Wavepacket dynamics in solid and its quantization

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- Review: wavepacket dynamics
  - QHE, AHE, SHE
- Multi-component wavepacket
  - Dirac electron
  - semiconductor electron
- Quantization
  - Peierls substitution
  - Effective Hamiltonian

Semiclassical electron dynamics in solid

(Ashcroft and Mermin, Chap 12)

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{E} - e\dot{\vec{r}} \times \vec{B}$$

$$\frac{d\vec{r}}{dt} = \frac{1}{\hbar} \frac{\partial E_0}{\partial \vec{k}}$$

- Lattice effect hidden in $E_0\,(k)$
- Derivation is harder than expected

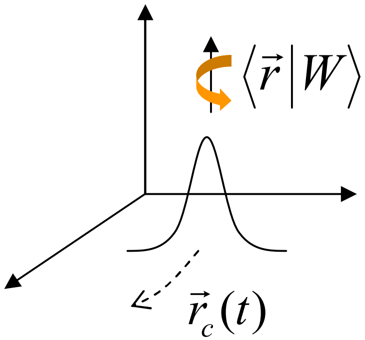
Limits of validity

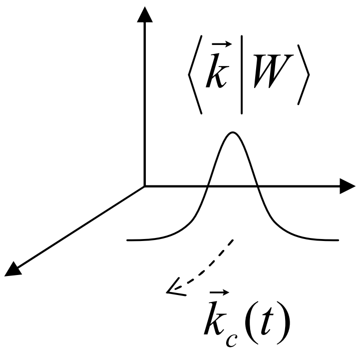
Negligible inter-band transition (one band approximation)
“never close to being violated in a metal”

Explains

- Bloch oscillation in electric field,
  quantization -> Wannier-Stark ladders
- cyclotron motion in magnetic field,
  quantization -> de Haas - van Alphen effect
- …

Semiclassical dynamics - wavepacket approach





1. Construct a wavepacket $|W\rangle$ that is localized in both the *r* space and the *k* space.

2. Using the time-dependent variational principle to get the effective Lagrangian

$$L_{eff}(\vec{r}_c, \vec{k}_c; \dot{\vec{r}}_c, \dot{\vec{k}}_c) = \langle W | i\hbar \frac{\partial}{\partial t} - H | W \rangle$$

3. Determine the trajectory ($r_c(t)$, $k_c(t)$) that minimizes the effective action

Equations of motion

$$\hbar \frac{d\vec{k}_c}{dt} = -e\vec{E} - e\dot{\vec{r}}_c \times \vec{B}$$

$$\frac{d\vec{r}_c}{dt} = \frac{1}{\hbar}\frac{\partial E}{\partial \vec{k}_c} - \dot{\vec{k}}_c \times \vec{\Omega}(\vec{k}_c)$$

"Anomalous velocity" due to the Berry curvature

Anomalous velocity

- (integer) Quantum Hall effect
- (intrinsic) Anomalous Hall effect
- (intrinsic) Spin Hall effect

- Berry curvature

$$\vec{\Omega}(\vec{k}) = i\left\langle \frac{\partial u}{\partial \vec{k}} \right| \times \left| \frac{\partial u}{\partial \vec{k}} \right\rangle$$

- spinning angular momentum

$$\vec{L}(\vec{k}_c) = m\langle W | (\vec{r} - \vec{r}_c) \times \vec{v} | W \rangle$$
$$= \frac{m}{i\hbar}\left\langle \frac{\partial u}{\partial \vec{k}_c} \right| \times (E_0 - H) \left| \frac{\partial u}{\partial \vec{k}_c} \right\rangle$$

Wavepacket energy

$$E(\vec{r}_c, \vec{k}_c) = E_0(\vec{k}_c) - e\phi(\vec{r}_c) + \frac{e}{2m}\vec{L}(\vec{k}_c) \cdot \vec{B}$$

Bloch energy

Quantum Hall effect

VOLUME 49, NUMBER 6 PHYSICAL REVIEW LETTERS 9 AUGUST 1982

Quantized Hall Conductance in a Two-Dimensional Periodic Potential

D. J. Thouless, M. Kohmoto,[a] M. P. Nightingale, and M. den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 30 April 1982)

The Hall conductance of a two-dimensional electron gas has been studied in a uniform magnetic field and a periodic substrate potential U. The Kubo formula is written in a form that makes apparent the quantization when the Fermi energy lies in a gap. Explicit expressions have been obtained for the Hall conductance for both large and small $U/\hbar\omega_c$.

$$\sigma_H = \frac{ie^2}{2\pi h}\sum\int d^2k\int d^2r\left(\frac{\partial u^*}{\partial k_1}\frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2}\frac{\partial u}{\partial k_1}\right)$$
$$= \frac{ie^2}{4\pi h}\sum\oint dk_j\int d^2r\left(u^*\frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j}u\right)$$

Semiclassical language

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{E}$$
$$\frac{d\vec{r}}{dt} = \frac{1}{\hbar}\frac{\partial E}{\partial \vec{k}} - \dot{\vec{k}}\times\vec{\Omega}(\vec{k})$$

(In one Landau subband)

$$\vec{J} = -e\int_{filled}\frac{d^2k}{(2\pi)^2}\dot{\vec{r}}$$
$$= 0 - \frac{e^2}{\hbar}\vec{E}\times\int_{filled}\frac{d^2k}{(2\pi)^2}\vec{\Omega}(\vec{k})$$
$$\Rightarrow J_x = -\left(\frac{e^2}{h}\frac{1}{2\pi}\int_{filled} d^2k\,\vec{\Omega}(\vec{k})\right)E_y$$

Anomalous Hall effect

PHYSICAL REVIEW VOLUME 95, NUMBER 5 SEPTEMBER 1, 1954

Hall Effect in Ferromagnetics*

ROBERT KARPLUS,† *Department of Physics, University of California, Berkeley, California*

AND

J. M. LUTTINGER, *Department of Physics, University of Michigan, Ann Arbor, Michigan*

(Received May 21, 1954)

Both the unusually large magnitude and strong temperature dependence of the extraordinary Hall effect in ferromagnetic materials can be understood as effects of the spin-orbit interaction of polarized conduction electrons. It is shown that the interband matrix elements of the applied electric potential energy combine with the spin-orbit perturbation to give a current perpendicular to both the field and the magnetization. Since the net effect of the spin-orbit interaction is proportional to the extent to which the electron spins are aligned, this current is proportional to the magnetization. The magnitude of the Hall constant is equal to the square of the ordinary resistivity multiplied by functions that are not very sensitive to temperature and impurity content. The experimental results behave in such a way also.

gives correct order of magnitude for Fe,
also explains $\rho_{AH} \sim \rho_L^2$

Modern language: $\sigma_{AH} = \frac{e^2}{\hbar} \int_{BZ} \frac{d^3k}{(2\pi)^3} \vec{\Omega}(\vec{k})$

Smit: KL’s (intrinsic) mechanism vanishes in a lattice w/o disorder

Alternative mechanisms (extrinsic):

- Smit’s skew scattering mechanism (1955)
- Berger’s side jump mechanism (1970)

“The difference of opinion between Luttinger and Smit seems never to have been entirely resolved.”
CM Hurd, *The Hall Effect in Metals and Alloys* (1972)

“It is now accepted that two mechanisms are responsible for the AHE: the skew scattering… and the side-jump…”
(Crepieux and Bruno, PRB 2001)

Spin Chirality, Berry Phase, and Anomalous Hall Effect in a Frustrated Ferromagnet

Y. Taguchi,[1] Y. Oohara,[2] H. Yoshizawa,[2] N. Nagaosa,[1,3] Y. Tokura[1,3]

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VOLUME 88, NUMBER 20 PHYSICAL REV

Anomalous Hall Effect in Fe

T. Jungwirth,[1,2] Qian Niu

[1]Department of Physics, The Unive

[2]Institute of Physics ASCR, Cukrovarnic

(Received 3 October 2001

We present a theory of the anomalous Hall effect in ferromagnetic (III, Mn)V semiconductors. Our theory relates the anomalous Hall conductance of a homogeneous ferromagnet to the Berry phase acquired by a quasiparticle wave function upon traversing closed paths on the spin-split Fermi surface. The quantitative agreement between our theory and experimental data in both (In, Mn)As and (Ga, Mn)As systems suggests that this disorder independent contribution to the anomalous Hall conductivity dominates in diluted magnetic semiconductors. The success of this model for (III, Mn)V materials is unprecedented in the longstanding effort to understand origins of the anomalous Hall effect in itinerant ferromagnets.

The Anomalous Hall Effect and Magnetic Monopoles in Momentum Space

Zhong Fang,[1,2*] Naoto Nagaosa,[1,3,4] Kei S. Takahashi,[5] Atsushi Asamitsu,[1,6] Roland Mathieu,[1] Takeshi Ogasawara,[3] Hiroyuki Yamada,[3] Masashi Kawasaki,[3,7] Yoshinori Tokura,[1,3,4] Kiyoyuki Terakura[8]

Science 2003

Efforts to find the magnetic monopole in real space have been made in cosmic rays and in particle accelerators, but there has not yet been any firm evidence for its existence because of its very heavy mass, $\sim 10^{16}$ giga–electron volts. We show that the magnetic monopole can appear in the crystal momentum space of solids in the accessible low-energy region ($\sim$0.1 to 1 electron volts) in the context of the anomalous Hall effect. We report experimental results together with first-principles calculations on the ferromagnetic crystal $SrRuO_3$ that provide evidence for the magnetic monopole in the crystal momentum space.

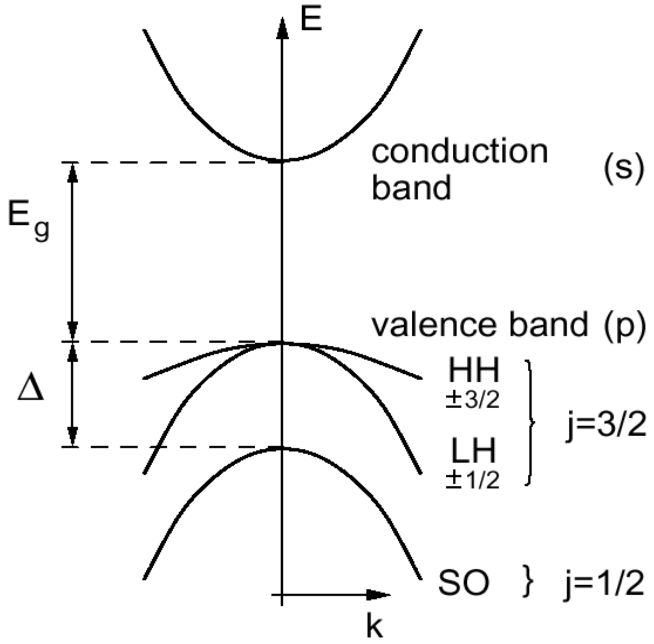
Karplus-Luttinger mechanism:

Mired in controversy from the start, it simmered for a long time as an unsolved problem, but has now re-emerged as a topic with modern appeal. -- Ong

Intrinsic spin Hall effect in p-type semiconductor

(Murakami, Nagaosa and Zhang, Science 2003; PRB 2004)

Valence band of GaAs:



Berry curvature in valence band,

$$\vec{\Omega}_\lambda(\vec{k}) = -2\lambda\left(\lambda^2 - \frac{7}{4}\right)\frac{\hat{k}}{k^2}$$

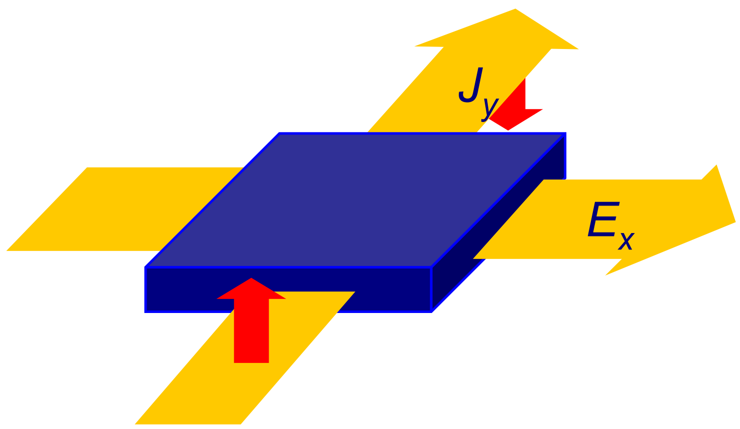
$$\lambda = \hat{k}\cdot\vec{J}$$

(helicity)

$$\hbar\frac{d\vec{k}}{dt} = e\vec{E}$$

$$\frac{d\vec{x}}{dt} = \frac{\partial E_\lambda(\vec{k})}{\hbar\partial\vec{k}} - \frac{d\vec{k}}{dt}\times\vec{\Omega}_\lambda(\vec{k})$$

Spin-dependent transverse velocity



No magnetic field required

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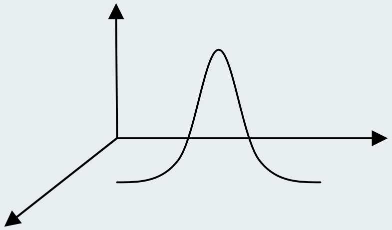
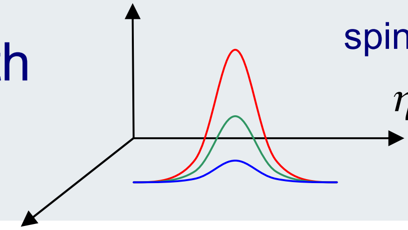
Wavepacket formulation

One band



A band with spin DOF



spinor $\eta = \begin{pmatrix} \eta_1 \\ \vdots \\ \eta_D \end{pmatrix}$

Basic quantities (scalar)

gauge potential and field: $\vec{R}(\vec{k}),\ \vec{\Omega}(\vec{k})$

angular momentum $\vec{L}(\vec{k})$

$$E(\vec{k}) = E_0(\vec{k}) - e\phi(\vec{r}) + \frac{e}{2m}\vec{L}(\vec{k})\cdot\vec{B}$$

Basics quantities (matrix, boldface)

gauge potential and field: $\vec{\mathbf{R}}(\vec{k}),\ \vec{\mathbf{F}}(\vec{k})$

angular momentum $\vec{\mathbf{L}}(\vec{k})$

$$\mathbf{H}(\vec{r},\vec{k}) = E_0(\vec{k}) - e\phi(\vec{r}) + \frac{e}{2m}\vec{\mathbf{L}}(\vec{k})\cdot\vec{B}$$

Dynamics

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{E} - e\dot{\vec{r}}\times\vec{B}$$

$$\hbar\frac{d\vec{r}}{dt} = \frac{\partial E}{\partial\vec{k}} - \hbar\dot{\vec{k}}\times\vec{\Omega}(\vec{k})$$

Dynamics

$$\begin{cases} \hbar\dfrac{d\vec{k}}{dt} = -e\vec{E} - e\dot{\vec{r}}\times\vec{B} \\ \hbar\dfrac{d\vec{r}}{dt} = \eta^{+}\left[\dfrac{\partial}{\partial\vec{k}} - i\vec{\mathbf{R}},\mathbf{H}\right]\eta - \hbar\dot{\vec{k}}\times\eta^{+}\vec{\mathbf{F}}\eta \end{cases}$$

$$\left\{ i\hbar\frac{d\eta}{dt} = \left(\mathbf{H} - \hbar\dot{\vec{k}}\cdot\vec{\mathbf{R}}\right)\eta \right.$$

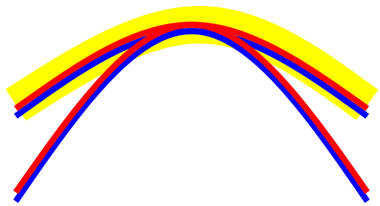
Chang and Niu, PRL 1995, PRB 1996
Sundaram and Niu, PRB 1999

Culcer, Yao, and Niu PRB 2005
Shindou and Imura, Nucl. Phys. B 2005

Emergence of curvature by projection

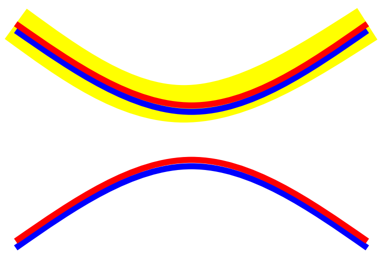
J.E. Avron, Les Houches 1994

- 4-band Luttinger model



(Murakami, Nagaosa and Zhang, Science 2003; PRB 2004)

- Free Dirac electron



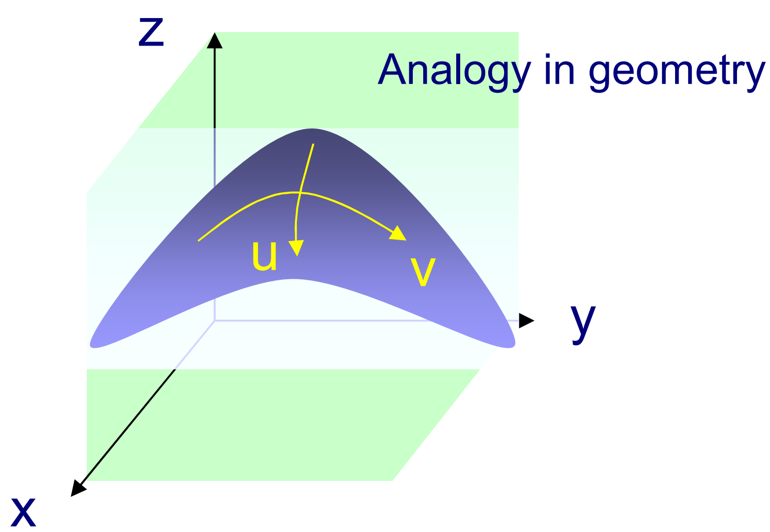
Non-Abelian $\vec{R}_{mn}(\vec{k}) = \langle u_m | i \frac{\partial}{\partial \vec{k}} | u_n \rangle$

Curvature for a complete space

$$\vec{\mathbf{F}} = \nabla \times \vec{\mathbf{R}} - i\vec{\mathbf{R}} \times \vec{\mathbf{R}} = 0$$

Curvature for a subspace

$$\vec{\mathbf{F}} = \nabla \times \tilde{\vec{\mathbf{R}}} - i\tilde{\vec{\mathbf{R}}} \times \tilde{\vec{\mathbf{R}}} \neq 0, \quad \tilde{\vec{\mathbf{R}}} \equiv P\vec{\mathbf{R}}P$$



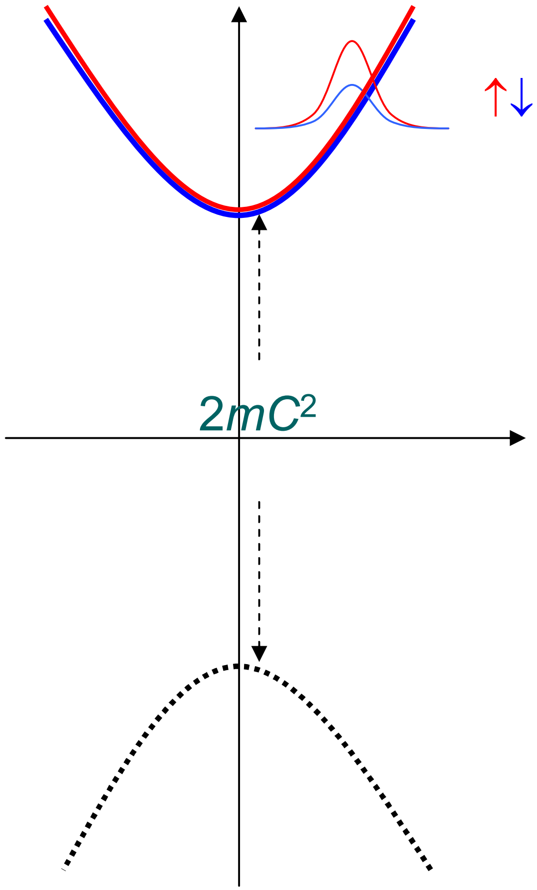
Dirac wavepacket as a trial case

(Free particle in external fields, positive-energy projection)

Positive branch

$$E_0(k) = \sqrt{m^2c^4 + c^2\hbar^2k^2}$$
$$\equiv \gamma(k) mc^2$$

$$\gamma(k) = \sqrt{1 + \left(\frac{\hbar k}{mc}\right)^2}$$
$$\left(\text{or } = \frac{1}{\sqrt{1-(\dot{r}/c)^2}}\right)$$



2-fold degeneracy

→ SU(2) gauge field

$$\vec{\mathbf{R}},\ \vec{\mathbf{F}},\ \vec{\mathbf{L}} = ?$$

$$\vec{R}_{mn}(\vec{k}) = \langle u_m | i\frac{\partial}{\partial \vec{k}} | u_n \rangle$$

$$\vec{\mathbf{F}} = \nabla \times \vec{\mathbf{R}} - i\vec{\mathbf{R}} \times \vec{\mathbf{R}}$$

• Angular momentum of the wave packet $\vec{L}_{mn}(\vec{k}_c) = \frac{m_0}{i\hbar}\left\langle \frac{\partial u_m}{\partial \vec{k}_c} \right| \times \left(E_0 - H\right) \left| \frac{\partial u_n}{\partial \vec{k}_c} \right\rangle$

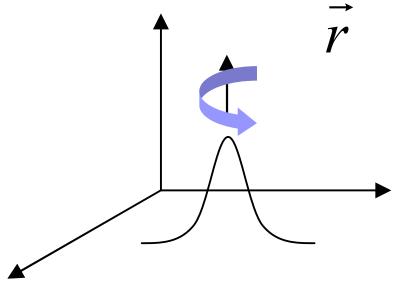
$$\Rightarrow \quad \vec{\mathbf{L}}(\vec{k}_c) = \frac{\hbar}{\gamma^2}\left[\vec{\sigma} + \frac{\lambda_c^2}{\gamma+1}\left(\vec{k}_c \cdot \vec{\sigma}\right)\vec{k}_c\right] \qquad \lambda_c = \frac{\hbar}{mc} \ \text{(Compton wavelength)}$$

$$= \frac{\hbar \vec{\tau}}{\gamma} \qquad \vec{\tau} = P\vec{\Sigma}P \ \text{(projected spin)}$$

• Zeeman energy

$$\vec{\mathbf{M}}(\vec{k}_c) = -\frac{e}{2m}\vec{\mathbf{L}}(\vec{k}_c) = -\frac{ge}{2\gamma m}\frac{\hbar\vec{\tau}(\vec{k}_c)}{2}$$

The spinning wavepacket gives the correct Zeeman energy with g_L =1 !



• Precession of spin (reproduces the BMT eq.)

$$\left(\vec{S} = \eta^{+}\frac{\vec{\sigma}}{2}\eta\right) \qquad \boxed{\frac{d\vec{S}}{dt} = \frac{e}{\gamma m}\left(\vec{B} + \frac{1}{\gamma+1}\vec{E} \times \frac{\hbar\vec{k}}{mc}\right) \times \vec{S}}$$

- Gauge structure   Ref: Bliokh, Europhys. Lett. 72, 7 (2005)

$$\vec{\mathbf{R}} = \frac{\lambda_c^2}{2\gamma(\gamma+1)} \vec{k} \times \vec{\sigma}$$

$$\vec{\mathbf{F}} = -\frac{\lambda_c^2}{2\gamma^3}\left[\vec{\sigma} + \frac{\lambda_c^2}{\gamma+1}\left(\vec{k}\cdot\vec{\sigma}\right)\vec{k}\right] \approx -\frac{\lambda_c^2}{2}\vec{\sigma} \quad \text{for } v<<c$$

(not monopole-like)

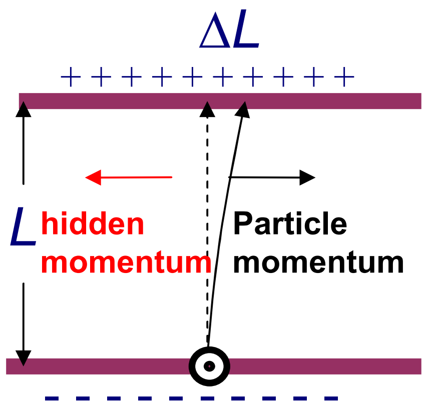
- Center-of-mass motion in E field

(for low v, linear in field)

$$\hbar\frac{d\vec{k}}{dt} = -e\vec{E}$$

$$\frac{d\vec{r}}{dt} = \frac{\hbar\vec{k}}{m} + \frac{e\lambda_c^2}{2\hbar}\langle\vec{\sigma}\rangle \times \vec{E}$$

Spin-dependent transverse velocity



for 1 GeV in 1 cm

$$\frac{\Delta L}{L} \sim \frac{\Delta E(\lambda_c)}{mc^2} \approx 10^{-6} \;!$$

Or,

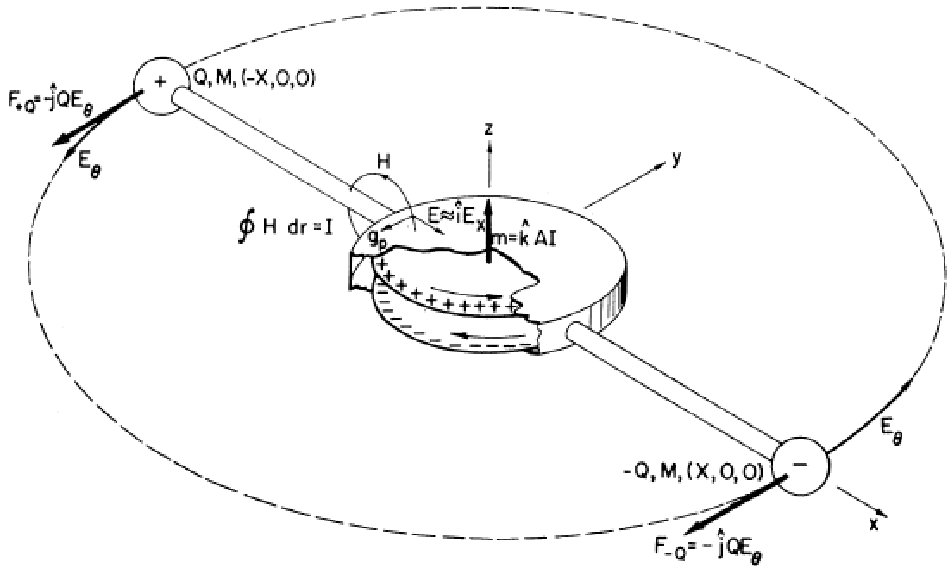
$$\hbar\vec{k} = m\dot{\vec{r}} + \vec{m}\times\vec{E}, \qquad \vec{m} = \frac{g(-e)}{2m}\vec{S}$$

"hidden" momentum
(Jackson, *Classical ED*, the 3rd ed.)

Transverse $\hbar\vec{k}$ remains conserved (= 0) !

Shockley-James paradox

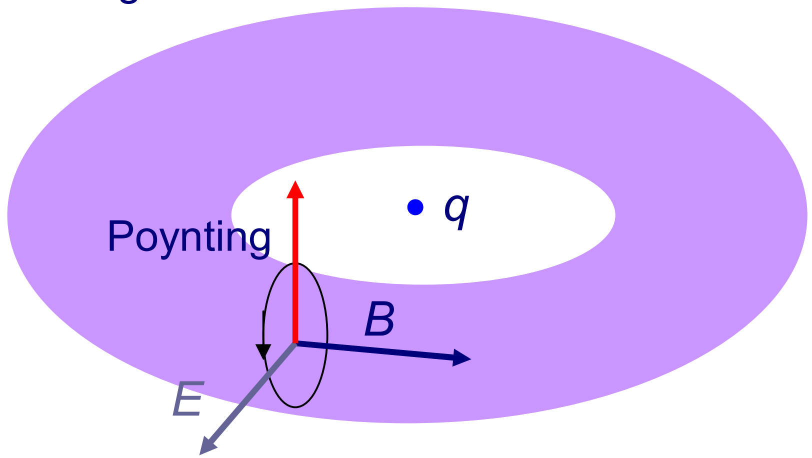
(Shockley and James, PRLs 1967)

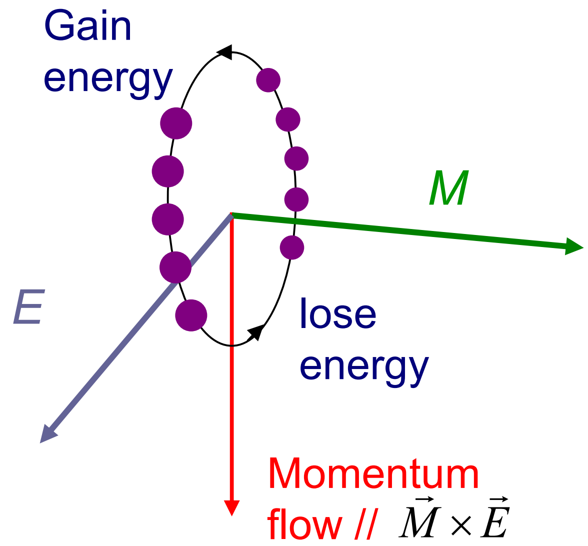


A simpler version

(Vaidman, Am. J. Phys. 1990)

A charge and a solenoid:





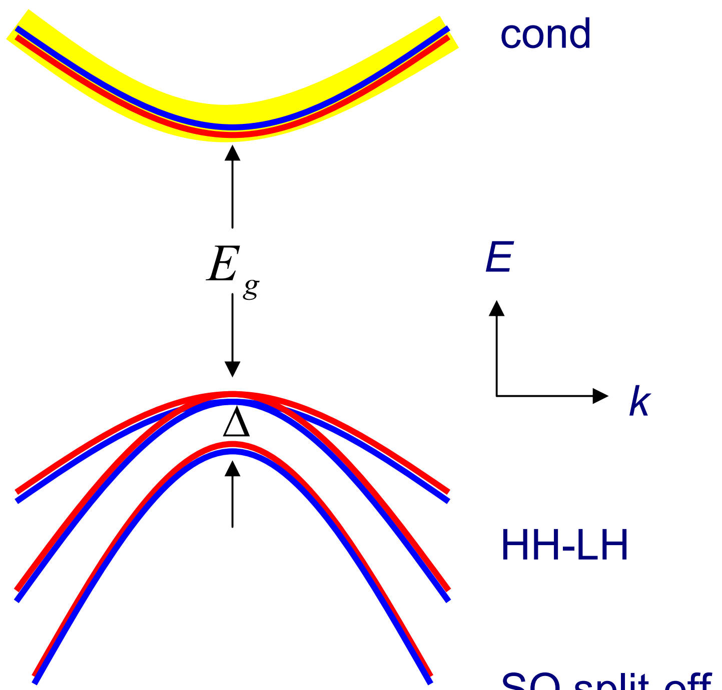
Resolution of the paradox

- Penfield and Haus, *Electrodynamics of Moving Media, 1967*
- *S.* Coleman and van Vleck, PR 1968

- semiconductor electron

Berry curvature in conduction band?

8-band Kane model



8-band Kane model $(\gamma_2=\gamma_3)$

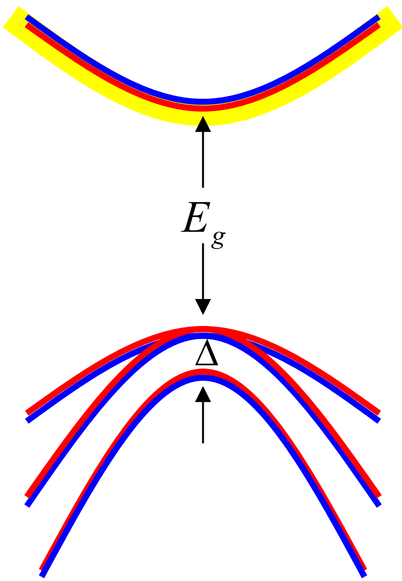
$$
\begin{array}{rcl}
 & \begin{array}{ccc}\text{Cond.} & \qquad\qquad\text{HH-LH}\qquad\qquad & \text{SO}\end{array} & \\
H = & \left(\begin{array}{cc|cccc|cc}
E_g+\frac{\hbar^2k^2}{2m'} & 0 & -\frac{1}{\sqrt{2}}Vp_+ & \sqrt{\frac{2}{3}}Vp_z & \frac{1}{\sqrt{6}}Vp_- & 0 & -\frac{1}{\sqrt{3}}Vp_z & -\frac{1}{\sqrt{3}}Vp_- \\
0 & E_g+\frac{\hbar^2k^2}{2m'} & 0 & -\frac{1}{\sqrt{6}}Vp_+ & \sqrt{\frac{2}{3}}Vp_z & \frac{1}{\sqrt{2}}Vp_- & -\frac{1}{\sqrt{3}}Vp_+ & \frac{1}{\sqrt{3}}Vp_z \\
\hline
-\frac{1}{\sqrt{2}}Vp_- & 0 & -(P+Q) & -L & -M & 0 & \frac{1}{\sqrt{2}}L & \sqrt{2}M \\
\sqrt{\frac{2}{3}}Vp_z & -\frac{1}{\sqrt{6}}Vp_- & -L^* & -(P-Q) & 0 & -M & -\sqrt{2}Q & -\sqrt{\frac{3}{2}}L \\
\frac{1}{\sqrt{6}}Vp_+ & \sqrt{\frac{2}{3}}Vp_z & -M^* & 0 & -(P-Q) & L & -\sqrt{\frac{3}{2}}L^* & \sqrt{2}Q \\
0 & \frac{1}{\sqrt{2}}Vp_+ & 0 & -M^* & L^* & -(P+Q) & -\sqrt{2}M^* & \frac{1}{\sqrt{2}}L^* \\
\hline
-\frac{1}{\sqrt{3}}Vp_z & -\frac{1}{\sqrt{3}}Vp_- & \frac{1}{\sqrt{2}}L^* & -\sqrt{2}Q & -\sqrt{\frac{3}{2}}L & -\sqrt{2}M & -\Delta-\gamma_1\frac{p^2}{2m} & 0 \\
-\frac{1}{\sqrt{3}}Vp_+ & \frac{1}{\sqrt{3}}Vp_z & \sqrt{2}M^* & -\sqrt{\frac{3}{2}}L^* & \sqrt{2}Q & \frac{1}{\sqrt{2}}L & 0 & -\Delta-\gamma_1\frac{p^2}{2m}
\end{array}\right) & \begin{array}{l}\text{Cond.}\\ \\ \\ \text{HH-LH}\\ \\ \\ \text{SO}\end{array}
\end{array}
$$

$$P=\gamma_1\frac{p^2}{2m}, \qquad Q=\gamma_2\frac{p_\parallel^2-2p_z^2}{2m}$$

$$L=-\sqrt{3}\gamma_3\frac{p_-p_z}{m}, \; M=-\sqrt{3}\frac{\gamma_2}{2m}\left(p_x^2-p_y^2\right)+2i\sqrt{3}\frac{\gamma_3}{2m}p_xp_y = -\sqrt{3}\frac{\gamma_2}{2m}p_-^2 \qquad V=\frac{1}{m}\langle S|p_x|X\rangle$$

R. Winkler, *SO coupling effect in 2D electron and hole systems*, App. C

Gauge structure in conduction band



- Gauge potential, correct to k^1

$$\vec{\mathbf{R}} = \frac{V^2}{3}\left[\frac{1}{E_g^2} - \frac{1}{\left(E_g+\Delta\right)^2}\right]\vec{\sigma}\times\vec{k}_c, \quad V = \hbar\left\langle S\middle|P_x\middle|X\right\rangle/m$$

- Gauge field, correct to k^0

$$\vec{\mathbf{F}} = \frac{2V^2}{3}\left[\frac{1}{E_g^2} - \frac{1}{\left(E_g+\Delta\right)^2}\right]\vec{\sigma}$$

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

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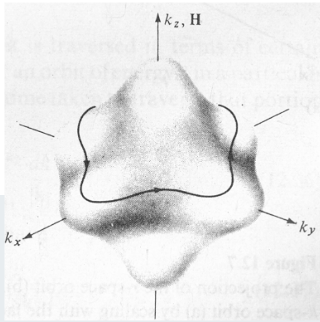
Re-quantize the wavepacket theory. Why bother?



Bohr-Sommerfeld quantization (Onsager, 1952)

Without Berry phase

$$\frac{1}{2}\oint_{C_m}\left(\vec{k}\times d\vec{k}\right)\cdot d\hat{z}=2\pi\left(m+\frac{1}{2}\right)\frac{eB}{\hbar}$$

With Berry phase

$$\frac{1}{2}\oint_{C_m}\left(\vec{k}\times d\vec{k}\right)\cdot d\hat{z}=2\pi\left(m+\frac{1}{2}-\frac{\Gamma(C_m)}{2\pi}\right)\frac{eB}{\hbar}$$

Berry phase $\Gamma(C_m)=\oint_{C_m}\vec{R}\cdot d\vec{k}$

Peierls substitution (1933)

Bloch energy E_0 (k)

$$\hbar\vec{k}\Rightarrow\hat{\vec{p}}+e\vec{A}(\vec{r})$$

Effective Hamiltonian

$$E_0(\vec{k})\Rightarrow H_{eff}\left(\hat{\vec{p}}+e\vec{A}\right)$$

With Berry phase?

Canonical variables in the semiclassical theory:

(everything valid to linear field only)

old variables,

$$\{r_{ci}, k_{cj}\} \neq \delta_{ij}$$

new "canonical" variables,

$$\{r_i, p_j\} = \delta_{ij}$$

$$\vec{r}_c = \vec{r} + \vec{R}(\vec{\pi});$$

$$\hbar\vec{k}_c = \vec{p} + e\vec{A}(\vec{r}) + e\vec{B}\times\vec{R}(\vec{\pi}),$$

$$\text{where } \vec{\pi} \equiv \vec{p} + e\vec{A}(\vec{r})$$

Energy in old variables

$$\mathbf{H}(\vec{r}_c,\vec{k}_c) = E_0(\vec{k}_c) - e\phi(\vec{r}_c) + \frac{e}{2m}\vec{\mathbf{L}}(\vec{k}_c)\cdot\vec{B}$$

Hamiltonian in canonical variables

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

SO coupling is now explicit !

The "Yafet" term

Chang et al, to be published

Roth, J. Phys. Chem. Solids 1962;
Blount, PR 1962

Effective Hamiltonian for Dirac wavepacket

Dirac Hamiltonian (4-component)

$$H_D = c\vec{\alpha}\cdot\left(\vec{p}+e\vec{A}(\vec{r})\right)+\beta mc^2-e\varphi(\vec{r})$$

Foldy-Wouthuysen transformation

$$H_P = U^\dagger H_D U$$

Seems strightforward, but nontrivial

• Semiclassical energy

• generalized Peierls substitution

Fool-proof

Quantum Pauli Hamiltonian (2-component)

Cf: Silenko, J. Math. Phys. 44, 1952 (2003)

$$H_P = \gamma(\vec{\pi})mc^2+\frac{\mu_B}{\gamma(\vec{\pi})[\gamma(\vec{\pi})+1]mc^2}\vec{\pi}\times\vec{\sigma}\cdot\vec{E}+\frac{\mu_B}{\gamma(\vec{\pi})}\vec{\sigma}\cdot\vec{B}-e\varphi(\vec{r})$$

correct to *first order* in fields,
exact to *all orders* of *v*/*c*!

C.P. Chuu et al, to be published

Effective Hamiltonian for conduction electron

$$\mathbf{H}(\vec{k}) = E_0(\vec{k}) + e\vec{E}\cdot\vec{\mathbf{R}}(\vec{k}) + \frac{e}{2m}\vec{B}\cdot\vec{\mathbf{L}}(\vec{k})$$

$$= E_0(\vec{k}) + \alpha\vec{E}\cdot\vec{\sigma}\times\vec{k} + \frac{g_{orb}}{2}\mu_B\vec{B}\cdot\vec{\sigma}$$

$$\alpha \equiv \frac{eV^2}{3}\left[\frac{1}{E_g^2} - \frac{1}{\left(E_g+\Delta\right)^2}\right]$$

$(= 0 \ \text{ if } \ \Delta = 0 \ )$

- Same form as the Rashba coupling
- But in the absence of BIA/SIA

$$g = 2 - \frac{4}{3}\frac{mV^2}{\hbar^2}\left(\frac{1}{E_g} - \frac{1}{E_g+\Delta}\right)$$

Spin part orbital part

Yu and Cardona, *Fundamentals of semiconductors*, Prob. 9.16

Effective Hamiltonians for other subspaces

$$\mathbf{H}(\vec{k}) = E_0(\vec{k}) + e\vec{E}\cdot\vec{\mathbf{R}}(\vec{k}) + \frac{e}{2m}\vec{B}\cdot\vec{\mathbf{L}}(\vec{k})$$

$$\mathbf{H}_{H/L}(\vec{k}) = E_0(\vec{k},\vec{J}) - \alpha_{H/L}\vec{E}\cdot\vec{J}\times\vec{k} - 2\kappa_{H/L}\mu_B\vec{B}\cdot\vec{J} \qquad (E_0 < 0)$$

$$\mathbf{H}_{SO}(\vec{k}) = E_0(\vec{k}) - \alpha_{SO}\vec{E}\cdot\vec{\sigma}\times\vec{k} - 2\kappa_{SO}\mu_B\vec{B}\cdot\vec{\sigma}$$

$$\alpha_{H/L} \equiv \frac{eV^2}{3}\frac{1}{E_g^2}, \quad \kappa_{H/L} = \frac{1}{3}\frac{mV^2}{\hbar^2}\frac{1}{E_g}$$

$$\alpha_{SO} \equiv \frac{eV^2}{3}\frac{1}{\left(E_g+\Delta\right)^2}, \quad \kappa_{SO} = \frac{1}{3}\frac{mV^2}{\hbar^2}\frac{1}{E_g+\Delta}$$

agree with those obtained using Löwdin partition.
R. Winkler, *SO coupling effect in 2D electron and hole systems*

Chang et al, to be published

summary

- gauge structure (gauge potential and gauge field) for Dirac electron and semiconductor carrier
- wavepacket dynamics for Dirac electron and semiconductor carrier
- generalized Peierls substitution
- effective quantum Hamiltonian