

## Reply to “Comment on ‘Self-assembly of magnetic balls: From chains to tubes’ ”

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The authors of the Comment [Phys. Rev. E **91**, 057201 (2015)] propose compact round clusters as, energetically, better candidates than stacked rings found in Messina *et al.* [Phys. Rev. E **89**, 011202 (2014)] (forming *open* tubes) at a pretty large number of constitutive magnets, typically for  $N \gtrsim 1300$ . Our new findings show that elongated rodlike structures can even outmatch the reported structures in Friedrich *et al.* [Phys. Rev. E **91**, 057201 (2015)] and in Messina *et al.* [Phys. Rev. E **89**, 011202 (2014)] from typically  $N \gtrsim 460$ .

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The main finding in the original article [1] deals with the newly discovered phase consisting of stacked rings that already rules when  $N > 14$ . We then used this phase to explore the regime of very large  $N$  in Ref. [1] that would not be possible by brute force minimization techniques. Our main conclusions in Ref. [1] still hold, except when  $N$  is very large. As a matter of fact, in this delicate regime, it is not possible to give a definite answer. This being said, in this Reply we shed light on the possibility of better geometries that yield to lower energies at large finite  $N$ .

In our numerical approach, the reduced potential energy of interaction  $U_N^{\text{tot}}$  has been minimized by evolving transient configurations on a discrete lattice [triangular lattices on the  $(x, z)$  and  $(y, z)$  planes] using a genetic algorithm. The genetic algorithm is especially well suited here since the objective function is discrete, high dimensional, and possesses an abundance of local minima.

In the present Reply, we were inspired by the idea that in the limit of  $N \rightarrow \infty$ , i.e., in the *bulk*, crystalline structures

with *parallel* dipoles are favored. Upon investigating a similar range of numbers of magnets (up to  $N \simeq 3000$ ) with that considered in Ref. [2], we found three relevant structures that are illustrated in Fig. 1. Thereby, straight long chains made up of parallel dipoles (here in the  $z$  direction) bind to build a rodlike structure with a narrow rectangular section, see Fig. 1. Interestingly, the beads do not locally exhibit a face centered cubic (fcc) packing, that is in qualitative contrast with the local fcc arrangement found in Ref. [2]. Hence these reported rodlike structures in Fig. 1, although dense, do not correspond to the highest (local) packing fraction.

To be more quantitative, we now monitor the reduced energy per magnet  $u_N$  for the filled tubular structures described in Fig. 1 as a function of  $N$ , see Fig. 2. Upon increasing  $N$ , the base of the rod tends to increase in size, see Fig. 1. Note that  $(2 \times 2)$ -row base structures are always beaten by larger bases. More specifically, for  $N = 767$  the  $(3 \times 3)$ -row rod wins with  $u_{767} = -2.773$ . For  $N = 1289$ , it is the  $(3 \times 4)$ -row rod that wins with  $u_{1289} = -2.810$ . At larger  $N$ , we see

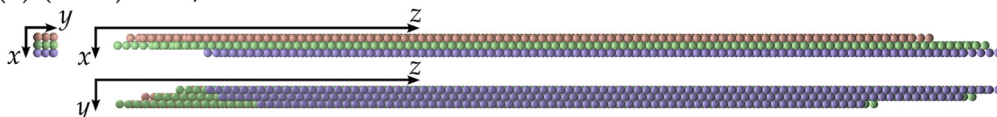
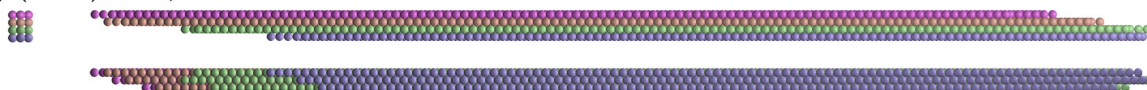
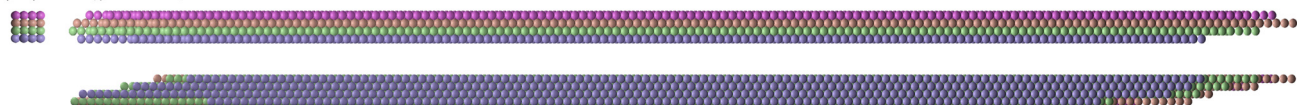
(a)  $(3 \times 3)$  row,  $N=767$ (b)  $(3 \times 4)$  row,  $N=1289$ (c)  $(4 \times 4)$  row,  $N=2093$ 

FIG. 1. (Color online) Typical rodlike structures made up of straight chains. A top view as well as two side views are provided in order to properly visualize the characteristics of the microstructures. (a)  $N = 767$  with a  $(3 \times 3)$ -row base, (b)  $N = 1289$  with a  $(3 \times 4)$ -row base, and (c)  $N = 2093$  with a  $(4 \times 4)$ -row base.

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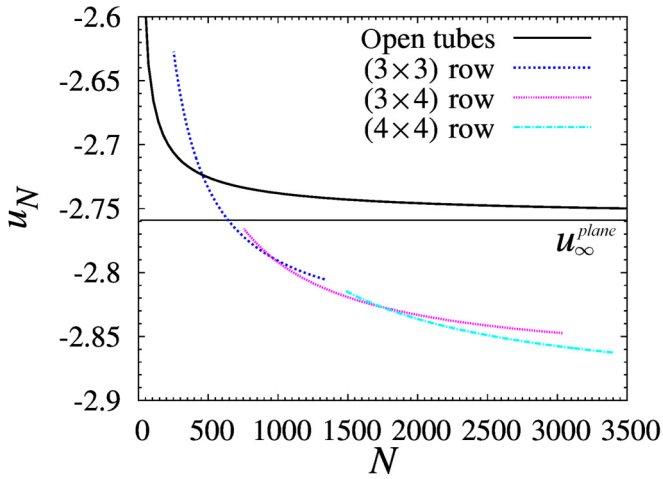


FIG. 2. (Color online) Reduced energy per magnet  $u_N$  for different rodlike structures, see Fig. 1 for the corresponding microstructures. Open tubes as considered in the original paper [1] are also shown. The constant value  $u_\infty^{\text{plane}} = -2.759$  corresponds to an infinite triangular lattice with parallel dipoles pointing in the dense direction [1].

the lowest energy for a  $(4 \times 4)$ -row rod with  $u_{2093} = -2.838$  and  $u_{3055} = -2.858$ . These four energy values have to be

compared with those stemming from the Comment [2]:  $-2.759$ ,  $-2.78$ ,  $-2.82$ , and  $-2.84$ , respectively. Rodlike structures are energetically comparable and even better than round clusters reported in Ref. [2] by roughly about 1%, which is non-negligible.

To summarize, we confirm, in agreement with the Comment, that at large  $N$  empty tubular structures made up of stacked rings can be easily beaten energetically. The pathway proposed in Ref. [2] is an interesting approach to understand the energy behavior for densely packed structures. This being said, strong anisotropic pair interactions can lead to counterintuitive results as again exemplified here. At this point we cannot firmly state that we found the global minima, but for sure we present an interesting new phase in the regime of large but finite  $N$ . Further insight could be gained by looking at the bulk case ( $N \rightarrow \infty$ ) in more detail to confirm the current findings and/or provide new ideas about the trends of the phase behavior at large finite  $N$ . Such a study will be properly addressed in a separate paper.

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[1] R. Messina, L. A. Khalil, and I. Stanković, *Phys. Rev. E* **89**, 011202 (2014).

[2] T. Friedrich, I. Rehberg, and R. Richter, previous paper, *Phys. Rev. E* **91**, 057201 (2015).