Mills's model of a surface spin-flop transition

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The coupled equations which result from Mills's model of a surface spin-flop (SSF) transition in an antiferromagnet in a uniform external magnetic field are solved exactly on a computer. The results are compared with Keffer's approximate analytical result. Also, an example of an SSF state is presented for the case when the magnetic field is confined to several layers of the crystal at the surface.

I. INTRODUCTION

Sometime ago Mills[1] analyzed a model of a semi-infinite antiferromagnet on which is imposed a uniform magnetic field. He searched for static spin structures in which the energy was a minimum. For small external magnetic fields, the lowest-energy state is the normal aligned antiferromagnetic (AF) state. Mills has demonstrated that as the magnetic field is increased the minimum-energy structure becomes one in which the spins near the surface turn through a larger angle than the spins deeper down inside the crystal. This state is called the surface spin-flop (SSF) state. The angle at which the spin turns goes to zero as its distance from the surface increases. But the angle between neighboring spins on adjacent layers remains very close to π throughout the crystal. As the magnetic field is further increased the SSF state changes abruptly to what is called the bulk spin-flop (SF) state. The SSF-SF transition is first order since the energy of the state also changes abruptly. After Mills's work Keffer[2] analyzed the same model more accurately and obtained a more reasonable scenario for what was happening to the minimum-energy structure as the magnetic field was increased. Mills later suggested to one of the present authors that it would be of interest to see if a ferromagnetic crystal joined to an antiferromagnetic crystal could cause the spins to turn and thereby produce a new minimum-energy static spin structure analagous to the SSF state. The mathematical analysis became somewhat unwieldy and it was decided to study the problem with the aid of a high-speed computer. The effect of a ferromagnet on the antiferromagnet was simulated by restricting the external magnetic field to only the first few layers of the antiferromagnet near the surface.

II. DISCUSSION OF THE NUMERICAL ANALYSIS AND RESULTS

Following Mills and Keffer, we start with their general expression for the energy of the spin structure which is

$$E=-\tfrac{1}{2}H_A\sum_{l=0}^{\infty}(\cos^2\alpha_{2l}+\cos^2\beta_{2l+1})+H\sum_{l=0}^{\infty}(\cos\alpha_{2l}+\cos\beta_{2l+1})$$
$$+\tfrac{1}{2}H_E\sum_{l=0}^{\infty}[\cos(\alpha_{2l}-\beta_{2l+1})+(1-\delta_{l,0})\cos(\alpha_{2l}-\beta_{2l-1})] \ . \quad (1)$$

The subscripts on α and β number the layers and α_{2l} and β_{2l} are the angles between the spins and the positive z axis. If the applied field H is greater than zero it points in the negative z direction. All spins on the same layer make the same angle with respect to the z axis. H_A and H_E are the effective anisotropy and exchange fields, respectively, in the molecular-field approximation. Following Mills we minimize (1) with respect to α_{2l} and β_{2l+1} to obtain, for $l\geq 0$,

$$\sin(\alpha_{2l+2}-\beta_{2l+1})+\sin(\alpha_{2l}-\beta_{2l+1})=2\xi\sin\beta_{2l+1}=\zeta\sin(2\beta_{2l+1}) \ , \quad (2)$$

$$\sin(\alpha_{2l}-\beta_{2l+1})+(1-\delta_{l,0})\sin(\alpha_{2l}-\beta_{2l-1})=-2\xi\sin\alpha_{2l}+\zeta\sin(2\alpha_{2l}) \ . \quad (3)$$

Here $\xi=H/H_E$ and $\zeta=H_A/H_E$.

In the numerical analysis it is not necessary to assume that $\zeta\ll\xi\ll1$ as Keffer and Mills did. Equations (2) and (3) apply to the infinite lattice when the Kronecker δ is dropped from (3). In this case $\alpha=\alpha_{2l}=-\beta_{2l+1}$ for all l is a solution to the equations with α given by

$$\cos\alpha=-\frac{\xi}{2-\zeta} \ . \quad (4)$$

This solution gives a spin structure called the SF state. When ξ and ζ satisfy Mills's criterion, α is close to $\frac{1}{2}\pi$. In the numerical analysis, of course, we dealt with a lattice containing N layers rather than with a semi-infinite lattice. We assumed that ξ was constant on the first n layers and zero on the rest of the layers and then searched for a minimum-energy structure. This was done and as a byproduct we solved Mills's equations exactly on the computer to compare with Keffer's analytical result. We have plotted a number of interesting graphs for comparison. Our procedure was to arrange Eqs. (2) and (3) in the following sequence starting with the first layer:

$$\begin{aligned}
\sin(\alpha_0-\beta_1) &= -2\xi\sin\alpha_0+\zeta\sin(2\alpha_0)\,,\\
\sin(\alpha_2-\beta_1)+\sin(\alpha_0-\beta_1) &= 2\xi\sin\beta_1-\zeta\sin(2\beta_1)\,,\\
&\vdots\\
\sin(\alpha_{2N}-\beta_{2N+1})+\sin(\alpha_{2N}-\beta_{2N-1}) &= -2\xi\sin\alpha_{2N}+\zeta\sin(2\alpha_{2N})\,,\\
\sin(\alpha_{2N}-\beta_{2N+1})+\zeta\sin(2\beta_{2N+1}) &= 2\xi\sin(\beta_{2N+1})\,.
\end{aligned} \tag{5}$$

The computer calculation consisted of choosing α_0 arbitrarily on the surface layer. The subsequent equations then determine β_1, α_1, $\beta_2, \ldots$, etc., in turn. The last equation becomes a consistency condition which must be satisfied since the α and β which appear in this equation have already been determined from the previous equations of the set (5). If it is not satisfied, α_0 is chosen to be a different value between 0 and π and the process repeated until the consistency condition is finally satisfied. Keffer determined analytically the functional dependence of α_{2l} on l and is given as follows:

$$\sin^2\alpha_{2l}=\{1+[1-(b^2/a^2)]\sinh^2(2al)\}^{-1}\,,$$

with

$$\begin{aligned}
a^2 &= 2\zeta+\zeta^2-\xi^2\,,\\
b^2 &= 2\zeta(\xi^2-\zeta)\,.
\end{aligned} \tag{6}$$

We now describe and discuss the results which are plotted in the figures. The first layer of spins is called the zeroth layer and the rest of the layers are numbered consecutively. The even-numbered layers are the α layers. The odd-numbered layers are the β layers. We also let α_{2l} be the angle which a spin in the $2l$th layer makes with the z axis, with a similar definition for β_{2l+1}. The angle between α and β in two neighboring layers is very closely equal to 180°. Therefore, we have plotted only α as a function of the numbered layer. This follows the convention of Mills and Keffer.

The curve labeled A in Fig. 1 is a plot of Keffer's approximate analytical result reproduced as Eq. (6). Keffer's result is for a semi-infinite crystal, i.e., for an infinite number of layers. Note that the spins in the zeroth layer (surface layer) are perpendicular to the magnetic field, while the spins gradually line up with the field as one moves towards the interior of the crystal. For the values of ζ and ξ chosen, almost complete alignment is attained by the 100th layer. This spin structure is called the SSF state. This state is obtained for only a narrow range of values of ζ and ξ. The value of ξ for curve A is 0.14000. For a slightly greater value of $\xi(=0.1407)$, we obtain curve B. Note that all of the spins in the deeper layers are beginning to turn perpendicular to the magnetic field. As the field is increased even further, this turning sweeps throughout the crystal until a value of ξ approximately equal to 0.1408 is reached. At this value α becomes imaginary in Eq. (6) because a becomes imaginary. Of course, there is a solution for any values of ζ and ξ, but it does not have the character assumed by Mills and Keffer. Curves C and D in Fig. 1 are the computer-generated exact solutions to the Mills-Keffer equations. Curve D is an exact solution calculated for $\xi=0.14000$ which is to be compared with curve A, Keffer's approximate analytical result. The two curves are quantitatively and qualitatively quite different. Both Mills and Keffer deduce that the spin in the surface layer is perpendicular to the magnetic field while the exact result gives that the spin is very close to 180°. The numerical results also indicate that as the number of layers increase, the spin in the surface layer approaches 180° as a limit. We have determined also the energy of our magnetic states per double layer in units of H_E. For curve D this energy is -1.008066. For a slightly larger value of $\xi=0.14124$ we obtain curve C, which still has the character of a surface spin-flop state with energy equal to -1.008140. Note that the energy has decreased when ξ increases in this range of H. But at $\xi=0.14125$ the minimum energy state is not the SSF state but the SF state with the energy increasing to -1.0075006.

In Fig. 2 we have plotted α vs l for the case when there is a constant applied magnetic field on the first six layers with zero field on the rest of the layers. The total number of layers is 98. Again both curves have $\zeta=0.01$. When $\xi=0.2$ (curve A) the minimum-energy structure is an SSF state with the energy equal to -1.0009762. When

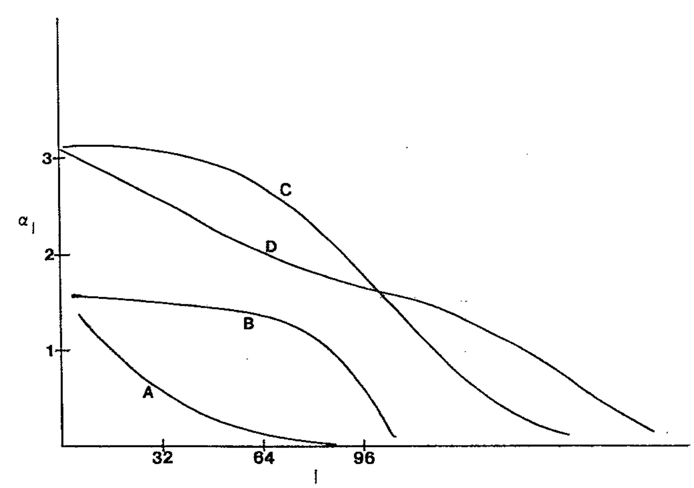

FIG. 1. A, Keffer's analytical result for $\zeta=0.01$ and $\xi=0.1400$; B, same as A except $\xi=0.1407$; C, exact solution for $\zeta=0.01$ and $\xi=0.14000$; D, same as C except $\xi=0.14124$.

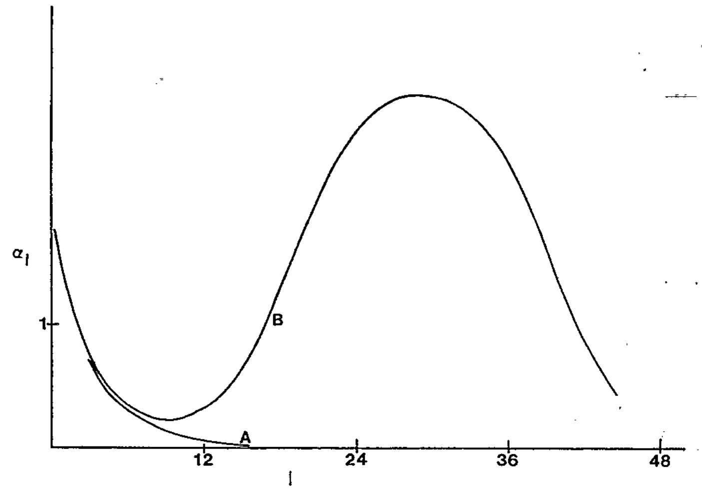

FIG. 2. Plot of spin angle vs even-numbered layer when external magnetic field is confined to the first six layers of a 98-layer crystal, with $\zeta=0.01$. Curve A, $\xi=0.2$. Curve B, $\xi=0.21$.

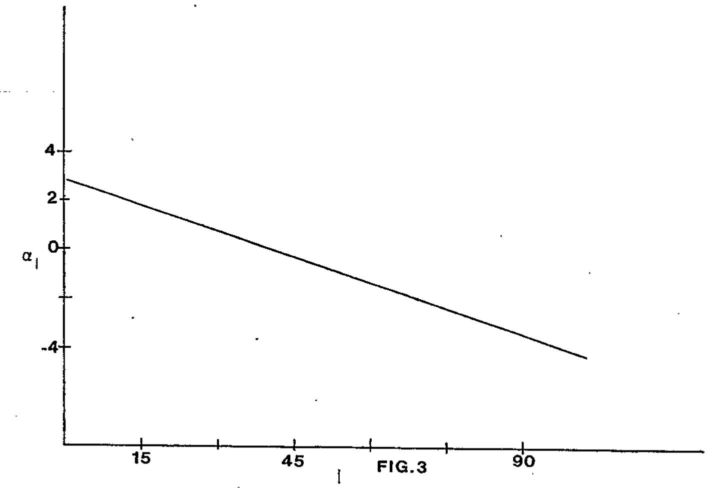

FIG. 3. Another SSF state not described by Keffer's analytical result. $\zeta=0.01$ and $\xi=0.1415$. The number of layers is 258 and the energy is -1.0062. Magnetic field has same value on all of the layers.

$\xi=0.21$ the SSF state goes through a maximum before the spin angle drops to zero on the other surface. It is interesting to note that the energy of this state (curve B) has increased to -0.9957 but is greater than the fully aligned state for the same value of the external magnetic field. It would appear that the SSF state is at a saddle point in the energy while the aligned state is a true minimum. Further analysis is warranted using for example the Morse critical-point theory.

Mills's model of a semi-infinite antiferromagnetic crystal permits other spin structures in which the energy is at least a relative minimum. For example, in Fig. 3 is a plot of α vs l for a minimum energy structure in which α goes negative. The calculations were also done in double precision so it does not appear that α going negative as the result of the propagation of any error. We have observed many minima of the kind seen in Fig. 3 and it appears that stable spin waves would develop around such minimum energy structures. We should point out that Eqs. (2) and (3) yield only extrema in the energy E. If the choice were only between a relative minimum or a relative maximum it would be easy to determine which it is by calculating E for values of α and β in the close proximity to the values which give the minimum energy. If it is a saddle point, a random number process to calculate E in the near vicinity could mistakenly indicate a relative minimum (or maximum). For example, if your choice of α_{2l} and β_{2l+1} solved all of the equations in (2) and (3) except one, the corresponding value of E would not be an extremum although it might appear to be one as you observed in a random manner the values of E in the neighborhood. All of our results were obtained for a crystal in which one side is bound by an α layer and the other side is bound by a β layer. In order to discount the possibility that an error was propagated through the equations as we passed from one side of the crystal to the other side we also solved the equations by starting from the opposite side. Finally, we mention that the model appears to have a richness of solutions which was unanticipated.

[1]D. L. Mills, Phys. Rev. Lett. **20**, 18 (1968).

[2]F. Keffer and H. Chow, Phys. Rev. Lett. **31**, 17 (1973).