Thermoelectric transport and quantum Hall effects in topological materials

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I. BACKGROUND

The electronic band structure of a solid gives the energy states which can be occupied by an electron of a given momentum. These energy states are usually obtained quantum mechanically as solutions of the Schrödinger equation. A band gap in the energy dispersion represents a region of energies where no electron states can exist. The energy range of the gap corresponds to the energy required to free an electron in the outer shell of an atom and allow it to propagate through the solid. Systems with such a gap are classified as insulators or semiconductors, depending on the size of the gap. While the presence of a band gap is a feature that characterizes such systems, it becomes important to classify the systems into **topologically equivalent groups**.

In mathematics topology is a way to distinguish objects that cannot be transformed into each other without tearing or cutting them. An example is that of a malleable sphere and torus. One can imagine deforming the sphere into the shape of a bowl. One could also imagine transforming the torus into a coffee cup where the hole in the torus becomes the handle of the cup. However, we could not turn the sphere into a torus without puncturing a hole in it. Thus, the sphere and bowl are said to be in the same topological class while the torus and cup are in a separate class. Mathematically, the two classes are distinguished by their **genus** (the number of holes).

The concept of topological equivalence can be extended to band structures [1]. In this context, topological equivalence means that the band structure of one system can be transformed to that of another system without closing the gap. While an atomic insulator (electrons bound to atoms in closed shells) and a semiconductor appear to be quite different, the Hamiltonian can be tuned to turn the band structure of one into the other without closing the band gap. In relativistic quantum theory the vacuum may also be described by a gapped band structure (i.e., a conduction band for electrons, a valence band for positrons, and an energy gap for pair production). So, the atomic insulator, semiconductor, and vacuum all belong to the same topological class.

How can these topologies be classified? It turns out that each band has an associated integer topological invariant n known as the **Chern invariant** [1], which is very much like the genus of a surface. This allows for a classification of the different topological phases. In fact, it can be related to the **Berry phase** [2] of the Bloch wave functions.

II. MSC PROJECT

The proposed project aims to explore some peculiar response properties of two-dimensional (2D) Dirac topological materials, such as the thermoelectric Nernst effect [3], anomalous Hall effect, and anomalous Nernst effect. The Nernst effect refers to the generation of a transverse electric field in the presence of a longitudinal temperature gradient. Conventionally, the Nernst effect can occur only in the presence of an external magnetic field, which provides a transverse velocity to the electrons by

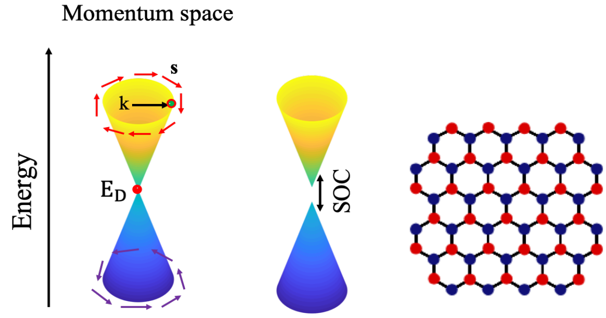

FIG. 1: Energy dispersion (E vs $\mathbf{k}$) for a two-dimensional Dirac-type material. The valence and conduction bands touch at the Dirac point E_D. In the presence of spin-orbit coupling (SOC) there is a gap.

the Lorentz force. However, a non-trivial Berry curvature $\mathbf{\Omega}$, can also give rise to a Nernst response as a result of an anomalous velocity term. This is the **anomalous Nernst effect** of topological origin. The Nernst effect is quite interesting; for example, it has been used as a probe for high-T_c curpate superconductors. There are several 2D materials that could exhibit Nernst and anomalous Nernst effects that the student could choose to work on; for instance, ferromagnetic graphene or silicene, bilayer graphene or bilayer WSe_2. The starting point of the investigation will be the calculation of the energy dispersion (as shown in Fig. 1) and of the eigenstates by solving a Dirac-type Hamiltonian including terms due to SOC. With the obtained eigenstates and energies the student will be able to calculate the Berry curvature of the system and consequently the Chern number, Hall and Nernst responses.

III. PHD PROJECT

There are many possible unexplored directions for expansion to PhD project. One direction could be the investigation of thermoelectric transport in topological Weyl semimetals. Despite the broken time-reversal and space-inversion symmetries, these materials can be topologically protected even without a bulk energy gap. These materials could lead to profound technological applications.

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[3] G. Y. Guo, Q. Niu, and N. Nagaosa, Phys. Rev B **89**, 214406 (2014).