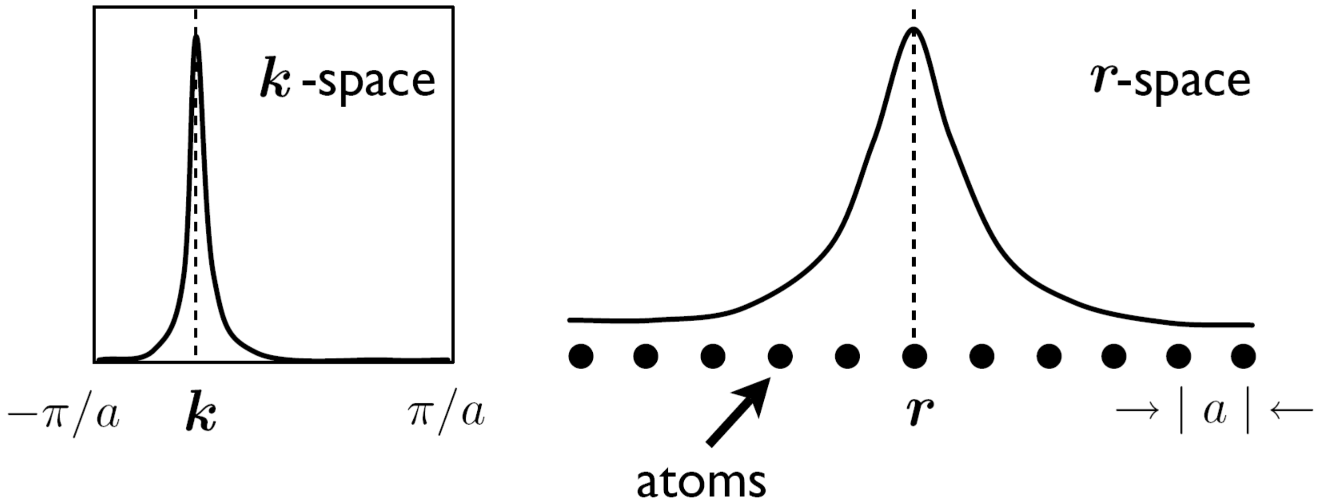
Lecture 4
Magnetic Properties

- Wave packet in electromagnetic field
- Field modified density of states
- Magnetic moment and Magnetization
- Cyclotron orbit and quantization
- Spin degenerate bands and effective Hamiltonian

Construction of Wave Packets



$$|W\rangle = \int_{\mathrm{BZ}} d\boldsymbol{k}\, a(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_c)} |u_n(\boldsymbol{k})\rangle$$

$$\boldsymbol{r}_c = \langle W|\hat{\boldsymbol{r}}|W\rangle$$

$$\boldsymbol{k}_c = \langle W|\hat{\boldsymbol{k}}|W\rangle$$

Equations of motion to first order in fields

Equation of motion

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

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

Berry curvature

$$\boldsymbol{\Omega}_n(\boldsymbol{k}) = \boldsymbol{\nabla}_{\boldsymbol{k}} \times \langle u_n(\boldsymbol{k}) | i \boldsymbol{\nabla}_{\boldsymbol{k}} | u_n(\boldsymbol{k}) \rangle$$

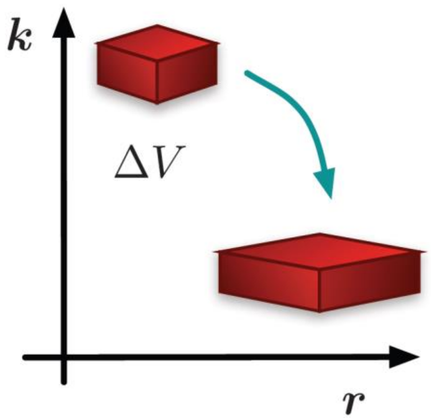
Energy correction

$$\varepsilon_n(\boldsymbol{k}) = \varepsilon_n^0(\boldsymbol{k}) - \boldsymbol{m}(\boldsymbol{k}) \cdot \boldsymbol{B}$$

$\boldsymbol{\Omega}_n(\boldsymbol{k})$ is nonzero in the presence of **broken** time-reversal (ferromagnets, magnetic Bloch bands) or space-inversion (GaAs) symmetry

Chang & Niu, PRL 1995, PRB 1996, Sundaram & Niu PRB 1999

Evolution of the Phase-Space Volume



Volume element $\Delta V = \Delta \boldsymbol{r} \Delta \boldsymbol{k}$

Conservation of phase space volume

$$\frac{1}{\Delta V}\frac{d\Delta V}{dt} = \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} + \boldsymbol{\nabla}_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}} = 0$$

With the Berry curvature field $\frac{1}{\Delta V}\frac{d\Delta V}{dt} \neq 0$

$$\Delta V = \frac{\text{constant}}{1 + (e/\hbar)\boldsymbol{B}(\boldsymbol{r}) \cdot \boldsymbol{\Omega}(\boldsymbol{k})}$$

Xiao, Shi & Niu, PRL 2005

Field-Dependent Density of States

Phase space volume of a quantum state

$$(2\pi)^d \quad \Rightarrow \quad \frac{(2\pi)^d}{1 + (e/\hbar)\boldsymbol{B} \cdot \boldsymbol{\Omega}}$$

Statistical physics – Density of states

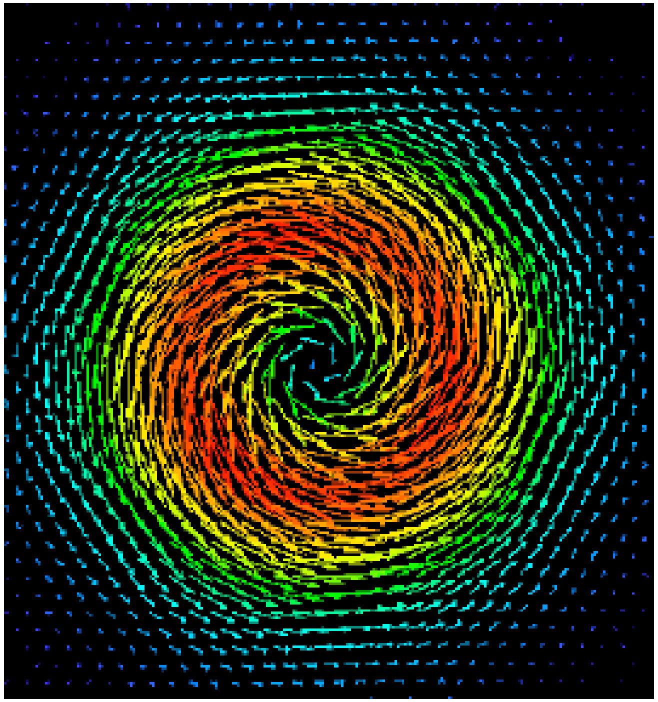
$$D(\boldsymbol{r}, \boldsymbol{k}) = \frac{1}{(2\pi)^d} \quad \Rightarrow \quad D(\boldsymbol{r}, \boldsymbol{k}) = \frac{1}{(2\pi)^d}(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})$$

Physical quantity

$$\langle \mathcal{O} \rangle = \sum_n \int d\boldsymbol{k}\, D_n(\boldsymbol{k}) f_n(\boldsymbol{k}) \mathcal{O}_n(\boldsymbol{k})$$

$f_n(\boldsymbol{k})$ - Occupation number

Orbital Magnetic Moment



A rotating wave packet

$$\boldsymbol{m}(\boldsymbol{k}) = -\frac{e}{2}\langle W|(\hat{\boldsymbol{r}} - \boldsymbol{r}_c) \times \boldsymbol{v}|W\rangle$$
$$= -i\frac{e}{2\hbar}\langle \boldsymbol{\nabla}_{\boldsymbol{k}} u| \times (\hat{H} - \varepsilon_{\boldsymbol{k}})|\boldsymbol{\nabla}_{\boldsymbol{k}} u\rangle$$

⇓

Correction to electron energy

$$\varepsilon_n(\boldsymbol{k}) = \varepsilon_n^0(\boldsymbol{k}) - \boldsymbol{m}(\boldsymbol{k}) \cdot \boldsymbol{B}$$

Orbital Magnetization

$$\boldsymbol{M} = -\left(\frac{\partial F}{\partial \boldsymbol{B}}\right)_{\mu,T}$$

$$F = -\frac{1}{\beta}\sum_{\boldsymbol{k}} \log(1 + e^{-\beta(\tilde{\varepsilon}-\mu)})$$

$$= -\frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^3}(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})(1 + e^{-\beta(\tilde{\varepsilon}-\mu)})$$

Xiao, Shi & Niu, PRL 2005
Xiao, Yao, Fang & Niu, PRL 2006

B **dependence**

Orbital magnetization

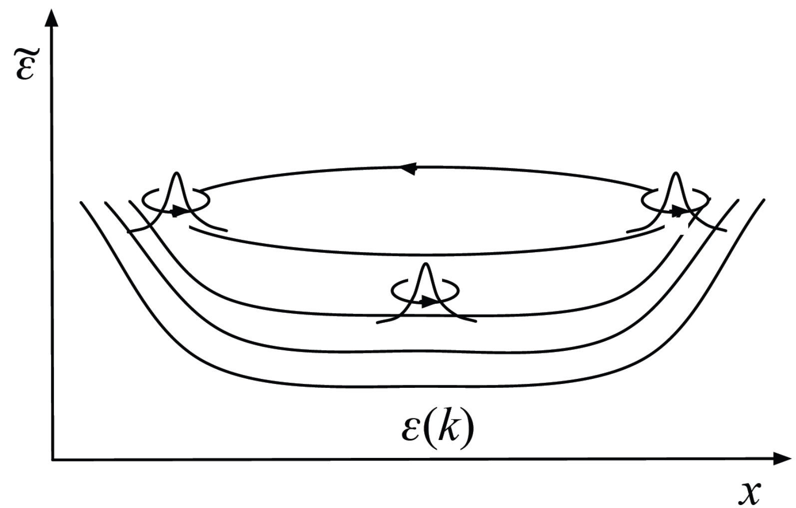
$$\boldsymbol{M}(\boldsymbol{r}) = \int \frac{d\boldsymbol{k}}{(2\pi)^d} f(\boldsymbol{r},\boldsymbol{k})\boldsymbol{m}(\boldsymbol{k}) + \frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})\log(1 + e^{-\beta(\varepsilon-\mu)})$$

A Pictorial Explanation

- Magnetic moment contribution (self-rotation)
- Berry-phase contribution (center of mass motion)

Anomalous velocity at boundary

$$\boldsymbol{v} = \frac{1}{\hbar} \boldsymbol{\nabla} V \times \boldsymbol{\Omega}(\boldsymbol{k})$$



$$M_z = \int \frac{d\boldsymbol{k}}{(2\pi)^3} f(\boldsymbol{k}) m_z(\boldsymbol{k}) - \frac{1}{e} \int d\varepsilon f(\varepsilon) \sigma_{xy}^{AH}(\varepsilon)$$

Cyclotron Motion

Equation of motion

$$\hbar \dot{\boldsymbol{k}} = -e \frac{\boldsymbol{v} \times \boldsymbol{B}}{1 + (e/\hbar)\boldsymbol{B} \cdot \boldsymbol{\Omega}}$$

Period

$$T = \oint_{t_1}^{t_2} dt = \oint \frac{d\boldsymbol{k}}{|\dot{\boldsymbol{k}}|}$$

Assume (1) energy dispersion ~ k^2; (2) rotational symmetry about z-axis:

Cyclotron frequency

$$\omega_c = \frac{eB}{m} \frac{1}{1 + (e/\hbar)\boldsymbol{B} \cdot \boldsymbol{\Omega}}$$

High-field Hall effect ($\omega_c \tau >> 1$)

In ferromagnets, the Hall current consists of the ordinary Hall current and the anomalous Hall current

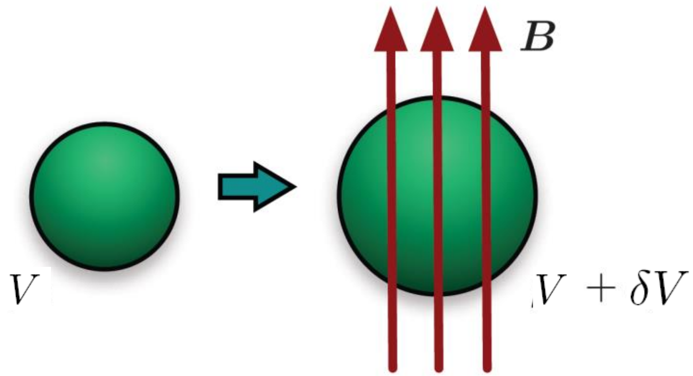
$$
\begin{aligned}
\boldsymbol{j}_H &= \boldsymbol{j}_{OH} + \boldsymbol{j}_{AH} \\
&= -e\frac{\boldsymbol{E}\times\boldsymbol{B}}{B^2}\int\frac{d\boldsymbol{k}}{(2\pi)^d}f(\boldsymbol{k}) - e\boldsymbol{E}\times\int\frac{d\boldsymbol{k}}{(2\pi)^d}\frac{e}{\hbar}\boldsymbol{\Omega}f(\boldsymbol{k}) \\
&= -e\frac{\boldsymbol{E}\times\boldsymbol{B}}{B^2}\int\frac{d\boldsymbol{k}}{(2\pi)^d}(1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})
\end{aligned}
$$

(Assume the magnetic field is parallel with the Berry curvature)

Electron density $\quad n = \int\frac{d\boldsymbol{k}}{(2\pi)^d}(1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})f(\boldsymbol{k})$

$$\boldsymbol{j}_H^{\text{electron}} = -e\frac{\boldsymbol{E}\times\boldsymbol{B}}{B^2}n_e \quad \Bigg| \quad \boldsymbol{j}_H^{\text{hole}} = -e\frac{\boldsymbol{E}\times\boldsymbol{B}}{B^2}n_h - e\boldsymbol{E}\times\int_{\text{BZ}}\frac{d\boldsymbol{k}}{(2\pi)^d}\boldsymbol{\Omega}$$

Field-Dependent Fermi Volume



Electron Density

$$n = \int_{V_F + \delta V_F} \frac{d\boldsymbol{k}}{(2\pi)^d}\left(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}\right)$$

Fixed electron density ⇒ Change of Fermi volume

$$\delta V_F = -\frac{e}{\hbar}\int_{V_F} d\boldsymbol{k}\, \boldsymbol{B}\cdot\boldsymbol{\Omega}$$

de Haas-van Alphen Oscillations

Quantization condition

$$A_n = \frac{2\pi eB}{\hbar}(n + \frac{1}{2} - \frac{\gamma_B}{2\pi})$$

Area of extremal orbits

$$A_f = A_f^0 - \frac{e}{\hbar}B\langle\gamma_B\rangle$$

$$\langle\gamma_B\rangle = \frac{D_2}{D_3}\int_{V_F} d^3k\,\Omega$$

$$A_f^0 = \frac{2\pi eB}{\hbar}(n + \frac{1}{2} - \frac{\gamma_B - \langle\gamma_B\rangle}{2\pi})$$

→ Phase shift to the oscillation

No Berry phase shift in 2D single band

Spin degenerate bands

- Internal degree of freedom η
- Non-abelian Berry curvature $\mathcal{F}$
- Non-abelian Berry connection $\mathcal{R}$
- Magnetic moment $\frac{e}{2m}\mathcal{L}$

$$\hbar \dot{\mathbf{k}}_c = -e\mathbf{E} - e\dot{\mathbf{r}}_c \times \mathbf{B},$$

$$\hbar \dot{\mathbf{r}}_c = \frac{1}{\mathrm{i}}\eta^\dagger \left[\mathrm{i}\frac{\partial}{\partial \mathbf{k}_c} + \mathcal{R}, \mathcal{H}\right]\eta - \hbar \dot{\mathbf{k}}_c \times \eta^\dagger \mathcal{F}\eta,$$

$$\mathrm{i}\hbar\dot{\eta} = \left(\frac{e}{2m}\mathcal{L}\cdot\mathbf{B} - \hbar\dot{\mathbf{k}}_c \cdot \mathcal{R}\right)\eta,$$

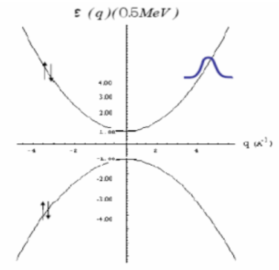
Culcer, Yao & Niu, PRB, 2005
Shindou & Imura, Nucl. Phys. B, 2005
Chang & Niu, 2008 (review)

Applications

- Dirac bands

$$\mathcal{R} = \frac{\lambda_c^2}{2\gamma(\gamma+1)} \mathbf{q} \times \boldsymbol{\sigma},$$

$$\mathcal{F} = -\frac{\lambda_c^2}{2\gamma^3} \left(\boldsymbol{\sigma} + \lambda_c^2 \frac{\mathbf{q} \cdot \boldsymbol{\sigma}}{\gamma + 1} \mathbf{q} \right)$$



- Semiconductor bands

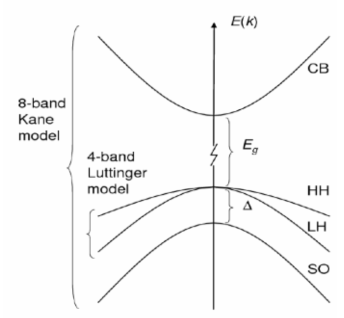


TABLE I: Berry connection, Berry curvature, and orbital angular momentum of the wavepacket in three disjoint subspaces of the 8-band Kane model. Only the leading order (in k) terms are shown. E_g and Δ are the conduction-valence band gap and the spin-orbit gap, σ and $\mathbf{J}$ are the spin-1/2 and spin-3/2 angular momentum matrices, and $V = \hbar\langle S|p_x|X\rangle/m_0$.

	conduction band	HH-LH band	split-off band
$\mathcal{R}$	$\frac{V^2}{3}\left[\frac{1}{E_g^2} - \frac{1}{(E_g+\Delta)^2}\right]\boldsymbol{\sigma} \times \mathbf{k}$	$-\frac{V^2}{3E_g^2}\mathbf{J} \times \mathbf{k}$	$-\frac{V^2}{3}\frac{1}{(E_g+\Delta)^2}\boldsymbol{\sigma} \times \mathbf{k}$
$\mathcal{F}$	$\frac{2V^2}{3}\left[\frac{1}{E_g^2} - \frac{1}{(E_g+\Delta)^2}\right]\boldsymbol{\sigma}$	$-\frac{2V^2}{3E_g^2}\mathbf{J}$	$-\frac{2V^2}{3}\frac{1}{(E_g+\Delta)^2}\boldsymbol{\sigma}$
$\mathcal{L}$	$-\frac{2m_0}{3\hbar}V^2\left(\frac{1}{E_g} - \frac{1}{E_g+\Delta}\right)\boldsymbol{\sigma}$	$-\frac{2m_0}{3\hbar}\frac{V^2}{E_g}\mathbf{J}$	$-\frac{2m_0}{3\hbar}\frac{V^2}{E_g}\boldsymbol{\sigma}$

Zeeman energy

Uniform $\vec{B}$ field, with $\vec{A}(\vec{r},t)=\frac{1}{2}\vec{B}\times\vec{r}$ $\quad\vec{k}=\vec{q}+\frac{e}{\hbar}\vec{A}(\vec{r},t)$

$$\hat{H}=\hat{H}_c+\delta\hat{H}_c$$
$$=H_c+\frac{1}{2}\left(\frac{\partial\hat{H}_c}{\partial\vec{r}_c}\cdot(\hat{r}-\vec{r}_c)+(\hat{r}-\vec{r}_c)\cdot\frac{\partial\hat{H}_c}{\partial\vec{r}_c}\right)$$

$$\langle\hat{\boldsymbol{H}}_c\rangle=\boldsymbol{E}=mc^2\sqrt{1+\lambda_c^2k_c^2}$$

$$\langle\delta\hat{\boldsymbol{H}}_c\rangle=-\frac{e}{2}\langle w\,|\,\vec{v}\times(\vec{r}-\vec{r}_c)\,|\,w\rangle\cdot\vec{\boldsymbol{B}}=-\vec{\boldsymbol{M}}\cdot\vec{\boldsymbol{B}}$$

$$\vec{M}=\frac{-e}{2}\langle w\,|\,(\vec{r}-\vec{r}_c)\times\vec{v}\,|\,w\rangle$$

Magnetic moment from self-rotation

$$\vec{L}=\langle w\,|\,(\vec{r}-\vec{r}_c)\times m\vec{v}\,|\,w\rangle$$

Spin is a spin after all !

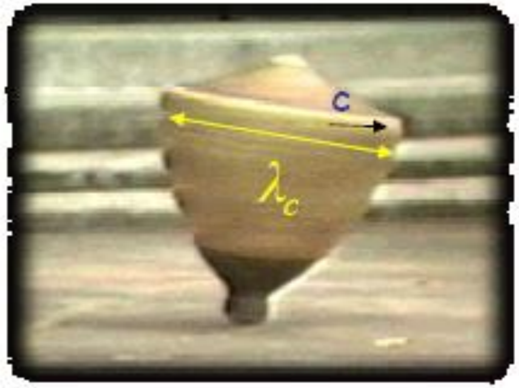
$$\vec{M} = -\frac{e\hbar c^2}{2\mathcal{E}}\left[\langle\vec{\sigma}\rangle + \frac{\hbar^2 c^2}{\mathcal{E}(\mathcal{E}+mc^2)}\vec{k}_c \times \left(\vec{k}_c \times \langle\vec{\sigma}\rangle\right)\right]$$

At rest $\left(\vec{k}_c = 0\right)$:

$$\vec{\boldsymbol{M}} = -\frac{e\hbar}{2\boldsymbol{m}}\langle\vec{\sigma}\rangle = -\mu_B\langle\vec{\sigma}\rangle$$

$$\vec{\boldsymbol{L}} = \hbar\langle\vec{\boldsymbol{\sigma}}\rangle$$

μ_B : Bohr magneton



A rotating top

$$M = I\vec{A} \sim \frac{-ec}{2\pi\lambda_c}\pi\lambda_c^{\ 2}$$
$$\sim \frac{-ec}{2}\lambda_c$$
$$\sim -\mu_B$$

Quantization of semiclassical dynamics

- Physical variables are not canonical
  - because of Berry curvature and magnetic field
- Canonical variables are not physical
  - Generalization of Peierls substitution
  - Gauge dependent

$$\mathbf{r} = \mathbf{r}_c - \mathbf{R}(\mathbf{k}_c) - \mathbf{G}(\mathbf{k}_c),$$

$$\mathbf{p} = \hbar\mathbf{k}_c - e\mathbf{A}(\mathbf{r}_c) - \frac{e}{2}\mathbf{B} \times \mathbf{R}(\mathbf{k}_c)$$

where $G_\alpha(\mathbf{k}_c) \equiv (e/\hbar)(\mathbf{R} \times \mathbf{B}) \cdot \partial\mathbf{R}/\partial k_{c\alpha}$.

M.C. Chang and QN (2008)

Effective Quantum Mechanics

- Wavepacket energy $\mathcal{H}(\mathbf{r}_c, \mathbf{k}_c) = E_0(\mathbf{k}_c) - e\phi(\mathbf{r}_c) + \frac{e}{2m}\boldsymbol{\mathcal{L}}(\mathbf{k}_c) \cdot \mathbf{B}$
- Energy in canonical variables

$$E(\mathbf{r}, \mathbf{p}) = E_0(\boldsymbol{\pi}) - e\phi(\mathbf{r}) + e\mathbf{E} \cdot \mathbf{R}(\boldsymbol{\pi}) + \frac{e}{2m}\mathbf{B} \cdot \left[\mathbf{L}(\boldsymbol{\pi}) + 2\mathbf{R} \times m\frac{\partial E_0}{\partial \boldsymbol{\pi}}\right].$$

$\boldsymbol{\pi} = \mathbf{p} + e\mathbf{A}(\mathbf{r})$

Spin-orbit

Spin & orbital moment

Yafet term

- Quantum theory

[r, p] = ih/2p

Summary

- Berry-phase modified electron dynamics
- Field-dependent density of states
- Orbital moment and magnetization
- Cyclotron orbit and quantization
- Spin degenerate bands and effective Hamiltonian