Geometric Phase in Quantum Physics of Solids

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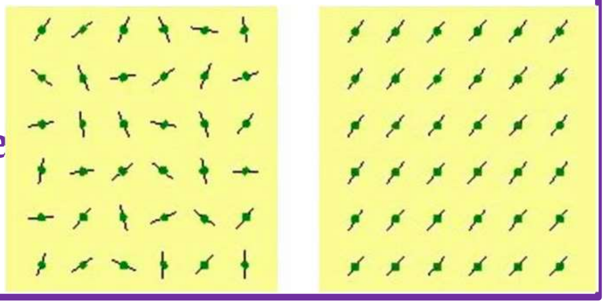
1980's have experienced a paradigm shift in our understanding of CMP

PRE 1980

In condensed matter physics, it's common to observe an ordered state at low temp undergoing phase transitions (1st or 2nd order) when the system spontaneously loses one of the symmetries present at high temp. i.e. symmetry breaking

<u>Examples</u> :

- crystals break translational & rotational symmetries of free
- ferromagnets break time-reversal symmetry
- superconductors break gauge symmetry.

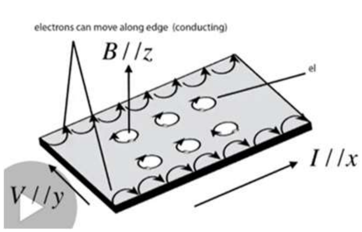


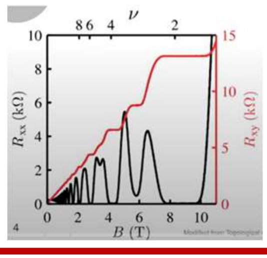
POST 1980

Subsequently it was found there are types of order occuring without symmetry breaking.

<u>Examples</u> :

- Integral Quantum Hall Efffect (IQHE) observed in 1980 in 2D electron gas at very low temp & strong magnetic field.
- Hall conductance, σ_{xy}, exhibits plateaus with the quantized value $n(e^2/h)$, accurate to 10^{-9}, a result of topological order.





→ 1980 : Von Klitzing's discovery of Quantum Hall Effect marks the advent of topology in CMP

→ 1984 : Michael Berry's discovery that besides the dynamical phase, there is an additional phase that can not be "gauged away" and whose origin is geometric or topological.

Plan of presentation :

- **Introductory remarks (some terminologies)**
- **Quantum Adiabatic Theorem**
- **Dynamical Phase & Geometrical Phase**
- **Berry phase and Berry curvature**
- **Generalizations and Physical Realizations**
- **Manifestation in Weyl Semimetals : IS and/or TRS preserved or broken**
- **Anomalous Thermal Hall Effect in Type-I Weyl Semimetal (TRS broken)**
- **Concluding remarks**

Non-holonomic System & Parallel Transport

Interesting Physics associated with quantities that fail to return to return after being taken round circuits --- called "nonholonomic".

There are several examples in classical as well as quantum world

$$\exp[i\theta] = \exp[i(\theta+2\pi)]$$

Angular Momentum of an electron :

$$J_z = -i\hbar\partial/\partial\phi$$

$$J_z |\psi> = m\hbar |\psi> \quad m=\pm 1/2$$

$$-i\hbar\partial/\partial\phi |\psi> = m\hbar |\psi>$$

$$\psi(\phi) \rightarrow \exp[im\phi]\, \psi(\phi)$$

$$\rightarrow \exp[i\phi/2]\, \psi(\phi)$$

Now if the angle ϕ is rotated by $2\pi=360°$

ψ does not return back to the same point

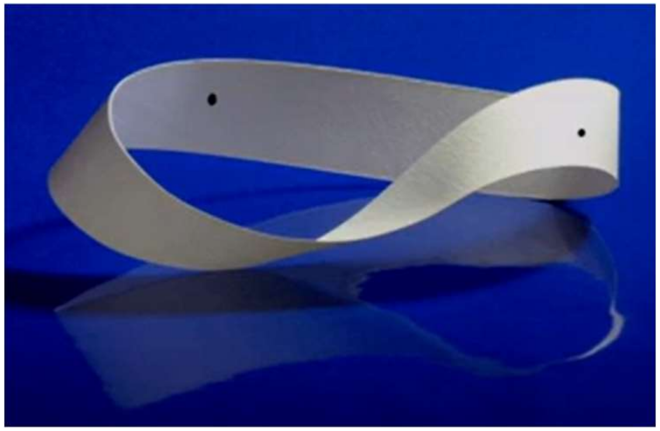
$$\exp[i\phi/2] = \exp[i\pi] = -1$$

However, if ϕ is rotated by $4\pi=720°$ then ψ returns back to the same point

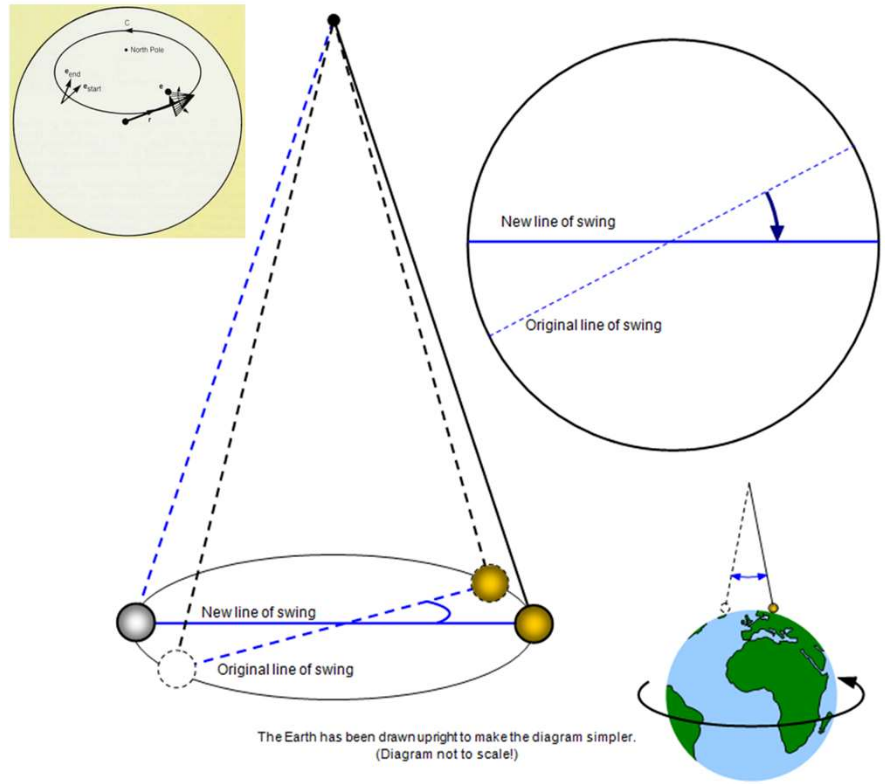
$$\exp[i\phi/2] = \exp[2i\pi] = 1$$

Möbius Strip :

If an ant crawls one full loop (4π) of the ribbon, it would find itself arriving at the other edge. Another trip (4π) across the ribbon will help in arriving at the same face.



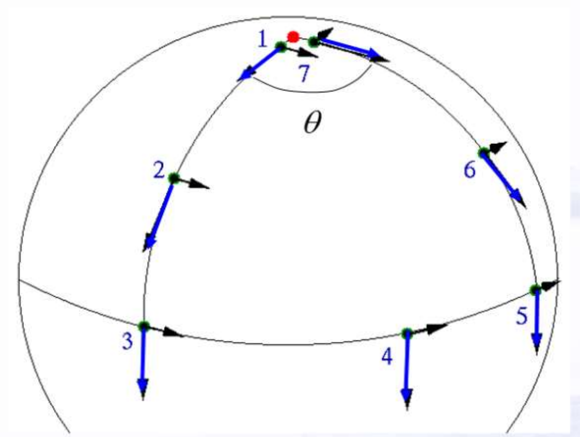
Foucault Pendulum : deceptively simple device illustrating earth's rotation



The direction of swing **e** does not return to its initial value when the pendulum completes its one-day trip around a circle of latitude; i.e. **e** is parallel-transported around the diurnal circuit C by the local vertical **r**.

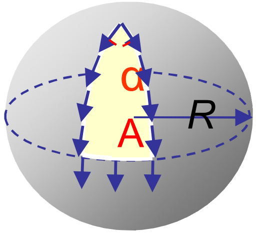
Geometric phase can be best understood in terms of parallel transport of a vector on the surface of a sphere along a closed loop.

Foucault Pendulum is a physical example of a *'global change without local change'*



B. Goss Levi, Phys. Today **46**, 17 (1993).

Why Berry Phase is often called a Geometric Phase ?



- **For a spherical triangle α=*A*/*R*²**
- **Gaussian curvature *G* ≡** $\lim_{A\to 0}\frac{\alpha}{A}=\frac{1}{R^2}$
- **Berry phase ≒ *anholonomy angle* in differential geometry**
- **Berry curvature ≒*Gaussian curvature***

Michael Berry first showed that this concept also applied to a quantum mechanical state when it makes a loop in parameter space when traversed adiabatically and acquires a 'phase' that is now referred as **Berry Phase.**

Quantum Adiabatic Theorem

Dynamical Phase and Geometric Phase

Quantum Adiabatic Theorem

"A physical system remains in its instantaneous eigenstates if a given perturbation is acting on it lowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum."

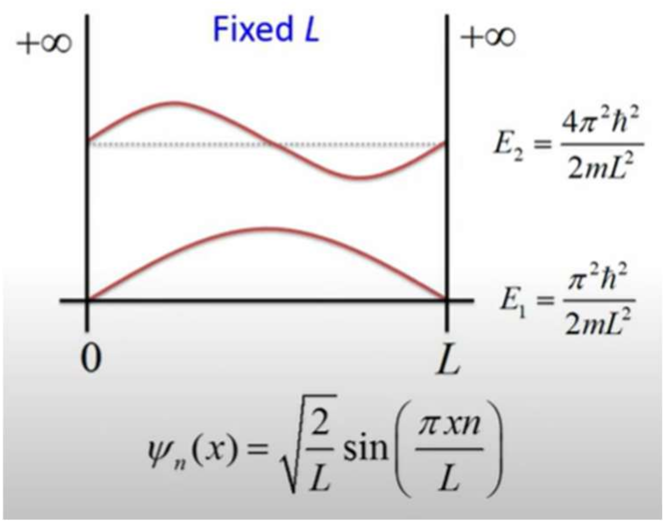
--- Max Born & Vladimir Fock

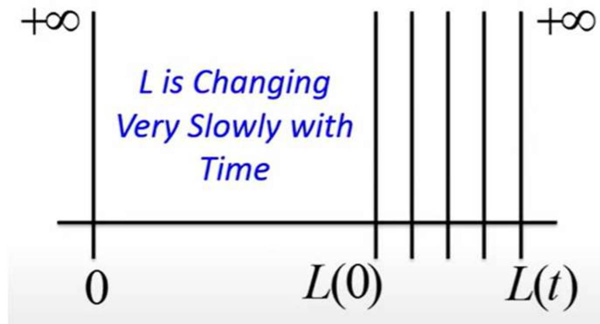
[Beweis des Adiabatensatzes (Proof of Adiabatic Theorem), Zeitschrift fur Physik 51, 165 (1928)]

- **Suppose the Hamiltonian of a quantum system changes very slowly with time from $\hat{H}(0)$ to $\hat{H}(t)$: So the quantum system which was initially (at t=0) in the non-degenerate n^{th} eigenstate of $\hat{H}(0)$ will remain in the non-degenerate n^{th} eigenstate of $\hat{H}(t)$.**
- **This means that a ground state system will remain in the ground state before and after the adiabatic change of the Hamiltonian without making transition to excited state. But the wave function will now have additional phases viz.**

$\exp[i\theta_n(t)]$ → Dynamical Phase $\exp[i\gamma_n(t)]$ → Geometric phase.

Example: Particle in 1D Box





L(0) → L(t)
adiabatically,
turned on at
t=0 and turned
off at t

The stationary state of the quantum system immediately after the process of adiabatic length change is turned off (with accumulated phase due to temporal change in the parameter L) can be written as :

$$\psi_n(x,t;L(t)) = \psi_n(x;L(t))\, e^{\frac{-i}{\hbar}\int_0^t E_n(t')dt'}$$

$$E_n(t')=(n^2\pi^2\hbar^2)/2m[L(t')]^2$$

Moral of the story :

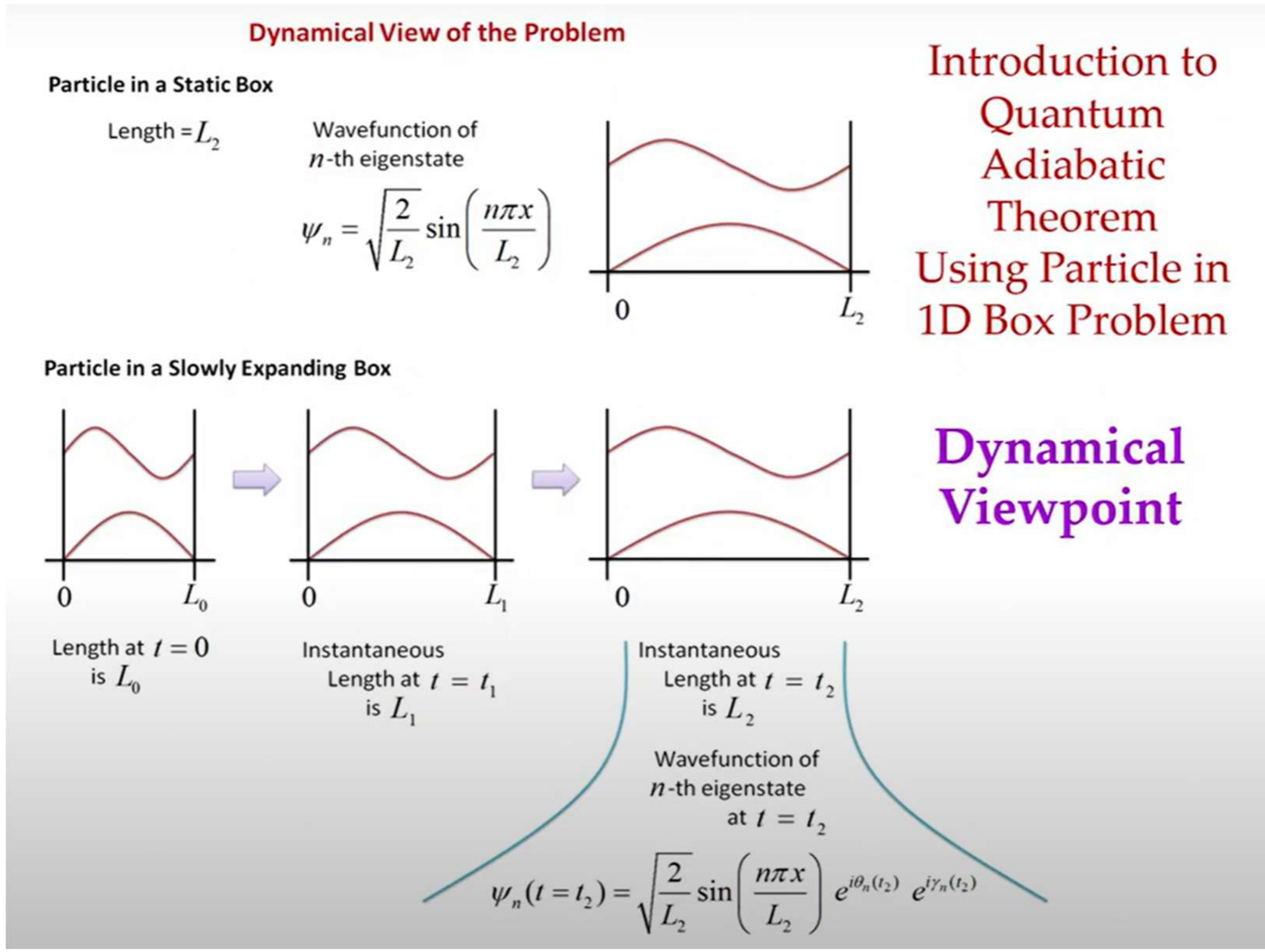
System started in state n, will remain in state of n of the new Hamiltonian under the adiabatic process

$$\Psi_n(t) = e^{i\theta_n t} e^{i\gamma_n t} \psi_n(t)$$

where

θ_n → dynamical phase

γ_n → geometric phase



Schrödinger Equation

In Born-Oppenheimer (Adiabatic) approximation the coordinates **R**(t) of the nuclei are regarded as parameters, to which quantum states of the electrons are 'slaved'.

Time-independent

$$\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$

$$|\psi_n(t)\rangle = |n\rangle\, e^{i\theta_n}$$

$$\theta_n = -\frac{1}{\hbar}\,E_n t$$

Time-dependent

(Adiabatic process*)

$$\hat{H}(t)\,|\psi_n(t)\rangle = E_n(t)\,|\psi_n(t)\rangle$$

$$\Psi(t) = \sum_n c_n(t)\,|n(\mathbf{R}(t))\rangle$$

$$c_n(t) = c_n(0)\,e^{i\theta_n(t)}\,e^{i\gamma_n(t)}$$

** "Adiabatic" means that the time scale of the system's evolution is much shorter than the time scale of the changing Hamiltonian*

Dynamical Phase

$$\boxed{\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt'}$$

Geometric Phase

$$\boxed{\gamma_n(t) = i\int_0^t \left\langle n(\mathbf{R}(t')) \middle| \frac{\partial}{\partial t'} n(\mathbf{R}(t')) \right\rangle dt' = \int_{R_i}^{R_f} i\left\langle n(\mathbf{R}) \middle| \frac{\partial}{\partial \mathbf{R}} n(\mathbf{R}) \right\rangle \cdot d\mathbf{R}}$$

Choosing a suitable gauge transformation $\mathcal{A}_n(\boldsymbol{R}) \rightarrow \mathcal{A}_n(\boldsymbol{R}) - \frac{\partial}{\partial \boldsymbol{R}}\zeta(\boldsymbol{R})$

θ_n can be vanished by not γ_n

How do we treat the nuclear coordinate R(t) in electron-ion problem ? --- as a parameter

Solving many body problem

Many body Hamiltonian

$$H = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 - \sum_{i,I}\frac{Z_I e^2}{|r_i - R_I|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i - r_j|}$$

$$-\sum_i \frac{\hbar^2}{2M_I}\nabla_I^2 + \frac{1}{2}\sum_{I\neq J}\frac{Z_I Z_J e^2}{|R_I - R_J|}$$

Schrödinger equation for coupled electron-ion system

$$H\psi_s(\{r,R\}) = E_s\psi_s(\{r,R\})$$

$$\psi_s(\{r,R\}) = \sum_i \chi_{si}(\{R\})\psi_i(\{r\}:\{R\})$$

What is gauge freedom ?

$$\vec{B} = \nabla \times \vec{A}$$

where $\boldsymbol{A}$ is vector potential and $\boldsymbol{B}$ is magnetic field.

Define another potential $\vec{A}'$ i.e.

$$\vec{A}' = \vec{A} + \nabla\alpha \qquad (1)$$

where α is an arbitrary differentiable function.

$$\Rightarrow \vec{B}' = \nabla \times (\vec{A} + \nabla\alpha) = \nabla \times \vec{A} = \vec{B}$$

So, $\vec{A}'$ and $\vec{A}$ are physically equivalent and thus, $\vec{A}$ is not measurable (i.e. it is unphysical).

Transformation (1) is known as gauge transformation and thus, $\vec{A}$ and $\vec{A}'$ are called **gauge equivalent.**

Geometric Phase

Starting with the time-dependent solution and the definitions of the two phases, it is now possible to calculate the geometric phase from what is known about the time evolution of the Hamiltonian

$$\Psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t), \quad \theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')dt', \quad \gamma_n(t) \equiv i\int_0^t \left\langle \psi_n(t') \middle| \frac{\partial}{\partial t'} \psi_n(t') \right\rangle dt'$$

the eigenstate depends on time because there is some parameter $R(t)$ in the Hamiltonian which is changing slowly with time

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R}\frac{dR}{dt}$$

the time integral for the geometric phase can thus be recast as an integral over the changing parameter, $R(t)$

$$\gamma_n(t) = i\int_0^t \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle \frac{dR}{dt'} dt' = i\int_{R_i}^{R_f} \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle dR$$

for a single evolving parameter, if the system returns to it's original value $(R_f \equiv R_i)$, then geometric phase is zero. However, this is not the case if there is more than one such parameter

Berry Phase

Thus with N parameters which are varying slowly, $R_1(t)$, $R_2(t)$, $\ldots R_N(t)$:

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_1}\frac{dR_1}{dt} + \frac{\partial \psi_n}{\partial R_2}\frac{dR_2}{dt} + \cdots + \frac{\partial \psi_n}{\partial R_N}\frac{dR_N}{dt} = (\nabla_R \psi_n) \cdot \frac{d\vec{R}}{dt}$$

the geometric phase can now be written

$$\gamma_n(t) = i \int_{\vec{R}_i}^{\vec{R}_f} \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R}$$

or if the Hamiltonian returns to its original form after a time T

$$\gamma_n(T) = i \oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R}$$

this is called Berry's phase and it depends only on the path taken, not the duration of traversal

the dynamic phase, on the other hand, *always* depends on the elapsed time

$$\theta_n(T) = -\frac{1}{\hbar}\int_0^T E_n(t')dt'$$

Dynamical Phase versus Geometric Phase, in very simple term

- **Dynamical phase describes the oscillations that occur even if the parameters don't change : $\exp(-i\omega t)$**
- **Geometric phase describes the additional phase, from the changing parameters**

- **After a cycle, dynamical phase answers the question : how long did your trip take ?**
- **While geometric phase answers the question; where have you been ?**

Proof of the evolution of Berry phase for a general slowly varying parameter $\lambda(t)$

Proof

TDSE

$$i\hbar \frac{\partial \psi(t)}{\partial t} = \hat{H}(t)\psi(t)$$

Ansatz

$$\psi(t) = \sum_n c_n(t)\ \psi_n(t)\ e^{i\theta_n(t)}$$

$$i\hbar \frac{\partial}{\partial t}\psi(t) = i\hbar \sum_n \frac{dc_n(t)}{dt}\psi_n(t)e^{i\theta_n(t)} + i\hbar \sum_n c_n(t)\frac{\partial \psi_n(t)}{\partial t}e^{i\theta_n(t)} + \cancel{\sum_n c_n(t)\psi_n(t)\left(-\hbar\frac{\partial \theta_n(t)}{\partial t}\right)e^{i\theta_n(t)}}$$

$$\hat{H}(t)\psi(t) = \cancel{\sum_n c_n(t)\left(-\hbar\frac{\partial \theta_n}{\partial t}\right)\psi_n(t)e^{i\theta_n(t)}}$$

Pre-multiplying by $\langle \psi_m(t) |$

$$\frac{dc_m(t)}{dt} = -\sum_n c_n(t)\left\langle \psi_m(t) \,\middle|\, \frac{\partial \psi_n(t)}{\partial t}\right\rangle e^{i[\theta_n(t)-\theta_m(t)]}$$

Taking time derivative of $\hat{H}(t)\psi_n(t) = E(t)\psi_n(t)$

$$\left\langle \psi_m(t) \left| \frac{\partial \hat{H}(t)}{\partial t} \right| \psi_n(t) \right\rangle + \left\langle \psi_m(t) \left| \hat{H}(t) \right| \frac{\partial \psi_n(t)}{\partial t} \right\rangle = \frac{\partial E_n(t)}{\partial t} \langle \psi_m(t) | \psi_n(t) \rangle + E_n(t) \left\langle \psi_m(t) \left| \frac{\partial \psi_n(t)}{\partial t} \right. \right\rangle$$

$$\frac{dc_m(t)}{dt} = -\sum_n c_n(t) \left\langle \psi_m(t) \left| \frac{\partial \psi_n(t)}{\partial t} \right. \right\rangle e^{i[\theta_n(t) - \theta_m(t)]}$$

$$\frac{dc_m(t)}{dt} = -c_m(t) \left\langle \psi_m(t) \left| \frac{\partial \psi_m(t)}{\partial t} \right. \right\rangle - \sum_{n \neq m} c_n(t) \frac{\left\langle \psi_m(t) \left| \frac{\partial \hat{H}(t)}{\partial t} \right| \psi_n(t) \right\rangle}{[E_n(t) - E_m(t)]} e^{i[\theta_n(t) - \theta_m(t)]}$$

For m = n, $c_m(t) = c_m(0)\,\mathrm{e}^{+i\gamma_m(t)}$ $\qquad \psi(t) = \sum_n c_n(t)\psi_n(t)\,\mathrm{e}^{i\theta_n(t)}$

Berry phase, Berry curvature, Berry connection

To summarize :

Berry phase

$$\gamma_n(t) = \int_{R_i}^{R_f} A_n(\mathbf{R}) \cdot d\mathbf{R}$$

$$A_n(\mathbf{R}) \equiv i \langle n(\mathbf{R})| \frac{\partial}{\partial \mathbf{R}} |n(\mathbf{R})\rangle$$

Fock (1928) found that, the phase can always be made zero by choosing a suitable gauge transformation

$$\mathcal{A}_n(\boldsymbol{R}) \to \mathcal{A}_n(\boldsymbol{R}) - \frac{\partial}{\partial \boldsymbol{R}} \zeta(\boldsymbol{R})$$

However, Berry (1984) showed that this is not in general true for a cyclic evolution

$$\boxed{\gamma_n = \oint A_n(\mathbf{R}) \cdot d\mathbf{R}}$$

Berry Phase & Berry Curvature

Berry Phase $\boxed{\gamma_n = \oint A_n(\mathbf{R}) \cdot d\mathbf{R}}$ $\gamma_n = \int_S \Omega_n(\mathbf{R}) \cdot d\mathbf{a}$

Berry Curvature $\boxed{\Omega_n(\mathbf{R}) = \nabla_R \times \mathbf{A}_n(\mathbf{R})}$

Berry Flux **is analogous to Magnetic flux :** $\Phi = \int_S \mathbf{B} \cdot d\mathbf{a} = \int_S (\nabla \times \mathbf{A}) \cdot d\mathbf{a} = \oint \mathbf{A} \cdot d\mathbf{r}$

Thus Berry's phase can be thought of as the "flux" of a "magnetic field" like qty.

Here $A_n(R)$ is called Berry potential, just like Vector potential

Berry field is just like magnetic field B

"Chern Number" is defined by : $C_m = \dfrac{1}{2\pi} \int_{BZ} \Omega_m(\mathbf{k}) \cdot d^2\mathbf{k}$ $\rightarrow$ **integer**

The integer C_m is non-zero only when the bands are topologically non-trivial.

Dynamical evolution of a quantum system $H(\vec{r}, \vec{p}; \vec{\lambda})$

$$H(\vec{r}, \vec{p}; \vec{\lambda})\psi_{n,\vec{\lambda}}(\vec{x}) = E_{n,\vec{\lambda}}\psi_{n,\vec{\lambda}}(\vec{x})$$

$\underline{x} \rightarrow \underline{(r, \lambda, t)}$ $\underline{r} \rightarrow$ Variable ; $\underline{\lambda} \rightarrow$ Parameter

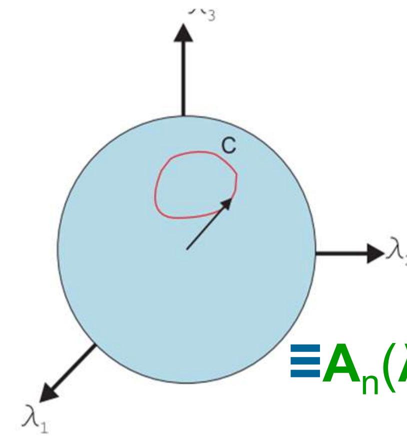
Time evolution of $\psi(t) \rightarrow \psi(0)\ \exp\{-\, i/\hbar \int dt' \,(\lambda(t) + i\,\gamma_n(t)\}$

For an arbitrary open path in the parameter space,
$\gamma_n(t) = 0$ under gauge transformation (Fock 1928)

For a closed path (cyclic evolution), the accumulated phase γ is gauge invariant & is a measurable quantity

Berry Phase

$$\gamma_n = \oint_C d\boldsymbol{\lambda} \cdot \mathbf{A}_n(\boldsymbol{\lambda})$$



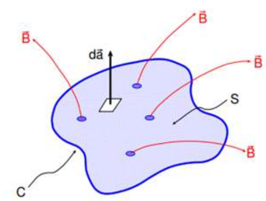
$\equiv \mathbf{A}_n(\boldsymbol{\lambda})$

Berry Connection or Potential $\rightarrow$ $\mathbf{A}_n(\boldsymbol{\lambda}) = i \int d^3r\, \Phi_n^*(\mathbf{r}, \boldsymbol{\lambda}) \nabla_{\boldsymbol{\lambda}} \Phi_n(\mathbf{r}, \boldsymbol{\lambda})$

Berry Curvature or Field $\rightarrow$ $\boldsymbol{\Omega}_n(\boldsymbol{\lambda}) = \nabla_{\boldsymbol{\lambda}} \times \mathbf{A}_n(\boldsymbol{\lambda})$

Analogous to Vector Potential and Magnetic Field respectively.

The Berry phase in terms of Ω : $\gamma_n = \int_S \Omega_n(\mathbf{R}) \cdot d\mathbf{a}$



Similar to "flux" of a "magnetic field" like quantity : $\Phi = \int_S \mathbf{B} \cdot d\mathbf{a} = \int_S (\nabla \times \mathbf{A}) \cdot d\mathbf{a} = \oint \mathbf{A} \cdot d\mathbf{r}$

Analogies with magnetic flux and vector potentials

Parameter Space	Real Space
Berry Curvature (or Field) Ω_n (Gauge independent)	Magnetic Field $\underline{B}$ (Gauge independent)
Berry Potential (or Connection) A_n (Gauge dependent)	Vector Potential $\underline{A}$ (Gauge dependent)
Berry Phase γ	Magnetic Flux ϕ
Chern Number	Dirac Monopole

The so-called "Chern Number" is defined by : $C_m = \frac{1}{2\pi}\int_{BZ} \Omega_m(\mathbf{k}) \cdot d^2\mathbf{k}$ → integer

Generalizations & Physical Realizations of Berry Phase

Berry's original approach assumed : Adiabatic, Cyclic, Unitary evolution of quantum systems

Generalizations : non-Adiabatic, non-Cyclic, non-Unitary

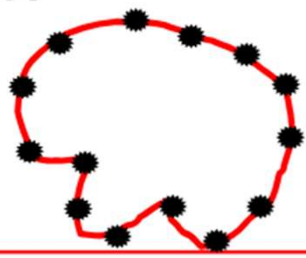
Generalizations of Geometric phase

	Condition	Space
Berry's Phase M. Berry, Proc. R. Soc. Lond. A, p. 45 (1984).	Adiabatic and cyclic	Parameter space
Aharonov-Anadan Phase (A-A Phase) Y. Aharonov and J. Anandan, PRL **58**, 1593 (1987).	Cyclic	Ray Space
Pancharatnam Phase S. Pancharatnam, Proc. Indian Acad. Sci., 247 (1956); J. Samuel and R. Bhandari, PRL **60**, 2339 (1988).	General **Non-Cyclic** **Non-Unitary**	Ray Space

Shivaramakrishnan Pancharatnam's work on interference of polarized light (that had anticipated Berry's finding in 1956 i.e. nearly 3 decades earlier !) was formulated in the language of differential geometry (interplay between connection & geodesics)

Discrete
(Pancharatnam)

$$\gamma = -\arg \prod_{i=1}^{M-1} \langle \psi(\xi_i) | \psi(\xi_{i+1}) \rangle$$



Continuous limit
(Berry)

$$\gamma = \int_C i \langle \psi(\xi) | \nabla_\xi \psi(\xi) \rangle d\xi$$

Berry's connection

$$i \langle \psi(\xi) | \nabla_\xi | \psi(\xi) \rangle$$

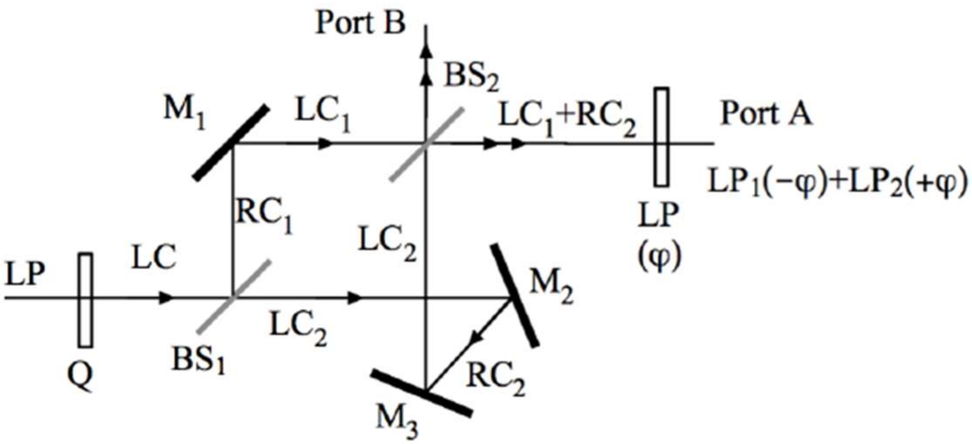
Shivaramakrishnan Pancharatnam
1934-1969

The Pancharatnam formulation is the most useful e.g. in numerics.

Trajectory C is in parameter space: one needs at least 2 parameters.

Polarization is a physical degree of freedom of an electromagnetic wave and like the dynamical phase of the wave, the evolution of wave polarization must be considered during propagation.

Pancharatnam's phase is a fascinating manifestation of this additional degree of freedom associated with the evolution of wave polarization.



$$\langle LC_1| = \begin{pmatrix} 1 \\ -i \end{pmatrix}, \qquad \langle RC_2| = \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\langle LP_1| = \begin{pmatrix} \cos^2\varphi & \sin\varphi\cos\varphi \\ \sin\varphi\cos\varphi & \sin^2\varphi \end{pmatrix} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} e^{-i\varphi},$$

$$\langle LP_2| = \begin{pmatrix} \cos^2\varphi & \sin\varphi\cos\varphi \\ \sin\varphi\cos\varphi & \sin^2\varphi \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} e^{+i\varphi}.$$

Both beams begin with the same initial polarization (LC) and end with the same final polarization LP (which is different from the initial polarization). Therefore, their polarization trajectories form a closed loop on Poincare sphere.

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Geometric Phase in Optics: From Wavefront Manipulation to Waveguiding

*Chandroth Pannian Jisha, Stefan Nolte, and Alessandro Alberucci**

The historical development of the geometric phase in the field of optics is clearly much more complicated than the short summary provided in the abstract. In fact, the concept of geometric phase (even though the name was not coined at that time) has been first introduced by Shivaramakrishnan Pancharatnam in 1956 while studying the interference between optical waves of different polarizations.[2] Even though at a first and distracted glance this problem could seem trivial, Pancharatnam unveiled its true complexity, discovering that an optical wave acquires a phase dependent on the path followed by the polarization on the Poincaré sphere. Even more surprisingly, he discovered that this phase is non-transitive. This path-dependent behavior requires that the evolution operator does not commute with itself at different instants, thus somehow resembling the motion of charged particles immersed in a rotating magnetic field.[3] Indeed, after discovering Pancharatnam's work through Ramaseshan and Nityananda,[4-6] Berry himself found the equivalence between his geometric phase and the phase introduced by Pancharatnam, thus giving origin to what is called today the Pancharatnam–Berry phase, abbreviated with PBP hereafter.

Geometric Phase (Chronologically): from Pancharatnam (1956) to Berry (1984) and beyond

- S Pancharatnam, Generalized theory of interference and its applications, Proc. Indian Acad. Sci. **A44**, 247 (1956), reprinted in Curr. Sci. **55**, 1225 (1986) article by S. Ramaseshan, R. Nityananda; also see articles in Pancharatnam memorial issue in Current Science Vol 67(4), 25 August 1994 https://www.jstor.org/stable/i24092525 ; also see the recent article by Luis Garza-Soto et al "Deciphering Pancharatnam's discovery of geometric phase", arXiv 2301.04359 (2023)
- A. Aharonov, Y. & D. Bohm, Significance of electromagnetic potentials in the quantum theory. Phys. Rev. **11**, 485 (1959)
- Y. Aharonov & J. Anandan, Phase change during a cyclic quantum evolution. Phys. Rev. Lett. **58**(16), 1593 (1987)
- M.V. Berry, Quantal phase factors accompanying adiabatic changes. Proc. R. Soc. A. **392**(1802), 45–57 (1984)
- M.V. Berry, The adiabatic phase and Pancharatnam's phase for polarized light. J. Mod. Opt. **34**(11), 1401–1407 (1987)
- M. V. Berry, Anticipations of the geometric phase. Phys. Today **43**(12), 34 (1990)
- V.C. Rakhecha & A.G. Wagh, Geometric Phase a la Pancharatnam, Pramana **46**, 315 (1996)
- R. Citro & O. Durante, The Geometric Phase: Consequences in Classical and Quantum Physics Lecture Notes in Physics **1000**, 63 (2023)

Following Berry's work, several experiments performed to observe geometric phases

- Neutron interferometry – spin ½ systems evolving in changing external fields eg. A. Wagh *et al*., PRL **78**, 755 (1997); B. Allman *et al*., PRA **56**, 4420 (1997); Y. Hasegawa *et al*., PRL **87**, 070401 (2001).
- Microwave resonators – real-valued wave functions evolving in cavity with changing boundaries
  eg. H.-M. Lauber, P. Weidenhammer, D. Dubbers, PRL **72**, 1004 (1994).
- Quantum pumping – time-varying potential walls (gates) for a quantum dot: geometric phase $\propto$ number of electrons transported eg. J. Avron *et al*., PRB **62**, R10618 (2000); M. Switkes *et al*., Science **283**, 1905 (1999).
- Level splitting and quantum number shifting in molecular physics
- Intimately connected to physics of fractional statistics, quantized Hall effect, and anomalies in gauge theory
-

PHYSICAL REVIEW LETTERS

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Experimental Separation of Geometric and Dynamical Phases Using Neutron Interferometry

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Atominstitut of Austrian Universities and Technical University of Vienna, Schuettelstrasse 115, A-1020 Vienna, Austria

B. E. Allman, H. Kaiser, K. Hamacher, D. L. Jacobson, and S. A. Werner

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(Received 5 February 1996)

We present results of the first experiment clearly demarcating geometric and dynamical phases. These two phases arise from two distinct physical operations, a rotation and a linear translation, respectively, performed on two identical spin flippers in a neutron interferometer. A reversal of the current in one flipper results in a pure geometric phase shift of π radians. This observation constitutes the first direct verification of Pauli anticommutation, implemented in neutron interferometry. [S0031-9007(96)02278-8]

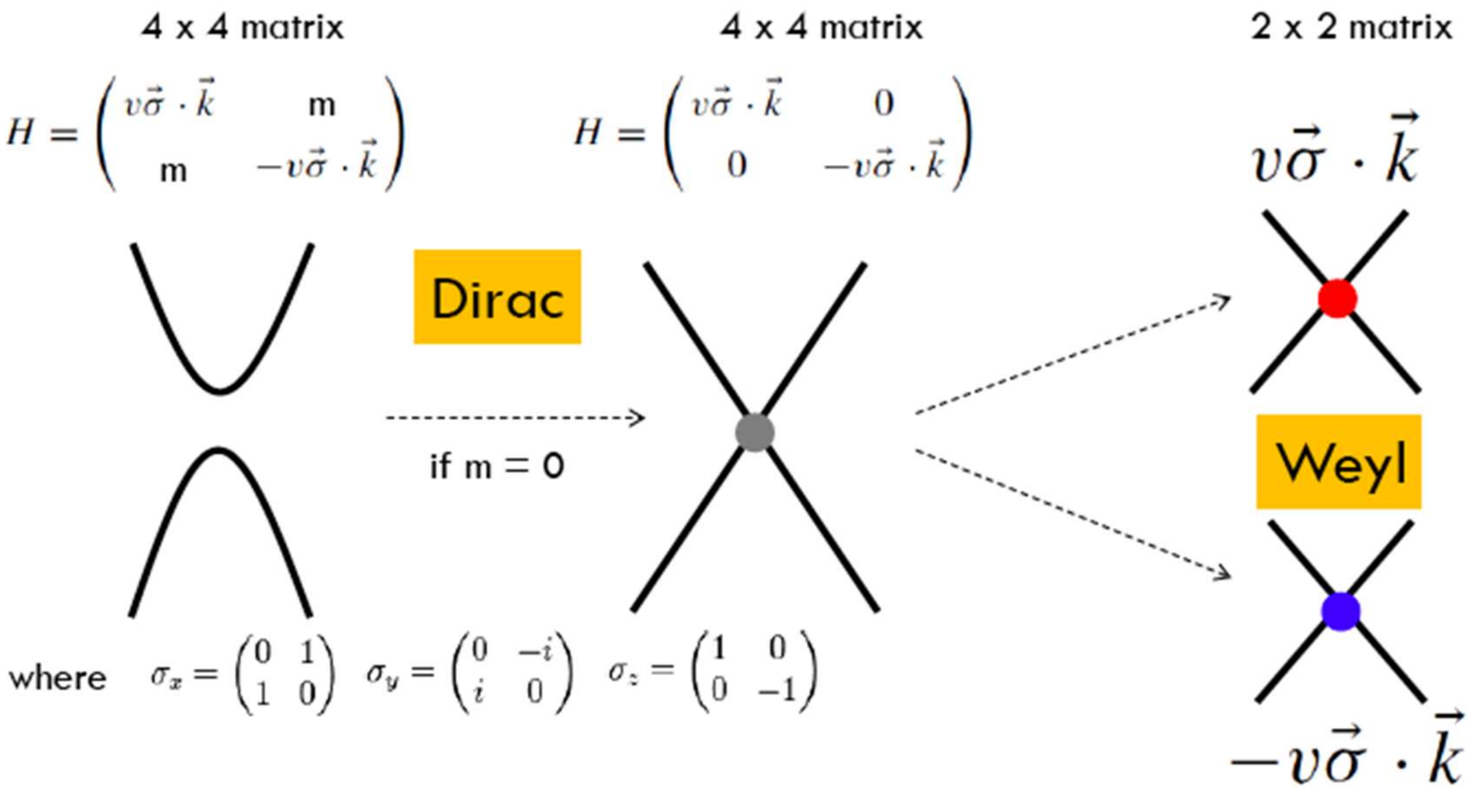
Manifestations Berry Curvature in Weyl Semimetals

Inversion Symmetry and / or

Time Reversal Symmetry preserved or broken

Abhirup Roy Karmakar :
PhD Thesis (2024)

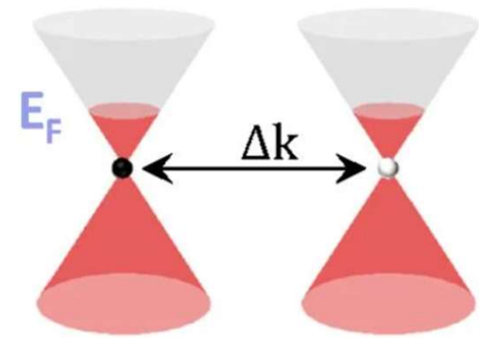
Dirac Fermions (Massive) versus Weyl Fermions (Massless)



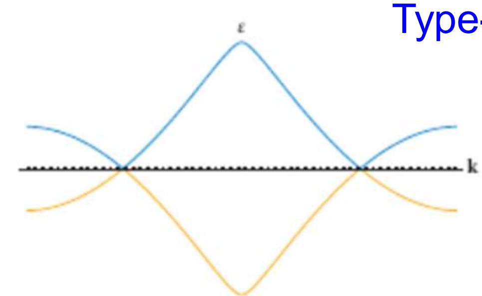
A Weyl fermion is one-half of a charged Dirac fermion of a definite chirality

Weyl semimetal (WSM)

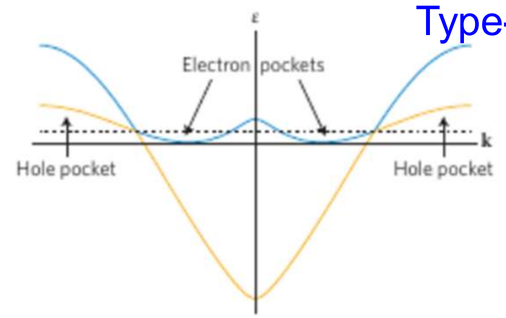
- Valence and conduction bands cross at discrete points
- Energy dispersion is linear near the crossings
- Weyl nodes always come in pairs with opposite chiralities
- Each Weyl node acts as source (+ve chirality) or sink (-ve chirality) of the Berry curvature (viewed as mag field in momentum space)
- IS broken but TRS preserved WSM : Ex. TaAs, ...
- IS preserved but TRS broken (magnetic WSM) Ex $Co_3Sn_2S_2$
- Type-I WSM : Zero DOS at Weyl node
- Type-II WSM : Supports Fermi pockets at node energy
- Unique and fascinating transport properties of WSM :
    - Anomalous Hall effect
    - Anomalous Nernst effect
    - Planar Hall effect
    - Negative longitudinal magnetoresistance
    - Chiral magnetic effect



Type-I WSM



Type-II WSM



Anomalous effects can be see only with broken Symmetries : IS & TRS

- Space inversion symmetry $\vec{\Omega}_n(-\vec{k}) = \vec{\Omega}_n(\vec{k})$
- Time reversal symmetry $\vec{\Omega}_n(-\vec{k}) = -\vec{\Omega}_n(\vec{k})$

Both symmetries

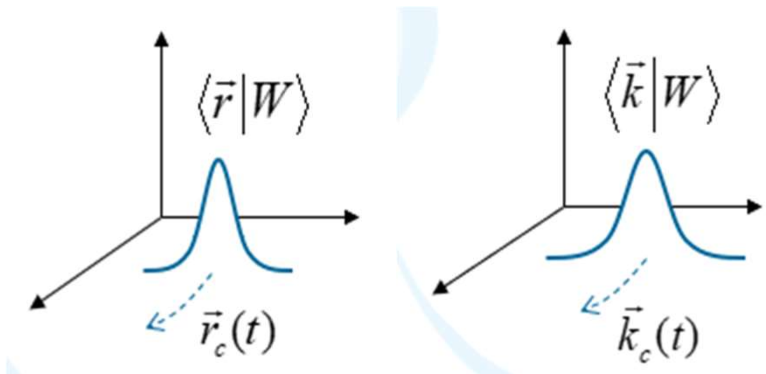
$$\vec{\Omega}_n(\vec{k}) = 0, \ \forall \vec{k}$$

- **IS preserved (TRS broken) :** $\sum_n \Omega_n(\mathbf{k}) \neq 0$
- **TRS preserved (IS broken) :** $\sum_n \Omega_n(\mathbf{k}) = 0$
- **Both are preserved (Ex Graphene) :** $\Omega_n(\mathbf{k}) = 0$

- SI symmetry is broken $\leftarrow$ Electric polarization
- TR symmetry is broken $\leftarrow$ QHE
- *Spinor* Bloch state (degenerate band) $\leftarrow$ SHE
- Band crossing $\leftarrow$ Monopole

Semiclassical electron dynamics in solids : Wave packet approach

Localized wave packet dynamics (r,k) :
Time evolution of $\underline{r}_c(t)$ & $\underline{k}_c(t)$ for a Bloch band in presence of E & B



$$\dot{\mathbf{r}}_c = \frac{1}{\hbar}\frac{\partial \mathcal{E}_{n\mathbf{k}}}{\partial \mathbf{k}}\bigg|_{\mathbf{k}=\mathbf{k}_c} = \mathbf{v}_n(\mathbf{k}_c),$$

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

$$\dot{\mathbf{r}}_c = \frac{1}{\hbar}\frac{\partial \mathcal{E}_{n\mathbf{k}}}{\partial \mathbf{k}}\Big|_{\mathbf{k}=\mathbf{k}_c} - \dot{\mathbf{k}}_c \times \boldsymbol{\Omega}_n(\mathbf{k}_c),$$

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

$$\vec{\Omega}_n(\vec{k}) = i\left\langle \nabla_k u_{n\vec{k}} \right| \times \left| \nabla_k u_{n\vec{k}} \right\rangle$$

Wave packet in magnetic Bloch band → the semi-classical dynamics gets modified with the additional contribution of "Anomalous" velocity originating from <u>Berry curvature</u>

[Chang & Niu, PRB 54, 7010 (1996)]

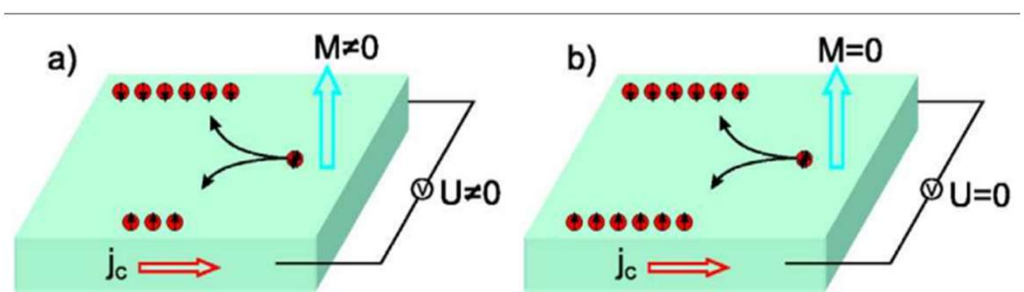
Equation of motion

Ref.: "Berry Phase, ... Semiclassical Dynamics in magnetic Bloch bands", M.-C. Chang and Q. Niu, Phys. Rev. B 53, 7010 (1996)

Magnetic field (Lorentz Force) : $$\boxed{\dot{\mathbf{k}} \rightarrow \dot{\mathbf{k}}_0 + q\,\dot{\mathbf{r}} \times \mathbf{B}}$$

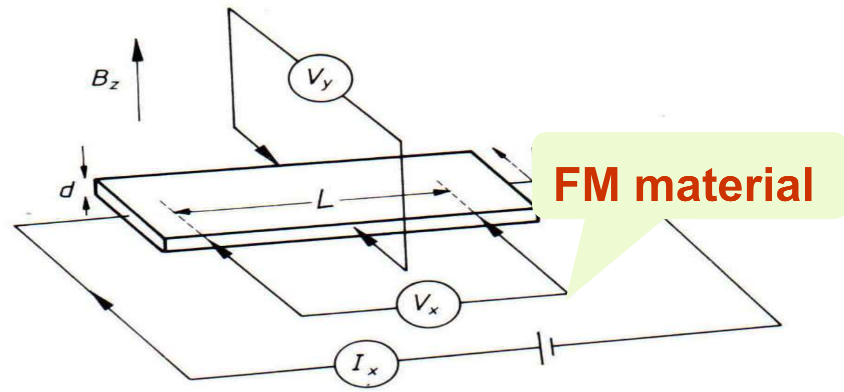
Berry curvature : $$\boxed{\dot{\mathbf{r}} \rightarrow \dot{\mathbf{r}}_0 + \dot{\mathbf{k}} \times \Omega_n(\mathbf{k})}$$

If B=0, then dk/dt // electric field → Anomalous velocity ⊥ electric field

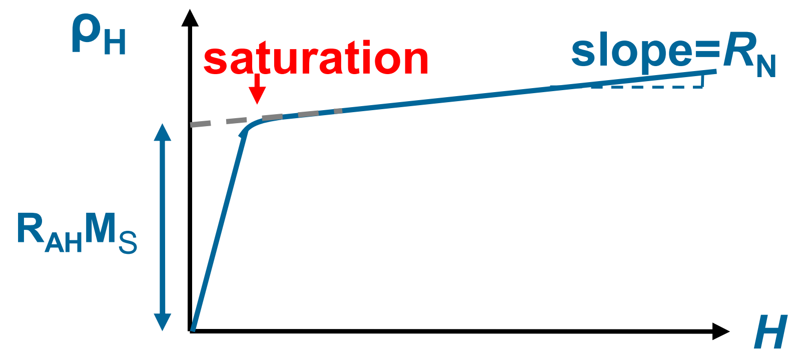


- (integer) Quantum Hall effect
- (intrinsic) Anomalous Hall effect
- (intrinsic) Spin Hall effect

Anomalous Hall effect (Edwin Hall 1881) :



Hall effect in ferromagnetic materials



The usual Lorentz force term

$$\rho_H = R_N H + \rho_{AH}(H),$$

Anomalous term

$$\rho_{AH}(H) \equiv R_{AH} M(H)$$

Is the anomalous term extrinsic & materials specific (imperfection induced scattering) ?

Answer : → Karplus & Luttinger (1954)
It is completely intrinsic in nature.

Electrons in a FM acquire a net anomalous velocity that is related to the Berry curvature.

Physical realizations of anomalous transports in Weyl Semimetals

(All expressions derived in terms of Berry curvature $\boldsymbol{\Omega}_n$)

The anomalous Hall conductivity :

Electrical current ⊥ electrical voltage

$$\boxed{L_{xy}^{EE} = \frac{e^2}{\hbar}\sum_n \int \frac{d^3k}{(2\pi)^3}\Omega_{n,z}(\mathbf{k})\, f_0(\mathbf{k})}$$

The anomalous thermoelectric conductivity :

Electrical current ⊥ thermal gradient

$$\boxed{L_{xy}^{ET} = \frac{k_B e}{\hbar}\sum_n \int \frac{d^3k}{(2\pi)^3}\Omega_{n,z}(\mathbf{k}) s(\mathbf{k})}$$

$$s(\mathbf{k}) = -f_0(\mathbf{k})\ln[f_0(\mathbf{k})] - [1 - f_0(\mathbf{k})]\ln[1 - f_0(\mathbf{k})]$$

The anomalous thermal Hall conductivity :

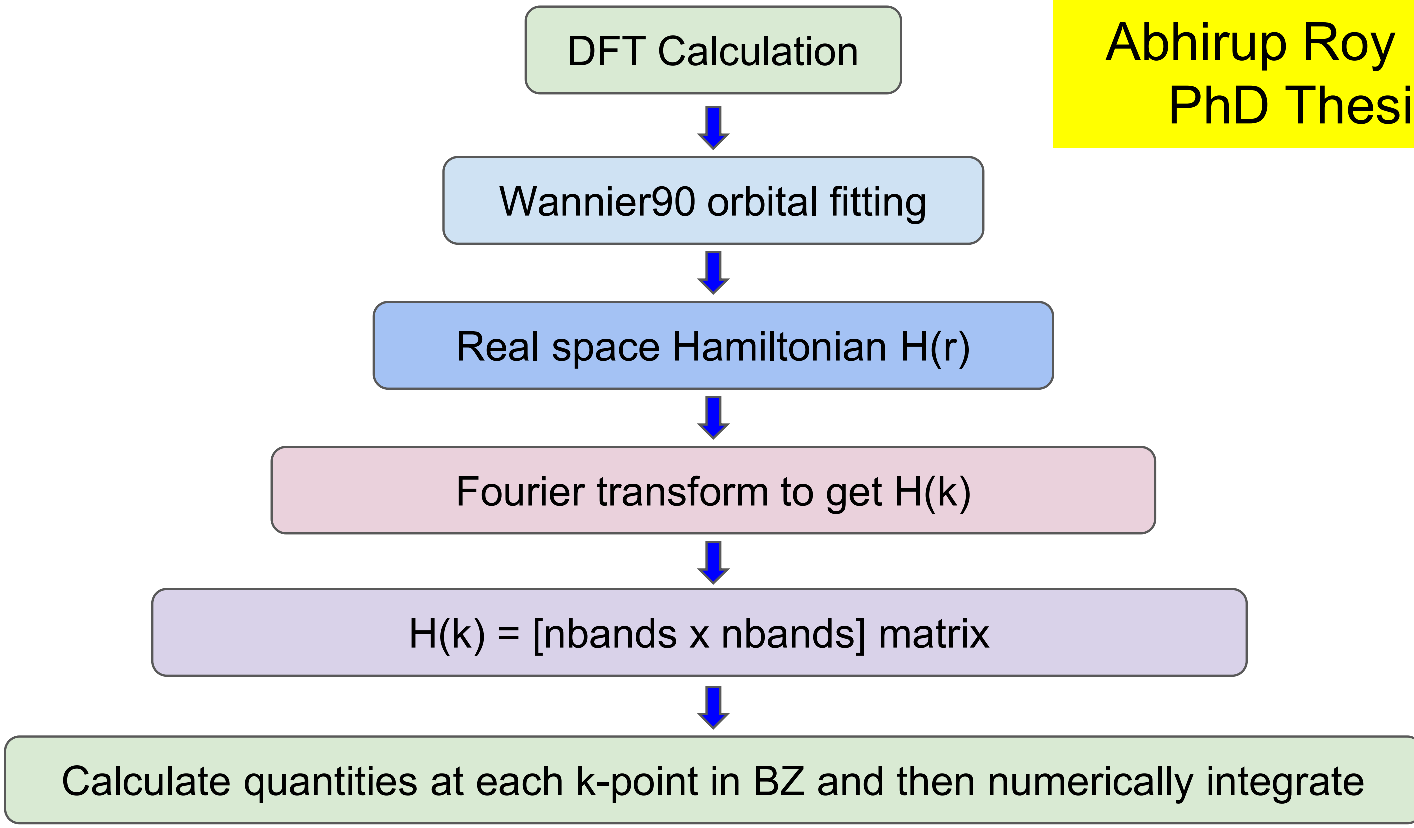
Heat current ⊥ thermal gradient

$$\boxed{\begin{aligned} L_{xy}^{TT} = \frac{k_B^2 T}{\hbar}\sum_n \int \frac{d^3k}{(2\pi)^3}\Omega_{n,z}(\mathbf{k})\Bigg(\frac{\pi^2}{3} + \frac{(\mathcal{E}-\mu)^2}{(k_B T)^2} f_0(\mathbf{k}) \\ - \ln\left(1 + e^{-\frac{\mathcal{E}-\mu(T)}{k_B T}}\right) + 2\mathrm{Li}_2(1 - f_0(\mathbf{k}))\Bigg) \end{aligned}}$$

Ref.: McCormick, McKay & Trivedi, Phys. Rev. B ***96****, 235116 (2017)*

Berry curvature-induced properties from first-principles DFT calculations
Tight-binding Hamiltonian

Abhirup Roy Karmakar :
PhD Thesis (2024)



Case study of $Co_3Sn_2S_2$: Type-I Weyl semi-metal

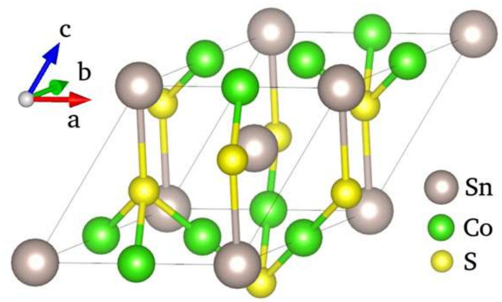
PHYSICAL REVIEW B **106**, 245133 (2022)

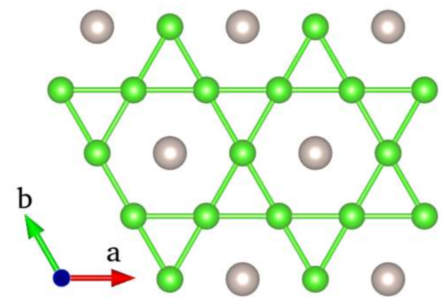
Giant anomalous thermal Hall effect in tilted type-I magnetic Weyl semimetal $Co_3Sn_2S_2$

Abhirup Roy Karmakar,[1,*] S. Nandy,[2] A. Taraphder,[1,†] and G. P. Das[3,‡]

Crystal structure of $Co_3Sn_2S_2$ (Shandite)

- Crystal
  - Rhombohedral (*R-3m*)
  - Co & Sn atoms form a kagome lattice
  - Quasi-2D layer of Co_3Sn forms the kagome plane
- Lattice parameters
  - a = b = c = 5.38 Å
  - $\alpha = \beta = \gamma = 60.128°$
- Symmetries
  - C_{3z} rotational symmetry
  - Inversion symmetry (Present)
  - Time-reversal symmetry (Broken)





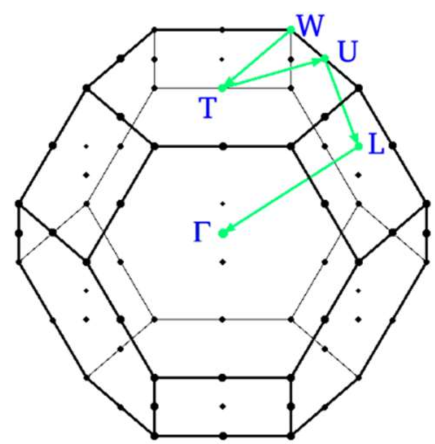
Ref.: Z. Anorg. Allg. Chem. **632**, 1531 (2006)

Methodology and properties

- **Tools**
  - DFT (VASP with PAW, PBE)
  - TB Hamiltonian **(Wannier90)**
  - Post-processing (Python)

- **Magnetic moment:**
  - Literature : 0.29 μ_B/Co [Experimental]
    0.33 μ_B/Co [Theory]
  - Our work : 0.33 μ_B/Co

- **Brillouin Zone :**
  - Truncated octahedral
  - **W $\rightarrow$ T $\rightarrow$ U $\rightarrow$ L $\rightarrow$ Γ**



Ref.: Solid State Sciences **11**, 513 (2009), Nature Physics **14**, 1125–1131 (2018)

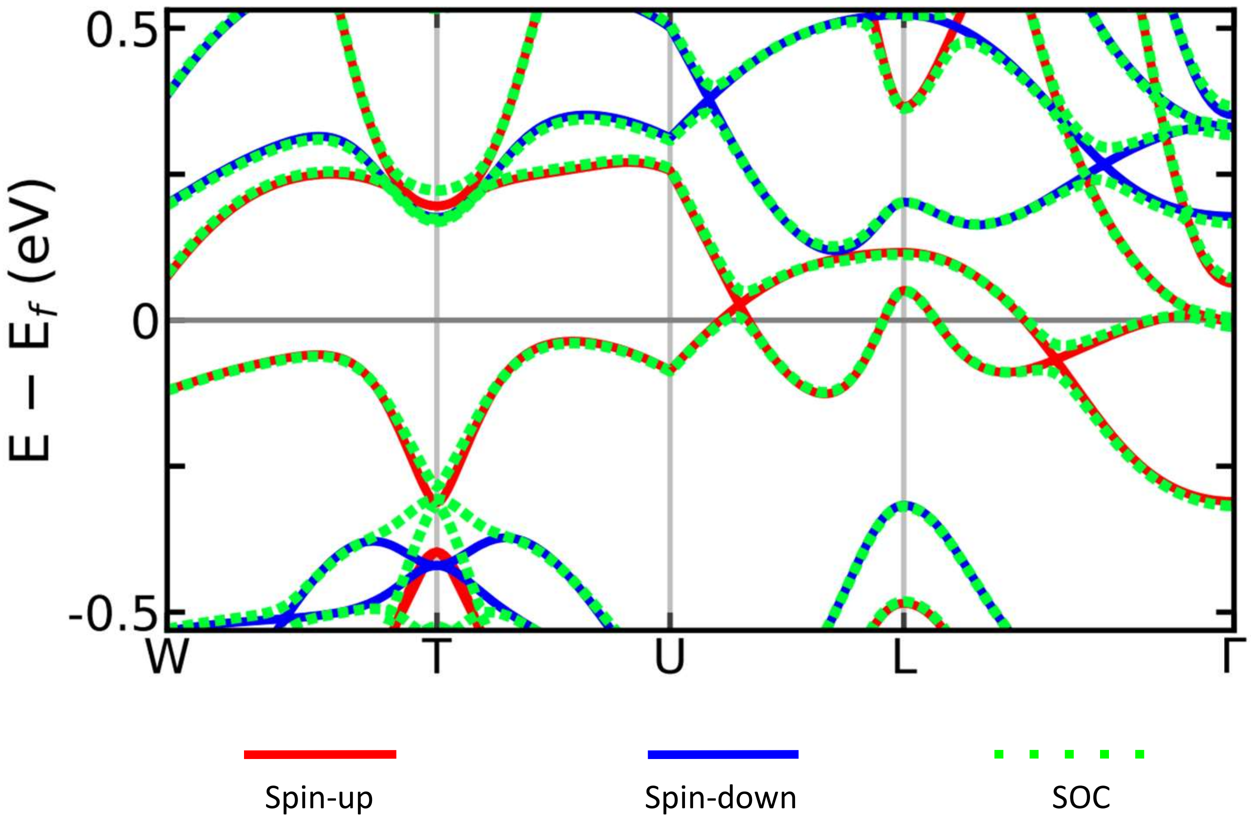
Calculation of Berry curvature

The Berry curvature in the momentum space can be calculated as :

$$\Omega_{n,\mu\nu}(\mathbf{R}) = i \sum_{n' \neq n} \frac{1}{(\varepsilon_n - \varepsilon_{n'})^2} \left(\langle n| \frac{\partial H}{\partial R_\mu} |n'\rangle \langle n'| \frac{\partial H}{\partial R_\nu} |n\rangle - \langle n| \frac{\partial H}{\partial R_\nu} |n'\rangle \langle n'| \frac{\partial H}{\partial R_\mu} |n\rangle \right)$$

where **n** is the eigenfunction, and **R** is the momentum vector

Spin-polarized Band structure



- Half metallic compound
- Spin-up channel is gapless
- Spin down channel has 0.44 eV gap
- There are two crossings along U-L-Γ line which are parts of closed nodal ring
- SOC gaps out the crossing which leads to 6 discrete Weyl nodes

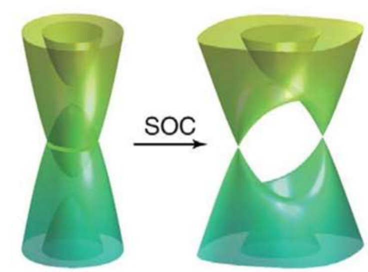
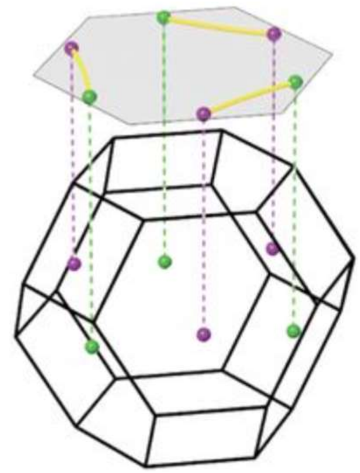


Image source: Science **365**, 6459

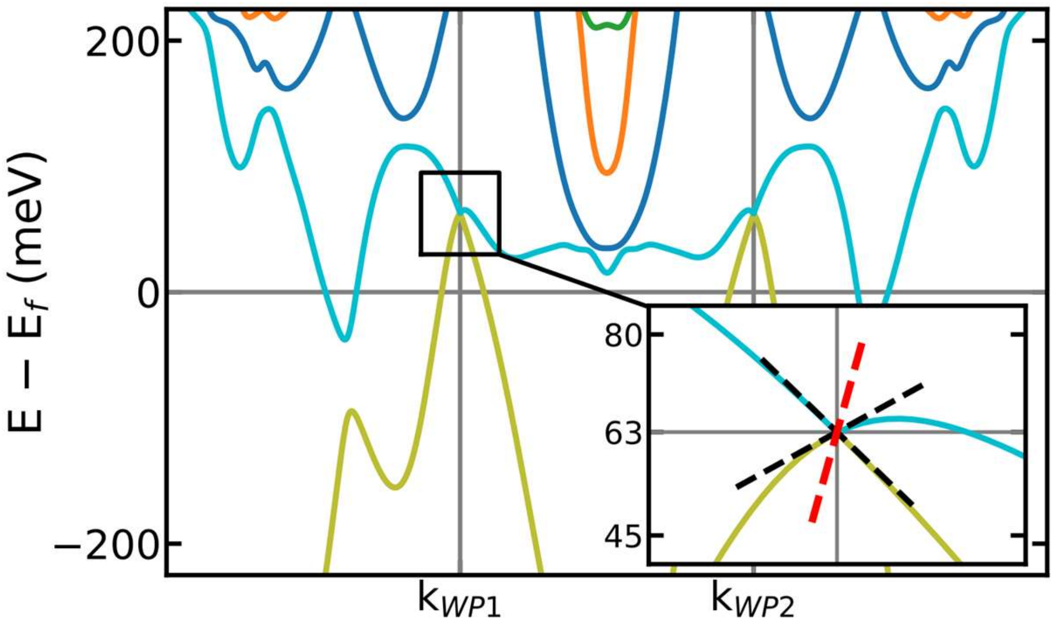
Weyl nodes

	k_1	k_2	k_3	$E - E_f(meV)$	$Chirality$
WP1	0.000	0.425	0.063	62.9	+1
	0.000	−0.425	−0.063	62.5	−1
WP2	0.425	0.000	0.063	62.3	+1
	−0.425	0.000	−0.063	62.6	−1
WP3	−0.425	−0.425	−0.365	62.7	+1
	0.425	0.425	0.365	62.5	−1



- ➔ There are three pairs of Weyl nodes with opposite chiralities
- ➔ Consequence of C_{3z} rotational symmetry and inversion symmetry
- ➔ All of the nodes are situated about 63 meV above the Fermi level

Tilted Weyl cones



- Weyl cones are plotted along k_y-axis
- Cones with opposite chirality are tilted in opposite directions
- Tilt parameter (i.e. slope) less than 1
- Hence classified as tilted type-I Weyl semimetal

Effective 2-band Hamiltonian

$$H = v\boldsymbol{k} \cdot \boldsymbol{\sigma} + \boldsymbol{t} \cdot \boldsymbol{k} + \epsilon_0,$$

k* : *momentum relative to the Weyl node; ***v* : *Fermi velocity;*** ***t* : *Tilt parameter;*** **ε_0 : Weyl node energy;**

Cones shown are tilted primarily along the k_y direction.

From our DFT calculation, the value of t_y and v as 0.19 and 0.65 eV; ratio t_y/v ~ 0.29 (< 1) ⇒ WSM of type-I

Anomalous thermal Hall conductivity

Equation for heat current:

$$\boldsymbol{J}_Q = T\alpha.\boldsymbol{E} - \kappa.\boldsymbol{\nabla} T$$

Transverse component of the thermal conductivity:

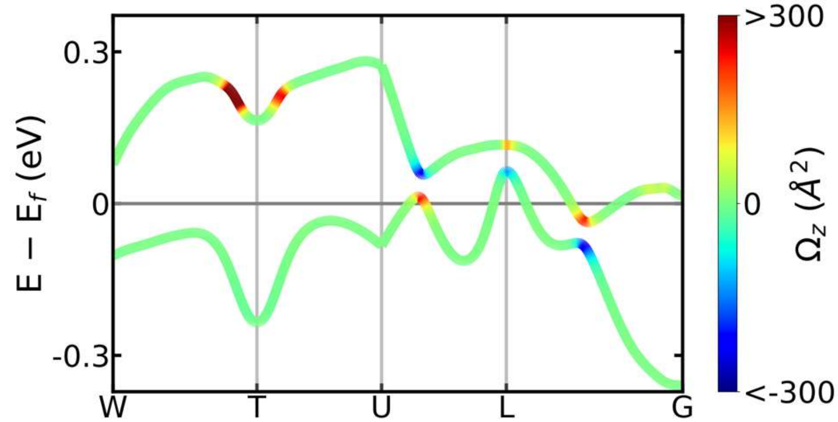
$$\kappa_{xy} = \frac{k_B^2 T}{h}\int \frac{d\boldsymbol{k}}{(2\pi)^3}\sum_n \Omega_{\mathbf{k}n}[\frac{\pi^2}{3}+\beta^2(\epsilon_{\boldsymbol{k}n}-\mu)^2 f(\epsilon_{\boldsymbol{k}n}-\mu)$$
$$-[ln(1+e^{-\beta(\epsilon_{\boldsymbol{k}n}-\mu)})]^2 - 2Li_2[1-f(\epsilon_{\boldsymbol{k}n}-\mu)]]$$

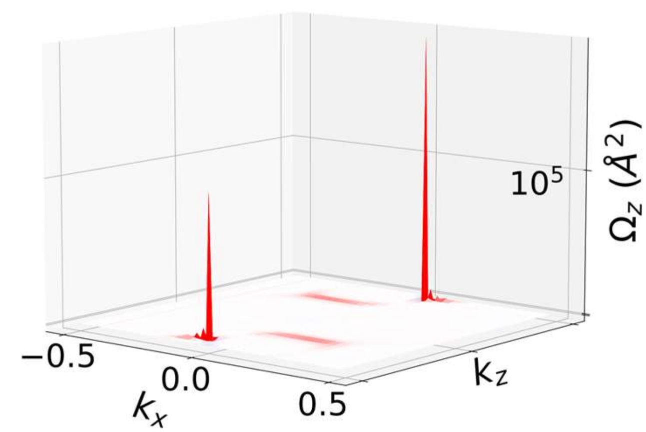
where, $\Omega_{\mathbf{k}n}$: **Berry curvature for *n*-th band**

f_{eq} : **Equilibrium Fermi function**

Ref.: Phys. Rev. Lett. **104**, 066601, Phys. Rev. B **83**, 161407(R)

Calculated Berry curvatures

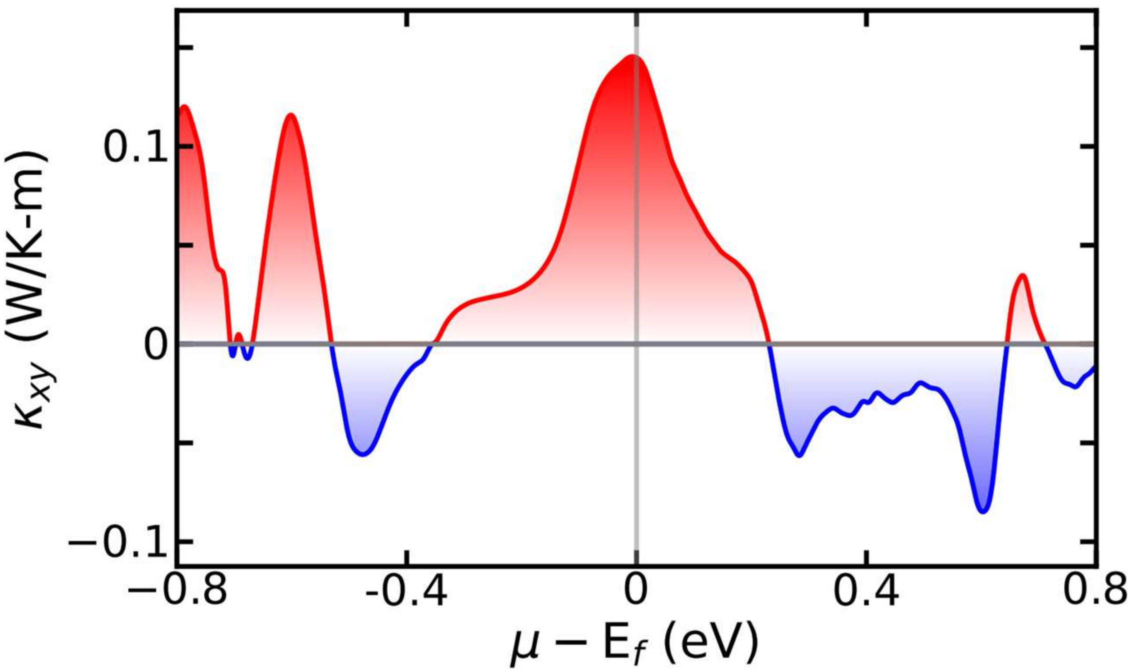




➔ **Left:** Color represents the value of the Berry curvature at different regions of the valence and conduction bands

➔ **Right:** The curvature attains very high values near the Weyl points

Anomalous thermal Hall conductivity

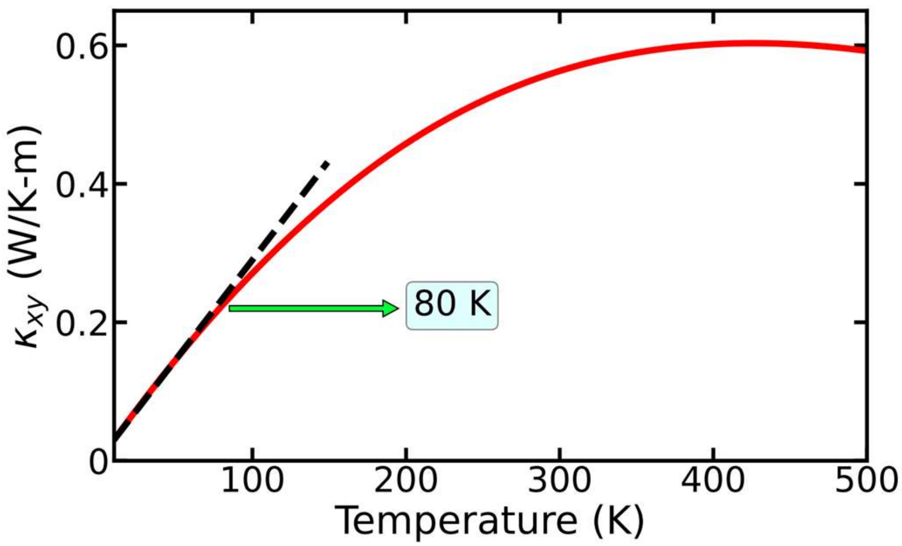


- ➔ **The conductivity is maximum at original Fermi level**
- ➔ **The peak value is 0.145 W/K-m which is quite large compared to other topological systems**
- ➔ **The thermal current can be tuned as well as reversed by varying the chemical potential**

Validation of the calculations

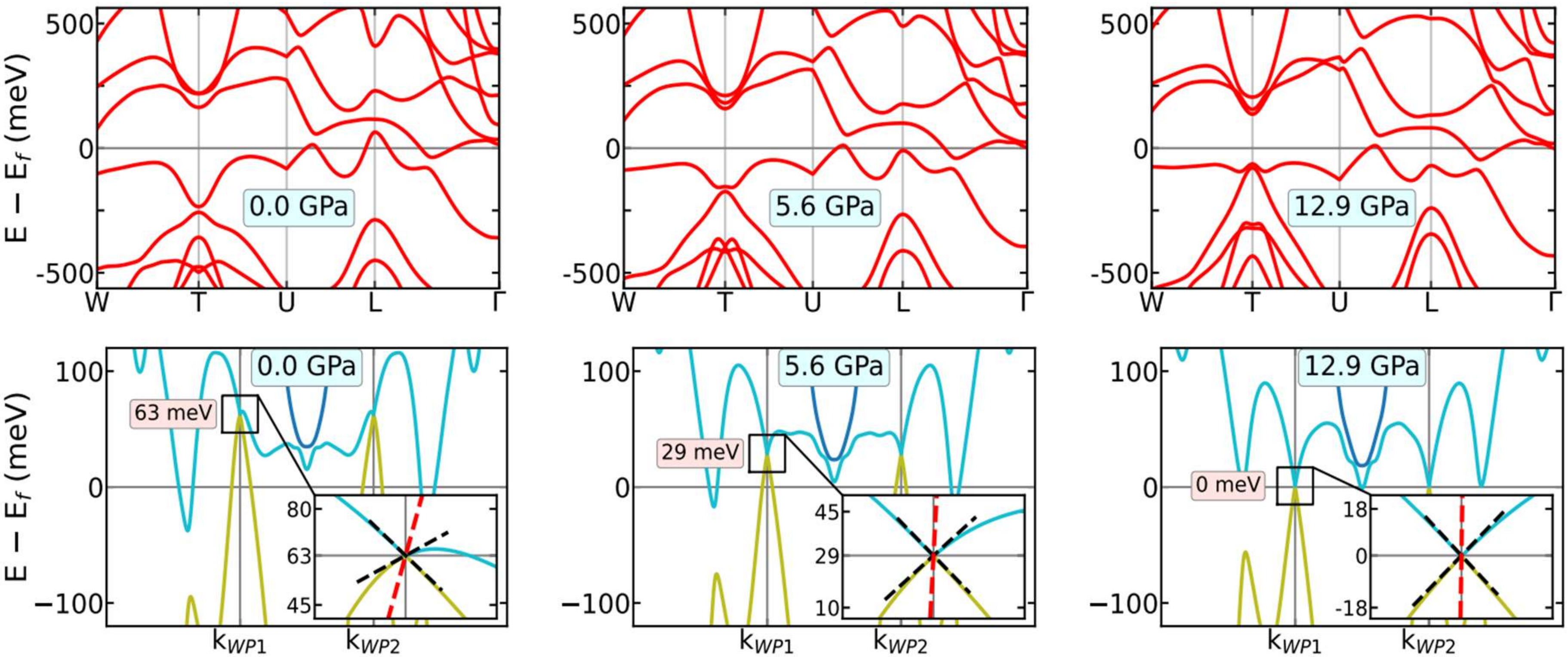
At low temperatures:

$$\kappa_{xy} = \frac{\pi^2}{3}\frac{k_B^2 T}{h}\int \frac{d\boldsymbol{k}}{(2\pi)^3}\sum_n \Omega_n \theta(\mu - \epsilon_{\boldsymbol{k}n}) = L_0 T \sigma_{xy}$$



- ➔ **Linear nature up to T = 80 K**
- ➔ **The values also satisfy the Wiedemann-Franz law**
- ➔ **The Lorenz number stays very close to the theoretical value which is 2.44×10^{-8} WΩK^{-1}**

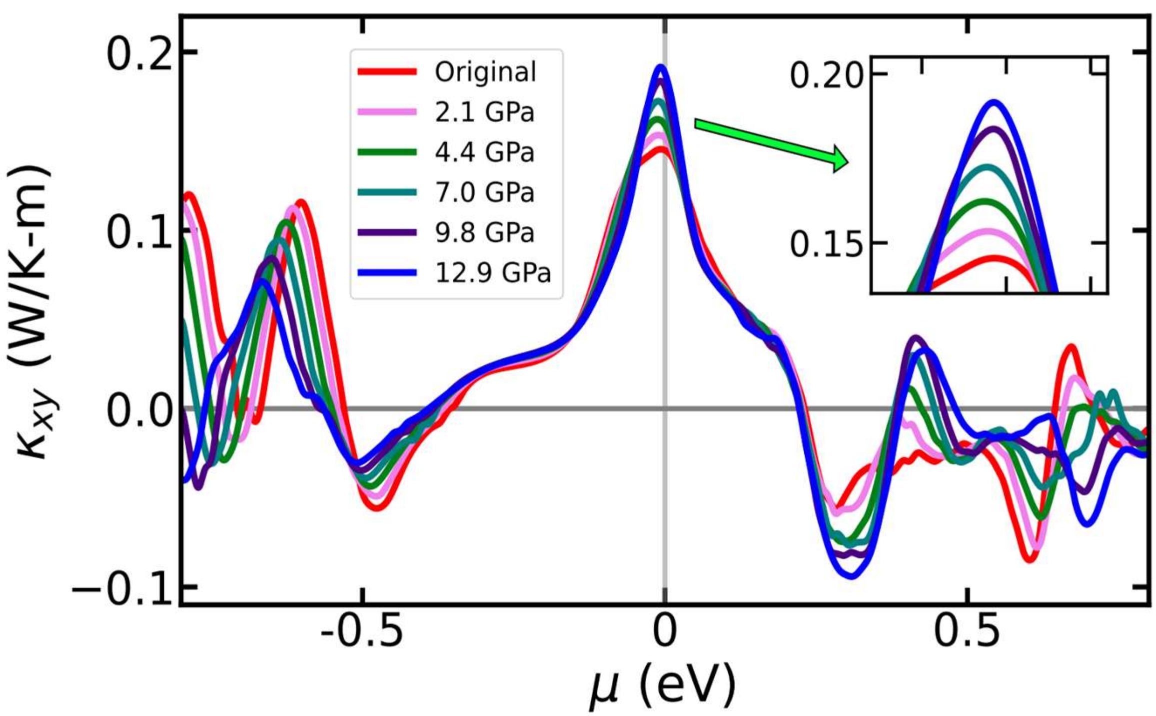
Strain-induced band dispersion



➔ **With application uniaxial compressive stress, Weyl nodes move towards E_f**

➔ **The material turns into a non-tilted WSM with 13 GPa stress**

Strain-enhanced anomalous thermal Hall conductivity



- ➔ The conductivity increases with uniaxial strain at original Fermi level
- ➔ The enhancement is about 33% for a compressive strain of 5% along *z*
- ➔ The reason for this effect is the shifting of Weyl nodes towards the Fermi level which in turn amplifies Berry curvature

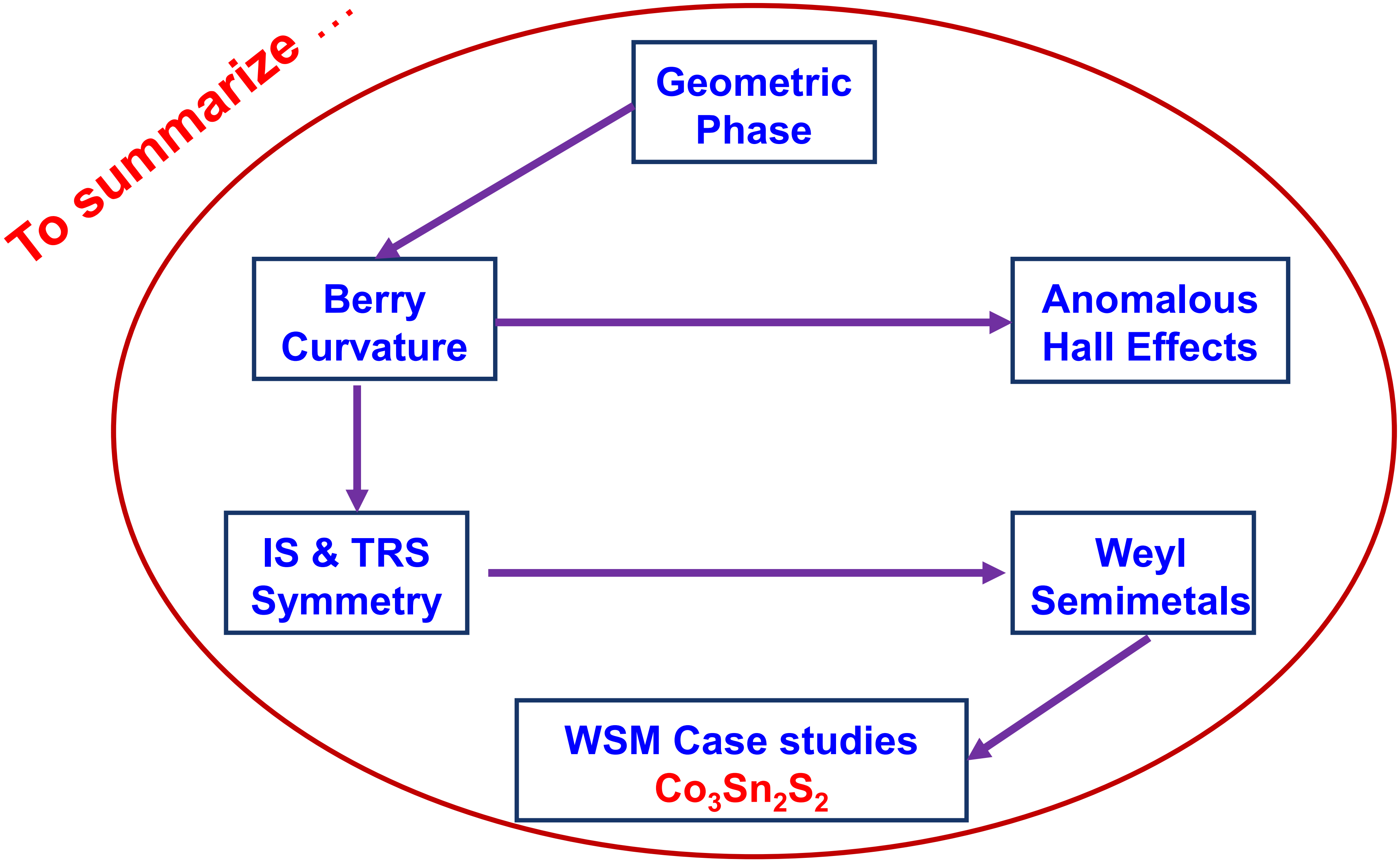
To summary the story of $Co_3Sn_2S_2$

- **Ferromagnetic half-metal $Co_3Sn_2S_2$ transits from a nodal line semimetal to a Weyl semimetal (WSM) upon incorporating spin-orbit coupling**
- **We identify from DFT calculation that the material is a tilted type-I WSM**
- **The anomalous thermal Hall conductivity came out to be quite high and can be tuned by varying the chemical potential**
- **Application of uniaxial strain drags the Weyl nodes towards the Fermi level which leads to a significant enhancement of the Hall conductivity**

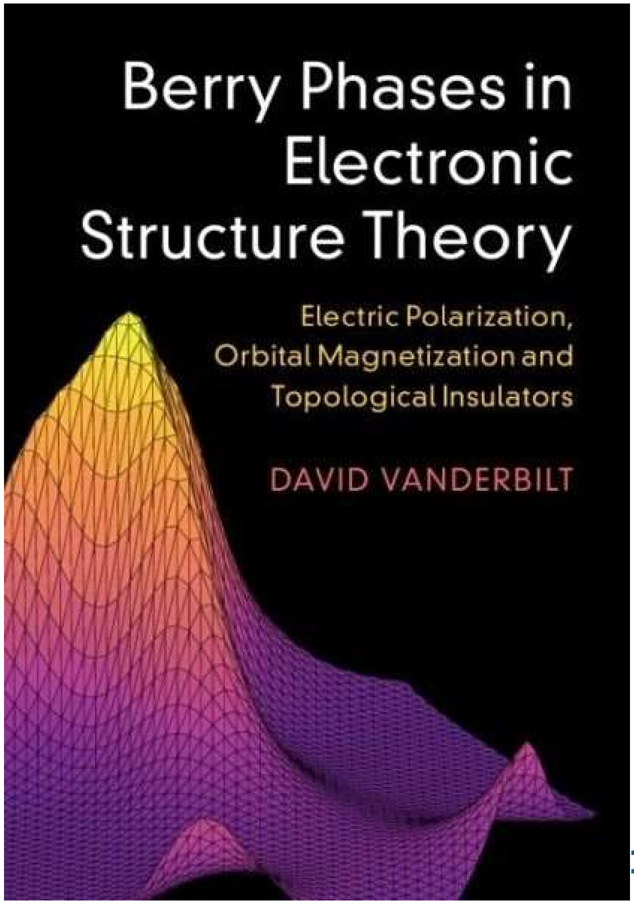
Ref. : Abhirup Roy Karmakar et al, Phys. Rev. B ***106****, 245133 (2022)*

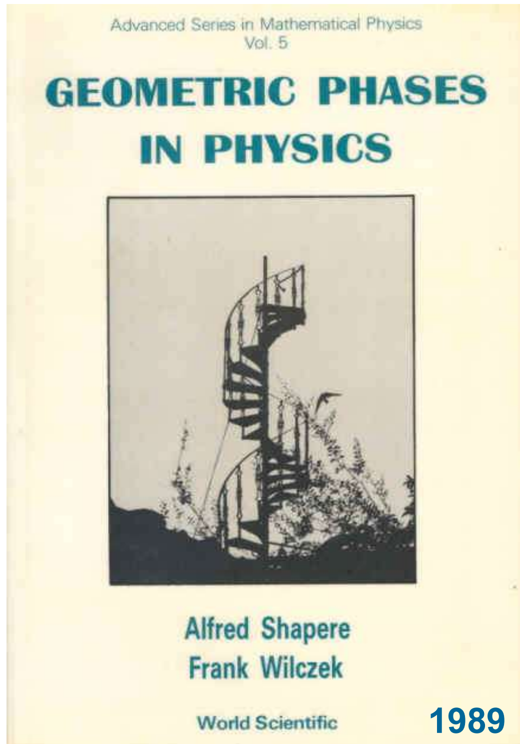
Berry phase in condensed matter physics, a partial list:

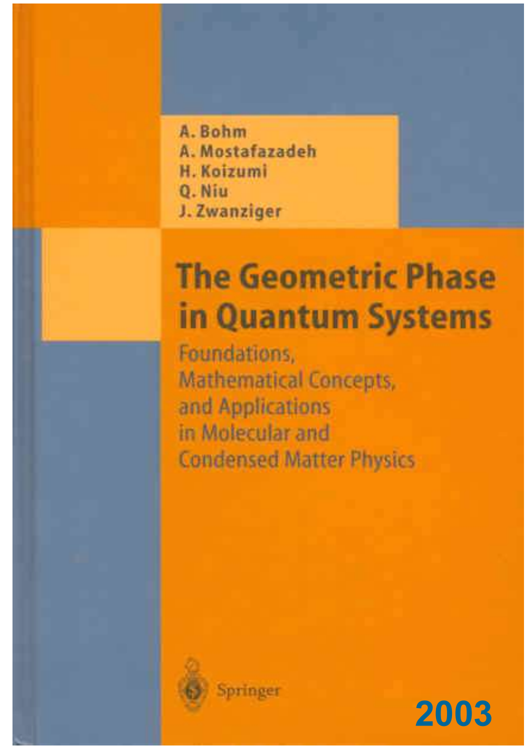
- 1982 Quantized Hall conductance **(Thouless et al)**
- 1983 Quantized charge transport **(Thouless)**
- 1984 Anyon in fractional quantum Hall effect **(Arovas et al)**
- 1989 Berry phase in one-dimensional lattice **(Zak)**
- 1990 Persistent spin current in one-dimensional ring **(Loss et al)**
- 1992 Quantum tunneling in magnetic cluster **(Loss et al)**
- 1993 Modern theory of electric polarization **(King-Smith et al)**
- 1996 Semiclassical dynamics in Bloch band **(Chang et al)**
- 1998 Spin wave dynamics **(Niu et al)**
- 2001 Anomalous Hall effect **(Taguchi et al)**
- 2003 Spin Hall effect **(Murakami et al)**
- 2004 Optical Hall effect **(Onoda et al)**
- 2006 Orbital magnetization in solid **(Xiao et al)**
- …


To summarize …
Geometric Phase
Berry Curvature
Anomalous Hall Effects
IS & TRS Symmetry
Weyl Semimetals
WSM Case studies
Co3Sn2S2

References on Geometric Phase Berry Phase



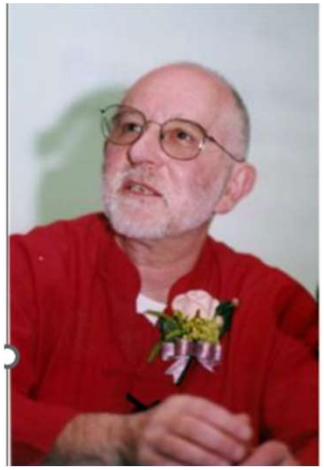




- **D. Xiao, M.C. Chang, and Q. Niu, Rev. Mod. Phys, (2010)** "In science we like to emphasize the novelty and originality of our ideas. This is harmless enough, provided it does not blind us to the fact that concepts rarely arise out of nowhere. There is always a historical context, in which isolated precursors of the idea have already appeared. What we call "discovery" sometimes looks, in retrospect, more like emergence into the air from subterranean intellectual currents."

--- Michael Berry

Geometric Phase is one such "discovery"



Thank you for your attention