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Simulation of an antiferromagnet by microcomputer

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Computer simulation of the behavior of the system, of which free energy is known to depend on a number of parameters and also on a running parameter, is exhibited. As an example, the induced magnetization of a uniaxial antiferromagnet under varying external field is shown. It has three phases: antiferromagnetic, spin-flopping, and ferromagnetic. Though the complexity of the expression of free energy makes it difficult to see when and how phase transition occurs, a simple device facilitates visualization of the processes.

INTRODUCTION

It is known that even a small computer can do a good job in simulating the behavior of a physical system; sometime ago this was emphasized, for example, by Bak.[1] In this Journal, too, in the same spirit, lattice gauge theory on microcomputers was handled by Dreher[2] as an instructive theme in a classroom. The situation is getting better, since nowadays we can have very efficient CPU and big RAM in our sophisticated home computers. In this article, we would like to show how we can see behavior of a system that evolves under a varying environment. If we know the value of free energy of the system as a function of a point in the configuration space of the system, we can see how the system evolves. But it is too much for us to calculate free energy of the system in so many sites of configuration space under varying environmental conditions. So we invented a device called SUR, which is the abbreviation for surroundings.

We take arbitrarily an initial point in our configuration space, and calculate free energy possessed by our system at this point. We surround this point by a closed surface in the configuration space and we calculate free energy of the system at every site in the region bounded by the closed surface. (Of course, our configuration space is a lattice.) We look for a point where the free energy is minimum, and if this point differs from the initial point, this point shall be a new initial point. This procedure is repeated until it is found that the free energy at the initial point is truly minimum among those in the bounded surrounding. This point represents a stable or metastable state of the system. If an external parameter controlling the system is changed, a new equilibrium point is searched again by the same procedure. Thus, under the varying external parameters, corresponding equilibrium points are found out successively, and we can follow a movement of the physical point on a CRT.

Though extremum of the free energy is not always fixed uniquely by the value of the parameter that determines the environment, we need not care about it explicitly. The case when the minimum value of free energy is not fixed uniquely occurs when the system is undergoing phase transition. If we use only a single bounded region under our continuous watch, the system makes a phase transition after being in a metastable state. On a CRT, the movement of a point showing the free energy of the system exhibits an abrupt change. In such a case, the state of the system evolves along a different route according to whether a parameter, which fixes the external environment, changes in this way or the other. Our procedure, which we call SUR, is useful to see the behavior of the system vividly on a CRT. In the following, this is exemplified for a uniaxial antiferromagnet in a varying external magnetic field. We have tried previously to obtain some graphical representation of the behavior of a uniaxial ferromagnet and antiferromagnet by analyzing their free energy.[3] We will present here some results on simulation of behavior of a uniaxial antiferromagnet in a varying external magnetic field.

I. SIMULATION OF UNIAXIAL ANTIFERROMAGNET

A. Free energy and three phases of magnetization

We consider a uniaxial antiferromagnet described by the two-lattice model, in which each lattice has magnetization $\mathbf{M}$ or $\mathbf{M}'$ of constant saturated magnitude $M(=M')$. We suppose that our crystal has a single axis of easy magnetization, and we take this as the z axis. Then the free energy is given by

$$E = \alpha \cos(\mathbf{M},\mathbf{M}') + [\sin^2(\mathbf{M},z\text{ axis}) + \sin^2(\mathbf{M}',z\text{ axis})] - \gamma[\cos(\mathbf{H},\mathbf{M}) + \cos(\mathbf{H},\mathbf{M}')],$$

where $(\mathbf{A},\mathbf{B})$ means the angle between the directions of $\mathbf{A}$ and $\mathbf{B}$, and since we need only the relative magnitude of energy, we normalized the coefficient of the second term to 1. The first term comes from the exchange energy, the second term from the anisotropy energy, and the final term is the Zeeman energy.

Such an aniferromagnet takes the following three phases of magnetization[4]: the antiferromagnetic phase (AF) in a weak external field, in which $\mathbf{M}$ and $\mathbf{M}'$ point in almost opposite directions; the spin-flopping phase (SF) in a rather strong field, in which $\mathbf{M}$ and $\mathbf{M}'$ make some angle between them; and the ferromagnetic phase (FE) in a strong field, in which $\mathbf{M}$ and $\mathbf{M}'$ are parallel.

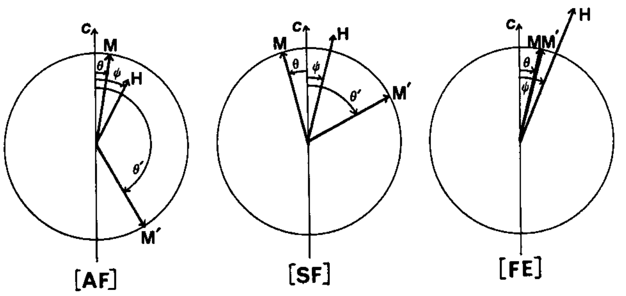

FIG. 1. Three phases of magnetization: Antiferromagnetic (AF); spin-flopping (SF); and ferromagnetic (FE).

We suppose that the direction of the external magnetic field stays always in the xz plane. We investigated carefully the generic case where magnetization vectors are not necessarily in the xz plane and found that the configuration in which those vectors are not in the plane is not stable. Therefore, we restrict ourselves in the following to the case where the z axis (axis of easy magnetization), external magnetic field, and both magnetization vectors are coplanar. So the three phases can be drawn as in Fig. 1 and the free energy of our system can be written simply as follows:

$$E = \alpha \cos(\theta - \theta') + (\sin^2\theta + \sin^2\theta') - \gamma[\cos(\psi - \theta) + \cos(\psi - \theta')].$$

Our object is to see magnetization vectors evolving according to change of environmental condition. To get the general idea, it is better first to have phase diagrams.

B. Stable or metastable region for each phase

In Fig. 2 we show which phase is stable or metastable when the direction of the external magnetic field is kept fixed and the coefficients α and γ are varied. Similarly, in Fig. 3, α is kept fixed and the coefficient γ and the direction of the external magnetic field are varied. In those figures, regions where AF, SF, and FE are stable are separated by lines l, m, and n. That is, FE is stable in the region above l and n, SF is stable in the region between m and n, and AF is stable below l and m. Except for the case $\psi = 0$, the line m terminates at a finite point c; so, in such a case, the stable SF and AF are not separated clearly in the region beyond c. Furthermore, some metastable regions are shown in these figures. In the region bounded by lines l and r, or m and r, AF is metastable. In the region bounded by lines l and p, FE is metastable. And in the region bounded by lines m, p, and q SF is metastable. Figure 2(a) is for $\psi = 0$ and it is easy to calculate the boundaries between two stable phases and find the region where the system is metastable: We need no SUR to draw this figure. Figure 2(b) and (c) are for $\psi \neq 0$, and to draw those figures we used SUR. The phase diagrams in Fig. 3 have γ as ordinate and ψ as abscissa, with α being kept fixed.

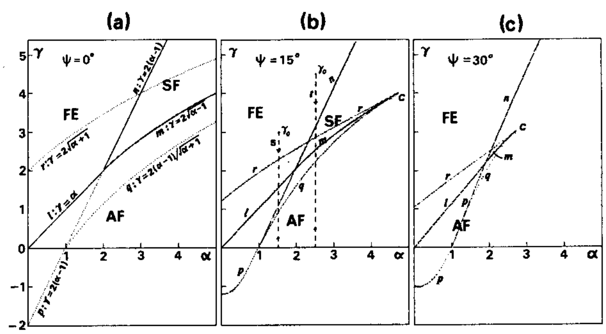

FIG. 2. Stable and metastable regions of each phase in the γ-α plane for the cases: (a) $\psi = 0°$; (b) $\psi = 15°$; (c) $\psi = 30°$. FE is stable in a region above l and n, and metastable in a region bounded by l and p. SF is stable in a region between n and m, metastable in a region bounded by m, q, and p. AF is stable in a region below l and m, and metastable in a region bounded by l, m, and r. Lines s and t in (b) are paths along which γ varies to produce Figs. 4(a) and (b).

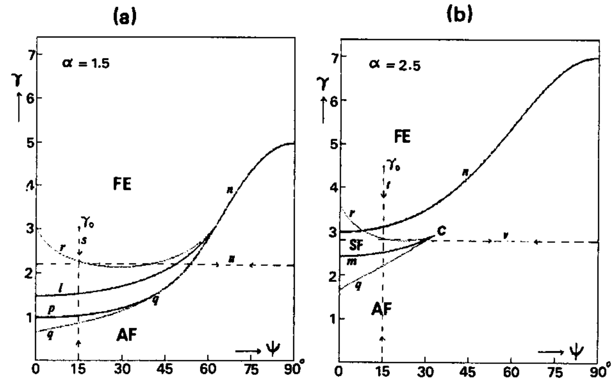

FIG. 3. Stable and metastable regions of each phase in the γ-ψ plane for the cases: (a) $\alpha = 1.5$; (b) $\alpha = 2.5$. Boundaries of regions where each of three phases is stable or metastable are named by the same letters as in Fig. 2. Line s in (a) and line t in (b) are the same as those in Fig. 2. u in (a) and v in (b) are paths along which ψ changes to produce Figs. 5(a) and (b).

C. Simulation of changing magnetization

In the simulation of magnetization under the varying external field, programming SUR exhibits especially its usefulness. We show some examples in which phase transitions occur accompanied by a jump at the boundary of phases and a hysteresis is seen when the external variable makes a return journey.

Figure 4 shows changes of (θ, θ'), and E when the magnitude of γ is varied. In Fig. 4(a), $\alpha = 1.5$, $\psi = 15°$, and γ is varied from 3 to 0 and then from 0 to 3 along the path s shown in Fig. 2(b) and in Fig. 3(a), in broken lines. The system changes its configuration as follows: When γ is decreasing, it changes from FE (which turns into metastable after s crosses the line l) to the metastable SF at (p) (where s crosses p), and then it jumps to stable AF at (q). [Marks (l), (p), etc. in Fig. 4 correspond to the points where s crosses the line l, p, etc.] When γ is increasing, the system continues to be AF (stable and then metastable) until it reaches (r), where it jumps to stable FE. Another example is shown in Fig. 4(b), where $\alpha = 2.5$, $\psi = 15°$, and γ changes along the path t in Fig. 2(b) or in Fig. 3(b) (from 4.5 to 0 and then from 0 to 4.5). Change of the configuration followed by the path t is vividly exhibited in Fig. 4(b). An example that does not show any clear-cut

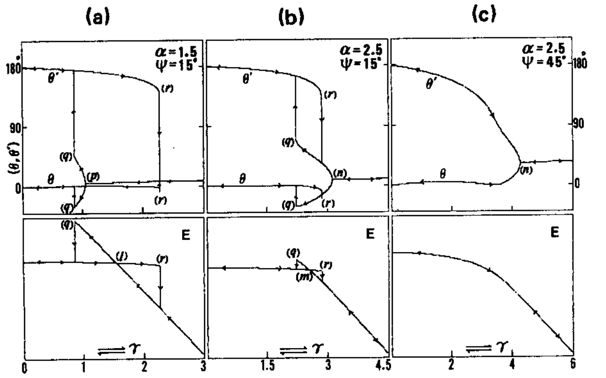

FIG. 4. Changes of configuration (θ,θ') and free energy E as γ varies along the path s or t in Figs. 2 and 3 from γ_0 to 0 and then from 0 to γ_0. Letters (l), (m),... represent the points where s or t crosses the line l, m,..... (a) $\alpha = 1.5$, $\psi = 15°$; when γ:3→0; FE(stable)→(l)→FE(metastable)→(p)→SF(metastable)→(q)*jump*→AF(stable); when γ:0→3, AF(stable)→(l)→AF(metastable)→(r)*jump*→FE(stable); (b) $\alpha = 2.5$, $\psi = 15°$; when γ:4.5→0, FE(stable)→(n)→SF(stable)→(m)→SF(metastable)→(q)*jump*→AF(stable); when γ:0→4.5, AF(stable)→(r)*jump*→SF(stable)→(n)→FE(stable); (c) $\alpha = 2.5$, $\psi = 45° > \psi_c$. A clear-cut transition between EF(stable) and SF(stable) occurs only at (n).

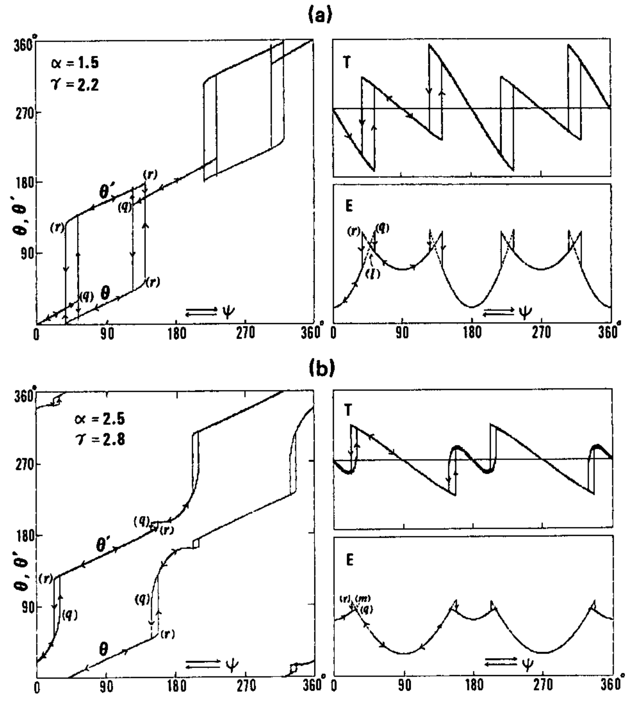

FIG. 5. Changes of (θ,θ'), E, and torque T as **H** rotates from $\psi = 0$ to 2π and then from 2π to 0, along the path u or v in Fig. 3. Marks (r), (l), etc. are points where u or v crosses r, l, etc., (a) $\alpha = 1.5$, $\gamma = 2.2$; when ψ:0→2π, FE(stable)→(l)→FE(metastable)→(q)*jump*→AF(stable)→(l)→AF(metastable)→(r)*jump*→FE(stable)→and so forth. (b) $\alpha = 2.5$, $\gamma = 2.8$; when ψ:0→2π, SF(stable)→(m)→SF(metastable)→(q)*jump*→AF(stable)→(r)*jump*→SF(stable)→and so forth.

boundary between SF and AF is given in (c) for $\alpha = 2.5$ and $\psi = 45°$.

Figure 5 shows the change of (θ,θ'), E, and the torque T $[T = (\partial E/\partial\psi)_{\text{equil}}]$ when the external field is rotated clockwise or counterclockwise while α and γ are kept fixed. In this case, the route of the representative point followed by the system in the configuration space is dependent on the direction of rotation. In Fig. 5(a), $\alpha = 1.5$, $\gamma = 2.2$, and ψ changes from 0 to 2π, and then from 2π to 0. A part of the path u that shows the change of ψ is drawn in a phase diagram, Fig. 3(a). Points where u crosses the boundary lines l, q, and r, (l) (q), and (r) are marked in Fig. 5. In this case, the system is first stable in FE and it transits to AF at (q). On its way back, when ψ is decreasing, the system transits from AF to FE at (r). The system is in a metastable state after it passes the point (l). The whole process is the repetition of this which occurs when ψ changes over $\pi/2$ rad. Another example is shown in Fig. 5(b), where transition occurs between SF and AF. A broken horizontal line v in Fig. 3(b) corresponds to u in Fig. 3(a).

To obtain those figures, when the surrounding domain is two-dimensional, we used only eight points on a circumference of the circle centering the point, of which the free energy of the system is to be compared. We examined in a generic case using as many as 5^4 points that fill the four-dimensional parallelepiped surrounding the point, and in the two-dimensional case 7^2 points. And we finally found that a small number of points are enough to represent surroundings.

II. CONCLUDING REMARKS

As is seen in the above examples, simulation by SUR is a very useful and expedient way to explore characteristic behavior of the system from its free energy and to represent it graphically. Under the varying external condition, an equilibrium point determines by itself its path in the configuration space and, when it comes to the end point of extremum of free energy [such as the point (q) in Fig. 4(a)], it looks for its destination and does jump. This is just the physical situation itself. The system in a metastable state always has some possibility to jump to a stable state, and what we have done is equivalent to assuming that the system stays on the metastable state as long as possible.

The phase transition shown in this article is very similar to that of a gas–liquid system. We applied SUR to the system, of which the equation of state is Van der Waals' equation. The p-v diagram satisfying Maxwell's law can be obtained with the aid of SUR. (Two disconnected domains, one in liquid phase, one in gaseous phase are needed for this purpose.) Our procedure should be useful for analyzing various other thermodynamic systems.

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