Two-dimensional array of magnetic particles: The role of an interaction cutoff

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(Received 28 May 2003; published 2 October 2003)

Based on theoretical results and simulations, in two-dimensional arrangements of a dense dipolar particle system, there are two relevant local dipole arrangements: (1) a ferromagnetic state with dipoles organized in a triangular lattice and (2) an antiferromagnetic state with dipoles organized in a square lattice. In order to accelerate simulation algorithms, we search for the possibility of cutting off the interaction potential. Simulations on a dipolar two-line system lead to the observation that the ferromagnetic state is much more sensitive to the interaction cutoff R than the corresponding antiferromagnetic state. For $R \gtrsim 8$ (measured in particle diameters) there is no substantial change in the energetical balance of the ferromagnetic and antiferromagnetic state and the ferromagnetic state slightly dominates over the antiferromagnetic state, while the situation is changed rapidly for lower interaction cutoff values, leading to the disappearance of the ferromagnetic ground state. We studied the effect of bending ferromagnetic and antiferromagnetic two-line systems and observed that the cutoff has a major impact on the energetical balance of the ferromagnetic and the antiferromagnetic state for $R \lesssim 4$. Based on our results we argue that $R \approx 5$ is a reasonable choice for dipole-dipole interaction cutoff in two-dimensional dipolar hard sphere systems, if one is interested in local ordering.

DOI: 10.1103/PhysRevE.68.041102 PACS number(s): 64.10.+h, 45.70.−n, 74.25.Ha, 75.40.Mg

I. INTRODUCTION

Long-range interaction represents a major challenge for computer simulations. The size of the tractable systems (N particles) is limited through the fact that the order of N^2 calculations are to be carried out at each step, though for many purposes large systems need to be studied. Periodic boundary conditions, which are often helpful, can be implemented only by using sophisticated summation algorithms (if possible due to screening).

In principle, the above problems occur in so called short-range interaction models as well, such as in the most extensively studied Lennard-Jones system. However, for these systems a cutoff is usually introduced making the original short-range model explicitly finite range. It is generally accepted that the error introduced by the cutoff is negligible provided the cutoff distance is large enough [1].

Frequently the long-range interaction potential falls off like r^{-1}, where r is the distance between the particles. This should be compared to the Lennard-Jones system where the potential decreases like r^{-6}, where it is assumed that the attractive part of that potential is due to induced dipole-dipole interaction.

In this study, we focus on the question of cutting off a potential which is in between the two above cases. We consider a two-dimensional ensemble of magnetic particles interacting with a r^{-3} potential, which however, has an orientation dependence as well. It is crucial from the point of view of efficient programing to know if a reasonable cutoff can be introduced in this system. We investigate this problem by comparing the stability of static configurations.

II. THE LUTTINGER-TISZA METHOD

The Hamiltonian of a system of spherical dipoles is

$$H = \frac{1}{2} \sum_{i \neq j} \mathbf{s}_i^T \mathbf{J}_{ij} \mathbf{s}_j , \tag{1}$$

where i and j are dipole indices, $\mathbf{s}$ denotes the dipole momentum vector, $\mathbf{s}^T$ denotes the transpose of $\mathbf{s}$, and

$$\mathbf{J}_{ij} = \frac{1}{\|\mathbf{r}_{ij}\|^3} \left(\mathbf{I} - 3 \frac{\mathbf{r}_{ij} \circ \mathbf{r}_{ij}}{\|\mathbf{r}_{ij}\|^2} \right), \tag{2}$$

where $\mathbf{I}$ denotes the identity matrix and $\mathbf{r}_{ij}$ denotes the relative position vector of two dipoles. The 1/2 factor in Eq. (1) avoids double counting of dipole pairs.

We can study the crystalline state of a dipole system using the Luttinger-Tisza method [2] based on the idea that in case of crystals it is a natural assumption that the ground state exhibits some discrete translational symmetry. If $\Gamma(i)$ denotes the points generated from i with discrete translations belonging to the Γ symmetry group, the mentioned symmetry corresponds to $\mathbf{s}_i = \mathbf{s}_{i'}$ for all $i' \in \Gamma(i)$. According to this, the system can be broken into identical cells and the summation in Eq. (1) can be limited to summation over one single cell. Accordingly, the energy per dipole can be expressed as

$$E = \frac{1}{2n} \sum_{i,j=1}^{n} \mathbf{s}_i^T \mathbf{A}_{ij} \mathbf{s}_j , \tag{3}$$

where n is the number of dipoles per cell and $\mathbf{A}_{ij}$ are symmetric matrices defined by

$$\mathbf{A}_{ij} = \sum_{j' \in \Gamma(j),\ j' \neq i} \mathbf{J}_{ij'} . \tag{4}$$

The expression of the energy per dipole in Eq. (3) can be simplified by considering the $\hat{\mathbf{s}} = (\mathbf{s}_i)_{i=1}^{n}$ hypervector and $\hat{\mathbf{A}} = (\mathbf{A}_{ij})_{i,j=1}^{n}$ hypermatrix. By construction $\hat{\mathbf{A}}$ is symmetric. Using these, E can be written as

$$E = \frac{1}{2n} \hat{\mathbf{s}}^T \hat{\mathbf{A}} \hat{\mathbf{s}}. \tag{5}$$

Solving the eigenvalue problem of the (nd)-dimensional symmetric matrix $\hat{\mathbf{A}}$, where d is the dimension of the dipoles, we find the λ_k eigenvalues and $\hat{\mathbf{x}}_k$ orthogonal eigenvector system with normalization $\|\hat{\mathbf{x}}_k\| = \sqrt{n}$. Using these we have

$$E = \frac{1}{2} \sum_{k=1}^{nd} \lambda_k b_k^2 , \tag{6}$$

where b_k denotes the components of $\hat{\mathbf{s}}$ in the $\hat{\mathbf{x}}_k$ orthogonal eigenvector system.

If the dipoles have identical scalar strength μ, i.e., $\|\mathbf{s}_i\| = \mu$, then b_k must satisfy for all $i = 1, \ldots, n$ the condition

$$\left\| \sum_{k=1}^{nd} b_k \mathbf{x}_k^i \right\| = \mu, \tag{7}$$

where $\mathbf{x}_k^i$ are the components of the $\hat{\mathbf{x}}_k$ hypervector which belong to dipole index i. Adding the square of the above equations and taking into consideration that $\{\hat{\mathbf{x}}_k\}_{k=1}^{nd}$ form an orthogonal system, we conclude that b_k must satisfy the condition

$$\sum_{k=1}^{nd} b_k^2 = \mu^2. \tag{8}$$

In the framework of the Luttinger-Tisza method, these two conditions are known as the strong [Eq. (7)] and the weak [Eq. (8)] conditions. From the weak condition and Eq. (6), it can be derived that the energy per dipole in the ground state is $E_{min} = 1/2\ \lambda_{min} \mu^2$, where λ_{min} denotes the smallest eigenvalue of $\hat{\mathbf{A}}$. If there is one single eigenvalue equal to λ_{min}, the ground state dipole arrangement is given by the corresponding eigenvector. If there are more eigenvalues equal to λ_{min}, the ground state dipole arrangement is given by the linear combinations of the corresponding eigenvectors which satisfy the strong condition.

III. TWO-DIMENSIONAL ARRAY OF MAGNETIC PARTICLES

The above method was applied to a system of two-dimensional dipole moments with identical scalar strength located at the sites of an infinite rhombic lattice with an arbitrary rhombicity angle by Brankov and Danchev [3]. They considered that the ground state of this system has a translational symmetry corresponding to discrete translations along the lattice lines with multiples of $2a$, where a is the lattice constant. They found that the ground state depends on the rhombicity angle.

TABLE I. Dipole arrangements corresponding to the lowest two energy values per dipole in a two-dimensional system of dipole moments with identical scalar strength located at the sites of an infinite rhombic lattice with rhombicity angles $\alpha = 60°$ and $\alpha = 90°$. The energy is measured in μ^2/a^3 units, where μ is the scalar strength of the dipole moments and a is the lattice constant.

$\alpha = 60°$	$E = -2.758$	Continuously degenerate ferromagnetic state
	$E = -2.047$	Sixfold degenerate antiferromagnetic state
$\alpha = 90°$	$E = -2.549$	Continuously degenerate microvortex state including a fourfold degenerate antiferromagnetic state
	$E = -2.258$	Continuously degenerate ferromagnetic state

We repeated their calculations with the consideration that the dipoles are carried by identical hard spherical particles of diameter equal to the lattice constant, and according to the geometrical constraint introduced by this consideration we limited the rhombicity angle to $60° \leqslant \alpha \leqslant 90°$. In accordance with their results, we found that the system has a ferromagnetic ground state for $60° \leqslant \alpha \lesssim 79.38°$, and an antiferromagnetic ground state for $79.38° \lesssim \alpha \leqslant 90°$. We also found that the ground state for $\alpha = 60°$ is a continuously degenerate ferromagnetic state, and for $\alpha = 90°$ is a continuously degenerate microvortex state including a fourfold degenerate antiferromagnetic state, where the microvortex state is defined as two antiferromagnetic sublattices making an arbitrary angle with each other. We also identified the states with the second lowest energy per dipole. The results for $\alpha = 60°$ and $\alpha = 90°$ are summarized in Table I.

We repeated the calculations taking into consideration the interaction of only two neighboring lines on the rhombic lattice. This corresponds to the interaction of two lines of dipolar hard spheres shifted according to the α rhombicity angle. The Luttinger-Tisza method can be applied in a straightforward way also in this case. We observed that the ground state depends on the rhombicity angle α similar to the previous case. We found that the system has a ferromagnetic ground state for $60° \leqslant \alpha \lesssim 75.67°$, and an antiferromagnetic ground state for $75.67° \lesssim \alpha \leqslant 90°$. The ground state for $\alpha = 60°$ is a twofold degenerate ferromagnetic state, and for $\alpha = 90°$ is a twofold degenerate antiferromagnetic state. We also identified the states with the second lowest energy per dipole, and we summarized the results for $\alpha = 60°$ and $\alpha = 90°$ in Table II.

It is not surprising that taking into consideration only two lines of the rhombic lattice reduces significantly the original symmetry of the system. This can be seen comparing the results in Tables I and II. It is important to note that the two-line system has no continuously degenerate ground state, and thus the ground state is always defined by the

TABLE II. Dipole arrangements corresponding to the lowest two energy values per dipole in a two-dimensional system of dipole moments with identical scalar strength located on two neighboring lines of an infinite rhombic lattice with rhombicity angles $\alpha=60°$ and $\alpha=90°$. The energy is measured in μ^2/a^3 units, where μ is the scalar strength of the dipole moments and a is the lattice constant.

$\alpha=60°$	$E=-2.582$	Twofold degenerate ferromagnetic state
	$E=-2.226$	Twofold degenerate antiferromagnetic state
$\alpha=90°$	$E=-2.477$	Twofold degenerate antiferromagnetic state
	$E=-2.331$	Twofold degenerate ferromagnetic state

Luttinger-Tisza basic arrangement with the lowest eigenvalue. In particular, there is a special ferromagnetic and an antiferromagnetic state, which—depending on the α rhombicity angle—define the ground state.

It can be also seen comparing the results in Tables I and II that the interaction of two neighboring lines almost saturates the long-range dipole-dipole interaction, furthermore it is widely known that dipolar spheres due to dipole-dipole interactions tend to aggregate into chainlike structures (see, for example, Refs. [4,5] and references therein) in which the energies of intrachain interactions are much greater than those of interchain interactions [6]. These confirm that studying a two-line system gives valuable results related to properties of dipole-dipole interaction in general.

IV. THE ROLE OF AN INTERACTION CUTOFF

Brankov and Danchev [3] observed that the ground state of a system of dipoles on an infinite rhombic lattice is sensitive to the dipole-dipole interaction range. An R interaction cutoff distance can be introduced in a natural way with a slight modification of Eq. (4) as

$$\mathbf{A}_{ij}=\sum_{j'\in\Gamma(j),\ j'\neq i}\mathbf{J}_{ij'}|_{r_{ij'}<R}, \tag{9}$$

where $r_{ij'}$ denotes the distance of two dipoles and the $r_{ij'}<R$ constraint represents the fact that the summation must only contain terms corresponding to pairs of spherical dipoles closer to each other than the R cutoff distance. We measure the interaction cutoff value in a units, where a is the lattice constant equal to the particle diameter.

It can be seen from Eq. (2) that the strength of the dipole-dipole interaction decays with $1/r_{ij'}^3$, and thus the above expression for large R can be arbitrarily close to the long-range limit in Eq. (4). This means that the numerical evaluation of Luttinger-Tisza states in general can be based on Eq. (9) if R is big enough.

Our numerical results for the two-line system at R equal to 10^6 (lines) and 8 (points) are shown on Fig. 1. The results corresponding to $R=10^6$ are close to the long-range interaction limit within the numerical errors of 64-bit floating point arithmetic. The upper panel of Fig. 1 shows the lowest energy per dipole of the ferromagnetic and the antiferromagnetic state as function of the rhombicity angle. The lower panel of Fig. 1 shows the angle of the dipoles with respect to the direction of the longest linear dimension of the system.

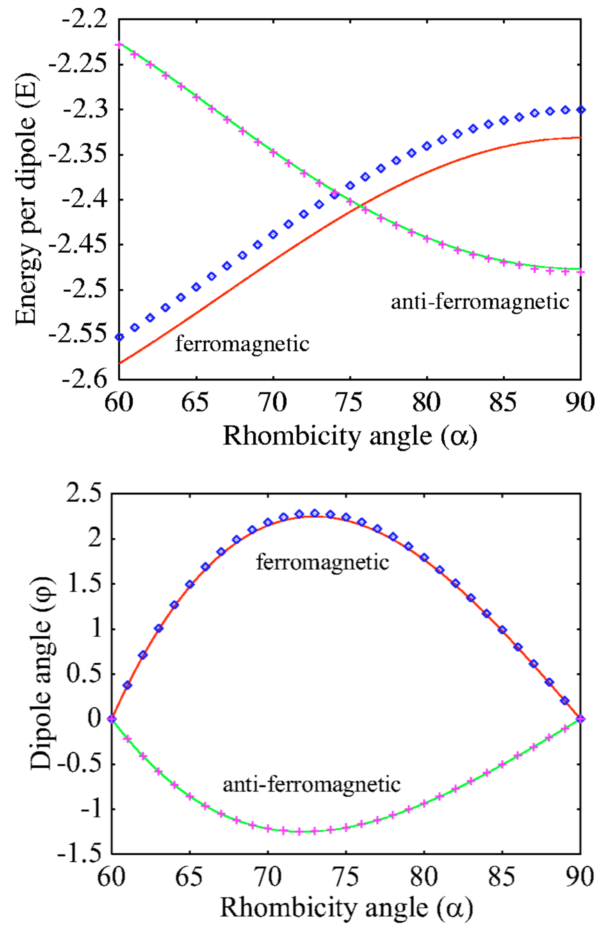

FIG. 1. Numerical results for the two-line system at R equal to 10^6 (lines) and 8 (points). The upper panel shows the lowest energy per dipole of the ferromagnetic and the antiferromagnetic state as function of the rhombicity angle (in degrees). The energy is measured in units μ^2/a^3. The lower panel shows the angle in degrees which the dipoles form with the direction of the longest linear dimension of the system.

Without any calculation, one might expect that in the ground state of the two-line system the dipoles are oriented parallel to the lines in both ferromagnetic and antiferromagnetic states. It is a surprising result of our calculations that this is true only for $\alpha=60°$ and $\alpha=90°$. For any other α the dipoles form a small angle with the lines. However, these angles are less than 2.5° so they cannot be neglected.

Below a certain α, as can be observed in Fig. 1, the ground state of the system corresponds to the ferromagnetic order, and above it to the antiferromagnetic order. The angle at which the transition from a ferromagnetic to an antiferromagnetic ground state takes place is shifted by only 3% due to the cutoff. That the antiferromagnetic state remains almost unchanged is a consequence of the strong coupling of neighboring dipoles of opposite orientation, which makes the interaction cutoff irrelevant.

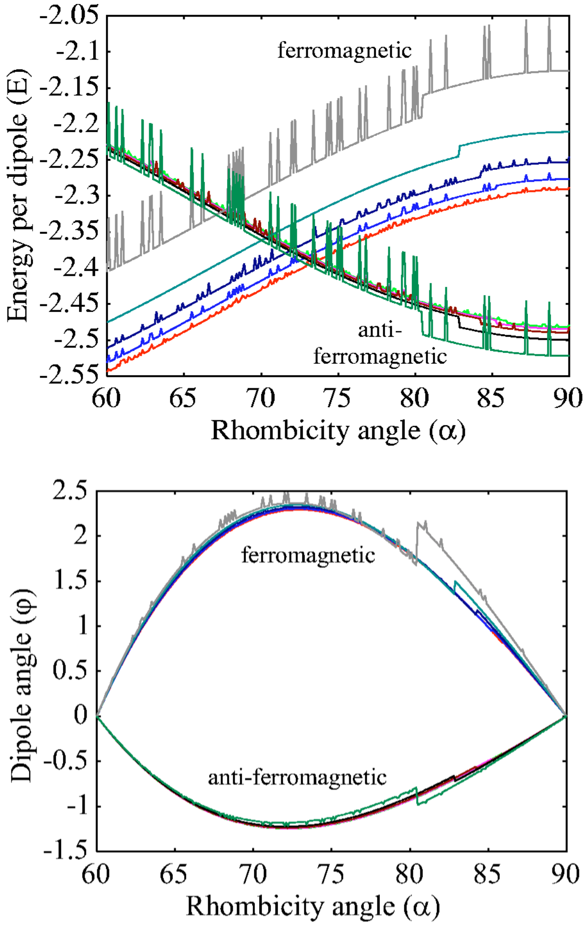

FIG. 2. Numerical results for the two-line system at R equal to 7, 6, 5, 4, and 3. The upper panel shows the lowest energy per dipole of the ferromagnetic and the antiferromagnetic state as function of the rhombicity angle (in degrees). In ferromagnetic states, the lines are shifted upward as R decreases. The lower panel shows the angle in degrees which the dipoles form with the direction of the longest linear dimension of the system.

As expected (see Fig. 1) the ferromagnetic state at $\alpha=60°$ and the antiferromagnetic state at $\alpha=90°$ are stable configurations of the two-line system of dipolar hard spheres independent of R, however as R decreases the crossover point gets slightly shifted.

At low interaction cutoff distances ($R\lesssim 8$), the discrete nature of the system becomes more and more relevant and both the ferromagnetic and the antiferromagnetic energy per dipole begin to exhibit sudden jumps in function of the rhombicity angle (see Fig. 2). As the interaction cutoff decreases, the energy jumps become more and more relevant. This behavior can introduce numerical instabilities in simulations using a badly chosen cutoff distance. It must be noted, however, that one should not overestimate this effect as the energy jumps are relatively small. It is an interesting observation that for some interaction cutoff values (e.g., at $R\approx 4$) the energy per dipole shows significantly lower anomalies.

The ferromagnetic line is shifted upward as R decreases (see Figs. 1 and 2), and according to this the antiferromagnetic state becomes more and more dominant. For large R the ferromagnetic state at $\alpha=60°$ has lower energy per dipole than the antiferromagnetic state at $\alpha=90°$. Our numerical results show that at $R\approx 4$ the situation is reversed, and at $R\approx 2$ the ferromagnetic ground state disappears. Brankov and Danchev [3] found that in case of an infinite rhombic lattice with rhombicity angle $\alpha=60°$ the ferromagnetic ground state disappears at $R\approx 3$.

V. FINITE SIZE CORRECTIONS

We investigated the finite size corrections of the energy per dipole of the two-line system in ferromagnetic and antiferromagnetic states. In these states the infinite system can be decomposed into identical finite segments. If N denotes the number of dipoles per line in a finite segment, the energy per dipole of the infinite system can be written as

$$E=\frac{1}{2N}\left[\frac{1}{2}\sum_{i,j\in\sigma(N),\ i\neq j}\mathbf{s}_i^T\mathbf{J}_{ij}\mathbf{s}_j\right]+\frac{1}{2N}\left[\frac{1}{2}\sum_{i\in\sigma(N),\ j\in\sigma(N)^c}\mathbf{s}_i^T\mathbf{J}_{ij}\mathbf{s}_j\right], \tag{10}$$

where $\sigma(N)$ denotes the dipoles belonging to one segment and $\sigma(N)^c$ denotes the complementer of $\sigma(N)$. The first part in the above expression can be recognized as the energy $\mathcal{E}(N)$ per dipole of a finite segment containing N dipoles per line.

We define the following quantity of energy dimension:

$$\partial\mathcal{E}(N)\equiv N[\mathcal{E}(N)-E]. \tag{11}$$

It can be seen that

$$\partial\mathcal{E}(N)=-\frac{1}{4}\sum_{i\in\sigma(N),\ j\in\sigma(N)^c}\mathbf{s}_i^T\mathbf{J}_{ij}\mathbf{s}_j, \tag{12}$$

where in case of an interaction cutoff R one may add the condition $r_{ij}<R$. As $\mathbf{J}_{ij}$ is proportional to $1/r_{ij}^3$ [see Eq. (2)], one may expect that for large system size $\partial\mathcal{E}(N)$ is independent of N, and thus the limit

$$\partial E=\lim_{N\to\infty}\partial\mathcal{E}(N), \tag{13}$$

exists and is finite. Our numerical investigations confirmed this expectation. The convergence of $\partial\mathcal{E}(N)$ is of order $1/N$ in the ferromagnetic case and is of order $1/N^3$ in the antiferromagnetic case. This proves that the above quantity is well defined. We refer to the above quantity as the finite size coefficient.

Numerical results showing the dependence of the energy per dipole $\mathcal{E}(N)$ of the two-line system on the system size in the long-range limit are presented in Fig. 3. The upper panel shows results for N equal to 10^5 (lines) and 100 (points), and the lower panel shows results for N equal to 10, 8, 7, 6, and 5. Both the ferromagnetic and antiferromagnetic lines are moved upward as N decreases. $\mathcal{E}(N)$ at $N=10^5$ is close to

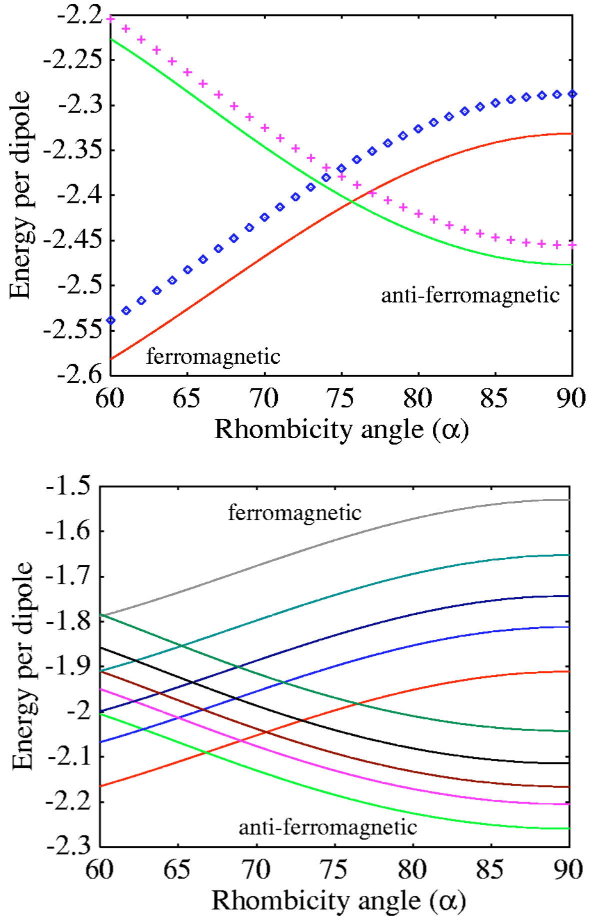

FIG. 3. Numerical results showing the dependence of the energy per dipole of the two-line system on the system size in the long-range limit. The upper panel shows results for N (number of particles per line) equal to 10^5 (lines) and 100 (points). The lower panel shows results for N equal to 10, 8, 7, 6, and 5. Both the ferromagnetic and antiferromagnetic lines are moved upward as N decreases. (Note the different scales on the vertical axes.)

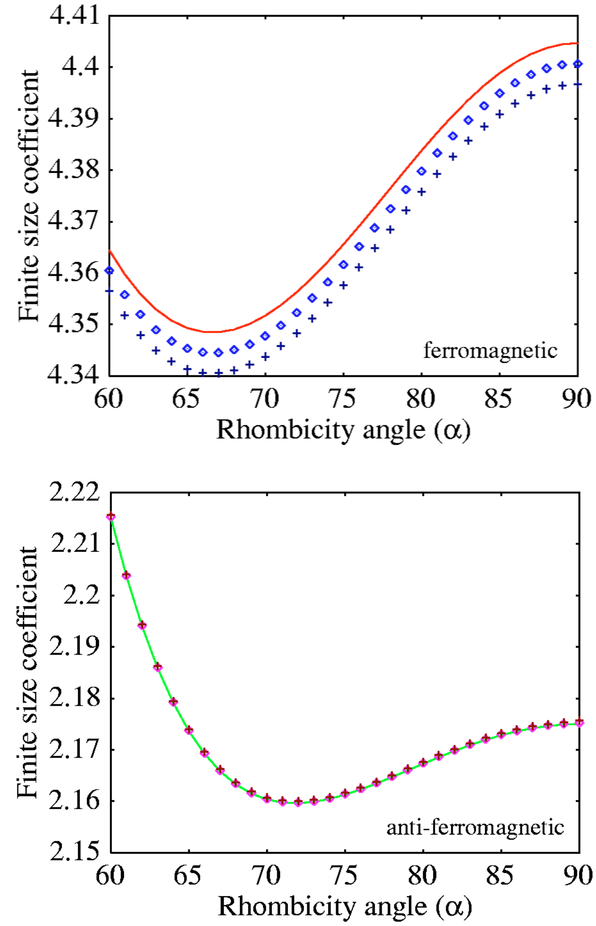

FIG. 4. Numerical results showing the dependence of the finite size coefficient for both ferromagnetic and antiferromagnetic states at $R=10^6$ (lines), for ferromagnetic state at R equal to 1000 and 500 (points), and for antiferromagnetic state at R equal to 100 and 50 (points). The upper panel shows results for the ferromagnetic state and the lower panel shows results for the antiferromagnetic state. The finite size coefficient is measured in units μ^2/a^3. In the ferromagnetic case, the lines are lowered as R decreases. (Note the different scales on the vertical axes.)

the energy per dipole E of the infinite two-line system within the numerical errors of 64-bit floating point arithmetic.

Based on the definition of the finite size coefficient for large N, the energy per dipole of a finite system can be approximated as

$$\mathcal{E}(N) \approx E + \partial E/N. \tag{14}$$

Our numerical investigations show that this approximation is reasonable even for $N \approx 10$. The finite size coefficient of the ferromagnetic state is approximately two times larger than the finite size coefficient of the antiferromagnetic state, and thus the ferromagnetic line moves upward approximately two times faster than the antiferromagnetic line (see Fig. 3). It can be observed that for large N the ferromagnetic state at $\alpha=60°$ has lower energy per dipole than the antiferromagnetic state at $\alpha=90°$. Our numerical results show that at $N=20$ the situation is reversed, and at $N=5$ the ferromagnetic ground state disappears.

VI. DEPENDENCE OF THE FINITE SIZE COEFFICIENT ON INTERACTION CUTOFF

We investigated the dependence of the finite size coefficient on the interaction cutoff distance R. Figure 4 shows the numerical results for ferromagnetic state (upper panel) at R equal to 1000 and 500 (points), for antiferromagnetic state (lower panel) at R equal to 100 and 50 (points), and for both ferromagnetic (upper panel) and antiferromagnetic states (lower panel) at $R=10^6$ (lines). The finite size coefficient is measured in units μ^2/a^3. We calculated its value by evaluating the expression in Eq. (12) at $N=10^5$. The results for $R=10^6$ are close to the long-range limit within the errors of 64-bit floating point arithmetic.

As R is lowered in the antiferromagnetic case, the finite size coefficient remains almost unchanged even for $R \approx 50$, while in the ferromagnetic case it decreases significantly already at $R \approx 1000$. This shows again that the ferromagnetic

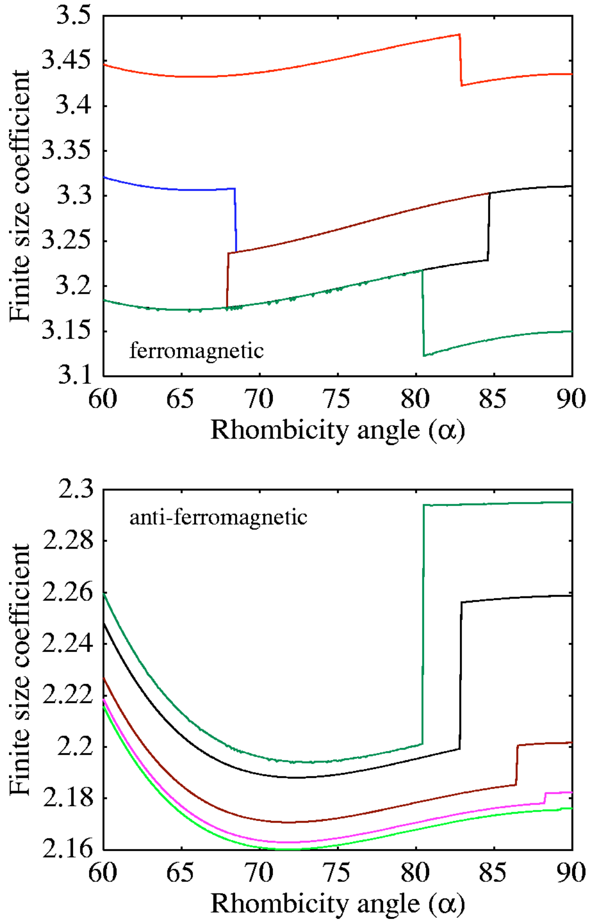

FIG. 5. Numerical results showing the dependence of the finite size coefficient at lower interaction cutoff distances. The upper panel shows the finite size coefficient of the ferromagnetic state as function of the rhombicity angle (in degrees) at R equal to 4, 3.75, 3.5, 3.25, and 3. The lines are lowered as R decreases. The lower panel shows the finite size coefficient of the antiferromagnetic state at R equal to 40, 16, 8, 4, and 3. The lines are shifted upward as R decreases. (Note the different scales on the vertical axes.)

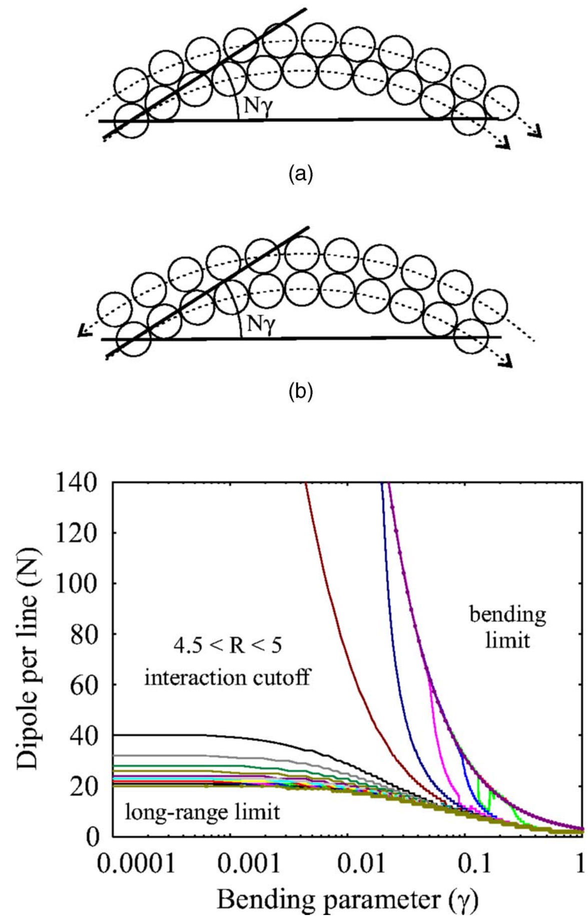

FIG. 6. Numerical results related to bending a two-line system at different interaction cutoff values. The upper panel shows a finite system of two lines of dipolar hard spheres in ferromagnetic and antiferromagnetic states. The lower panel shows (γ,N) state diagrams (see text for description) for R ranging from 2 to ∞. The lines are moved upward and lower as R decreases.

state is much more sensitive to the interaction cutoff than the antiferromagnetic state.

At lower interaction cutoff distances (at $R \lesssim 50$), the discrete nature of the system manifests itself in sudden jumps in the finite size coefficient (see Fig. 5).

The upper panel of Fig. 5 shows the finite size coefficient of the ferromagnetic state as function of the rhombicity angle at R equal to 4, 3.75, 3.5, 3.25, and 3. The lines are lowered as R decreases. The lower panel shows the finite size coefficient of the antiferromagnetic state at R equal to 40, 16, 8, 4, and 3. The lines are shifted upward as R decreases.

The jumps in the finite size coefficient become bigger as the interaction cutoff decreases (see Fig. 5). These jumps are not relevant at large N, but can introduce energy jumps at lower dipole numbers, and thus can introduce local numerical instabilities in simulations, but this effect should not be overestimated as the introduced energy jumps are relatively small.

VII. BENDING TWO LINES OF MAGNETIC PARTICLES

The finite size behavior presented before gives a good description of finite dipole systems at large N, but it is not too helpful at lower N. For a better understanding of the system, we studied numerically finite systems (at small N) investigating the effect of bending two lines of dipolar hard spheres in ferromagnetic and antiferromagnetic states [see Figs. 6(a) and 6(b)]. In unbent case these correspond to the previously studied ferromagnetic state at $\alpha=60°$ and antiferromagnetic state at $\alpha=90°$. We introduce the γ bending parameter and define the bent system as composed of particles placed on an arc of angle $2N\gamma$ with dipole vectors tangential to the arc [see definition of γ on Figs. 6(a) and 6(b)]. This definition involves a so called ''bending limit'' as the arc's angle is limited to 2π, and thus γ must satisfy the $\gamma \leqslant \pi/N$ condition.

Our numerical results show that for bending either a ferromagnetic or antiferromagnetic two-line system, some physical effort is needed. We observed that the two-line system in ferromagnetic state can be bent easily than in the corresponding antiferromagnetic state. This is a consequence of the strong coupling of neighboring dipoles oriented antiparallelly. We also observed that as the antiferromagnetic state is bent it becomes less and less stable. Figure 6 shows numerical results related to bending a two-line system at different interaction cutoff values. As function of the bending parameter γ and system size N, we compared the energy per dipole of the ferromagnetic and antiferromagnetic states and identified the points (γ,N) at which these two states are energetically equivalent. We repeated this procedure at different R interaction cutoff values. The lower panel of Fig. 6 shows corresponding (γ,N) state diagrams.

In the long-range limit for small system size and low bending parameter, the antiferromagnetic state has lower energy per dipole. This is in accordance with our previous results, and remains valid up to $R\approx 5$. It is a surprising result that this behavior changes rapidly for interaction cutoff values between 4 and 5. For $R\lesssim 4$, the antiferromagnetic state remains more stable at large N values even for large bending parameters. This means that at this point the general characteristics of an arbitrary dipole system is substantially changed. Based on Fig. 6 and on our previous results, we argue that $R\approx 5$ is a reasonable choice for dipole-dipole interaction cutoff for two-dimensional systems of dipolar hard spheres, if one is interested in local ordering.

VIII. CONCLUSIONS

Based on the fact that dipolar spheres due to dipole-dipole interactions tend to aggregate into chainlike structures in which the ratio of interchain-to-intrachain interactions is small, and that moreover the interaction of parallel chains of dipolar hard spheres almost saturates the dipole-dipole interaction in two-dimensional dense systems, we argue that the study of a dipolar two-line system gives valuable results for general dipolar particle systems.

Theoretical results and simulations show two relevant dipole arrangements: (1) a ferromagnetic state with dipoles organized in a triangular lattice and (2) an antiferromagnetic state with dipoles organized in a square lattice. Numerical results on a dipolar two-line system show that the ferromagnetic state is much more sensitive to the interaction cutoff than the corresponding antiferromagnetic state. This can be explained by the efficient coupling of dipoles oriented antiparallelly. For $R\gtrsim 8$, there is no substantial change in the energetical balance of the ferromagnetic and antiferromagnetic states and the ferromagnetic state slightly dominates over the antiferromagnetic state, while the situation is changed rapidly for lower interaction cutoff values, leading to the disappearance of the ferromagnetic ground state. Our numerical results show that the ferromagnetic ground state disappears at $R\approx 2$. Brankov and Danchev [3] found that in case of an infinite triangular lattice the ferromagnetic ground state disappears at $R\approx 3$.

For characterizing the finite size behavior of the two-line system, we introduced a finite size coefficient and observed that it is sensitive to the interaction cutoff for both ferromagnetic and antiferromagnetic states. We also observed that at low interaction cutoff values the discrete nature of the system leads to small energetical anomalies. These anomalies increase as the interaction cutoff is lowered and can introduce instabilities in numerical simulations. We argue, however, that this effect becomes relevant only at first or second neighbor interaction and it can be neglected at higher interaction cutoff values.

Finally, we studied the effects of bending ferromagnetic and antiferromagnetic two-line systems. We characterized the bending of a two-line system with the parameter γ, while N is the number of dipoles per line. We created (γ,N) state diagrams separating energetically favorable ferromagnetic and antiferromagnetic states. We observed that there is a substantial change of these state diagrams for $R\lesssim 4$, and—in accordance with our previous results—we argue that $R\approx 5$ is a reasonable choice for dipole-dipole interaction cutoff in two-dimensional dipolar hard sphere systems, if one is interested in local ordering.

It is a surprising result that the reasonable interaction cutoff is independent of the strength of the dipole-dipole interaction and the particle size. This is a consequence of the fact that there are two relevant dipole arrangements (a ferromagnetic and an antiferromagnetic), and their energetical balance can be reduced to geometrical factors. If there are any other interactions in the system (e.g., friction), this study must be revisited and it may turn out that the reasonable interaction cutoff is dependent on the interaction strength and particle size. We envision, however, that in some cases (e.g., in case of friction) the presence of another short-range interaction keeps or even lowers the value of the reasonable interaction cutoff found above.

In this paper, we focused on the local dipole ordering. In the ferromagnetic case, however, domain structures become important, which can reduce external magnetic stray fields. These global structures should depend on the long-range part of the interaction. For magnetic granular systems, the formation of such domains may be hindered, e.g., by friction, though, as it requires the reorientation of particles.

We did not address the response to an external magnetic field. The reason is that long-range correlations and hence the response functions will be more strongly affected by a dipolar interaction cutoff than the local structures and energy densities considered in this paper. In principle, an Ewald summation method [7,8] would allow us to explore the response properties in the thermodynamic limit in terms of large but finite systems with periodic boundary conditions. However, here again friction may be an important factor to be taken into account: An external magnetic field trying to orient the magnetic moments would exert a stress on the particle arrangement, if particle rotations would be hindered by friction. Then the magnetic response of the system would crucially depend on the relative strength of the magnetic anisotropy of the particles, i.e., the coupling between particle and magnetic moment orientations, and friction forces between the particles.

ACKNOWLEDGMENTS

This research was carried out within the framework of the ‘‘Center for Applied Mathematics and Computational Physics’’ of the BUTE, and it was supported by BMBF, Grant No. HUN 02/011, and Hungarian Grant No. OTKA T035028.

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