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Phase transition in dimer liquids

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Abstract
We study the phase transition in a system composed of dimers interacting with each other via a nearest-neighbor (NN) exchange J and competing interactions taken from a truncated dipolar coupling. Each dimer occupies a link between two nearest sites of a simple cubic lattice. We suppose that dimers are self-avoiding and can have only three orientations, which coincide with the x, y or z direction. The interaction J is attractive if the two dimers are parallel to each other at the NN distance, zero otherwise. The truncated dipolar interaction is characterized by two parameters: its amplitude D and the cutoff distance r_c. Using the steepest descent method, we determine the ground-state (GS) configuration as functions of D and r_c. We then use Monte Carlo simulations to investigate the nature of the low-temperature phase and to determine characteristics of the phase transition from the ordered phase to the disordered phase at high temperatures at a given dimer concentration. We show that as the temperature increases, dimers remain in the compact state and the transition from the low-T compact phase to the disordered phase where dimers occupy the whole space is of second order when D is small, but becomes of first order for large enough D, for both polarized and nonpolarized dimers. This transition has a resemblance to the unfolding polymer transition. The effect of r_c is discussed.

(Some figures may appear in colour only in the online journal)

1. Introduction

The problem of the phase transition in polymers is one of the most important domains not only for fundamental sciences such as statistical physics but also in many interdisciplinary areas such as biophysics and biochemistry [1]. Since the introduction of the renormalization group [2, 3] (RG), the understanding of the nature of the phase transition in many systems has become clear. With its concepts, we understand that the nature of the phase transition in a system depends on a very few parameters, such as the symmetry of the order parameter and the space dimension. Phase transitions in various systems which are very different in nature can belong to the same universality class. However, there are complicated systems where the RG presents much difficulty in application. One can mention frustrated systems where competing interactions cause highly degenerate ground states with a combination of several symmetries [4]. Polymers and moving interacting species such as dimers are another category of systems which cannot be easily treated with conventional methods.

We are interested here in the phase transition of a system composed of interacting dimers, a kind of axial molecule moving in space. At low temperatures these dimers are in an orientationally ordered phase and at high temperatures they are in a liquid state. There is thus a resemblance to liquid crystals. We recall that liquid crystals are somewhere between solid and liquid states where molecules have some spatial orientations which under some conditions can order themselves into some ordered structures. There are two kinds of ordering in the liquid state: (i) the smectic phase where axial molecules are ordered in planes but there is no order between planes and (ii) the nematic phase where molecules are oriented in the same direction but there is no spatial ordering between them. The smectic phase is divided into subcategories according to the molecular orientation with

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respect to the normal axis of the planes. Of course, at very high temperatures, molecules are completely orientationally disordered: we have the so-called isotropic phase. Liquid crystals have been a subject of intense investigations for more than 50 years due to their numerous applications [5, 6]. Systems of interacting dimers have also been recently studied [7–12].

We study in the present paper a model of a dimer liquid by taking into account an exchange interaction between nearest neighboring (NN) dimers. In addition, in order to create competing interactions between dimers we introduce a truncated dipolar interaction. Our purpose is not to investigate the effect of the infinite-range dipolar interaction, but to use the competing interactions generated by the two terms of the dipolar interaction within a cutoff distance instead of putting by hand competing interactions between NN, next NN, third NN, etc. The dipolar interaction in spin systems—in particular, in thin films—has been widely studied (see references in [13]). In two dimensions, a liquid of dipoles under an applied field was investigated by Monte Carlo (MC) simulation a long time ago [14], which showed already an orientational ordering of chains of dipoles along the applied field.

Our aim is to investigate the nature of the ordering and of the phase transition in a liquid crystal described by our dimer model. This is motivated by recent experiments on periodic layered structures of ordered phases [15–20] and on orientational phase transitions in various liquid crystals [21–27]. Some numerical investigations on orientational order have also been published: stability of liquid crystalline phases in the phase-field-crystal model has been investigated [29], molecular simulation of hierarchical structures in bent-core nematic liquid crystals has been carried out [28] and numerical evidence for nematic and smectic behavior of two-dimensional hard models has been found [30]. Note that aggregation of nanoparticles in a block copolymer bilayer has been numerically studied as functions of various kinds of interactions present in the system [31, 32]. For systems of dimers interacting via an anisotropic exchange between first neighbors in three directions of a cubic lattice, the work of Papanikolaou *et al* [12] showed a first-order transition in some region of parameters. It summarized very well previous works [7–11] which demonstrated the difficulty in constructing an appropriate Landau–Ginzburg–Wilson (LGW) theory to describe the phase transition in classical dimer liquids, which are still far from being well understood.

The absence of MC simulations in the literature for dimer liquids with dipolar interactions in three dimensions has motivated our present work. Our model is described in detail in section 2. The ground-state (GS) analysis of polarized dimers is shown in section 3 and results of MC simulations are shown and discussed in section 4. The case of nonpolarized dimers is shown in section 5. Concluding remarks are given in section 6.

2. Model

We consider a system of dimers, each of which lies on a link between two nearest sites on a simple cubic lattice. By definition, dimers do not touch each other. The dimer axis can be in the x, y or z direction. The Hamiltonian is given by the following 3-state Potts model [33]:

$$\mathcal{H} = -\sum_{(ij,mn)} J(ij,mn)\delta(\sigma_{ij},\sigma_{mn}) \tag{1}$$

where σ_{ij} is a variable defined for the link between nearest lattice sites i and j. σ_{ij} is equal to 1 if the dimer axis is x, 2 if it is y, and 3 if it is z. We suppose that the interaction between two dimers (ij) and (mn) is $J(ij,mn)$ and it is equal to J ($J > 0$) if they occupy two parallel links on a square face of a cubic lattice cell, zero otherwise. For description purposes, we shall adopt the following notation to define a dimer: the dimer on the link (ij) is always written with i being the first end. In the case where the dimer is oriented (or polarized), the dimer is considered as a vector. In the case of nonpolarized dimers, each dimer is a nonoriented segment. Periodic boundary conditions (PBC) are applied in all directions.

As said in the Introduction, we want to introduce competing interactions between dimers. One way to do is to take the dipolar interaction between dimers within a cutoff distance r_c. The dipolar term is written as

$$\mathcal{H}_d = D\sum_{(ij,mn)}\left\{\frac{\mathbf{S}(\sigma_{ij})\cdot\mathbf{S}(\sigma_{mn})}{r^3_{(ij,mn)}} - 3\frac{[\mathbf{S}(\sigma_{ij})\cdot\mathbf{r}_{(ij,mn)}][\mathbf{S}(\sigma_{mn})\cdot\mathbf{r}_{(ij,mn)}]}{r^5_{(ij,mn)}}\right\} \tag{2}$$

where $\mathbf{r}_{(ij,mn)}$ is the vector of modulus $r_{(ij,mn)}$ connecting the middle point A of the dimer (ij) and the middle point B of the dimer (mn). One then has: $\mathbf{r}_{(ij,mn)} \equiv \mathbf{r}_B - \mathbf{r}_A$. In equation (2), D is a positive constant depending on the material, the sum $\sum_{(ij,mn)}$ is limited at pairs of dimers within a cutoff distance r_c. A discussion on the dipolar interaction and the cutoff distance is given in the next section. The dimer state is defined by a quantity $\mathbf{S}(\sigma_{ij})$ given by

$$\mathbf{S}(\sigma_{ij}) = (S_1, 0, 0) \qquad \text{if } \sigma_{ij} = 1 \tag{3}$$

$$\mathbf{S}(\sigma_{ij}) = (0, S_2, 0) \qquad \text{if } \sigma_{ij} = 2 \tag{4}$$

$$\mathbf{S}(\sigma_{ij}) = (0, 0, S_3) \qquad \text{if } \sigma_{ij} = 3. \tag{5}$$

There are two cases:

(i) the nonpolarized dimers: $\mathbf{S}(\sigma_{ij})$ is defined by one of the following nonalgebraic components $S_1 = a$, $S_2 = a$, $S_3 = a$, a being the lattice constant.

(ii) The polarized dimers: $\mathbf{S}(\sigma_{ij})$ is defined by one of the three-component vectors given above, with $S_1 = \pm a$, $S_2 = \pm a$ and $S_3 = \pm a$.

In this paper we study both nonpolarized and polarized dimers. a will be taken to be 1 in the following.

3. Polarized dimers: ground-state analysis

3.1. Without dipolar interaction ($D = 0$)

Without the dipolar interaction, the interaction between neighboring molecules will give rise to an orientational order

of molecular axes at low temperatures. This situation is similar to a 3-state Potts model in three dimensions (3D), but the difference resides in the fact that dimers are moving from one bond to another, while in the Potts model the particle stays at its lattice site. The dynamics which leads to excited states is not the same: dimers have self-avoiding constraints. Note that the phase transition of the q-state Potts model in 3D is of first order for $q > 2$ [33]. We will see that the 3-state dimer crystal described above undergoes a second-order transition in the absence of a dipolar interaction.

It is easy to see that in the GS of the above Hamiltonian all dimers are parallel, as shown by the dimer configuration of type 1 in figure 2. Note that if the lattice size is $L \times L \times L$, the number of links is $3L^3$, but the number of dimers N_d in a lattice of linear size L should be less than or equal to $N_\mathrm{d}^\mathrm{max} = L^3/2$ because each dimer takes two lattice sites and they do not touch each other. The dimer concentration n_d is defined as

$$n_\mathrm{d} \equiv \frac{N_\mathrm{d}}{N_\mathrm{d}^\mathrm{max}}. \tag{6}$$

If $N_\mathrm{d} = N_\mathrm{d}^\mathrm{max}$, i.e. $n_\mathrm{d} = 1$, then the dimers occupy the whole lattice as shown in figure 2. Now if we use a number of dimers less than $N_\mathrm{d}^\mathrm{max}$, for instance $N_\mathrm{d} = N_\mathrm{d}^\mathrm{max}/2$ ($n_\mathrm{d} = 0.5$), then in the GS the dimers will fully occupy the half of the lattice in which they are parallel, leaving the remaining half empty. In other words, in the GS dimers occupy the lattice space in a most compact manner. This GS is similar to that of a polymer on a lattice where it is 'folded' to get a minimal energy at temperature $T = 0$ [5, 6]. We emphasize that when $N_\mathrm{d} = N_\mathrm{d}^\mathrm{max}$, dimers cannot move, and the system is blocked. In order to study excitations of a dimer system at a finite temperature T, it is necessary to take N_d less than $N_\mathrm{d}^\mathrm{max}$. As we will see later, the phase transition temperature as well as some low-T behaviors depend on N_d in both cases $D = 0$ and $D \neq 0$.

3.2. With dipolar interaction ($D \neq 0$)

At this stage, it is worth discussing the dipolar interaction. The infinite-range dipolar interaction has been used for a long time ago in theories and in simulations. Often, for the electric dipolar interaction, the sum was treated by using the Ewald sum [34, 35], which consists in writing the sum as two sums: the short-range real-space sum and the long-range sum in reciprocal space. The necessity in performing the second sum is to choose a central unit and making its translation in the whole space to realize a periodic system. The central unit and its translated images have the same average properties. With some careful techniques to ensure the charge neutrality of the central unit, Ewald's method can be used with some success. However, unlike the electric dipolar interaction, where there is a sum of $1/r^3$ terms, the magnetic dipolar interaction has two sums with $1/r^3$ terms: the second one depends on the spin orientations as seen in equation (2). In spin systems, the choice of the central unit is not obvious because the magnetic ordering is no longer periodic in the vicinity of the phase transition: spin clusters of all sizes exist in the critical region. A choice of a periodic unit can alter the nature of the phase transition because replacing the long-range part by a periodic system is more or less equivalent to replacing surrounding spins beyond a short distance by the same average. This is indeed a mean-field approach. It is well known that low-level mean-field theories do not correctly take into account critical fluctuations near the phase transition [3], the critical behavior cannot be thus correctly determined.

In the present work, as said in the Introduction, our objective is not to treat the infinite-range dipolar interaction. Our aim is to introduce some competing interactions between dimers. One way to do is to introduce, by hand, competing interactions between NN, NNN, third NN, ... and to study their effects. Another way is to choose competing interactions coming from the dipolar formula within a cutoff distance. We have chosen the second way and we looked for the effect of the two competing terms of equation (2) and of the cutoff on physical quantities. We are convinced that many aspects found here remain in models with limited-range competing interactions. Results of NN interactions in models of statistical physics allow us to qualitatively understand experimental systems which are not always of short-range interaction [3].

We see hereafter that when a dipolar interaction between dimers is introduced, the GS depends on D and r_c. In the uniform dimer configuration, such as the configuration of type 1 in figure 2, the dipolar energy is zero: when there is only one kind of dimer orientation, say axis z, the dipolar energy of σ_{ij} is

$$E_i = D \sum_{mn} \left[\frac{1}{r_{ij,mn}^3} - 3 \frac{(u_{ij,mn}^z)^2}{r_{ij,mn}^3} \right]. \tag{7}$$

If we transform the sum into an integral, the sum in the first term gives $4\pi \ln r_\mathrm{c}$ (integrating from 1 to r_c), while the second term gives $-4\pi \ln r_\mathrm{c}$, which cancels the first term. This is valid for r_c larger than 1. The energy of the system comes from the short-range exchange term, equation (1).

In order to understand the GS found below as functions of D and r_c, let us consider a dimer σ_{ij} interacting with its neighbor σ_{mn}. If they have the same orientation, say the x axis for instance, the energy calculated with equation (2) is

$$E_i = D \left[\frac{1}{r_{ij,mn}^3} - 3 \frac{x_{ij,mn}^2}{r_{ij,mn}^5} \right] \tag{8}$$

in which the first term is positive and the second one is negative. However, when the first dimer is on x and the second one on y, for example, the first term in equation (2) is zero, the dipolar energy for the perpendicular dimer pair is given by

$$E_i = D \left[-3 \frac{S_1 x_{ij,mn} S_2 y_{ij,mn}}{r_{ij,mn}^5} \right] \tag{9}$$

where $S_1 = \pm 1$ and $S_2 = \pm 1$. This term can be positive or negative, depending on the signs of $x_{ij,mn}$, $y_{ij,mn}$, S_1 and S_2 of the dimer pair (ij, mn). So, in the GS, S_1 and S_2 take their signs which minimize this term. The difficulty of determining the GS comes from the choice of each dimer pair so as to have the minimum of the global energy. This cannot be analytically

r_c \ D	0.30	0.40	0.45	0.48	0.50	0.60
1.5	1	1	1	1	3	3
1.8	1	1	4	4	4	4
2.3	1	1	4	4	4	4
2.5	1	1	5	5	5	5
2.8	1	1	5	5	5	5
3.2	1	2	2	6	6	6
3.6	1	2	6	6	6	6

Figure 1. Ground-state configurations numbered from 1 to 6 obtained by the steepest descent method in the space (D, r_c). These configurations are displayed in figures 2 and 3.

done. To determine the GS, we therefore use the numerical steepest descent method, which works very well in systems with uniformly distributed interactions. This method is very simple [36, 37]: (i) we generate an initial dimer configuration at random; (ii) we calculate the local field created at a given dimer by its neighbors using (1) and (2); (iii) we change the dimer axis to minimize its energy (i.e. align the dimer in its local field); (iv) we go to another dimer and repeat until all dimers are visited, in doing this we say we make one sweep; (v) we do a large number of sweeps until a good convergence is reached.

Using the steepest descent method, we have calculated the GS configurations for various sets of (D, r_c). The results are shown in figure 1. For each set (D, r_c), the configuration is indicated by a number. The configurations corresponding to the numbers from 1 to 6 are shown in figures 2 and 3. For descriptive convenience, let us call z the vertical axis of these figures, and x the horizontal axis. Note that the GS degeneracy is determined by the number of permutations of the dimer axes. Let us now comment on figure 1. For small D and small r_c, the GS is of type 1, which is uniform as in the case $D = 0$ discussed above. Larger values of D and r_c yield complicated configurations: for instance, type 2 consists of a three-layered structure of opposite dimer polarizations with a shift in z at their interface, type 3 consists of a single-layered structure of parallel polarization but with a shift in z. Types 4, 5 and 6, which are more complicated with larger dimer lattice cells, will be presented below.

It is important to note that all the presented GSs are compact where dimers occupy a portion of the lattice. The term 'compact' indicates that there are no free links between dimers. Such GSs are very similar to the folded polymers at low T. The 'volume' of the occupied space with respect to the total lattice volume depends on the dimer concentration n_d. In the figures showing the GSs, only the occupied portion of the lattice is displayed.

4. Polarized dimers: phase transition

We consider a sample size of $L \times L \times L$, where L varies from 12 to 24. The NN exchange interaction is used as the unit of energy, i.e. $J = 1$. For the dipolar term, a cutoff distance r_c is taken up to $\sqrt{10} \simeq 3.15$ lattice distance. At this value, each lattice site has 146 neighboring sites.

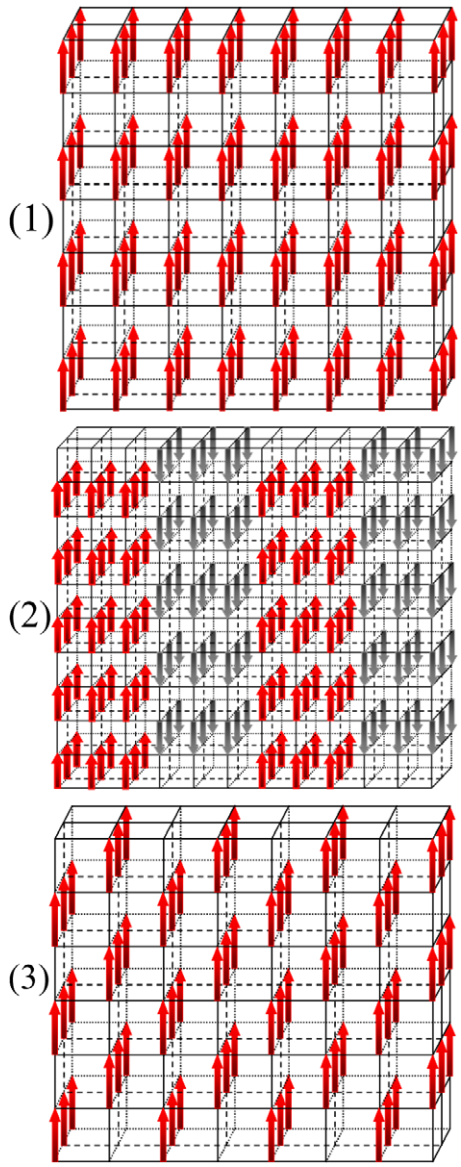

Figure 2. Ground-state dimer configurations of type 1, 2 and 3 as indicated in figure 1 in the polarized case are shown.

The algorithm is described as follows: we consider a dimer and calculate its interaction energy E_1 with other dimers within r_c using equations (1) and (2). We move this dimer to one of the links surrounding its two ends. There are such 10 links in the simple cubic lattice, but not all of them are 'free' at the other end, namely unoccupied by another dimer. A random free link is chosen, and the new energy E_2 is calculated. If $E_2 \leq E_1$, the new position of the dimer is accepted, otherwise it is accepted with a probability $\exp[-(E_2 - E_1)/(k_B T)]$. This is the well-known Metropolis algorithm [38]. We go next to another dimer and repeat the procedure until all dimers are visited: we say we accomplish one MC step/dimer. We use several millions of MC steps/dimer for equilibrating and for averaging. The averaged energy and the specific heat are

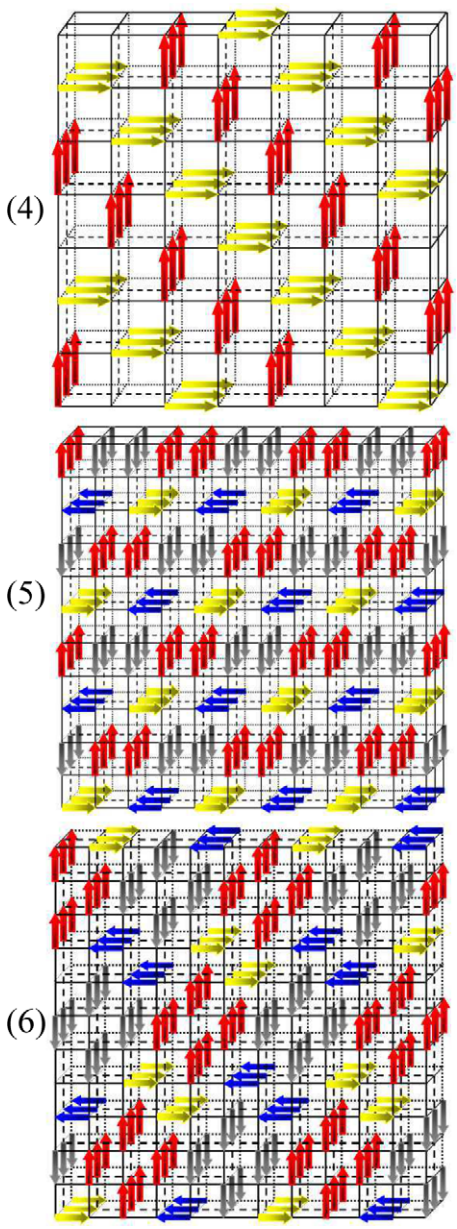

Figure 3. Ground-state dimer configurations of type 4, 5 and 6 as indicated in figure 1 in the polarized case are shown.

defined by

$$\langle U\rangle = \langle \mathcal{H} + \mathcal{H}_{\rm d}\rangle \tag{10}$$

$$C_V = \frac{\langle U^2\rangle - \langle U\rangle^2}{k_{\rm B}T^2} \tag{11}$$

where $\langle\cdots\rangle$ indicates the thermal average taken at T.

We define the order parameter Q by

$$Q = [q\max(Q_1, Q_2, Q_3) - 1]/(q-1) \tag{12}$$

where Q_n is the spatial average defined by

$$Q_n = \sum_j \delta(\sigma_{ij} - n)/L^3 \tag{13}$$

n ($n = 1, 2, 3$) being the value attributed to denote the axis of the dimer σ_{ij} at the link (ij). The susceptibility is defined by

$$\chi = \frac{\langle Q^2\rangle - \langle Q\rangle^2}{k_{\rm B}T}. \tag{14}$$

For each lattice size we choose the dimer concentration $n_{\rm d}$ small enough to allow the dimers to move on free links with increasing T. In the following, we shall use $n_{\rm d} = 5/6 \simeq 0.833$, except in section 4.3 where we study the effect of $n_{\rm d}$. Since we work at finite sizes, for each size we have to determine the 'pseudo' transition which corresponds in general to the maximum of the specific heat or of the susceptibility. The maxima of these quantities need not to be at the same temperature. Only at infinite size should they coincide. The theory of finite-size scaling [39–41] permits one to deduce properties of a system at its thermodynamic limit. We also use the histogram technique to distinguish first- and second-order transitions. The main idea of this technique is to make an energy histogram at a temperature T_0 as close as possible to the transition temperature [40, 41]. Using this histogram in the formulas of statistical physics for a canonical distribution, one obtains energy histograms in a range of temperature around T_0. In second-order transitions, these histograms are Gaussian. They allows us to calculate averages of physical quantities as well as critical exponents using the finite-size scaling. In first-order transitions, the energy histogram shows a double-peak structure.

4.1. Without dipolar interaction $D = 0$

We show first in figure 4 the energy per site $E \equiv \langle U\rangle/L^3$, the order parameter $M = \langle Q\rangle$ and the energy histogram, for $J = 1$ and $D = 0$. Several remarks are in order:

(i) At very low T (<0.4), the dimers are frozen in the GS configuration.

(ii) For $0.45 < T < 0.95$ dimers are unfrozen (cf peak of χ at $T \simeq 0.45$), they move to occupy free links in the nearby empty lattice space but they remain compact and orientationally ordered.

(iii) For $T > 0.95$, they are disordered both in their orientations and spatial positions. The dimers occupy the whole space in the way a polymer does in a solvent at the unfolding transition. We find an aspect of a second-order transition at $T = T_C \simeq 0.95$ indicated by a Gaussian peak. Note that we should check the order of the phase transition by making a finite-size scaling up to a very large size since it is known in some cases that the Gaussian shape at small sizes can become a double-peak structure (first-order transition) at large sizes. However, this huge task, which needs long calculations, is left for the near future.

We show the snapshots of these phases in figure 5. In the low-T phase, the upper part of the lattice is empty (not fully shown) and the lower part is compactly occupied by the dimers. Only in the disordered phase do the dimers occupy all the lattice space with vacancies uniformly distributed.

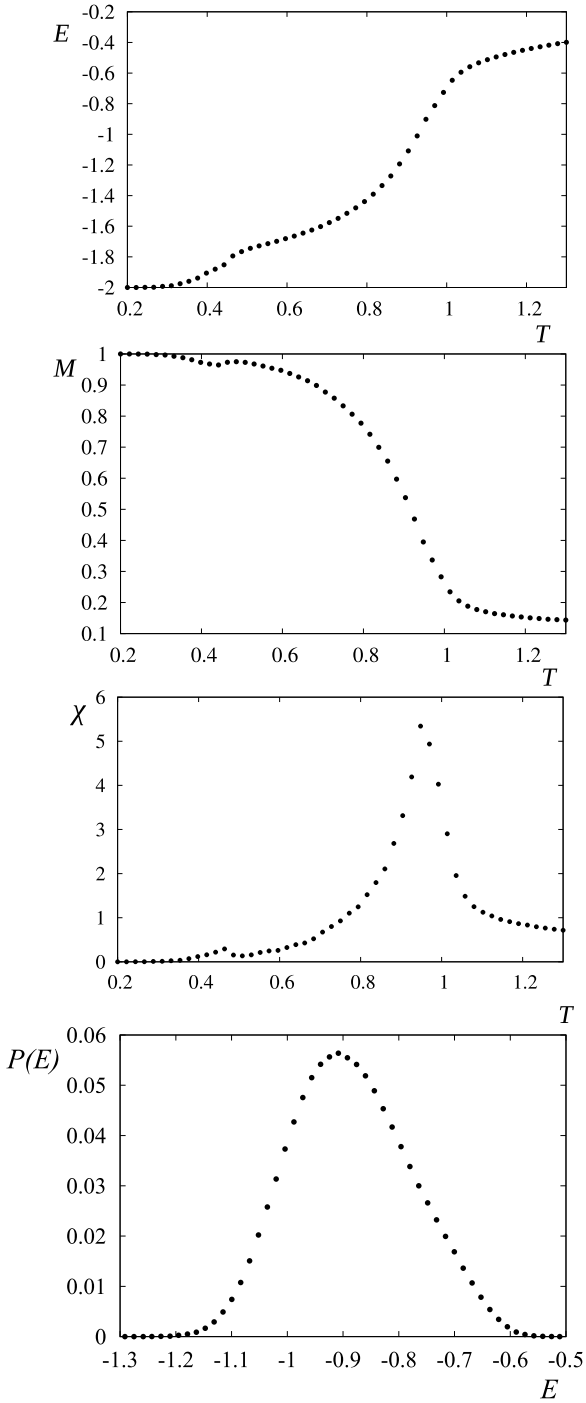

Figure 4. Energy per dimer E, order parameter $M = \langle Q \rangle$ and susceptibility χ versus T in the case $D = 0$. The bottom figure is the energy histogram at the transition temperature.

4.2. With dipolar interaction $D \neq 0$: polarized case

The energy versus T for $D = 0.6$ and the energy histogram are shown in figure 6 for several values of r_c. One observes a discontinuous transition and a double-peak structure which is a signature of a first-order transition, for all r_c.

Let us discuss the case of $r_c = 2.3$. The transition to the disordered phase takes place at $T \simeq 0.33$. Note that the system is unfrozen at $T \simeq 0.12$. We show in figure 7 the snapshots of the frozen phase, the compact phase and the isotropic phase, similarly to the $D = 0$ case shown above. Note that the 'surface' separating occupied and unoccupied parts in the GS is not flat as in the $D = 0$ case shown above. In the compact phase, a few dimers move to this empty space: the system is excited but remains compact. After the 'unfolding transition', dimers are uniformly distributed over the whole lattice (figure 7(c)).

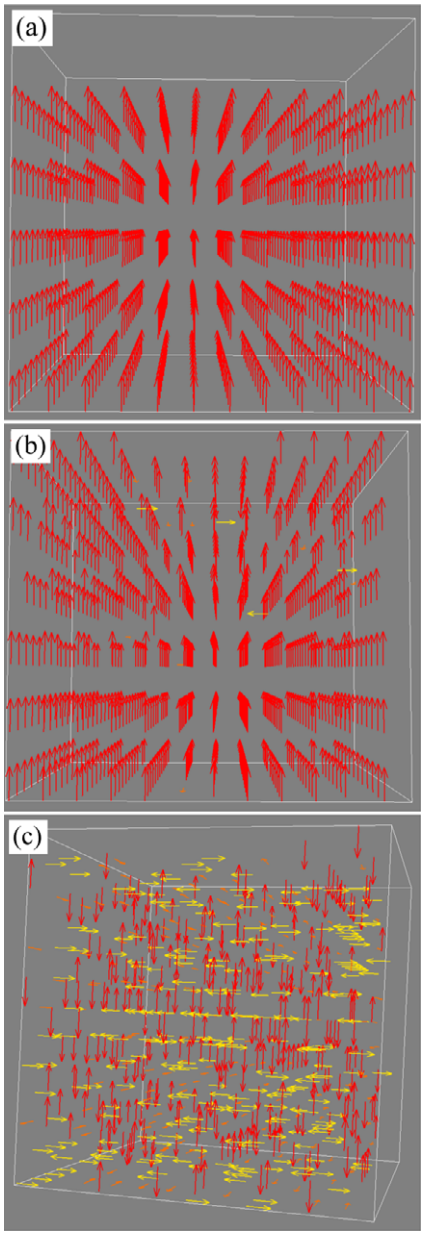

Figure 5. Snapshots of the dimer configuration for $D = 0$ at (a) $T = 0$, ground state, (b) $T = 0.508$, compact state, (c) $T = 1.19$, disordered (isotropic) phase. See text for comments.

4.3. Effect of dimer concentration

In this paragraph, we show that the dimer concentration n_d strongly affects the system. The main points are:

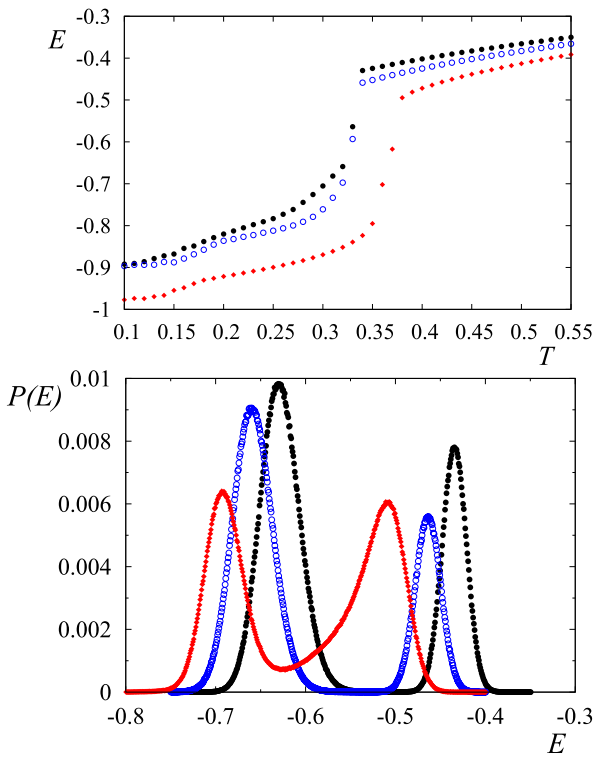

Figure 6. Energy versus T and energy histogram at the transition temperature for $D = 0.6$ with $r_c = 2.3$ (black circles), $r_c = 2.5$ (open blue circles) and $r_c = 3.2$ (red diamonds).

(i) Without dipolar interaction: there is a decrease of the transition temperature with decreasing n_d. This is because the number of neighbors decreases so that the energy per dimer decreases, therefore lowering the disordering temperature. This is shown in figure 9.

(ii) With dipolar interaction: there is a decrease of the transition temperature with decreasing n_d as in the $D = 0$ case, but the first-order character observed above remains (see figure 10).

(iii) There is a softening of the unfreezing process at low T ($\simeq$0.42) in the case where $D = 0$: the magnetization becomes smoother for smaller n_d as seen in figure 9. This can be qualitatively understood by observing that the more empty space is available the more easily the unfreezing is realized. The case of $D \neq 0$ is less visible due to the fact that in this case the interface between occupied and empty spaces in the GS is much larger—it has a paraboloid form as seen above—making the unfreezing process easy even at high n_d.

Note that to decrease n_d we can increase L while keeping N_d unchanged (see equation (6)). We show in figure 8 that the transition temperature decreases with increasing L but it remains finite as $L \to \infty$.

5. Nonpolarized dimers: ground state and phase transition

The main difference of polarized and nonpolarized dimers resides in the fact that a polarized dimer has an additional internal degree of freedom which makes more abundant the number of the GS and more excited states at finite T. As a consequence, the number of GS in the nonpolarized case is smaller, the GS configurations are simpler and the transition temperature is higher than in the polarized case.

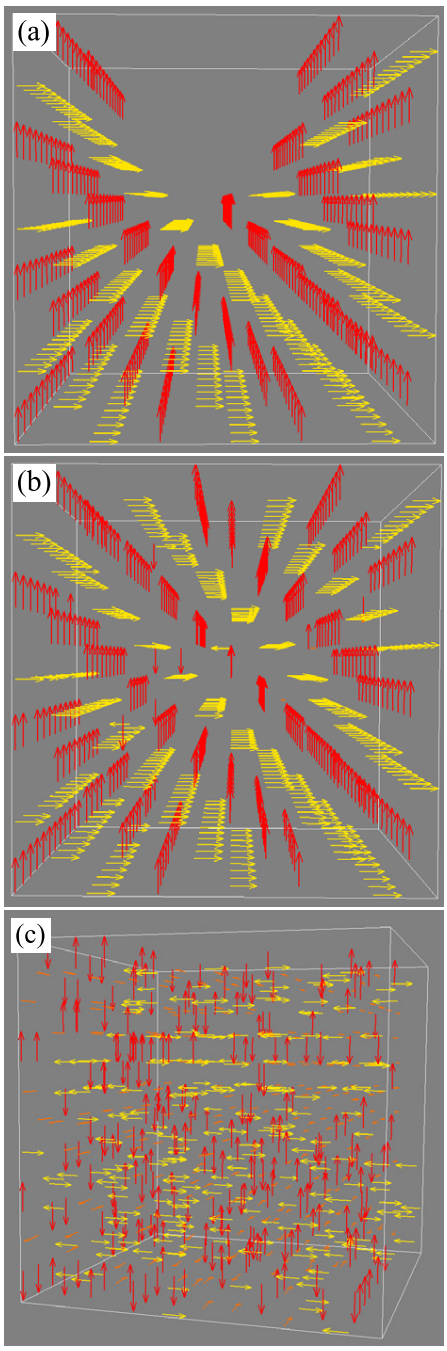

Figure 7. Snapshots of the dimer configuration for $D = 0.6$ at several temperatures: (a) $T = 0$, ground state, (b) $T = 0.17$, compact phase, (c) $T = 0.45$, disordered (isotropic) phase ($r_c = 2.3$). See text for comments.

5.1. Ground state

In the following we show results for the dimer concentration $n_d = 5/6$ similar to main results shown for the polarized case above.

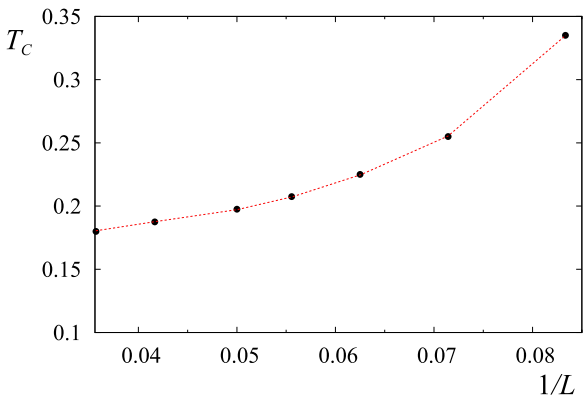

Figure 8. Transition temperature T_C versus $1/L$ with $L = 12$, 14, 16, 18, 20, 24 and 28 ($J = 1$, $D = 0.6$, $r_c = 2.3$). See text for comments.

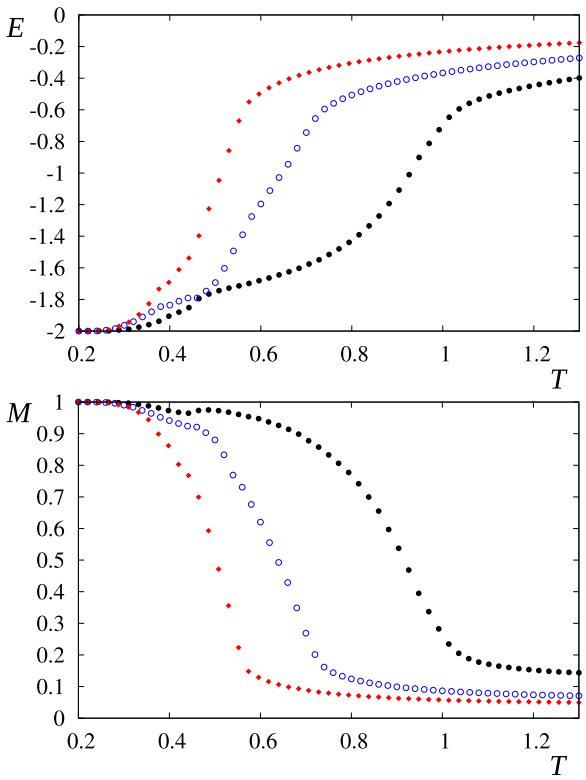

Figure 9. Energy per dimer E and order parameter $M = \langle Q \rangle$ versus T are shown in the case $D = 0$ for concentrations $n_d = 5/6 \simeq 0.833$ (black circles), $5/8 = 0.625$ (open blue circles) and $5/12 \simeq 0.417$ (red diamonds).

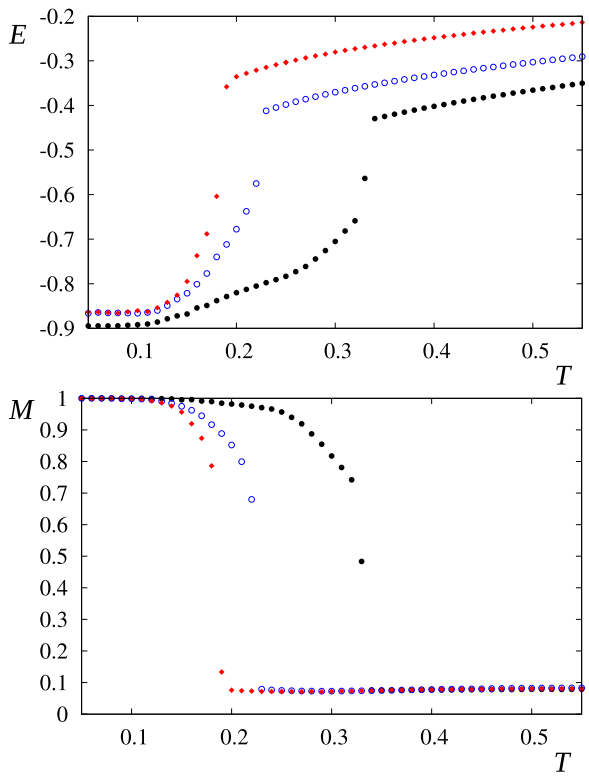

Figure 10. Energy per dimer E and order parameter $M = \langle Q \rangle$ versus T are shown in the case $D = 0.6$ with $r_c = 2.3$ for concentrations $n_d = 5/6 \simeq 0.833$ (black circles), $5/8 = 0.625$ (open blue circles) and $5/12 \simeq 0.417$ (red diamonds).

r_C \ D	0.30	0.40	0.45	0.48	0.50	0.60
1.5	1	1	1	1	3	3
1.8	1	1	1	2	2	2
2.3	1	1	1	2	2	2
2.5	1	1	1	2	2	2
2.8	1	1	1	2	2	2
3.2	1	1	2	2	2	2
3.6	1	1	4	4	4	4

Figure 11. Nonpolarized dimers: ground-state configurations numbered from 1 to 4 obtained by the steepest descent method in the space (D, r_c). These configurations are displayed in figure 12.

For non-zero D, the results obtained from the steepest descent method are shown in figure 11. The configurations 1–4 are shown in figure 12. Note that for $D = 0$, the GS is the uniform configuration of type 1, similar to that in the polarized case. We note the diagonal ordering of types 3 and 4.

5.2. Phase transition

The energy versus T is shown in figure 13 for two typical cases $D = 0.4$ and 0.6. Again here, we observe three successive phases with increasing T: for $D = 0.4$, for example, the frozen phase is at ($T < 0.25$), the 'compact' phase at ($0.25 < T < 0.7$) and the isotropic phase at ($T > 0.7$). For small D (as shown with $D = 0.4$), the transition is of second order, while for larger D ($D = 0.6$ for example) the transition becomes of first order. The energy histograms at the respective transition temperatures show a Gaussian peak for $D = 0.4$ and a double-peak structure for $D = 0.6$ (not shown). As said in the previous section, a second-order transition indicated by a Gaussian peak here should be checked with simulations using very large sizes. This formidable task is left for a future study.

As in the polarized case, the transition temperature decreases with decreasing n_d. Note that the unfreezing is not a phase transition, it is a gradual process in which the

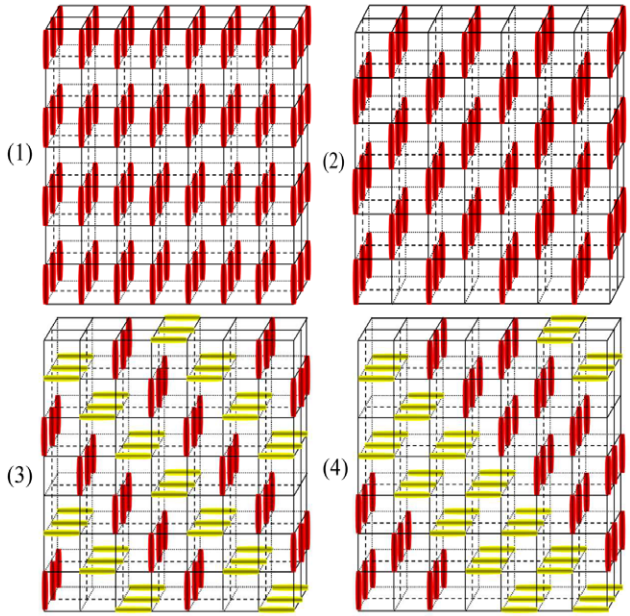

Figure 12. Nonpolarized dimers: ground-state dimer configurations of the type 1, 2, 3 and 4 indicated in figure 11 are shown.

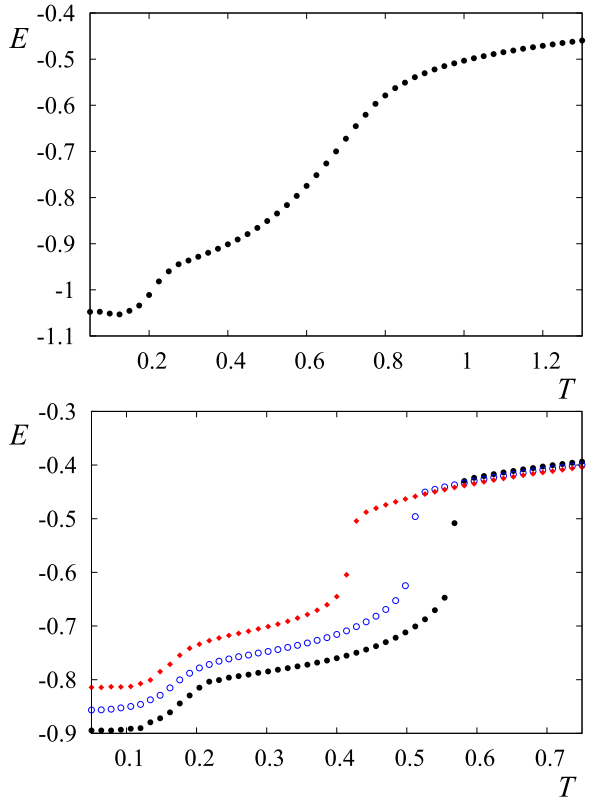

Figure 13. Nonpolarized dimers: energy per dimer E versus T for (i) top: $D = 0.4$ with $r_c = 2.5$, (ii) bottom: $D = 0.6$ with several r_c: 2.3 (black solid circles), 2.5 (blue open circles), 2.8 (red diamonds).

maximum of the specific heat and the susceptibility as well as its unfreezing temperature do not depend on the lattice size, unlike in a true phase transition where these quantities depend on L. As in the polarized case, the unfreezing is smoother in the case of smaller n_d (not shown).

6. Concluding remarks

Previous studies on interacting dimers in three dimensions have shown that the phase transition in this system is far from being well understood [7–12]. There are contradictions between LGW theories and numerical results [11, 12]. Note that these previous works have examined the case of a short-range interaction, limited to first neighbors. In order to contribute to this domain, we have studied in this paper a model of dimers moving on the simple cubic lattice and interacting with each other via the nearest-neighbor 3-state Potts model of strength J and competing interactions taken from a truncated dipolar interaction of amplitude D and cutoff distance r_c. This model has never been considered before. The numerical steepest descent method has been used to determine the GS dimer configuration and MC simulations have been carried out to determine the ordered phase at finite T and the nature of the phase transition. We have found for both polarized and nonpolarized dimers complicated GS configurations as functions of (D, r_c). They are all compact, occupying a portion of the lattice. For small D, the GS is uniform, and the surface separating the empty part of the lattice is flat. For large D, the GS is nonuniform, the empty lattice space is a 'paraboloid hole'. With increasing T, the dimers remain in the compact phase at low T. They undergo a transition to the spatially 'extended' isotropic phase at high T. This transition bears some resemblance to the unfolding transition of polymers in a solvent. Note that the change from the compact phase to the isotropic phase is of second order for small D (at least up to the largest sizes we have studied here) and of first order for large D. The first-order transition observed here is due to the competition of the two terms in equation (2) for large enough D. We believe that other types of competing interactions which give rise to frustration and instability of the dimer configuration would cause a similar first-order 'unfolding' transition.

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