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Introduction

MATERIALS AND METAMATERIALS consist of fundamental units called particles. The material properties of these *microscopic* components often determine the *macroscopic* properties of the resulting material. In many cases, however, it turns out that the underlying *geometrical* and *topological* properties of the many-body system or confining space also have a tremendous impact on the macroscopic properties of matter. From a solid understanding of how materials and metamaterials achieve their properties one can start designing materials and metamaterials with useful and novel functionalities [18, 19, 34, 37].

Chiral symmetry

The concept of spontaneous symmetry breaking is one of the cornerstones of modern physics. Spontaneous symmetry breaking occurs when the laws of physics are invariant under a certain symmetry. One of these symmetries is *chirality* – or handedness. Spontaneous symmetry breaking due to chirality is often referred to as chiral symmetry breaking. The concept of chirality is perhaps easily understood when observing our hands. Our right hand cannot possibly be superimposed on our left hand, unless the palms are facing the opposite directions. Our hands are each other's mirror image. Chiral objects are all around us: examples are screws, fusilli pasta, guitars, bikes, cars, etc. The test for chirality is simple: as long as we cannot recreate the mirror image of the object by translating and/or rotating the object in its entirety, the object is chiral; otherwise it is not. For example, a coffee mug is not chiral as its mirror image can be found by rotating the mug by half a turn. A simple system showing chiral symmetry breaking is depicted in fig. 1 where we find that both chiral states are energy symmetric yet can not be transformed into one another.

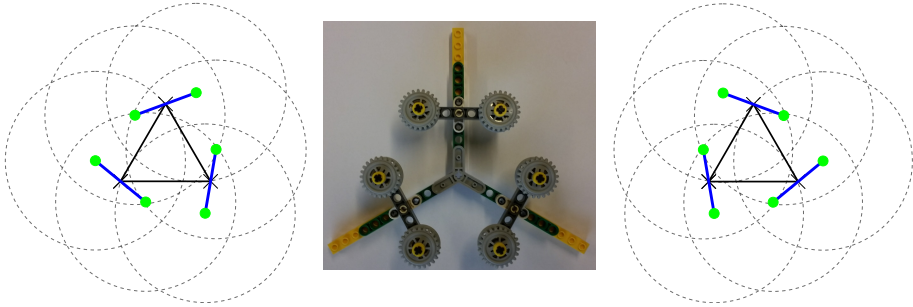


Figure 1: A simple setup showing chiral symmetry breaking. **Center:** an unstable-state achiral state made with LEGO gray bars can rotate freely. Gears are equally magnetized such that they repel one another. **Left–right:** two stable chiral states found using a numerical minimization. Both states have an equal energy lower than the unstable state. Both chiral states can be found in the LEGO setup as well.

The chirality of our hands is a spatial asymmetry. Chirality, however, can also exist as a *temporal* asymmetry. Imagine an analog clock. The second hand moves in a clockwise direction. A clock therefore possesses left-handed temporal chirality.[♠] When we mirror the arrow of time, meaning that time now goes backwards, the second hand of the clock moves backwards too. In such an event, the orbit of the second hand becomes anti-clockwise. There is, however, a class of systems imaginable where the chirality does not change upon time reversal. Suppose the clock is driven by a digital signal, and the second hand represents a time interval as measured by a crystal oscillator. Then, regardless of the arrow of time, the clock’s chirality is defined by the internal mechanics of the device. An experimental system with temporal chiral particles is depicted in fig. 2.

Naively, the macroscopic chirality of systems follows from the microscopic chirality of the particles of which they consist. Remarkably, however, this is not necessarily the case. Achiral particles confined in an *achiral* geometry may still spontaneously manifest a *chiral* macroscopic state. This means that due to the achiral nature of the microscopic particles, the particular choice of chirality — left-handed or right-handed — is energetically indifferent and

[♠]Some may argue that canonical clock is left-handed. This is purely semantical and mostly concerned with how we label things, hence irrelevant for this discussion. Physics would not change if we consistently relabeled left as right and right as left. We have implicitly assumed here that the unit vector \hat{z} points from the book towards your eyes as this is the canonical *right* way — and incidentally also the right-handed way.

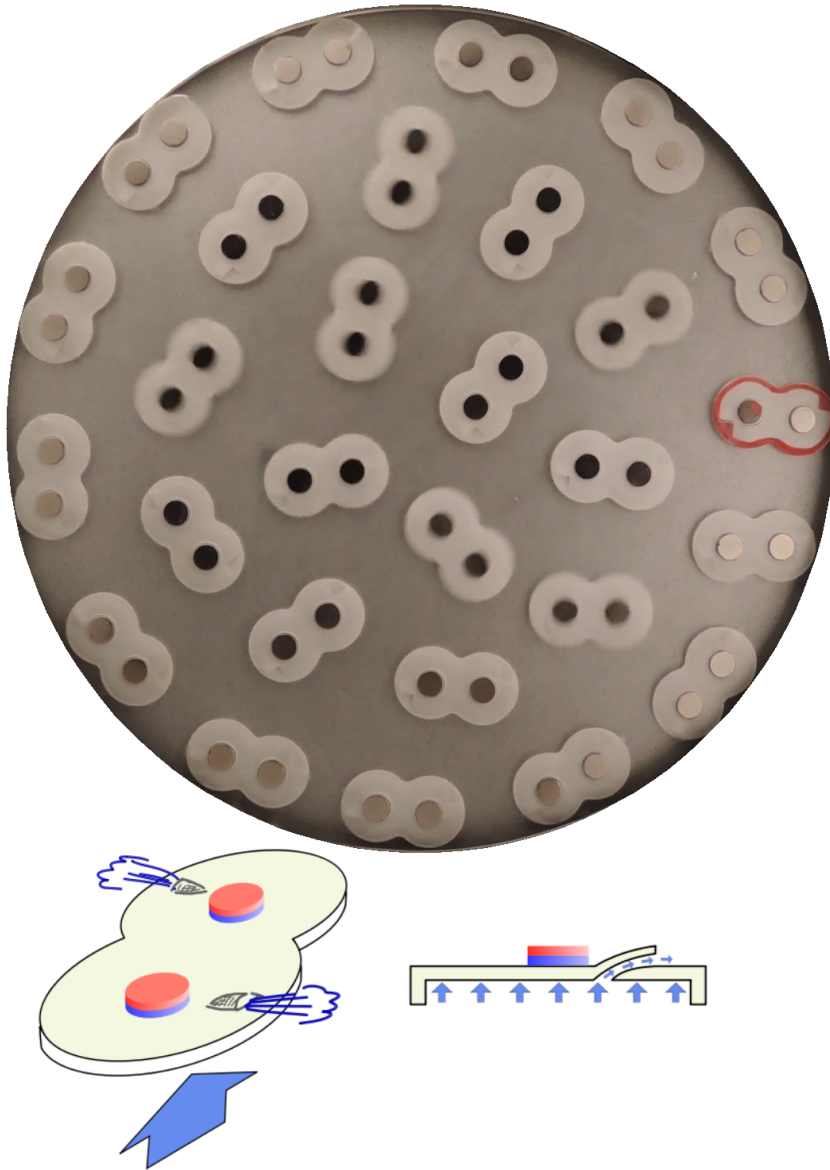


Figure 2: A setup showing temporal chiral symmetry. **Top:** a custom-built air hockey table with 3D-printed chiral pucks floating and rotating due to airflow. Pucks may appear blurred as some are rotating fast. **Bottom:** illustration of the airflow through the puck causing both lift and spin, the latter breaking temporal chiral symmetry.

hence a chiral state is spontaneously chosen. In this thesis, we will examine two examples of this effect: one spatial, chapter 1, and one temporal, chapter 2. Additionally, we will give an example of how the temporal chirality of particles determines the temporal chirality of the system in chapter 3.

Active matter

Particles are often thought of as static units. In recent attempts to understand the collective behavior of biological and robotic systems, however, physicists have researched particles which are internally or externally driven. Systems containing such particles manifest much more complex physics [52, 110, 148, 149]. These self driven systems are often called *active* systems, as energy is actively pumped into to the system at the microscale. Hence, the system consumes energy. Unlike *passive* systems, which tend to reside in *equilibrium*, active systems often reside in *steady states*, where the energy pumped into the system is on average equal to the energy dissipated from the system. In addition, as the fundamental units that form matter become increasingly more complex, so may their interactions. For instance, while a simple charged particle merely exchanges positional information with other particles – and possibly information about its velocity as well – a more complex particle may also exchange non-trivial information like a list of its neighbors, the availability of nutrition or other resources in its surroundings, etc. On the receiving end, more complex particles with a little processing power may use all this information to decide on their course of action – which likely also requires energy. These active systems offer exciting possibilities for more complex material and metamaterial design.

The canonical toy model for active matter is called the Vicsek model [133, 142, 149]. This model can be used to describe a school of fish, a flock of birds, a large group of bacterial swimmers, a swarm of robots etc. There are two assumptions the Vicsek model makes. First, particles are self-driven, yielding some stationary speed. Second, particles try to align the direction of that speed with the velocity of their neighbors. Additionally, the Vicsek model allows for noise in the alignment procedure, mimicking temperature, communication errors or similar perturbations. It relies on an overdamped version of Newton's equations of motion[♣] where inertia does not play a role. The result is that, if the noise term is sufficiently low, the particles align and flock, swarming around through their confinement space, never in equilibrium but possibly in a

[♣]Newton's equations of motion are briefly introduced in appendix A.

steady state. In two dimensions, mean field theory finds that the model defies the Mermin–Wagner theorem, stating that long-range order cannot exist in two-dimensional equilibrium systems at finite temperature. It is therefore possible for the alignment of the self-driven particles to spontaneously emerge throughout the system.

As active matter is driven externally or internally, it naturally breaks time reversal symmetry.[♣] Time reversal symmetry is the property that enables the mapping of t to $t \rightarrow -t$. As time reversal symmetry breaking is a key ingredient for a class of topological insulators, active matter might be a perfect candidate to achieve a classical topological insulator [16, 31, 82], as we will see in chapter 2.

Topology and geometry

The macroscopic properties of materials are tremendously impacted by the geometrical and topological properties of the confinement space [5, 38, 115, 132]. For passive matter this means that the ground state structure often fails to propagate throughout the system, often introducing defects or changing the structure altogether. An example of the latter will be shown in chapter 1. For active matter it means the flow of the particles is dominated by the topology and geometry of its confining space. If the confinement is for instance tubular, particles will likely flow along the long axis of the tube. Similarly, if the confinement is circular or annular, particles will tend to flow along the circle. The chirality of the flow in a circular confinement is chosen spontaneously; the same goes for an annular confinement, as we will see in chapter 2.

The concept of topology has changed both modern mathematics and physics. Topology is roughly a way to characterize a mathematical space in such a way that the characterization is invariant under continuous transformations. Suppose we have an inflated bicycle inner tube. The number of handles or holes in such a system is conserved regardless of linear transformations, geometrical irregularities and/or different embeddings. In fact, the number of handles serves as a *topological index*, an integer number that allows us to topologically characterize objects. As our bicycle tire has exactly one handle, we classify its index as one. Comparing this to, for instance, a ball which has exactly zero handles, we conclude that there is no possible way to continuously transform an inner tube into a ball – or vice versa. It is, however, possible to

[♣]Strictly speaking, a system with just a damping term already breaks time reversal symmetry although such a system might also demonstrate somewhat dull physics.

continuously transform an inner tube into a coffee mug — and vice versa — as the number of handles in both objects is equal. The number of handles is one of the many imaginable topological indices. A more sophisticated topological index for spatial objects is the Euler characteristic. In momentum space one may use the Chern number to conclude if certain band gaps are topologically protected, as these band gaps cannot be closed by smoothly deforming the system.

Computational physics

Performing analytical calculations on passive systems in equilibrium often requires complicated mathematics. As activity and complexity are introduced to these systems, calculations become increasingly harder. Fortunately, the discipline of computational physics may often help. Numerical methods have shown both to be an excellent way to validate analytical theories, as well as revealing new hidden physics from known analytical theories — the latter often unreachable from the analytical point of view. Combined with analytical methods and possibly experiments, the computer allows us to make great leaps forward in science as a whole.

One of the powerful numerical methods we will employ in this thesis is called molecular dynamics. Molecular dynamics is, very briefly, a method to solve the classical N -body problem numerically — in general, N bodies with arbitrary defined interactions. At its core, molecular dynamics employs one of the most validated equations in physics: Newton's equations of motion, eq. (A.2). A brief explanation of how molecular dynamics works is given in appendix O.

For this thesis a custom molecular dynamics computer library called `libmd` was written; see appendix P for more details. The library differs from other libraries as it is specifically designed to solve problems in passive and active matter with geometrical and topological constraints. More explicitly, it contains an implementation of a novel symplectic integrator that solves Newton's equation in the presence of curvature numerically, as described in chapter 4. Additionally, it employs computational techniques like automatic differentiation, appendix section G.3, to make simulations more accurate, simpler and more reliable.

Outline of this thesis

In this thesis we will study the interplay of topology and geometry with chirality for several passive and active systems, employing both analytical and numerical methods. Specifically, this thesis discusses the systems briefly mentioned here.

In chapter 1 we explain how nematic liquid crystals confined in toroidal geometries undergo structural phase transitions depending on the slenderness of the confining toroid. We will see that, although the nature of the nematic liquid crystal is achiral, the toroidal geometry will force the system to choose a chiral state. As both states yield the same Frank free energy the choice of chirality is spontaneous. This structural phase transition falls in the same universality class as the famous Ising model, a model for ferromagnetism: both are perfect examples of spontaneous symmetry breaking. For a schematic see fig. 3.

In chapter 2 we consider a system of active polar swimmers that align with their neighbors. When confined in the right geometry, the system will self-assemble into a state with topologically protected chiral acoustic modes. The chirality in this system manifests itself as a temporal one, rather than a spatial chirality. For a schematic see fig. 4.

Chapter 3 shows how systems of Yukawa charged active spinning dimers self-assemble into a crystal phase with spatiotemporal order, a liquid phase or a glass phase depending on the density. The chirality in this system is determined by the handedness of spin of the dimers. Depending on the phase and the confinement geometry of these systems of actively spinning dimers, the system will allow for rigid body rotations or edge currents. The chirality of rotations and edge currents are set by the chirality of the spinning dimers. For a schematic see fig. 5.

Finally, in chapter 4 we introduce a novel method of doing molecular dynamics on curved surfaces by developing a symplectic integrator. Although this new method can be applied to many topics, see for instance fig. 6, we present preliminary results on two-dimensional crystal melting in the presence of curvature. As melting in two dimensions is mediated by topological defects which are spatially positioned by the curvature, we find that the crystal may melt inhomogeneously.

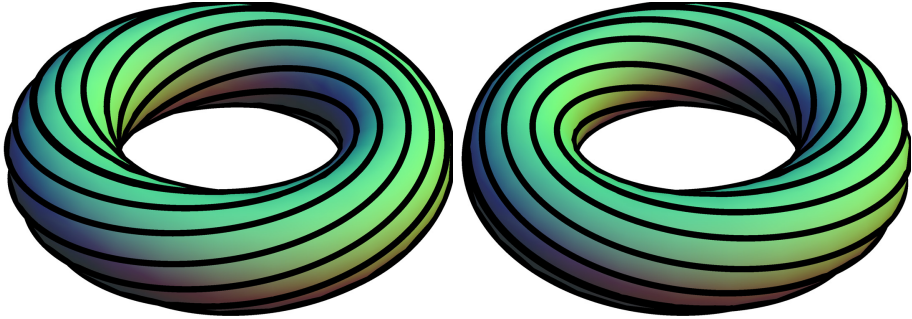


Figure 3: Schematic of left-handed (**left**) and right-handed (**right**) toroidal nematic liquid crystals.

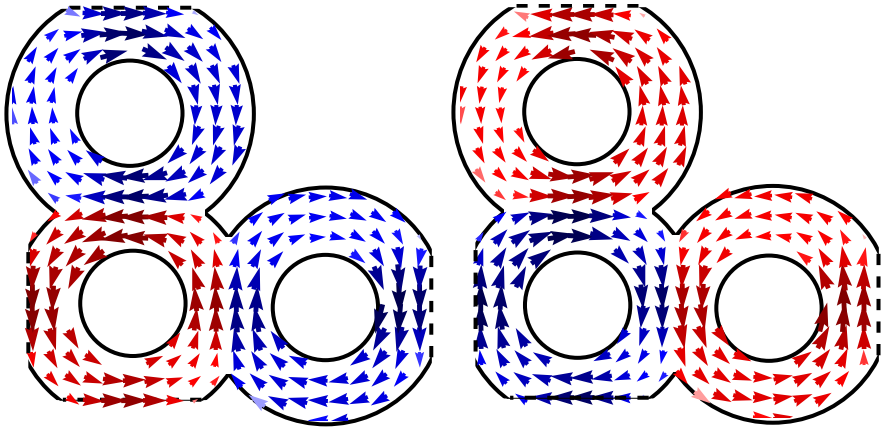


Figure 4: Schematic of a confined polar active liquid flow field with spontaneously broken chirality and left-handed (**left**) or right-handed (**right**) polarization.

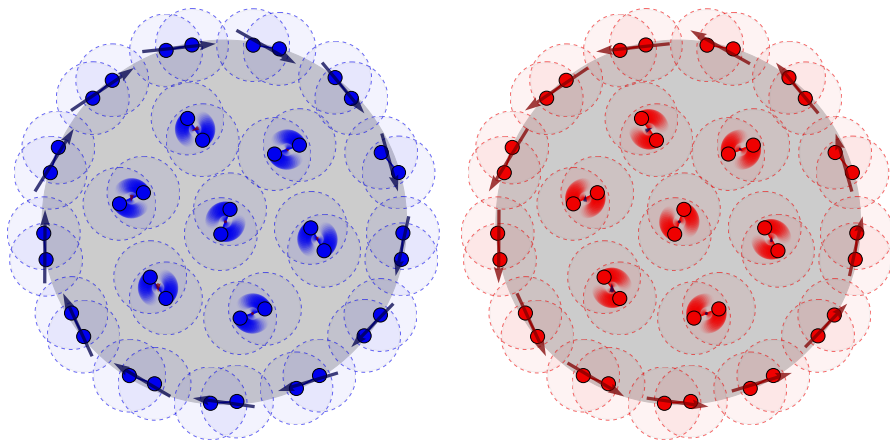


Figure 5: Snapshots of simulations done with 20 chiral dimers confined in a disk. We observe spatiotemporal order and edge currents. **Left:** a left-handed spinning system. **Right:** a right-handed system.

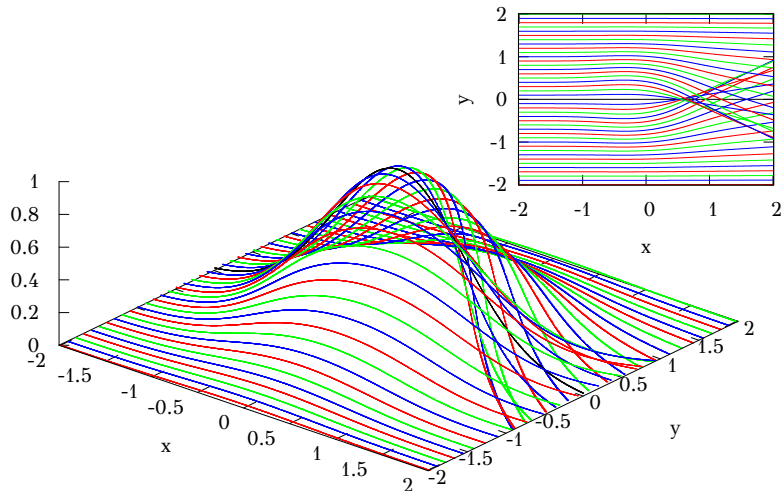


Figure 6: Geodesic lines on a Gaussian bump found using our developed integrator. The integrator solves Newton's equations of motion in the presence of Riemannian curvature symplectically. In the absence of a force term Newton's equations of motions are equal to the geodesic equation.

