Alternative paradigm for physical computing

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We identify a different class of physical systems that are able to form universal logic gates. By analogy with Si(100) surface dimers, we present a model to analyze the trajectories of the fixed points (interpreted as logic states) under variation of the basic parameters. Using the perspective of catastrophe theory, we show that information processing is the result of cycling the parameters of such systems through a path containing a cusp-type catastrophe. We apply this analysis to the construction of an example based on magnetic memory.

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I. INTRODUCTION

Because current bulk semiconductor-based designs are incapable of miniaturization past a closely approaching limit, we must look to different physical systems capable of logic operations as replacements. Research in this area has focused on molecular electronics [1], cellular automata [2], nanotubes [3], DNA [4], etc. In choosing new avenues to explore, it would be helpful to have a guiding principle and a general mechanism for information processing. In other words, we would like to search not only for specific alternative physical systems, but an entirely different paradigm for logic operations evident in a wide range of physical systems. Once we have identified which ones satisfy the requirements of the paradigm, technology can choose for us which system is most likely to succeed in practice.

In this paper we propose an alternative information-processing paradigm that utilizes a class of inherently bistable systems. The bistability persists regardless of the inputs to the logic gate; a system parameter must be cycled to force the computation. We exploit an analytic model of a system within this class to analyze the parametrized motion of the fixed points (which represent the distinct digital states) in a bifurcation diagram. The analysis shows that the effect of forcing the system past ''catastrophic points,'' where one of these fixed points disappears, can be interpreted as a NOR universal logic gate. After identifying further general requirements for equivalent systems, we construct an example from a ferromagnetic cluster array.

II. MODEL

Cho and Joannopoulos originally proposed the use of the Si(100) surface as an ultrahigh density memory storage medium by interpreting the up/down buckled states of individual dimers as digital bits of information [5].

Based on this idea, Appelbaum *et al.* have shown, using density functional theory (DFT) calculations of total energy, that the system of three colinear buckled Si(100) surface dimers and an asymmetrically placed tungsten (W) scanning tip can be used to produce a NOR logic gate under proper adiabatic variation of tip position [6]. The two dimers on the side are inputs to the gate and the center is the output. The tip lowering and raising cycle forces the output dimer to a state determined by the inputs in the case that they are in the same state, or to a state determined by the tip asymmetry in the case that they are different. The important insight, and the point of this paper, is that the mechanism for logic processing here is not necessarily unique to this system. In fact, the general features responsible may show themselves in a possibly wide and varying class of phenomena. We here attempt to outline the requirements for such an equivalent system.

We would like to analyze the motion of the fixed points (the states called ''0'' and ''1'') of the dimer potential under variation of the system parameters, in order to generalize the requirements for a *class* of similar systems. However, to do so by dense calculation of total energy with DFT would be prohibitively expensive. Therefore, we have modeled the dimer potential by a straightforward analytic expression that retains its important features.

The Si(100) dimer buckles because, after the surface reconstructs, there are only enough electrons to form one set of sp^3 (tetrahedral) hybridized orbitals. The remaining dimer atom, electron deficient, can only form sp^2 (planar) orbitals. The planar configuration of the latter atom forces it lower than the former, with respect to the bulk. Thus, the dimer buckling is directly controlled by the location of one electron orbital that can move from one dimer atom to the other, flipping the dimer. A model to predict the dimer buckling orientation, therefore, can focus on the equilibrium positions of the electron potential (in the semiclassical sense). This potential is formed from the sum of the local interatomic potentials from the dimer atoms themselves, the bulk Si, the nearby dimers on the surface, and a weakly interacting W tip.

Our model for the dimer is based on a purely mechanical bistable system [7]. The electron orbital is modeled by a bead that is constrained to move on a wire between the dimer atoms, and is held by a fixed, pivoted spring of relaxed length L and spring constant k. See Fig. 1. If the spring is compressed when $x=0$, two equivalent stable minima will appear for $x<0$ and $x>0$. However, the dimer energy minima are *not* equivalent. This evident asymmetry is a result of the influence of the orientation of nearby dimers. The potential due to this interaction may be quite complicated owing to the fact that it is coupled through intermediate lattice atoms. However, we can model it sufficiently by retaining just the first-order term of an expansion, which is assumed to be the dominating term. (The mechanical analog to

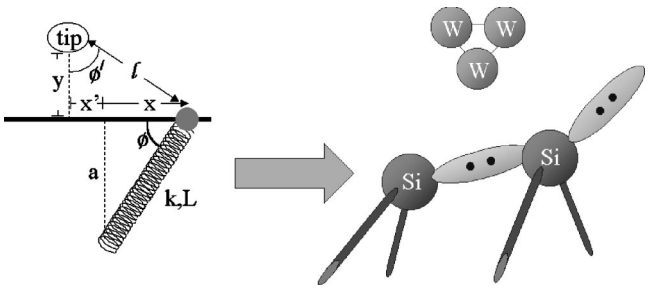

FIG. 1. *Left*: The mechanical analog to Si(100) surface dimers we analyze, with appropriate variables labeled. *Right*: A schematic of a buckled dimer and tungsten scanning probe system, with filled electron orbitals shown as ovals with two dots.

this interaction is a constant force like gravity, which becomes important if the wire is at an angle from horizontal.) This parameter may be determined by fitting the potential to that obtained using DFT calculations.

The remaining interaction is from the W tip. From DFT calculations of total energy we deduce that the interaction is attractive. The W tip atom forms a partial bond with the Si atoms, by ''sharing'' valence electrons. We take our basic model from the Morse molecular potential [8]:

$$U(x)=D_e[1-e^{-(x-r_e)/L'}]^2$$
$$=D_e(1-2e^{-(x-r_e)/L'}+e^{-2(x-r_e)/L'}).$$

Assuming the Si-W distance remains much larger than the equilibrium distance r_e, we can, to a good approximation, discard the second-order term. To first order then,

$$U(x)\approx D_e(1-2e^{-(x-r_e)/L'}).$$

Thus our model for the total force on the electron orbital is (neglecting constant terms)

$$F=F_{inputs}+F_{spring}+F_{tip}=ka(h_{inputA}+h_{inputB})$$
$$-k(x-L)\cos(\phi)-D'e^{-l/L'}\sin(\phi').$$

In unitless variables, we have

$$F=ka\left(h_{inputA}+h_{inputB}-u\left(1-\frac{R}{\sqrt{1+u^2}}\right)\right.$$
$$\left.-Te^{-[\sqrt{(u+v)^2+w^2}]/R'}\frac{u+v}{\sqrt{(u+v)^2+w^2}}\right). \qquad (1)$$

where $u=x/a$, $w=y/a$, $v=x'/a$, $R=L/a$, and $R'=L'/a$. T and $h_{inputA/inputB}$ are tunable parameters that represent the strength of the Si-W interatomic potential and the influence of the input dimers, respectively.

III. DYNAMICS

To illustrate information processing with this system, refer to Fig. 2. Here we have numerically integrated Eq. (1) with Gaussian quadrature to obtain a potential energy curve

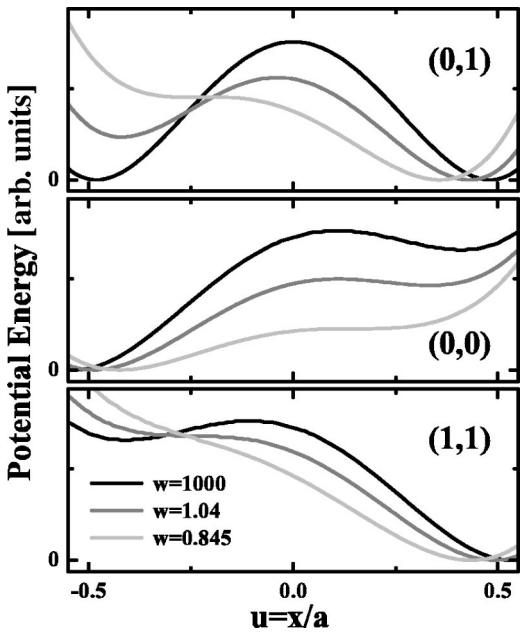

FIG. 2. The potential energy curves for inputs A and $B=(0,1)$ *(top)*, (0,0) *(middle)*, and (1,1) *(bottom)* for the Si(100) dimer model. At large tip distance w, the system is always bistable. Past a critical value, however, one stable minimum disappears.

as a function of electron orbital position u. We use parameter values of $R=1.11$, $R'=0.305$, $v=-0.1$, and $T=1.0$. The asymmetry that depends on the nearby input dimer configuration has a value of $h_{inputA/inputB}=0.0055$ for 1, and $h_{inputA/inputB}=-0.0055$ for 0. (We define 0 to correspond to the minima at $x>0$ and 1 to the minima at $x<0$.) These parameters have been chosen such that the energy of this mechanical system as a function of u has similar features as the energy of the Si-dimer system as a function of dimer angle (see Fig. 2 of Ref. [6]).

Interpreting the minima of each curve at constant w as distinct states, we see that as the tip is lowered (parameter w is decreased), the potentials are reduced to one unique stable state. Raising the tip completes a cycle. Regardless of which state the system started in at large w, the final state will be the one that survived the ''catastrophe'' when the other disappeared.

Let us now analyze the trajectories of these critical points as the tip height parameter is varied. See, for example, Fig. 3 *top*, corresponding to $(inputA,inputB)=(0,1)$. Here we have numerically solved for the roots of Eq. (1), using the Van Wijngaarden–Dekker–Brent algorithm [9]. The parameters are the same as above, with $h_{inputA}+h_{inputB}=0$. We see that reducing the tip height parameter adiabatically forces the system past a catastrophe near $w=0.85$ where one stable minimum and the unstable maximum annihilate each other. Starting on this stable branch 1 at large w, the system will follow the path towards this point. Past this cusp-type catastrophe, only one stable state remains i.e., 0. The system quickly relaxes to this new branch.

When the cycle reverses its path, there is no way for the system to deviate from this locus of connected critical points. At the end of the cycle, the system does not return to its starting point, but remains in the other stable minimum. This

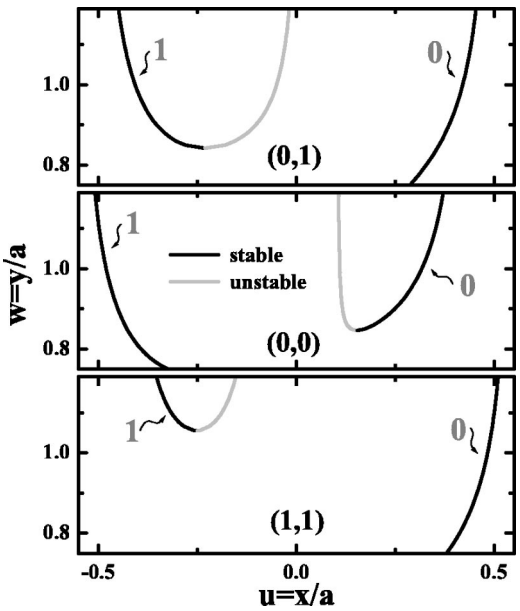

FIG. 3. Bifurcation diagrams corresponding to the potential energy curves in Fig. 2. As *w* adiabatically decreases, a stable minimum and an unstable maximum annihilate each other, leaving only one fixed point. When *w* increases, the system stays on that stable branch. This hysteresis is determined by the inputs in a way that is equivalent to a NOR logic gate.

hysteresis is responsible for information processing; the result of the logic operation with inputs 0 and 1 is 0. Comparison of Fig. 3 *top*, *middle*, and *bottom* shows that the same tip lowering cycle results in a final state determined solely by the inputs. The association between the input and output states for all possibilities is analogous to the logical NOR gate,[1] whose ''truth table'' is shown in Fig. 4 *top*. The NOR gate is a universal logic gate that can be used to form any other logic gate.

IV. DISCUSSION

We now discuss the salient features of this model in order to generalize the requirements for similar systems.

Clearly, we require a bistable system with antiferromagnetic[2] interaction with the inputs (in this case Si dimers). We also require a mechanism for destroying the bistability of the output without removing the asymmetry (W tip). However, the influence of the inputs are additive, so when the inputs are opposite (0,1), we need a residual asymmetry to pin the system to a definite state. In the model above, this asymmety is provided by the shift of the tip lowering axis from the center of the wire. These requirements result in a bifurcation diagram with the general topology of connected minima shown in Fig. 3.

[1]By switching the definition of 0 and 1, this gate becomes a NAND gate. We choose the current convention for comparison with Ref. [6].

[2]A ferromagnetic interaction would result in the noninverting (and thus nonuniversal) logic gates AND or OR.

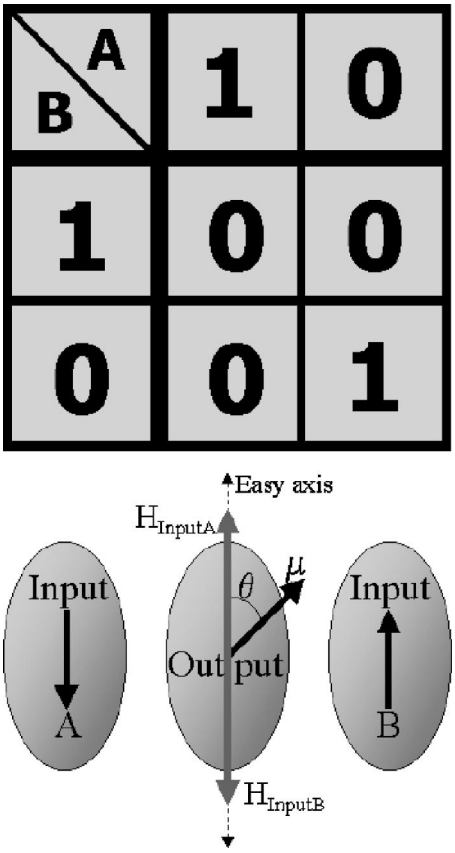

FIG. 4. *Above*: The truth table for a NOR gate. *Below*: Three collinear, antiferromagnetically coupled, anisotropic magnets are an example of a system that fulfills the requirements of the alternative paradigm. The geometry and model variables are shown here.

Since the input values are arbitrary, the parameter that is cycled must pass through the catastrophe points of all possible bifurcation diagrams. In the model discussed above, therefore, the tip height parameter *w* must cycle from a value of at least 1.06 to a value of at most 0.84.

Taking the above requirements into consideration, we can now give an example based on a very familiar bistable system, the uniaxial magnet.

Consider three such antiferromagnetically coupled magnets in close proximity along a one-dimensional array [10]. See Fig. 4 *bottom*. The easy magnetization axis of the magnets is along the direction perpendicular to the array dimension. The information is stored in the up/down orientation of the magnetization of these magnets.

The stray field from its neighbors (the inputs) determines the asymmetry in the energy diagram of the middle magnet (the output). To remove the energetic barrier between the two stable magnetization states, and cause the necessary catastrophe, a local *H* field perpendicular to the easy axis can be turned on adiabatically. When the input magnets are antialigned, their influences cancel. To provide a residual asymmetry, a biasing background magnetic field aligned with the easy axis can be used.

We use the Stoner-Wohlfarth model [11] to describe the energy of the middle (output) magnet as a function of its magnetization orientation:

$$E \propto E_0 \sin^2\theta - \mu(H_{inputA} + H_{inputB} - H_{bias})\cos\theta - \mu H_\perp \sin\theta,$$

where $H_{inputA}+H_{inputB}$ is the sum of the magnitudes of the stray fields from nearby input magnets, H_{bias} is the magnitude of the parallel bias field, and $H_\perp$ is the magnitude of the perpendicular field. θ is the angle between the easy axis and the magnetic moment $\vec{\mu}$. The first term represents the shape or crystal anisotropy effect, and the other terms are simply dipole interaction energies. The roots of the derivative of this function are the stable points; they are shown in Fig. 5 in a bifurcation diagram, parametrized by the magnitude of $H_\perp$. For this example, we use parameters $E_0=1$, $\mu=1$, $H_{bias}=0.1$, and $H_{inputA/inputB}=-0.075$ for 1 and 0.075 for 0. Comparison with Fig. 3 reveals that the basic topology of the branches is identical. Therefore we see that this well known system is capable of being used as a universal NOR gate; one has only to cycle the perpendicular field $H_\perp$ at the output magnet from the lowest catastrophe point (≈ 1.25) through the highest catastrophe point (≈ 1.75).

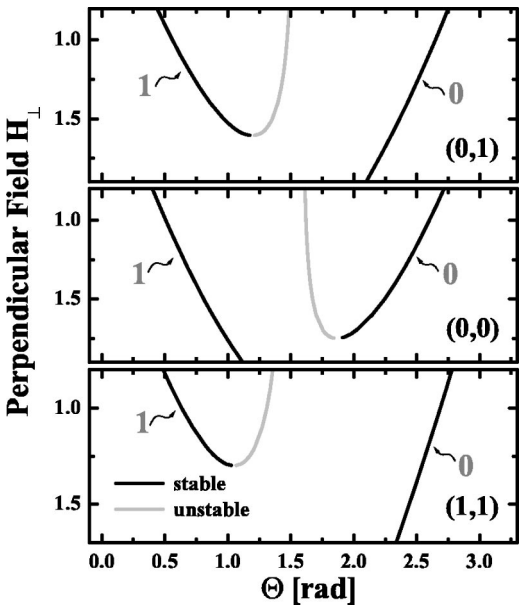

FIG. 5. Bifurcation diagram of the magnet system, parametrized by a perpendicular field. The topology of connected fixed points in this parameter space is exactly the same as in the Si(100) dimer model. Therefore, this system can also be interpreted as a NOR logic gate.

V. CONCLUSION

We have shown the generalization of a system capable of forming a universal NOR gate, and analyze it from the perspective of catastrophe theory. After establishing basic requirements, we give a simple and well-known example that can be interpreted as a physical NOR gate.

We conclude on an interesting but speculative note. There is no reason to assume that this mechanism for information processing should be unique to just bistable systems. Systems with more minima and the features outlined above should be capable of three- or higher-valued logic operations. It remains to be seen if the correct topology of the bifurcation diagrams involved is a physical possibility.

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