## 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 pontential 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 indistinghisable particles are allowed to move freedly 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  $-k_BTN \ln \frac{V}{N}$  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.