

Since X_{SPS} in this formula is calculated only from the pairs whose graph variables are one, it can be calculated with very short computational time as \tilde{E}' and $\frac{\partial \tilde{E}'}{\partial \beta}$ in eqs. (32) and (33) are.

V. THE CASE WHEN LONG-RANGE INTERACTIONS AND SHORT-RANGE INTERACTIONS COEXIST

When long-range interactions $\{V_{ij}^{(L)}\}$ and short-range interactions $\{V_{ij}^{(S)}\}$ coexist, we do not need to use the SCO method for short-range interactions because it does not reduce the computational time significantly. In other words, we can switch $V_{ij}^{(L)}$ to 0 or $\tilde{V}_{ij}^{(L)}$ with $V_{ij}^{(S)}$ unchanged. This can be realized by setting $\tilde{V}_{ij}^{(L)} = 0$ and $\tilde{V}_{ij}^{(S)} = V_{ij}^{(S)}$. In this case, we can decompose E_{const} , \tilde{E} , $\frac{\partial \tilde{E}}{\partial \beta}$, and X_{SPS} in eqs. (27), (28), (29), and (40) as

$$E_{\text{const}} = E_{\text{const}}^{(L)} + E_{\text{const}}^{(S)}, \quad (43a)$$

$$\tilde{E} = \tilde{E}^{(L)} + \tilde{E}^{(S)}, \quad (43b)$$

$$\frac{\partial \tilde{E}}{\partial \beta} = \frac{\partial \tilde{E}^{(L)}}{\partial \beta} + \frac{\partial \tilde{E}^{(S)}}{\partial \beta}, \quad (43c)$$

$$X_{\text{SPS}} = X_{\text{SPS}}^{(L)} \times X_{\text{SPS}}^{(S)}, \quad (43d)$$

where the first terms and the second terms in the right hand sides denote contributions from long-range interactions and those from short-range interactions, respectively. As we have already mentioned, the first terms are given by eqs. (31), (32), (33), and (42), respectively. On the other hand, by substituting $\tilde{V}_{kl} = V_{kl}^{(S)}$ and $\Delta V_{kl}^* = 0$ into eqs. (27), (28), (29), and (40), we readily obtain

$$E_{\text{const}}^{(S)} = 0, \quad (44a)$$

$$\tilde{E}^{(S)} = - \sum_{\langle kl \rangle} V_{kl}^{(S)}, \quad (44b)$$

$$\frac{\partial \tilde{E}^{(S)}}{\partial \beta} = 0, \quad (44c)$$

$$X_{\text{SPS}}^{(S)} = \prod_{\langle kl \rangle} \exp[(\beta_m - \beta_n)(V_{kl}(\mathbf{S}_k, \mathbf{S}_l) - V_{kl}(\mathbf{S}'_k, \mathbf{S}'_l))] = X_{\text{B}}^{(S)}, \quad (44d)$$

where we have used the fact that all the potentials are switched to \tilde{V}_{kl} . Note that $P_{kl} = 1$ when $\tilde{V}_{kl} = V_{kl}$ and $\Delta V_{ij}^* = 0$. These results are quite natural because they coincide with the results in the usual MC procedure.

VI. NUMERICAL TESTS

A. Internal energy and heat capacity measurements

In order to check the validity of the formulae for internal energy and heat capacity measurements, we perform

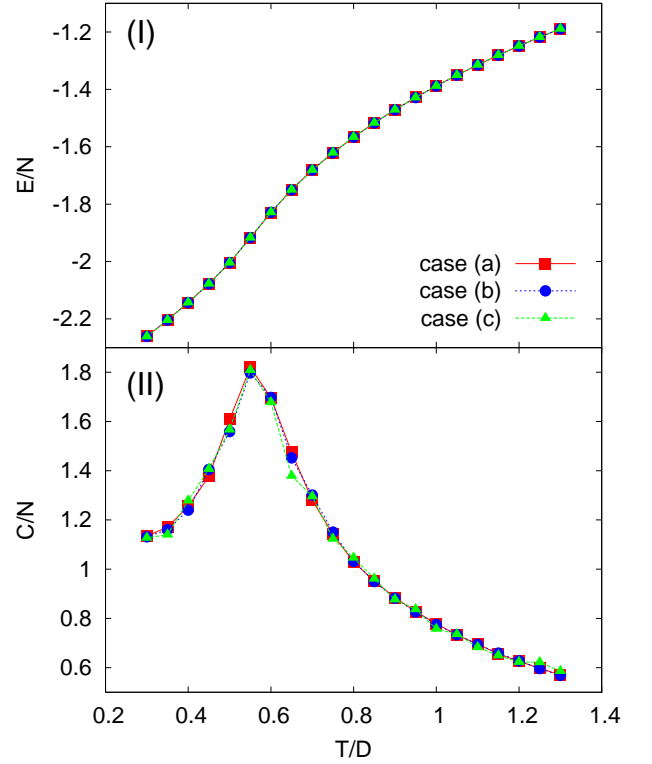


FIG. 1: (Color online) Temperature dependence of (I) internal energy E/N and (II) heat capacity C/N in the purely dipolar system. Simulated annealing method is used for the measurement. The size N is 10^3 . Measurements are done in the three cases (see text).

MC simulations of a three dimensional magnetic dipolar system on a L^3 simple cubic lattice. The boundary condition is open. The Hamiltonian of the system is described as

$$\mathcal{H} = \mathcal{H}_{\text{dip}} = D \sum_{i < j} \left[\frac{\mathbf{S}_i \cdot \mathbf{S}_j - 3(\mathbf{S}_i \cdot \mathbf{r}_{ij})(\mathbf{S}_j \cdot \mathbf{r}_{ij})}{r_{ij}^3} \right], \quad (45)$$

where \mathbf{S}_i is a classical Heisenberg spin of $|\mathbf{S}_i| = 1$, \mathbf{r}_{ij} is the vector spanned from a site i to j in the unit of the lattice constant a , $r_{ij} = |\mathbf{r}_{ij}|$, and $D = (g\mu_B S)/a^3$. We hereafter call the system *purely dipolar system*.

In simulations with the SCO method, we regard each term in the right hand side of eq. (45) as V_{ij} . Since $\tilde{V}_{ij} = 0$ in the SCO method, ΔV_{ij} defined by eq. (3) is equal to V_{ij} . Interaction V_{ij} has the maximum value $2D/r_{ij}^3$ when \mathbf{S}_i and \mathbf{S}_j are anti-parallel along \mathbf{r}_{ij} . We therefore set ΔV_{ij}^* , which should be equal to or greater than ΔV_{ij} over all \mathbf{S}_i and \mathbf{S}_j , to $2D/r_{ij}^3$. By substituting these into eq. (2), we obtain

$$P_{ij} = \exp \left[\beta D \left\{ \frac{\mathbf{S}_i \cdot \mathbf{S}_j - 3(\mathbf{S}_i \cdot \mathbf{r}_{ij})(\mathbf{S}_j \cdot \mathbf{r}_{ij}) - 2}{r_{ij}^3} \right\} \right], \quad (46)$$