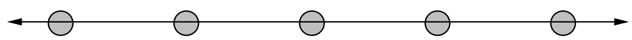
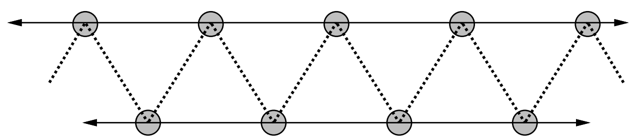
Mathematics 14: Magnetism: Long-range order and energy gaps.

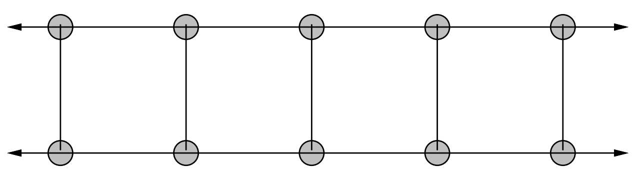
In project2 and project3 the topic of interest is magnetism, and in particular the demise of magnetism. You should all be aware of ‘bar’ magnets, and have some conception of atoms having magnetic moments from your course on atomic physics. Magnetism involves an array of atoms, each with an unquenched magnetic moment. These moments interact with each other via forces which prefer to align the moments either parallel (ferromagnetism) or anti-parallel (antiferromagnetism). Although the energetics prefers the ordering of the moments, other phenomena are in direct competition. Temperature induces fluctuations in the spin configurations which can eliminate the order, and this is investigated in project 2. Also, the so-called ‘zero-point motion’ inherent to quantum mechanics, involves fluctuations of the spins and in project 3 you can investigate whether or not these fluctuations can be strong enough to eliminate the order even at zero temperature.



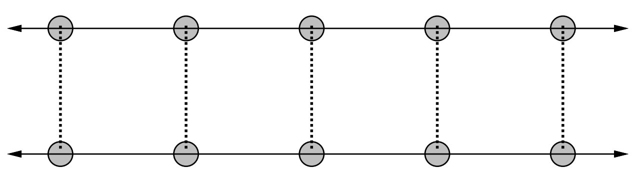
LINEAR CHAIN



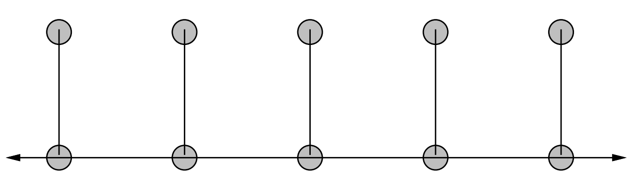
RAILROAD TRESTLE



LADDER

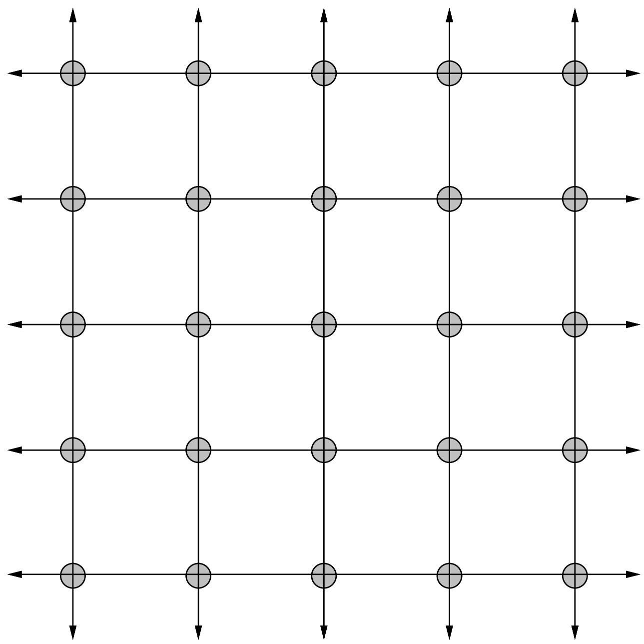


SQUARE ANALOGUE LADDER



COMB

A study of *magnetism* involves a collection of atoms together with a network of bonds which compose the geometry. Examples are depicted above for one dimension and below is the simplest two-dimensional system:



SQUARE LATTICE

Single bond

Double bond

where the filled circles denote atoms and the double bond denotes a bond with double strength.

Magnetism involves the spins becoming related or correlated to each other over long distances. For the Ising model the z-axis is *special*, and one need only look at this component, but for the x-y or Heisenberg models there is a *continuous* symmetry (ie rotation about the z-axis) which complicates the search for order.

The order in the Ising system can be studied with a z-component of total spin:

$$S^z_{total} = \sum_i (-1)^{\chi_i} \hat{S}^z_i$$

where $\chi_i = 0$ or 1 promotes either parallel or anti-parallel spins, enabling a study of either ferromagnetism or antiferromagnetism.

For the x-y or Heisenberg systems we need to consider:

$$< \hat{\mathbf{S}}^\alpha_i . \hat{\mathbf{S}}^\alpha_j >$$

with $\alpha = \|, \perp$ or is blank. These quantities measure the *relative* orientation between spins and are known as *correlation functions.* The quantity which exhibits any order is now:

$$< \hat{\mathbf{S}}^\alpha_{total} . \hat{\mathbf{S}}^\alpha_{total} > = \sum_{ij} (-1)^{\chi_i + \chi_j} < \hat{\mathbf{S}}^\alpha_i . \hat{\mathbf{S}}^\alpha_j >$$

and long-range order in the system occurs when:

$$S^z_{total} \sim N$$

or

$$< \hat{\mathbf{S}}^{\alpha}_{total}.\hat{\mathbf{S}}^{\alpha}_{total} > \sim N^2$$

For the *x*-*y* or Heisenberg models there is a second method of looking for order: Magnetic order is associated with low-energy excitations associated with the continuous degeneracy, known as *Goldstone modes.* If there is a *gap* to excitations then there cannot be long-range order.

The quantities to analyse are:
$\epsilon = E_0/N$ the energy per spin
$\Delta E_n = E_n - E_0$ the gap to the n'th excitation
$< \hat{\mathbf{S}}^{\alpha}_1.\hat{\mathbf{S}}^{\alpha}_{N/2} >$ the correlations half-way around the system

$$M^{\alpha} = \frac{1}{N}\sum_{ij}(-1)^{\chi_i+\chi_j} < \hat{\mathbf{S}}^{\alpha}_i.\hat{\mathbf{S}}^{\alpha}_j >$$

the magnetisation or 'number of particles in the condensate'.

These quantities can be calculated for finite N, the number of atoms in the system, and then scaled towards $N \mapsto \infty$: so-called *finite-size scaling.*