Comment on "Self-assembly of magnetic balls: From chains to tubes"

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The paper states that magnetic balls preferably assemble in a tube geometry if the number of particles exceeds $N \ge 14$. We find that for substantially higher particle counts, such as N > 1300, a round cluster of densely packed magnetic balls with an fcc lattice can outmatch the described tube structure.

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The paper [1] considers the problem of stable arrangements of magnetic balls (with diameter d). In particular, it demonstrates that a tube geometry is superior over a ring arrangement, provided that the number of particles N is larger than 15. It concludes: "The essential finding is the stacking of rings with curling dipole vectors as minimal energy configurations." That statement is correct but could be misinterpreted: Namely, in the sense that for sufficiently large N the tubular stacks described with the reduced potential energy u_N (defined by Eq. (2) of Ref. [1]) of about -2.759 are the energetically favored configuration.

Playing with those magnetic balls experimentally (as indicated in the lower left inset of Fig. 1), however, triggers the idea that a close packing in the form of some three-dimensional cluster might be superior in that respect.

To test this idea, we have numerically checked the reduced potential energy $u_N(R)$ of round clusters of densely packed spheres in a face-centered cubic arrangement. The magnets are centered around the middle ball within a radius R.

The energy is minimized by adjusting the orientations of the dipoles via a mixed relaxation strategy switching among three procedures: (i) to follow the torques on each dipole in an overdamped fashion, (ii) to adjust each dipole according to the local field sequentially, and (iii) to perturb all dipole orientations slightly in order to check the stability of the solution. With this strategy, the configuration ends up in a local energy minimum, but it cannot be guaranteed that this is also the global minimum.

The resulting upper bound of the energy is displayed in Fig. 1, together with two corresponding dipole configurations. Although indeed $u_N(R < 5d) > -2.759$ (R = 5dcorresponds to N = 767), sufficiently large clusters are energetically favored with respect to the tube configuration:



FIG. 1. An upper bound of the reduced potential energy as a function of the cluster size. The circles indicate the value obtained by the numerical procedure, the gray connecting curves should guide the eye, the short dashed line indicates the energy for an infinitely long chain for comparison (Eq. (4) of Ref. [1]), and the long dashed line is the asymptotic value for a tube (Eq. (8) of Ref. [1]). The lower left inset shows the experimental realization of a cluster with R = d = 5 mm (N = 13). The inset above is the corresponding computed dipole arrangement. The inset on the right hand side shows N = 767 dipoles obtained for R = 5d.

 $u_N(6d) < -2.78$, (R = 6d corresponds to N = 1289), and the energy becomes even smaller for bigger clusters: $u_N(7d) < -2.82$ (N = 2093), $u_N(8d) < -2.84$ (N = 3055), etc.

Thus it is safe to conclude that a dense packing of magnetic balls is energetically favored over a tube arrangement, provided that N > 1300.

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