}$$

$$\nabla\cdot\vec{B} = 0$$

$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\nabla\times\vec{B} = \mu\vec{J} + \epsilon\mu\frac{\partial\vec{B}}{\partial t}$$

$$\vec{F} = q\vec{E} + \mathrm{q}\vec{v}\times\vec{B}$$

量子

$$E = \hbar\omega$$

$$\vec{p} = \hbar\vec{k}$$

$$i\hbar\frac{\partial}{\partial t}\psi = \widehat{H}\,\psi$$

$$\rho(\vec{r},t) = |\psi(\vec{r},t)|^2$$

$$[\hat{x},\hat{p}] = i\hbar$$

热统

$$\mathrm{d}U = \delta Q + \delta W$$

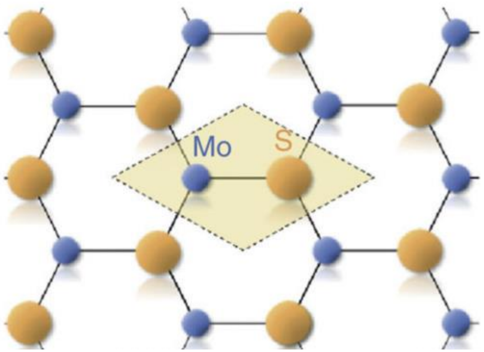
$$\oint\frac{\delta Q}{T} \le 0$$

$$S = k_B\ln\Omega$$

$$Z = \sum e^{-\beta H}$$

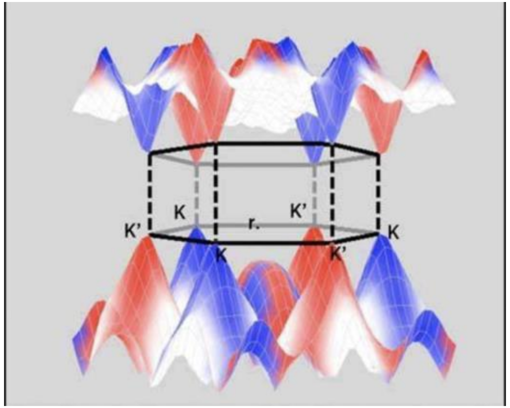
$$f = \frac{1}{e^{\beta(\varepsilon-\mu)} \pm 1}$$

Crystal properties



- Structure and ordering
- Electronic bands
- Collective excitations
- Equilibrium and transport responses

Microscopic to macroscopic properties



Newtonian Dynamics (1687)

- Absolute space and time: continuous and flat
  - Gravity is just another force
  - Einstein (1916): gravity reflects space-time deformation
- Canonical phase space (1834)
  - Hamilton’s equations and Liouville’s theorem
  - Basis for statistical and quantum mechanics

$$\dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}} \qquad \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}}$$

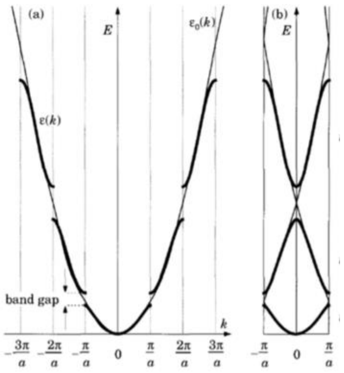
Bloch dynamics (1928)

- Real space becomes homogeneous beyond atomic scales: meta space
- Momentum space becomes a finite torus for each band
  - Band energy is periodic in k

$$\varepsilon(k+2\pi/a)=\varepsilon(k)$$

  - Particle dynamics in a band

$$\dot{x} = \partial_k \varepsilon,$$
$$\dot{k} = -eE - e\dot{x} \times B$$



- Can be made canonical and quantized by the Peierles substitution (1933)
  k --> k + eA, ε --> ε-eϕ
- Provide a basic theory for metals, semiconductors, and insulators (Luttinger &Kohn 1955).

Postdoc life with Walter Kohn

- 1987-1990 UC Santa Barbara

Walter Kohn’s 10 most cited papers

1 KOHN, W; SHAM, LJ. **Cited:** 31952
Self-consistent Equations Including Exchange and Correlation Effects

2 HOHENBERG, P; KOHN, W **Cited:** 26305
Inhomogeneous Electron gas

3 LUTTINGER, JM; KOHN, W. **Cited:** 2354
Motion of Electrons and holes in perturbed periodic Fields

4 Kohn, W; Becke, AD; Parr, RG **Cited:** 1569
Density functional theory of electronic structure

5 LANG, ND; KOHN, W **Cited:** 1523
Theory of Metal Surfaces-Charge Density and Surface Energy

6 KOHN, W; ROSTOKER, N **Cited:** 1119
Solution of the Schrodinger Equation in Periodic Lattices with an Application to Metallic Lithium

7 LANG, ND; KOHN, W **Cited:** 1031
Title: Theory of Metal Surfaces – Work Function

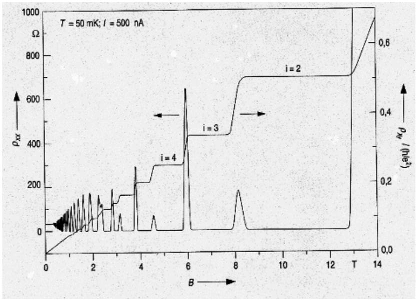
8 Kohn, W **Cited:** 1035
Nobel Lecture: Electronic structure of matter-wave functions and density functionals

9 Kohn, W **Cited:** 903
Shallow impurity States in Silicon and Germanium

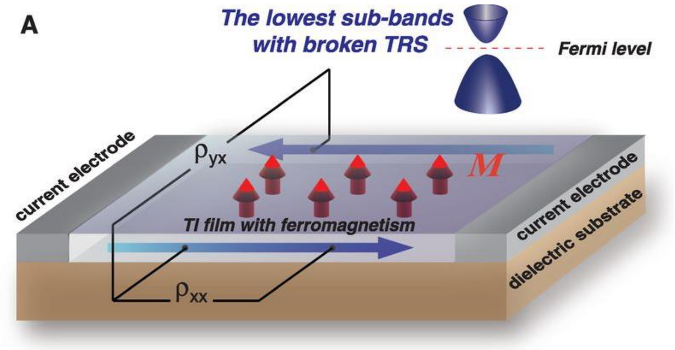
10 KOHN, W **Cited:** 885
Cyclotron Resonance and de Haas-van Alphen Oscillations of an Interacting Electron Gas

Topological phases of matter

- Quantum Hall effects



von Klitzing 1980



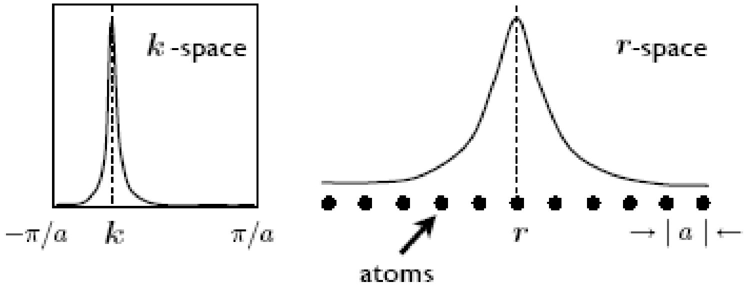
Q.K. Xue 2013

- Topological insulators and superconductors

David Thouless
2016 Nobel prize

Semiclassical Equations of Motion

Wave-packet
Dynamics
(r, k)



Chang and Niu (1995)

$$\dot{r} = \frac{\partial \varepsilon_n(k)}{\hbar \partial k} - \dot{k} \times \Omega_n(k)$$

$$\hbar \dot{k} = -eE(r) - e\dot{r} \times B(r)$$

Nonzero if either time-reversal or inversion symmetry is broken

Berry Curvature

$$\Omega_n(k) = \mathrm{i}\langle \nabla_k u_n(k) | \times | \nabla_k u_n(k) \rangle$$

Magnetic field in momentum space

Berry curvature in k space

magnetic Bloch bands

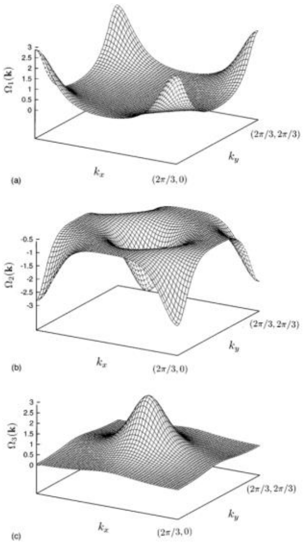
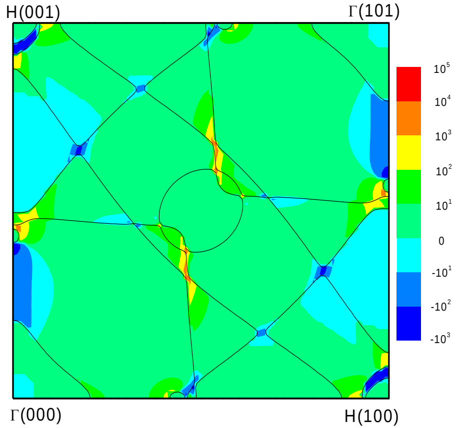


FIG. 5. Distributions of Berry curvature $\Omega_n(\mathbf{k})$ (in units of e^2/h). $\Omega_1(\mathbf{k})$ is equal to $\Omega_3(\mathbf{k})$ shifted by $(\pi/3, \pi/3)$.

Ferromagnetic bcc Fe



Yao et al, PRL (2004)

Anomalous Hall effect

- velocity $$\dot{\mathbf{x}} = \frac{\partial \mathcal{E}}{\partial \mathbf{k}} + e\,\mathbf{E}\times\boldsymbol{\Omega},$$
- distribution $$g(\mathbf{k}) = f(\mathbf{k}) + \delta f(\mathbf{k})$$
- current $$-e^2\,\mathbf{E} \times \int d^3\mathbf{k}\;\, f(\mathbf{k})\,\boldsymbol{\Omega} \;-e \int d^3\mathbf{k}\;\, \delta f(\mathbf{k})\,\frac{\partial \mathcal{E}}{\partial \mathbf{k}}$$

Intrinsic

Remarks

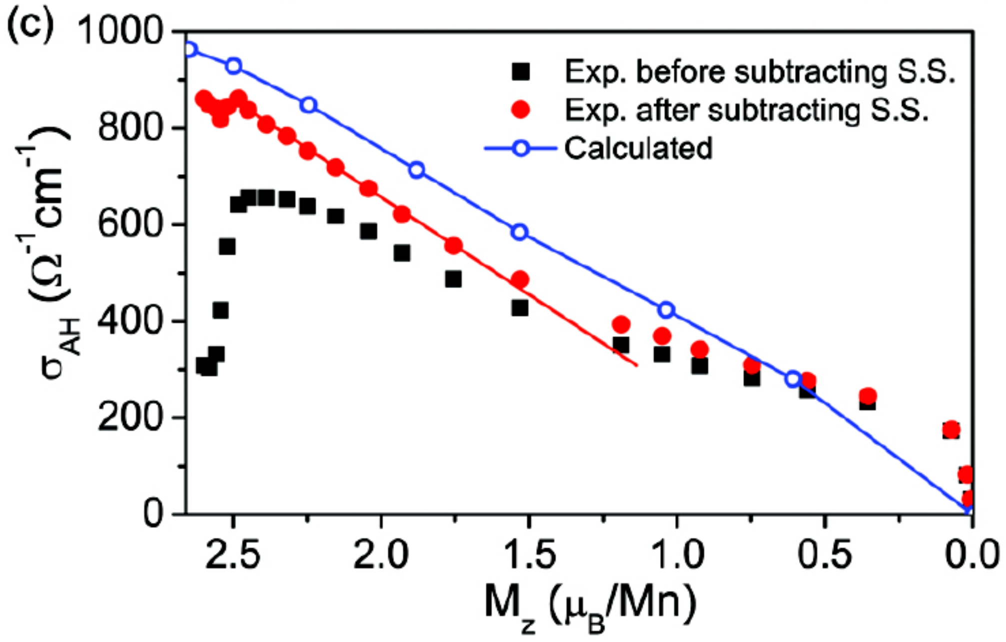
- For band insulators, we have the Chern number.
- In metals, the Berry curvature gives an intrinsic contribution: Karplus-Luttinger (1954)
- There are also extrinsic contributions
  - Smit: Skew Scattering (1955)
  - Berger: side jump (1970)
- Theoretical understanding of AHE was dominated by the extrinsic mechanisms until 2002.

Intrinsic AHE in ferromagnets

- Semiconductors, $Mn_xGa_{1-x}As$
  - Jungwirth, Niu, MacDonald , PRL (2002) , J Shi’s group (2008)
- Oxides, $SrRuO_3$
  - Fang et al, Science , (2003).
- Transition metals, Fe
  - Yao et al, PRL (2004),Wang et al, PRB (2006), X.F. Jin’s group (2008)
- Spinel, $CuCr_2Se_{4-x}Br_x$
  - Lee et al, Science, (2004)
- First-Principle Calculations-Review
  - Gradhand et al (2012)

Anomalous Hall Effect in Metal

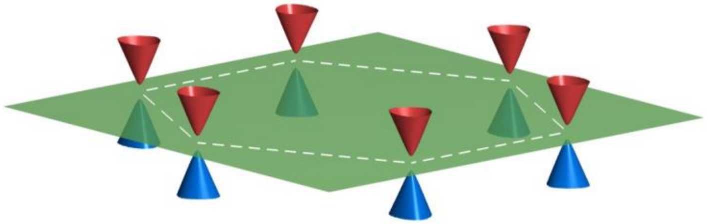
Mn5Ge3 : Zeng, Yao, Niu & Weitering, PRL 2006



Berry curvature from inversion symmetry breaking

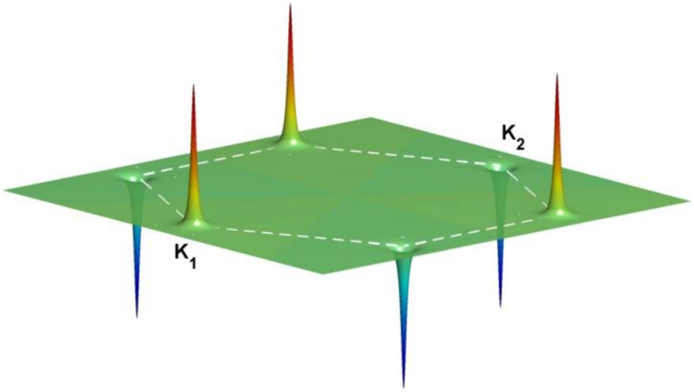
- Honeycomb lattice with sublattice bias
- Energy bands

$$\varepsilon(q) = \pm\sqrt{\Delta^2 + 3t^2q^2/4}$$



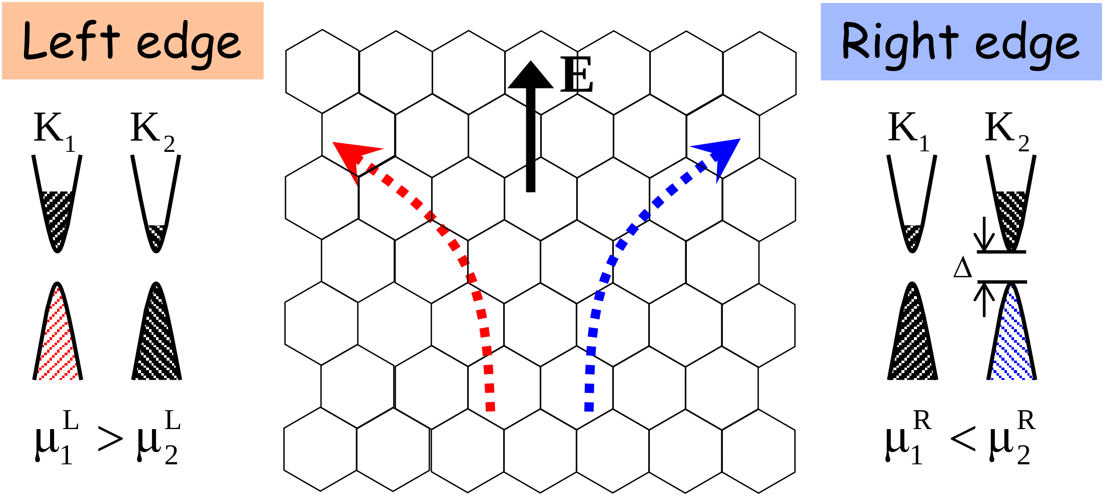
- Berry curvature

$$\Omega(\boldsymbol{q}) = \pm\tau_z \frac{3a^2\Delta t^2}{2(\Delta^2 + 3q^2a^2t^2)^{3/2}}$$



- Xiao,Yao, Niu (2007)

Valley Hall Effect



Observed 2014-2015:

- MoS2 (Mak et al)
- Graphene on hBN (Gorbachev et al)
- Graphene bi-layer (Sui et al)

Summary

Our world view of solid state has been greatly shaped by quantum mechanics:

Old particle view fails on the atomic scale
Energy momentum structure is modified into Bloch bands in crystals
New particle view re-emerges in Bloch bands beyond atomic scales
Berry curvature effects further modifies the dynamics
with dramatic effects including topological effects