THE TALE OF THE TAIL THAT WAGS THE DOG BREAKING EQUALITY VIA SYMMETRY AND TOPOLOGY



Even a preschooler knows that when heated, ice will first melt into water before it evaporates into a gas. But what about the fundamental mechanism behind this everyday phenomenon, in other words the so-called phase transition?

In crystalline solids like ice, chemical bonds hold all the molecules together in tight, regular patterns. Since the molecules in this state can only vibrate or rotate, the formation of a rigid crystal is determined by the internal energy and entropy of the molecules. Or more specifically, the configuration of the molecules with minimum internal energy (E) and maximum entropy (S) in the system. Recall that the entropy of a system directly determines how many internal configurations it can have. The higher its disorder or randomness (i.e. the more configurations), the higher its entropy. So solids with very low entropy such as diamonds are very rigid, well ordered structures, whereas solids with higher entropy such as graphite (e.g., cores of pencils) are softer and more malleable.

On the other hand, in liquids like water all the molecules are densely packed together in the shape of the liquid's container, without forming any underlying microscopically-regular pattern. Since the molecules are continuously breaking apart and binding to one another as they move around

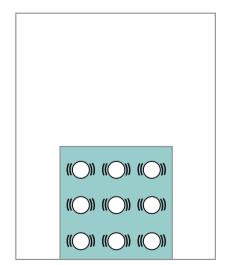
out of equilibrium, as the substance is heated the liquid configuration has a higher internal energy than the solid one and a much higher entropy due to the enhanced mobility of the molecules.

The melting temperature (T) of the material is determined by the competition between the free energies (F) of the solid and liquid phases. In other words thermal stability is governed by a conflicting demand of minimum internal energy together with a maximum entropy. Here, the thermodynamic free energy of a system [Fsys=Esys-T Ssys] refers to the amount of energy that can be converted to do useful work. Upon heating the solid, the molecules retain their crystalline structure as long as the free energy of the solid remains less than that of its liquid state (Fsolid<Fliquid). This continues until the melting point which is determined by the equilibrium condition Fliquid=Fsolid. Once the free energy of the system passes this equilibrium, melting occurs. Likewise, going beyond the melting point the liquid phase is eventually superseded by the gas phase once the temperature

reaches the boiling point determined by Fgas=Fliquid. Thus, the fundamental mechanism behind the interplay of solid and liquid phases of a material turns out to be a matter of their entropies, a physical quantity which is intrinsically associated with their macroscopic orders or symmetries.

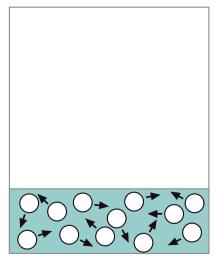
A symmetry of a system is a property that remains the same after an applied transformation. For instance. while a circle is symmetric under arbitrary rotations around an axis passing through its center, a square is symmetric only under four-fold (90 degree) rotations. Likewise, when a crystalline solid melts into a liquid it changes from an ordered, and hence, lower entropy phase (which is invariant under some discrete translations and rotations depending on the material) to a disordered, and hence, higher entropy phase where the molecules are arranged randomly. Thus, the melting point of a material may well be characterized by changes in some of its geometric symmetries, i.e., the stability of its solid and liquid phases are discriminated against one another

SOLID

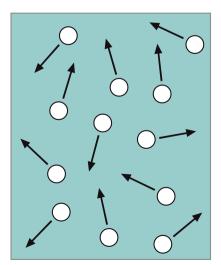


Crystalline solid versus liquid and gas phases.

LIQUID



GAS



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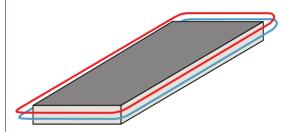
via symmetry breaking. While the atoms and molecules are locked in like a spider's web in solids, they are free to move around in liquids. On the other hand, even though the liquid and gas phases seem strikingly different from each other, they are exactly the same thing from the stand point of symmetry.

THE QUANTUM DIFFERENCE

While such a symmetry-based elementary division of solids into groups sheds some light on understanding their mechanical and structural differences, it is way too primitive to describe their electronic properties. This includes not only modern quantum materials but also rudimentary ones. For instance, this division cannot explain what causes the enormous

difference between the thermal and electrical properties of different categories of solids, for example, metals, semi-conductors, insulators, superconductors, etc.

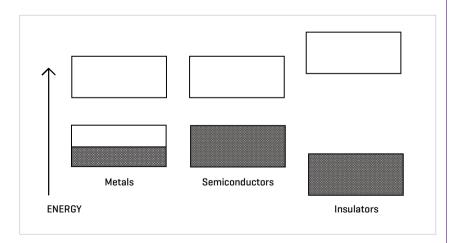
Instead, the electrical properties of a solid may be understood with quantum mechanics by solving the Schrödinger equation for the allowed energy spectrum of a single electron. By finding the allowed energy levels of the system we can determine how electrons will behave when an electric field is applied to the material. Heavily depending on the symmetries of the underlying crystal, it turns out that a typical electronic spectrum is not continuous in energy. Consecutive allowed regions [energy bands] are separated by



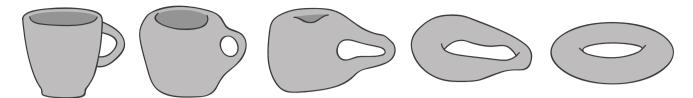
▲ A two-dimensional topological insulator conducts electricity along their edges but not through its bulk.

forbidden ones (band gaps).

If any one of these bands is only partially occupied by the electrons then the corresponding solid is a metal. What makes a metal amenable to electrical conduction is the availability of unoccupied energy states which can be enjoyed by its electrons upon the application of an electric field. In simple terms, since the electrons can switch seats, they are mobile and compressible. In contrast, the solid is a semi-conductor if its energy bands are completely occupied by the electrons, requiring some extra energy to compensate for the relevant band gap to generate an electric current. In simple terms, since all of the seats are taken, the electrons are immobile and incompressible unless they can sit on top of each other with the extra help from a battery. In this respect,



▲ In solids, electronic spectrum is not continuous in energy and exhibits a band structure.



• One cannot simply change the topology [here, it is the number of handles] of an object through a continuous deformation.

insulators are very similar to semiconductors but with significantly larger band gaps, forbidding them from carrying any current.

WHERE IS THE TAIL? WHERE IS THE DOG?

The accidental discovery of the socalled 'integer quantum Hall effect' back in 1980, and a plethora of other discoveries which followed in the last decade or so, have revealed a much richer hierarchy of modern quantum materials. For instance, the so-called 'topological insulators' are electrical insulators which can conduct electricity along their edges and surfaces. In other words, they behave like a block of wood entirely covered with a metal surface. Additionally, irrespective of their size and shape, cutting a topological insulator into pieces does not spoil its electrical properties, hence the name topological. It turns out that their real space features are nothing more than a reflection of some special quantum mechanical properties. Think of it as trying to demagnetize a magnet by ruining its shape and size. It is impossible of course, the magnetic north and south poles always appear no matter what. In simple terms, one cannot change an object by manipulating its shadow.

Now we come to the title. The dog is indeed wagged by its tail. The wondrous electrical properties we observe in our real physical space are controlled by the geometric topology of their reciprocal or Fourier space. This is what prevented the synthesis of a broad range of topological materials up until this century. Since what happens in the reciprocal space stays in the reciprocal space, topological materials are robust against real space disturbances,

offering greater promises in quantum information technology. Such possibility of band-structure engineering have kept numerous physicists like myself busy all around the world with disclosing their well-kept secrets.

MORAL OF THE TALE

By giving an overview of the historical development of modern solid-state theory, and uncovering the cunning role played by the geometric topology of the reciprocal space, I would like to convey the idea that even though some

things may look similar and equivalent for all practical purposes in our physical domain, they may still be distinguished and classified based on their shadows from a reciprocal domain, the one which is yet to be thought of or still waiting to be discovered.

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