Phase transition in a two-dimensional system of dipoles

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The problem of a phase transition in a square lattice of dipoles with a dipole–dipole interaction and a fourfold symmetry axis reduces to a two-dimensional Ising model. An exact analytic solution is thus possible.

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An example of a two-dimensional system of dipoles with a finite commutative symmetry group is the system of surface groups having a rotational degree of freedom. If the number of symmetrically arranged surface atoms nearest the group is m, the group has an m-fold symmetry axis, and a phase transition occurs against the background of random rotational reorientations between azimuthal potential wells.[1]

In two-dimensional systems with a continuous symmetry group, the long-range order disappears as the thermodynamic limit is approached, while the dipole interaction stabilizes this long-range order.[1] It is thus not surprising to find that there is a long-range order even in the specific model with a dipole-dipole interaction which we will discuss here:

$$U_{nm,\,n+1m} = J\,[\,e_{nm} \cdot e_{n+1m} - 3\,(e_{nm} \cdot i)(e_{n+1m} \cdot i)]\,,$$

$$U_{nm,\,nm+1} = J[\,e_{nm} \cdot e_{nm+1} - 3\,(e_{nm} \cdot j)(e_{nm+1} \cdot j)].$$

(1)

Here J is the energy of the dipole-dipole interaction, e_{nm} is a unit vector which specifies each of the four possible orientation directions of the dipole at site (nm) of the square lattice (Fig. 1), and i and j are unit vectors along the x and y axes. We resolve the vector e_{nm} into its components,

$$e_{nm} = \frac{1}{\sqrt{2}}\,(\sigma^x_{nm}\,i + \sigma^y_{nm}\,j\,).$$
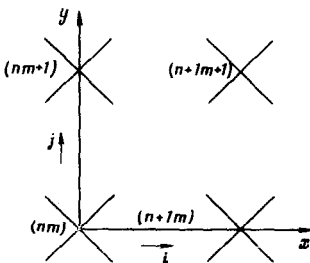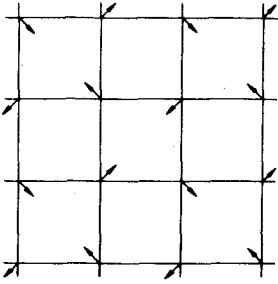
(2)

FIG. 1.

FIG. 2.

Each of the four orientation directions can thus be specified by a pair of independent components $\sigma_{nm}^x = \pm 1$, $\sigma_{nm}^y = \pm 1$. Substituting (2) into (1), we find the following expression for the complete Hamiltonian of the system:

$$\mathcal{H} = \mathcal{H}^x + \mathcal{H}^y ,$$

$$\mathcal{H}^x = -J \sum_{nm} \sigma_{nm}^x \sigma_{n+1m}^x + \frac{1}{2} J \sum_{nm} \sigma_{nm}^x \sigma_{nm+1}^x ,$$

$$\mathcal{H}^y = \frac{1}{2} J \sum_{nm} \sigma_{nm}^y \sigma_{n+1m}^y - J \sum_{nm} \sigma_{nm}^y \sigma_{nm+1}^y . \tag{3}$$

The original system has broken up into two noninteracting subsystems, each described by a two-dimensional Ising model, with different coupling constants within a column (n) and within a row (m) (Ref. 2). Figure 2 shows the configuration of dipole orientations in the ordered phase which corresponds to the minimum of Hamiltonian (3). The critical temperature for the transition to this phase, T_c, is determined by the equation

$$\text{sh} \frac{2J}{k T_c} \ \text{sh} \frac{J}{k T_c} = 1, \tag{4}$$

from which we find $kT_c \cong 1.641J$.

If the angle between the orientations e_{nm} and the x and y axes were different from 45°, a term $\mathcal{H}^{xy}$ would appear in (3) and describe the interaction of the two Ising subsystems. This discussion can also be generalized to n-dimensional square lattices with 2^n dipole orientations (along the principal diagonals).

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[1] A phase transition in a specific system, of hydroxyl groups on a silica surface, was studied in Ref. 3.

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