

# AMA4004 Statistical mechanics: Understanding phase transitions

The following problem should be solved by writing a computer program. This is a hard project and thus, if it is submitted for the portfolio, there is the potential to get marks of 9/10 out of 12 for it.

We can introduce a very simple model for the transition between a fluid and a gas phase of some substance as follows.  $N$  indistinguishable particles are allowed to move freely on a two dimensional square lattice with  $V$  sites (where  $1 \ll N \ll V$ ). The particles are subject to a short ranged attractive interaction, which makes the energy of the system  $E$  equal to  $-\epsilon$  times the number of particle pairs of neighbouring lattice sites. The kinetic energy of the particles is completely neglected in this model. In the fluid phase the particles condense into a single connected block, while in the gas phase the particles are distributed randomly on the lattice.

1. Write a program to generate all the possible microstates for a version of this model with 16 lattice sites and 4 particles. Calculate the energies of all these microstates and hence draw a graph showing how the ensemble average of the energy changes with temperature. Discuss the behavior you observe.
2. Calculate the histogram showing the most likely configurations that this system will adopt at two distinct temperatures
3. Give a justification for why the free energy of the fluid and gas phases are  $-2N\epsilon$  and  $-k_B T N \ln \frac{V}{N}$  respectively. Try to determine the temperature at which the transition between the fluid and the gas phase takes place.
4. Discuss how this system would behave if the interactions between particles were turned off.