Comment on “Magnetism of Nanowires Driven by Novel Even-Odd Effects”

In a recent Letter [1], S. Lounis et al. find that the ground state of finite antiferromagnetic nanowires deposited on ferromagnets depends on the parity of the number \( N \) of atoms and that a collinear-noncollinear transition exists for odd \( N \). Authors use \textit{ab initio} results and a Heisenberg model, which is studied numerically with an iterative scheme. In this Comment we argue that the Heisenberg model can much easier be investigated in terms of a two-dimensional map, which allows to find an analytic expression for the transition length, a central result of Ref. [1] (see their Fig. 3).

Heisenberg model in Ref. [1] corresponds to Eq. (1) of Ref. [2] for \( H_A = 0 \), which describes antiferromagnetic superlattices in a magnetic field. If we introduce the variable \( s_n = \sin(\theta_n - \theta_{n-1}) \), minimization of

\[
H = |J_1| \sum_{i=1}^{N-1} \cos(\theta_i - \theta_{i+1}) - J_2 \sum_{i=1}^{N} \cos \theta_i
\]

\[
s_{n+1} = s_n - h \sin \theta_n, \quad \theta_{n+1} = \theta_n + \sin^{-1}(s_{n+1}) \tag{1}
\]

where \( h = J_2/|J_1| \). This is an iterative two-dimensional map whose fixed points of order two \((s_{n+2} = s_n \text{ and } \theta_{n+2} = \theta_n)\) correspond to the ferrimagnetic (FI) configuration \((0,0) \leftrightarrow (\pi,0)\) and to the bulk spin-flop state \(((\bar{\theta}, \sin 2\bar{\theta}) \leftrightarrow (-\bar{\theta}, -\sin 2\bar{\theta})\), with \(\cos \bar{\theta} = h/4\). In Fig. 1 we plot the evolution of the map for different initial conditions and \( h = 0.376 \), the special value considered in [1].

Boundary conditions for chains of \( N \) atoms are taken into account [2] imposing \( s_1 = 0 = s_{N+1} \). The determination of the ground state therefore corresponds to find the value \( \theta_1 \) such that iterating the map \( N \) times from \((\theta_1,0)\) we get a point on the axis \( s = 0 \). The \( N \) values \( \theta_1, \ldots, \theta_N \) then give the sought-after configuration. In Fig. 1 we also plot the first \( N \) steps of the map evolution giving the ground states for \( N = 9 \) (red squares) and \( N = 10 \) (blue circles), showing different behaviors for odd and even \( N \). This difference is also visible from Fig. 6 (\( N = 52 \)) and Fig. 10 (\( N = 53 \)) in Ref. [3]. Different ground states also reflect on different behaviors for the spin wave excitations [4].

The existence of a minimum length to get a non-collinear configuration for odd \( N \) is clear from the inset of Fig. 2 where we plot \( s_{N+1}(\theta_1) \), assuming \( s_1 = 0 \), for different values of \( N \). Arrow points to the value \( \theta_1 \) for the first atom of the \( N = 9 \) chain.

In conclusion, the map method allows to have a direct graphical overview of the system, to get equilibrium configurations in a fast and reliable way (Fig. 1), and to find the analytical expression for the transition length (Fig. 2).

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