A Note on Stable States of Dipolar Systems at Low Temperatures

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1 Introduction

In the past several years, many important innovations in nanotechnology were made. Today it becomes possible to make nanosize magnetic particles, and development of high storage-density magnetic device is desired. Though dipole interaction plays the main role in these magnetic particle systems, there is little systematic study of dipolar systems \cite{1}.

Luttinger and Tisza (LT) discussed the ground states of three-dimensional dipole cubic lattices in their pioneering work \cite{2}. They assumed $\Gamma^2$ symmetry that ground states are constructed by the translations of the dipoles on $2 \times 2 \times 2$ cubic unit, and examined its dipole configurations. In addition, since the dipole interaction energy is a quadratic form, even though dipole moment has $O(3)$ symmetry, it is sufficient to consider only eight arrays for each component of the moment. We define eight arrays by

$$A_{b_x b_y b_z}(l) = (-1)^{b_x l_x + b_y l_y + b_z l_z}, \quad (b_x, b_y, b_z, l_x, l_y, l_z = 0, 1). \quad (1)$$

Here $b_x, b_y, b_z$ are indices for a dipole configuration, and an array $(l_x, l_y, l_z)$ represents a corner of the unit cube. An eight-dimensional vector $A$ corresponds to $X$, $Y$, or $Z$ depending on its component of moments. In Fig. 1, we show the eight basic arrays. For the simple cubic (SC) lattice, Luttinger and Tisza predicted the columnar antiferromagnetic state,

$$aX_{011} + bY_{101} + cZ_{110}, \quad (a^2 + b^2 + c^2 = 1), \quad (2)$$

has the lowest energy. For the body centered cubic (BCC) lattice, lowest energy states predicted by LT are tabulated in Table 1.

2 Results

In order to examine the lowest energy states predicted by LT, we simulate dipolar systems on the SC lattice and the BCC lattice at low temperatures. The Hamiltonian for system size $L$ is given by

$$H = \sum_{n_x, n_y, n_z} \sum_{i<j} \frac{\mu_i \cdot \mu_j}{(r_{ij} + nL)^3} - 3 \frac{(\mu_i \cdot (r_{ij} + nL))(\mu_j \cdot (r_{ij} + nL))}{(r_{ij} + nL)^5}. \quad (3)$$
Table 1. Lowest energy states are tabulated below. The states of lattice points (l.p.) and body centers (b.c.) are commutative. The condition, \(a^2 + b^2 + c^2 = 1\), is satisfied for the first line, and others satisfy the condition, \(a^2 + b^2 = 1\).

|                      | At l.p.(b.c.) | At b.c.(l.p.) |
|----------------------|--------------|--------------|
| \(aX_{101} + bY_{110} + cZ_{011}\) | \(bX_{110} + cY_{011} + aZ_{101}\) |
| \(aX_{101} + bZ_{101}\)               | \(bX_{101} + aZ_{101}\)           |
| \(aY_{110} + bX_{110}\)               | \(bY_{110} + aX_{110}\)           |
| \(aZ_{011} + bY_{011}\)               | \(bZ_{011} + aY_{011}\)           |

We employed heat bath method for Monte Carlo spin update, and Ewald summation method [3–5] is used for counting long range dipolar interaction. As expected, for the SC and BCC of \(L = 2\) lattice systems, dipole configurations produced by simulations well agree with the prediction by LT. The dipole configurations are consistent with the lowest energy state described in (2) for the SC of \(L \geq 4\) lattices. On the other hand, for the BCC of \(L \geq 4\) lattices, the stable dipole configuration that we obtained are different from the states in Table 1, which is shown Fig. 2(b). The dipole configuration in Fig. 2(b) is characterized by stacked dipole layers in which all dipoles align in the same direction. Such stacked dipole layer configurations can be constructed from LT’s predicted state, although ferromagnetic layer is single (Fig. 2(a)), but not double as in Fig. 2(b). We calculate the zero temperature internal energy as a function of thickness of ferromagnetic layer to check our result of MC simulation. The results are shown in Table 2. At least till \(L = 8\), the internal energy becomes lower as the thickness of ferromagnetic layer increases. Furthermore the values of these internal energies are lower than that
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Fig. 2. Stable states for the body centered cubic lattice. (a) A stable state which is consistent with LT’s predicted ground states. (b) A stable state obtained by MC simulation which is not consistent with the states in Table 1.

Table 2. The zero temperature internal energy dependence on thickness of ferromagnetic layer.

| Thickness of FM layer | $L = 2$ | $L = 4$ | $L = 6$ | $L = 8$ |
|-----------------------|--------|--------|--------|--------|
| 1                     | -7.94368 | -7.94368 | -7.94368 | -7.94368 |
| 2                     | —       | -8.16968 | —       | -8.16968 |
| 3                     | —       | —       | -8.23896 | —       |
| 4                     | —       | —       | —       | -8.27087 |

of LT calculated. This means that one cannot assume $I^2$ symmetry to dipole systems on the BCC lattice.

We set up a simplified model to obtain an intuitive understanding of stable states of dipolar systems at low temperatures. In some cases, consideration of low dimensional system provides insights into physics of the system. So we start looking at two-dimensional systems.

Typical ground states of the square lattice and triangular systems are depicted in Fig. 3. In order to investigate the stable state at low temperatures, we simplify the model as follows: we treat the system as interacting ferromagnetic dipole chain system, and ferromagnetic chain can take only two values (rightward or leftward as in Fig. 3). Then, Hamiltonian becomes

$$\mathcal{H} = \sum_{i \neq j} f(r_{ij}) \sigma_i \sigma_j, \quad (\sigma = \pm 1),$$

that is, the model is mapped to a one-dimensional Ising chain with long-range interaction $f(r)$. We estimate $f(r)$ by numerical calculation with $L/2$ cut off. At the zero temperature internal energy of the square lattice and the triangular lattice was calculated for several ferromagnetic dipole chain configurations. For the square lattice, antiferromagnetic state is the most stable, whereas for the triangular lattice, antiparallel two ferromagnetic domains structure is the most stable. This difference comes from the shape of $f(r)$, that is, $f(r)$ for square lattice is positive and monotonically decreas-
ing function. For the triangular lattice, on the other hand, except for nearest neighbor, \( f(r) \) is positive and its absolute value decreases monotonically. That is to say, ordering in the same direction gains energy in short range, while ordering in opposite direction gains energy in long range; as a consequence, ferromagnetic domains structure is realized at low temperatures.

Since the simplified model succeeded in explaining dipole configurations on two-dimensional lattices at low temperatures, we extend the model to three-dimensional systems. In Fig. 4, we show typical ground states for the SC lattice and the BCC lattice. If one notes dipole configuration on the gray sheet is merely reversed configuration on the white sheet, it is natural to apply the same tactics which is employed in the two-dimensional system to the three-dimensional systems: there are magnetic sheets interacting each other, and a magnetic sheet can take only two values as like Ising variable. Then, we obtain simplified Hamiltonian, \( \mathcal{H} = \sum_{i \neq j} f(r_{ij}) \sigma_i \sigma_j \). Again, the model is mapped to a one-dimensional Ising chain with long-range interaction.

In Fig. 5, we show the results of the SC lattice and the BCC lattice. The result of the SC lattice supports the one of LT. On the other hand, the result of the BCC lattice is not consistent with the LT result, but with our results of MC simulation. It is notable that ferromagnetic domains structure is stable for the BCC lattice, even though interaction \( f(r) \) is positive. We also examined \( L = 64 \) chain model, and we confirmed the four ferromagnetic domains structure is the most stable.
Fig. 5. (a) The internal energy at each site (layer) of the SC lattice ($L = 16$). The internal energy per site is $E_{FM} = 0.2437$, $E_{AF} = -0.2437$, and $E_{MD} = 0.1907$ for ferromagnetic dipole configuration, antiferromagnetic dipole configuration, and magnetic domain dipole configuration respectively. (b) The internal energy at each site (layer) of the BCC lattice ($L = 16$). The internal energy per site is $E_{FM} = 3.9016$, $E_{AF} = 0.1488$, and $E_{MD} = -0.4508$ for each dipole configuration.

3 Summary

To summarize, we showed “antiferromagnetic structure” is stable for the square lattice and the SC lattice as LT predicted. On the other hand, for the triangular lattice and the BCC lattice, magnetic domain structure is stable. Theoretical approach which assumes $P^2$ symmetry fails in the triangular lattice and the BCC lattice. For future works, examination of the face centered cubic lattice and estimation of critical temperatures and exponents for several lattices are remained.

References

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