1
Topological Materials
2
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Topology
Different in shape,
‘something’ is equivalent
and one shape can be transformed into other by ‘smooth deformation’
Topologically same
Topologically same
Transformation is not possible by
smooth deformation
- They are topologically different
Topology is a branch of mathematics concerned with geometrical properties that are insensitive to smooth deformation.
3
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How to characterize topology of an object?
By determining a “topological invariant”
“Topological invariant” = quantity that does not
change under continuous deformation
Objects with same topological invariant are have same topology, they may have different shapes.
It will be different for objects with different topology.
Let’s define a topological invariant: Gauss Bonnet theorem
=
1
2 −(1)2 =
Where, = = T
1 1 2
g = “genus”
g = 0 g = 1, g = n for “n-holed torus”.
χ or g →topological invariant here
4
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Topological phases
Nobel Prize in Physics 2016
David J. Thouless, F. Duncan M. Haldane and J. Michael Kosterlitz

for theoretical discoveries of topological phase transitions and topological phases of matter.
Topological phase transition
(one topological phase to other)
g=0
g=1
g=2
5
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Topology in condensed matter physics
Single electron wave function in a crystal of
energetically isolated bands in crystalline solids can
carry topologically quantized numbers — known as
topological invariants — that correspond to

experimentally measurable quantized response effects
These properties remain intact even if
the object undergoes deformation or
impurity or doping (as long as the lattice
symmetry, and hence the topology
remains unchanged)
How to determine the topological invariant (band topology) ?
Bloch's theorem: One-electron wavefunctions in a crystal (i.e., periodic potential) can be written
= . ( )
where k is "crystal momentum" and u a periodic function with same periodicity as the lattice.
Crystal momentum k can be restricted to the Brillouin zone, a region of k-space with periodic boundaries.
As k changes, we map out an "energy band". Set of all bands = "band structure".
So, the Brillouin zone will play the role of the "surface" as in the previous example.
A quantum mechanical property, the Berry phase, will give us the "curvature".
6
Berry phase in solid
= . ( )
Berry connection is defined as
=< − >
Berry curvature is defined as
= ×
Then, the Berry phase is
=

. =

2
Berry phase, calculated over a 2D closed manifold in k space (Brillouin zone)
2 = 2
is an integer, called the "Chern number" or "Chern index" of the surface, and can be regarded as a "topological index" or "topological invariant" attached to the manifold of states defined over the surface.
Just for your reference
No need to remember
7
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Ordinary materials (trivial band topology)
8
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Nontrivial band topology
Physical
mechanism
9
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Nontrivial band topology
Topological insulator
An insulator, but topologically
different than normal insulator.
Topological semimetal
Very small band overlap, so semimetal,
but topologicallydifferent than normal
semimetal.

Physical
mechanism
10
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Edge state of topological materials
A topological phase always has metallic edges/surfaces when put next to vacuum or an ordinary phase.
Imagine a “smooth” edge where the system gradually evolves from TI to ordinary insulator.
The topological invariant must change across the surface.
But the definition of our “topological invariant” means that, if the system remains insulating even at surface (so that every band is either full or empty), the invariant cannot change.
The system must not remain insulating at the surface. There must be metallic (gapless) surface/edge states
The trefoil knot (left) and the simple loop (right) represent different insulating materials: the knot is a topological insulator, and the loop is an ordinary insulator. Because there is no continuous deformation by which one can be converted into the other, there must be a surface where the string is cut, shown as a string with open ends (centre), to pass between the two knots.
11
Edge state in topological insulator
Physical
mechanism
Metallic edge state in topological insulator.
Bulk is insulating but the surface is conducting !!!
Example of topological insulator: Bi_2Te_3, Bi_2Se_3 and Sb_2Te_3 alloys
12
Dirac points
For ordinary solids, well inside the Brillouin zone

There may be special points in k space
around which

Such point is called Dirac point
3D analog, cone shaped E-k diagram
4 bands at the Dirac point
At one particulate energy value
2 states (with two opposite spin
configurations)
2 bands
Schematic representation: green
and purple color represent bands
with opposite spin configuration.
(They are overlapped on each
other)
13
Dirac points in real materials
Six Dirac points in graphene band structure
Band structure of graphene
Example of materials having Dirac points: Graphene, Cd_3As_2, BaAuSb, and SrAgBi etc.
14
Weyl points
If the two bands are separated in k space

Dirac point separates into a pair of band touching points → each point is a Weyl point

Dirac point
Dirac points separated into a pair of Weyl points
Weyl point
Example of materials with Weyl points: TaAs, NbAs, NbP, TaP, $Co_3Sn_2S_2$
15
Dirac and Weyl semimetals
How are they different from ordinary semimetals?
Dirac or Weyl points are topologically different than band structure of ordinary semimetals.
Topologically protected surface states appear → Arc-like segments of the Fermi surface
(connecting the projections of Weyl points onto the surface)
Dirac and Weyl semimetals: Materials hosting Dirac or Weyl points in band structure
In Dirac semimetal
In Weyl semimetal
16
Novel properties of Dirac and Weyl semimetals
Each of the Dirac or Weyl points associate fictitious magnetic field in k space →
Anomalous behavior in physical properties observed
For example, Hall effect observed in Weyl semimetals in absence or very small
external field (due to the fictitious magnetic field)→ Anomalous Hall effect
=

=

Anomalous Hall effect in $Co_3Sn_2S_2$, a Weyl semimetal
17
Not many quantum and/or topological materials are explored so far
Usually, low temperature phenomena
Yet to understand the underlying physics clearly
How to overcome:
Experimental
observation
Experimental
validation
Theoretical
explanation
Theoretical
prediction
Challenges in quantum materials