5. The lattice gas and the Ising model

It is common with models that are defined on a lattice instead for on the continuum.

- An important reason is that the computations then may be much simpler and thereby also considerably faster.
- A lattice model of a gas cannot reproduce all results from the continuum.
- Certain features are, however, not sensitive to the details of the model and if the goal is to examine such properties, the lattice model is superior to the continuum gas.

Coexistence region and the critical point

The gas changes to a liquid at temperatures and densities where the attractive interaction becomes important.

One way to examine this transition is to start from the gas phase and then decrease the volume at a fixed temperature.

- At a certain specific volume (volume per particle) there appears a small region with a higher density – a liquid.
- This is a coexistence between liquid and gas.
- The specific volume of the gas, v_{gas}, is then higher than the specific volume of the liquid, v_{liq}.

$$\Delta v = v_{\mathrm{gas}} - v_{\mathrm{liq}},$$

The critical point

At the critical point— (T_c, v_c, p_c) — Δv vanishes.

When approaching the critical temperature the volume difference vanishes with a power law,

$$\Delta v \sim (T_c - T)^\beta,$$

where $\beta \approx 0.3$ is a "critical exponent".

Close to the critical point there are large regions with a lower density coexisting with other regions with a higher density. This is a behavior that is both difficult to analyze with analytical methods and difficult to study with high precision in simulations.

The lattice gas

- The variables in the lattice gas are $n_i = 0, 1$, corresponding to the presence or absence of a particle at lattice point i.
- Attraction is given by assigning energy $-\epsilon$ for each neighboring pair of particles.
- Since two particles cannot be on the same lattice point this is in effect a repulsive term.

The energy for a certain configuration is

$$E = -\epsilon \sum_{\langle ij \rangle} n_i n_j,$$

where $\sum_{\langle ij \rangle}$ denotes a sum over all nearest neighbors.

Clearly, the number of particles is not a constant in this model.

The Ising model

The Ising model is usually thought of as a model of a magnet. This is in many ways similar to the lattice gas, the variables (the "spins") are now $s_i = \pm 1$, corresponding to spin up and spin down. The energy for the Ising model (with zero applied field) is

$$E = -J \sum_{\langle ij \rangle} s_i s_j.$$

The course *Monte Carlo simulations of critical phenomena in physics* is about the Ising model and other critical phenomena.

The Ising model has been called "the Drosophila of statistical physics" because it has been so thoroughly studied and manipulated in all conceivable ways.

Drosophila

From Wikipedia:

One species of Drosophila in particular, D. melanogaster, has been heavily used in research in genetics and is a common model organism in developmental biology. The terms "fruit fly" and "Drosophila" are often used synonymously with D. melanogaster in modern biological literature.