

### **POEM: Physics of Emergent Materials**

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L1: Spin Orbit Coupling L2: Topology and Topological Insulators

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### Scope of Lectures and Anchor Points:

- 1.Spin-Orbit Interaction
- atomic SOC
- band SOC: dresselhaus and rashba
- symmetries: time reversal, inversion, mirror

### 2.Berry Phase and Topological Invariant

- two level system
- graphene

### 3.Hall effects

• integer qhe and chern #

### Recap



Wednesday, May 24, 2017 10:15 PM

 $\frac{NO}{H} = \sum_{\vec{k}\sigma} E(\vec{k}) C_{\vec{k}\sigma}^{\dagger} C_{\vec{k}\sigma}$  $= \sum_{\vec{k}} \left( C_{\vec{k}\uparrow}^{\dagger} C_{\vec{k}\downarrow}^{\dagger} \right) \left( \frac{E(\vec{k}) O}{O E(\vec{k})} C_{\vec{k}\downarrow}^{\dagger} \right)$ 

$$\frac{\text{Soc} \neq 0}{\mathcal{H}} = \sum_{\vec{k}} \begin{pmatrix} c_{\kappa\uparrow} & c_{\kappa\downarrow} \end{pmatrix} \begin{pmatrix} h_{\uparrow\uparrow}(\vec{k}) & h_{\uparrow\downarrow}(\vec{k}) \\ h_{\downarrow\uparrow}(\vec{k}) & h_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} c_{\kappa\uparrow} \\ c_{\kappa\downarrow} \end{pmatrix}$$

$$\frac{\underline{Soc} \neq 0}{H} = \sum_{\vec{k}} \left( C_{K\uparrow} C_{K\downarrow} \right) \left( \begin{array}{c} h_{\uparrow\uparrow}(\vec{k}) & h_{\uparrow\downarrow}(\vec{k}) \\ h_{\downarrow\uparrow}(\vec{k}) & h_{\downarrow\downarrow}(\vec{k}) \end{array} \right) \left( \begin{array}{c} C_{K\downarrow} \\ C_{K\downarrow} \end{array} \right)$$
Effect of Soc:
In real space as election holps from
our site to another its spin can flip:
Using Pauli matrices
 $\vec{h}(\vec{k}) = \epsilon(\vec{k})I + \vec{d}(\vec{k}) \cdot \vec{\sigma}$ 
 $= \epsilon(\vec{k}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + d_{\chi}(\vec{k}) \sigma_{\chi} + d_{\chi}(\vec{k}) \sigma_{\chi} + d_{\chi}(\vec{k}) \sigma_{\chi}^{2}$ 
 $\left( \begin{array}{c} suppress \vec{k} \\ = \epsilon \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + d_{\chi} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + d_{\chi} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + d_{\chi} \begin{pmatrix} 1 & 0 \\ i & 0 \end{pmatrix} + d_{\chi} \begin{pmatrix} 1 & 0 \\ i & 0 \end{pmatrix} + d_{\chi} \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \right)$ 
 $= \begin{pmatrix} \epsilon + d_{\chi} & d_{\chi} - id_{\chi} \\ d_{\chi} + id_{\chi} & \epsilon - d_{\chi} \end{pmatrix}$ 

ln



Bands SOC



**Bands SOC** 

small Zeeman field along x Apply ٤ n=0 spin momentum locking 个  $p \rightarrow$ Gap opens up at the degenerate point. Traverse the BZ always remaining in the lowest band. (adiabatic evolution). -> The electron spin will twist from ↓ for - p to 1 for + p



**Bands SOC** 



No Winding: hence topologically trivial

Why is all this important? Interesting? Useful? Fundamentally important? Game changer? Can we get a device out of this? ...much more than a device! A whole new paradigm for information storage that is topologically protected!





## Topology: Shapes and invariants

### quantum hall effect

precise quantization of Hall conductance to one part in billion even though system is disordered

$$\sigma_{xy} = rac{e^2}{h}n$$
 Chern number

SOC is a source of "magnetic field" in momentum space k What kinds of Hall effects can it produce? What kinds of invariants does it lead to?



## ?

# How large is the effective magnetic field arising from SOC?

$$\mu_B \approx 10^{-4} \frac{\text{eV}}{\text{Tesla}}$$
$$\lambda_{\text{soc}} \approx 0.1 \text{eV}$$
$$\Rightarrow b_{\text{soc}}^{\text{eff}} \approx 1000 \text{Tesla}$$

#### insulators

#### Ordinary insulator (atomic or band)

#### Hall insulator





What is a topological insulator?

Bulk insulator Conducting edge or surface states Does not break TR





Hall

#### Topology and Topological Insulators

- Topology and Invariants: Gauss Bonnet formula
- Dynamic (usual) vs Geometric Phase
- Berry phase (topological invariant), can be measured
- Chern number and Quantum Hall Effect
- Degenerate bands, Berry Monopoles and Chern Number
- Spin Hall Effect

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### Toys: Playdoh $cup \simeq donut$





#### Topology and geometry: Gauss-Bonnet formula

- Topological (quantized) numbers can be written as integrals of local quantities
- Gauss-Bonnet theorem. The Gaussian curvature K of a 2D surface M of genus g integrated over the surface gives the Euler characteristic  $\chi = 2 2g$

$$2 - 2g = \frac{1}{2\pi} \int_M K dA$$

- Can locally change the curvature, but the integral is quantized
- Relate such integrals to quantized Hall effects



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#### Topology and band theory

• Bloch theorem: states are labeled by a crystal momentum k:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$$

 $u_{n\mathbf{k}}(\mathbf{r})$  • are lattice-periodic and are eigenstates of the Bloch Hamiltonian

$$H(\mathbf{k})|u_{n\mathbf{k}}\rangle = E_n(\mathbf{k})|u_{n\mathbf{k}}\rangle, \quad H(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{r}}He^{i\mathbf{k}\cdot\mathbf{r}}$$

k

 $\mathcal{BZ}\simeq\mathbb{T}^d$ 

- n labels bands. Fully filled bands are separated by a gap from empty bands
- Lattice symmetry implies periodicity in the reciprocal (momentum) space  $H({f k}+{f G})=H({f k}) \ \Rightarrow \ {f k}+{f G}\equiv {f k}$
- Crystal momenta lie in a periodic Brillouin zone



Main question: Consider an electron spin in a magnetic field:



At each time to the electron spin aligns itself to the local "up" direction.



Phase acquired by wave function as the Hamiltonian is changed adiabatically Remain on some eigenindex H(d) set of parameters {d,,...dm}∈M eg {d} > F eg {a} > k in the BZ n(x) is the nth eigenstate for a M~Td set of parameters a  $H(\alpha)|n(\alpha)\rangle = E_n(\alpha)|n(\alpha)\rangle |\Psi_n(k)\rangle$ 

consider the evolution of the state  $|n(\alpha)\rangle$ as the parameters  $\alpha(t)$  evolve in time.

Adiabatic  
time scale for  
evolution of 
$$\alpha(t)$$
  
is slow compared  
to energy gaps:  
 $n(\alpha(t))$  remains an eigenstate  
but the wavefunction acquires a phase  
 $|\Psi_n(t)\rangle = e^{i\Theta_n(t)} e^{iY_n(t)} |n(\alpha(t))\rangle$ 

Dynamic "usual" phase: t  

$$\Theta_n(t) = -\frac{1}{h} \int_0^L E_n(\alpha(t')) dt'$$

Geometric phase:  

$$\Im_n(t) = i \int_{all}^{t} (n(\alpha(t')) \frac{d}{dt'}) n(\alpha(t')) dt'$$
  
(real)  
\* assume state is non-degenerate "Quantum Mechanics"

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Berry connection  
overlap of two wavefunctions infinitesimally  
separated in 
$$\alpha$$
 - space  
 $\langle n(\alpha) | n(\alpha + \Delta \alpha) \rangle = 1 + \Delta \alpha \langle n(\alpha) | \nabla | n(\alpha) \rangle$   
 $-i \Delta \alpha \cdot \vec{a}_n(\alpha)$   
 $\simeq e^{-i \Delta \alpha \cdot \vec{a}_n(\alpha)}$ 

vector potential  $\vec{a}_n(a) = i \langle n(a) | \nabla_a | n(a) \rangle$ 



As 
$$\vec{k}$$
 is changed over the Brillouin zone  
the phase picked up by the electron is  
 $\vec{Y}_n = \oint \vec{a}_n \cdot d\vec{k} = \int \vec{n}_n \cdot d\vec{s}$   
 $K = \int \vec{a}_n \cdot d\vec{k} = \int \vec{n}_n \cdot d\vec{s}$   
(00)  
BEERRY = total Berry flux within  
PHASE a Brillouin zone  
opeometric  
phase  $a_{n\mu}(\vec{k}) = i \langle u_{n\bar{k}} | \frac{\partial}{\partial K_{\mu}} | u_{n\bar{k}} \rangle$   
around  $\vec{T}_{along \mu}$  direction  
 $\vec{a}_n(\vec{k}) = i \langle n\bar{k} | \vec{\nabla}_k | n\bar{k} \rangle$   
• Berry phase is gauge invariant  
and is measurable.

Berry Flux  $\vec{\Omega}_n = \vec{\nabla} \times \vec{a}_n$ Chern #  $C_n = \vec{n}_n$ # occ bands  $N = \sum_{n=1}^{\infty} C_n$ 

 $\sigma_{xy} = \left(\frac{e^2}{h}\right) N$ 

n=

[First derived by Pancharatnam (1955) in optics]

#### Dictionary

Aharonov Bohm		
Quality	AB	Beary
vector potential	式(ド)	An(K) = (Unk   i Vk Unk) [Berry connection]
magnetic field	$\vec{B}(\vec{r}) = \vec{\nabla} \times \vec{A}(\vec{r})$	$\vec{\Omega}_{n}(\vec{k}) = \vec{\nabla}_{k} \times A_{n}(\vec{k})$ [Berry curvature]
flux	$\overline{\Phi} = \oint_{e} \overline{\Lambda} \cdot d\overline{e}$	
integrated phase	$= \int \vec{B} \cdot d\vec{a}$ $\gamma = 2\pi \vec{\Phi} / \phi_0$ $\phi_0 = h/e$	$= \int \Pi_{n}(\mathbf{k}) \cdot d\mathbf{a}$ [Boxy flux] $\mathcal{T}_{n} = 2\pi \Phi_{n}/\Phi_{0}$ [Berry phase] $C_{n} = \Phi_{n}/\Phi_{0}$ [Chern #]

Degeneracies and two level systems  
Berry curvature 
$$\vec{\Pi}_{n}(\vec{k})$$
 is large  
near degeneracy points  $\vec{R}_{o}$  where  
energy levels cross  
 $E_{n}(\vec{R}_{o}) = E_{m}(\vec{R}_{o})$   
generically when two levels cross denote a  
 $E_{+}(\vec{R}) \ge E_{-}(\vec{R})$   
Expand  $H(\vec{R}) \approx H(\vec{R}_{o}) + (\vec{R} \cdot \vec{R}_{o}) \cdot \vec{\nabla} H(\vec{R})$   
 $\vec{\Omega}_{+}(\vec{R}) = i \langle +, k | \vec{\nabla} H(k_{o}) | -, k \rangle \times \langle -, k | \vec{\nabla} H(k_{o}) | +, k \rangle$   
 $(E_{+}(\vec{R}) - E_{-}(\vec{R}))^{2}$   
 $\vec{\Pi}_{+}(\vec{R}) = -\vec{\Omega}_{-}(\vec{R})$ 

• Berry curvature :  

$$\vec{\Omega}_{+}(\vec{R}) = i \langle \pm, \vec{R} | \vec{\sigma} | \pm, \vec{R} \rangle \times \langle \pm, \vec{R} | \vec{\sigma} | \pm, \vec{R} \rangle$$
  
 $4k^{2}$   
Choose  $\hat{\Xi}$  along  $\vec{R}$   
then  $\vec{\Omega}_{\pm} | \pm \rangle = \pm | \pm \rangle$   
 $\vec{\Omega}_{x} | \pm \rangle = \pm | \pm \rangle$   
 $\vec{\Omega}_{x} | \pm \rangle = | \mp \rangle$   
 $\vec{\Omega}_{y} | \pm \rangle = \pm i | \mp \rangle$ 



Berry curvature is large near the degeneracy points

Berry curvature = Monopole



$$\mathcal{X}_{\pm}(\mathcal{L}) = \int_{S} \vec{\Omega}_{\pm} \cdot \vec{dk} = \mp \frac{1}{2} \int_{S} \frac{\vec{k}}{k^{2}} \cdot \vec{dk} = \mp \frac{1}{2} \left( \frac{\text{solid angle}}{\text{substanded}} \right)$$
  
If we integrate the Berry curvature over a sphere containing the monopole we get  $2\pi$ 

Chern # 
$$C_n = \frac{o_n}{2\pi}$$

. .

#### d vector to Berry Curvature





For a generic 2-level system  
Berry flux (or Berry curvature)  
$$\vec{\Pi}_{\pm}, jk = \mp \frac{1}{2} \hat{d} \cdot (\partial_j \hat{d} \times \partial_k \hat{d})$$
  
= solid angle on unit sphere  $\hat{d}$   
 $\hat{d}(\vec{R})$  maps the manifold  $M \rightarrow S^2$   
 $e:q T^2$   
 $(torus)$ 

#### Honey comb with sublattice potential



Berry curvature (analog of local magnetic field ) on the lower band shows high density at the originally degenerate points. The mass terms have opened a gap at these points and created a monopole. However you see that the Berry curvature at the K and K' points have opposite sign so if you add up the total Berry curvature or total magnetic field on this band adds up to zero.



be combed straight up.

#### Honey comb with time reversal breaking



Berry curvature on the lower band shows high density at the originally degenerate points. The mass terms have opened a gap at these points and created a monopole. For the TR breaking case the Berry curvature at the K and K' points have the same sign so if you add up the total Berry curvature or total magnetic field on this band adds up to 1.



#### Honey comb with time reversal breaking



#### Now include spin $\rightarrow$ spin hall effect:





### Can the Berry phase be measured? Directly?

#### Berry Curvature in Graphene





L. Duca, T. Li, R. Reitter, M. Schleier-Smith, U. Schneider, *Science* **347**, 6219 (2015).



Ultracold <sup>87</sup>Rb in graphene-like honeycomb lattice

Three linearly polarized bluedetuned running waves at 120° at  $\omega_L$ 

Lattice acceleration from  $\Delta \omega$ provides spin-independent force

**B**-field gradient creates spin-

L. Duca, T. Li, R. Reitter, M. Schleier-Smith, U. Schneider, Science **347**, 6219 (2015).



(i) Resonant  $\pi/2$ -pulse creates coherent superposition of  $|\uparrow\rangle$  and  $|\downarrow\rangle$  states

(ii) *B*-field gradient and lattice acceleration move atoms adiabatically along spindependent paths

(iii)  $\pi$ -pulse swaps the  $|\uparrow\rangle$  and  $|\downarrow\rangle$  states

(iv) Each cloud experiences opposite force from *B*-field gradient in the *x*-direction

(v) Second  $\pi/2$ -pulse closes interferometer and converts phase information into spin populations  $n_{\uparrow,\downarrow} \propto \cos(\phi + \phi_{MW})$ 

L. Duca, T. Li, R. Reitter, M. Schleier-Smith, U. Schneider, *Science* **347**, 6219 (2015).



L. Duca, T. Li, R. Reitter, M. *Science* **347**, 6219 (2015).





#### QH vs. QSH





### Topological Insulator

- if two inequivalent insulators are in contact with each other, the gap must vanish at the boundary.
- Gapless states must exist at the boundary between inequivalent insulators
- The gapless states can also be classified topologically using the bulk-boundary correspondence
- Topological Invariant: Z<sub>2</sub> index (odd/even)





Trivial Insulator:  $Z_2$ =even



Kramer's Theorem → Degenerate Pairs at TR invariant momenta

Topological invariant is Z<sub>2</sub>: Either 0 or 1 Calculated as product of parity eigvalues at TRIM Time reversal invariant momenta (for systems with P symmetry)

On boundary the  $Z_2$  index corresponds to the numbers of pairs of edge modes

Topological Insulator: Z<sub>2</sub>=odd



#### Quantum Spin Hall Effect:



....sheer poetry

#### Idea $\rightarrow$ prediction $\rightarrow$ discovery $\rightarrow$ precise quantization

ш

1.0

[7]

T = 1.8 K

T = 0.03 K

G=2e2

 $G = 2 e^{2}/h$ 

1.5

2



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#### Spinors

Suppose the magnetic field keeps the same magnitude but changes its direction t=0t=T/2 t=T

$$\theta = 0 \qquad \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_- = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

$$\theta = \pi/2, \phi = 0$$
  $\chi_{+} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}$   $\chi_{-} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}$ 

At each time to the electron spin aligns itself to the local "up" direction.

After time 
$$t = T$$
 the  $\vec{B}(t)$  returns to its  
original value  
What is the net phase picked up by the electron  
 $\gamma = 0$ ?

Overlap of wave function at two nearby times:  
$$\langle \chi_{+}(\Theta, \phi) | \chi_{+}(\Theta + \Delta \Theta, \phi + \Delta \phi) \rangle$$

)|

$$a_{\phi} = \langle \chi_{+} | \vec{\nabla} \chi_{+} \rangle = i \frac{\sin^{2} \theta/2}{B \sin \theta} \hat{\phi}$$

$$\vec{\Omega} = \vec{\nabla} \times \vec{a} = \frac{i}{ar^2} \hat{r}$$

$$\gamma(T) = i \left( \vec{\Omega} \cdot \vec{dS} \right)$$

$$f(T) = r \int \Delta z \cdot \Delta s$$
  
+  $s r^2 d\omega \hat{r}$ 

$$= -\frac{\Omega}{2}$$
  
 $\Omega$  = solid angle subtended  
by the changing magnetic  
field once 1 time beried.

Berry



Next we want to evaluati  

$$\overrightarrow{\nabla} \times \langle \chi_{+} | \overrightarrow{\nabla} \chi_{+} \rangle$$
 only has a  $\widehat{\phi}$  component  
Now in general we have  
 $\overrightarrow{\nabla} \times \overrightarrow{A} = \frac{1}{r} \left[ \frac{\partial}{\partial \theta} A_{\phi} \sin \theta - \frac{\partial}{\partial \phi} A_{\theta} \right] \widehat{r}$   
 $+ \frac{1}{r} \left[ \frac{1}{2 \sin \theta} \frac{\partial A_{r}}{\partial \phi} - \frac{\partial}{\partial r} (r A_{\phi}) \right] \widehat{\theta}$   
 $+ \frac{1}{r} \left[ \frac{\partial}{\partial r} (r A_{\theta}) - \frac{\partial}{\partial r} A_{r} \right] \widehat{\phi}$ 

$$\vec{\nabla} \times \langle \chi_{+} | \vec{\nabla} \chi_{+} \rangle = \vec{\nabla} \times \left\{ i \frac{\sin^{2} \theta/2}{r \sin \theta} \right\} \hat{\phi}$$

$$= \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[ \frac{i \frac{\sin^{2} \theta/2}{r \sin \theta}}{s \sin \theta} \right] \hat{r} + \frac{1}{r} \left( \frac{\partial}{\partial r} \left\{ \frac{r i \sin^{2} \theta}{r \sin^{2} \theta} \right\} \right]$$

$$= \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[ \frac{i}{r} \frac{\sin^{2} \theta/2}{r \sin^{2} \theta} \right] \hat{r} + \frac{1}{r} \left( \frac{\partial}{\partial r} \frac{i \frac{\sin^{2} \theta}{2}}{s \sin^{2} \theta} \right) \hat{\theta}$$

$$= \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left[ \frac{i}{r} \frac{\sin^{2} \theta/2}{r \sin^{2} \theta} \right] \hat{r} + \frac{1}{r} \left( \frac{\partial}{\partial r} \frac{i \frac{\sin^{2} \theta}{2}}{s \sin \theta} \right) \hat{\theta}$$

$$= \frac{1}{r \sin \theta} \frac{i}{r} \frac{\beta}{2 \sin \theta} \sin \theta \cos \theta \sin \theta \sin \theta \sin \theta}{r}$$

$$\begin{split} \gamma_{+}(\tau) &= i \int \vec{\nabla} \times \langle \chi_{+} | \vec{\nabla} \chi_{+} \rangle , d\vec{a} \\ &= -\frac{i}{2} \int \frac{1}{r^{2}} \hat{r} , d\vec{a} \\ &= -\frac{i}{2} \int \frac{1}{r^{2}} \hat{r} , d\vec{a} \\ &\text{integral is over an area on the hyber out by  $\vec{B}$  in 1 cycle.   
  $d\vec{a} = r^{2} d\Omega \hat{r} \\ &\vec{a} = r^{2} d\Omega \hat{r} \\ &\gamma_{+}(\tau) = -\frac{i}{2} \int d\Omega = -\frac{1}{2} \Omega \\ &\Omega = Dolid angle Dubtended by the purface S \\ &at the enign. \end{split}$$$

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