Statistical Mechanics
from microscopic to macroscopic

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Statistical mechanics at Rutgers (math)

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What is Statistical Mechanics?

- Phenomena that are directly observable are Macroscopic: for example
  - Ideal gas law:
    $$pV = Nk_BT$$
  - Freezing and other phase transitions.
  - Ohm's law:
    $$V = RI$$
- How to understand these? Microscopic theories!

What is Statistical Mechanics?

- Phenomena that are directly observable are Macroscopic: for example
  - Ideal gas law: free molecules

$$pV = Nk_BT$$

  - Freezing and other phase transitions: ordering of particles.
  - Ohm's law: electrons moving through a metal

$$V = RI$$

- How to understand these? Microscopic theories!

What is Statistical Mechanics?

- Statistical mechanics: understanding how the macroscopic properties follow from the microscopic laws of nature ("first principles").

The arrow of time

- The microscopic dynamics are reversible.
  - Consider the motion of a point particle, which follows the laws of Newtonian mechanics.
  - If time is reversed, the motion still satisfies the same laws of Newtonian mechanics.
- Many macroscopic phenomena are irreversible.
  - For example: friction: the law of friction is not invariant under time reversal.
  - Or, consider the expansion of a gas in a container.

The thermodynamic limit

- One mole $\approx\ 6.02 \times 10^{23}$.
- Whereas a finite number of microscopic particles behaves reversibly, an infinite number of microscopic particles does not.
- Fundamental tool of statistical mechanics: the thermodynamic limit, in which the number of particles $\to \infty$.

Putting the Statistics in Statistical Mechanics

- To understand these infinite particles interacting with each other, we use probability theory.
- Simple example: the free gas:
  - Each particle is a point, and no two particles interact with each other.
  - Probability distribution: Gibbs distribution

$$p(\mathbf{x}, \mathbf{v}) = \frac{1}{Z} e^{-\beta H(\mathbf{x}, \mathbf{v})}, \quad \beta := \frac{1}{k_B T}$$

    where $H(\mathbf{x}, \mathbf{v})$ is the energy of the configuration where the particles are located at $\mathbf{x} \equiv (x_1, \cdots, x_N)$ with velocities $\mathbf{v} \equiv (v_1, \cdots, v_N)$.

The free gas

- The energy is the kinetic energy:
$$H(\mathbf{x}, \mathbf{v}) = \frac{1}{2} m \sum_{i=1}^{N} v_i^2.$$
- Denoting the number of particles by N and the volume by V, we have
$$Z = V^N \left(\frac{2\pi}{\beta m} \right)^{\frac{3}{2} N}.$$
- The pressure can be computed to be
$$p = \frac{N}{\beta V} \equiv \frac{N k_B T}{V}$$
that is, the ideal gas law.

Hard sphere model

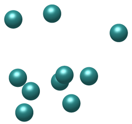
- Let us now consider a system where the microscopic particles interact: the hard sphere model, in which each particle is a sphere of radius R, and the interaction is such that no two spheres can overlap.
- Probability distribution:

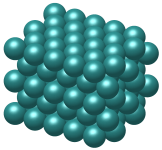
$$p(\mathbf{x}) = \frac{1}{Z} e^{\beta \mu N}$$

where μ is the chemical potential and $\beta = \frac{1}{k_B T}$.

Hard sphere model

- We expect, from numerical simulations, to see two phases: a gaseous phase and a crystalline one.





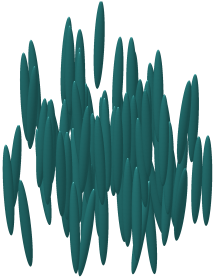
- In the gaseous phase, the particles are almost decorrelated: they behave as if they did not interact.
- In the crystalline phase, they form large scale periodic structures: they behave very differently from the non-interacting gas.

Hard sphere model

- The gaseous phase is very well understood. Much about it can be computed using analytic expansions (called "cluster expansions" or "Mayer expansions").
- The crystalline phase is much more of a mystery: we still lack a proof that it exists at positive temperatures!
- Open Problem: prove that hard spheres crystallize at sufficiently low temperatures.

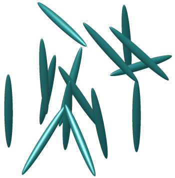
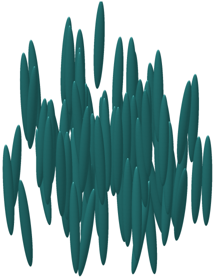
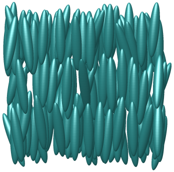
Liquid crystals

- Phase of matter that shares properties of liquids (disorder) and crystals (order).
- Nematic liquid crystals: order in orientation, disorder in position.



Liquid crystals

- Model: hard cylinders.
- Expected phases: gas, nematic, smectic

Liquid crystals

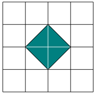
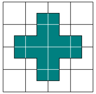
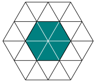
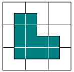
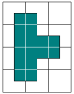
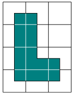
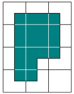
- Here again, the gas phase is well understood, but neither the nematic nor the smectic have yet been proved to exist.
- Open Problem: Prove the existence of a nematic or smectic phase.

Continuous symmetry breaking

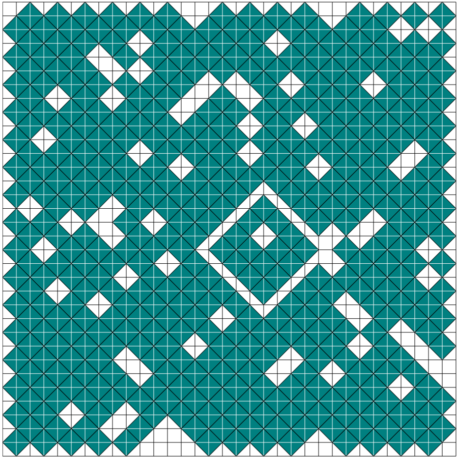
- Difficulty for both the hard spheres and liquid crystals: breaking a continuous symmetry (translation for the hard spheres, rotation for the liquid crystals).
- Continuous symmetries cannot* be broken in one or two dimensions.
- Continuous symmetry breaking can, so far, only be proved in very special models.

Lattice models

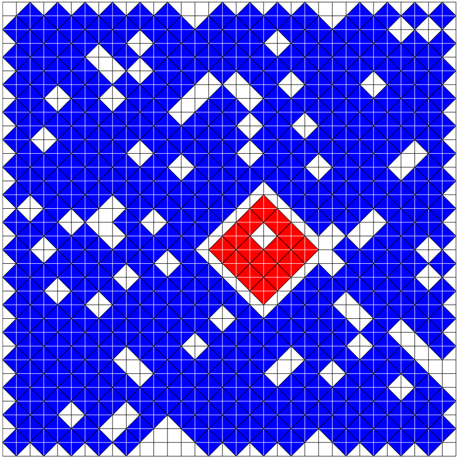
- Many examples:

Hard diamond model



Hard diamond model

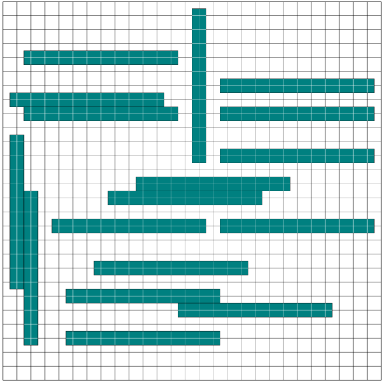


Hard diamond model

- Idea: treat the vacancies as a gas of “virtual particles”.
- Can prove crystallization for a large class of lattice models.

Hard rods on a lattice

- Model: rods of length k on $\mathbb{Z}^2$.



Hard rods on a lattice

- Can prove that, when $k^{-2} \ll \rho \ll k^{-1}$, the system forms a nematic phase.
- For larger densities, one expects yet another phase, in which there are tiles of horizontal and vertical rods.
- Open Problem: generalization to 3 dimensions.

Conclusion

- Statistical Mechanics establishes a link between Microscopic theories and Macroscopic behavior.
- (In equilibrium) it consists in studying the properties of special probability distributions called Gibbs Measures.
- Even simple models pose significant mathematical challenges.
- Still, much can be said about lattice models, even though there are many problems that are still open!