Letters

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CHUA'S ATOM

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The response of a chaotic Chua's electronic circuit and that of an atom show interesting common features. Starting from the comparison of the qualitative behavior of bifurcation diagrams and electronic spectroscopic series of atoms we associate *order–chaos* transition with those of an electron passing from a quantized to a continous energy spectrum. The resulting atomic model suggests an analogy between the synchronization of two *Chua's atoms* and chemical covalent bonding.

1. Introduction

Due to stimulating interaction with many different aspects of real life, Physics is in continous development. A rather new and interesting feature is the contemporary use of theory and experiment associated in computer numerical simulations. This allows us to extend the range of interest to many fields such as nonlinear dynamics. We thus have a new way of examining and explaining phenomena through techniques leading to many interconnections. This interdisciplinary way of studying allows the setting of many physical phenomena in scenarios up to now unimaginable. Recently, experimental and theoretical works have stressed the effects of chaotic mechanics on solid state devices such as semiconductor heterostructures [Fleishmann *et al.*, 1992]. In this way we can, for example, correlate different fields such as condensed matter and nonlinear chaotic dynamics.

In this work we present a chaotic model to describe the behavior of bound electrons in an atom and to give a physical analogy between the synchronization of two identical nonlinear systems and the covalent bonding picture.

The starting point is the resemblance between the bifurcation diagram and the electronic energy spectrum of a neutral, not excited atom. Our aim is to simulate order–chaos transitions by the electron passing from the bound state, with a quantized energy spectrum, to the free one with a continuous energy spectrum. To do this we study Chua's circuit [Madan, 1993], a nonlinear circuit showing chaotic behaviors. Since its realization is easy and inexpensive, it has been comprehensively studied in the field of electronic engineering where the control of chaos is a problem of great interest. Chua's circuit, because of its theoretical and practical simplicity, has become a very useful tool of investigation.

The first aim of the present work is to define the physical electronic parameters capable of simulating the properties of *Chua's chaotic atom*. This will be done for different atoms belonging to the first row of the Periodic Table, namely, Lithium, Berillium, Boron, Carbonium and Nitrogen. We choose this set of atoms because of the simplicity of their $1s^2$, $2s$, $2p$ electronic configuration.

The validity of the present model was tested through synchronization of two *chaotic atoms*. We found a correspondence between the *synchronization resistances* of pairs of coupled identical circuits and the values of the covalent bond energies of homonuclear diatomic molecules.

The paper is organized as follows: A schematic description of Chua's circuit and its bifurcation diagrams will be given in Sec. 2, and Sec. 3 will

introduce the model of *Chua's atom*. Section 4 presents *Chua's molecule*, and some conclusions will close the work.

2. Chua's Circuit

On examining circuits and signal processing systems we find phenomena that we can explain only in terms of nonlinear models. Nevertheless the study of nonlinear dynamics is still a great uncharted territory in system analysis. Chua's circuit is one of the simplest systems with nonlinear behavior; the detailed analysis of its components is reported extensively elsewhere [Madan, 1993]. Chua's circuit is a third-order system. Its state equations, reduced to the first order, are:

$$\begin{cases} C_1 \dfrac{dv_1}{dt} = \dfrac{1}{R}(v_2 - v_1) - f(v_1) \\ C_2 \dfrac{dv_2}{dt} = \dfrac{1}{R}(v_1 - v_2) + i_3 \\ L \dfrac{di_3}{dt} = -v_2 - R_0 i_3 \end{cases} \tag{1}$$

where v_1, v_2 are the voltages of the two capacitors, i_3 is the current in the inductor, R_0 is the internal resistance of the inductor and $f(v)$ is the piecewise-linear function:

$$f(v) = G_b v + \frac{1}{2}(G_a - G_b)(|v + B_p| - |v - B_p|) \tag{2}$$

Using the following normalization of variables the equations become dimensionless:

$$x \equiv \frac{v_1}{B_p} \qquad y \equiv \frac{v_2}{B_p} \qquad z \equiv \frac{Ri_3}{B_p}$$

$$\tau \equiv \frac{t}{RC_2} \qquad a \equiv RG_a \qquad b \equiv RG_b$$

$$\alpha \equiv \frac{C_2}{C_1} \qquad \beta \equiv \frac{R^2 C_2}{L} \qquad \gamma \equiv \frac{C_2 R R_0}{L} \tag{3}$$

$$\begin{cases} \dot{x} = \alpha(y - x - f(x)) \\ \dot{y} = x - y + z \\ \dot{z} = -\beta y - \gamma z \end{cases} \tag{4}$$

with $\dot{x} = dx/d\tau$ and

$$f(x) = bx + \frac{1}{2}(a - b)(|x + 1| - |x - 1|)\,. \tag{5}$$

In this work we have made a careful analysis of two circuit–parameter bifurcation diagrams. We studied the voltage of the C_1 capacitor versus the resistance R, the bifurcation parameter. We restricted our analysis to the first two period-doubling bifurcations.

3. The Model of the Neutral Atom

At first we considered searching for an analogy between the subsequent doublings of the orbits in the circuit and the atomic transitions. Unfortunately, this method is complicated in view of the rapidly increasing number of bifurcations that suddenly lead to a chaotic regime. This chaotic state is characterized by an attractor densely filling some region of the phase space, where the doubling of orbits is no longer observed and the plot becomes an almost continuous figure. It suggests a resemblance with atomic energy level schemes.

Since our model establishes a connection between the behavior of an electronic circuit and that of an atom, each circuit element will be assigned a value taken from the Periodic Table of elements.

In particular, we define $\Delta R = R_2 - R_1$ as the first ionization energy, where R_1 is the value when passing from the fixed point to the period-one orbit and R_2 the value when the period-one orbit bifurcates into a period-two orbit. The R_1 and R_2 values are collected in Table 1.

We will simulate the behavior of Li, Be, B, C, N atoms.

Firstly we trace the plot of their first ionization energy versus the atomic number Z. We then assume a special choice of circuit parameters, as shown in Table 2, to represent the Lithium atom.

The parameters, once inserted into Chua's equations, give rise to a bifurcation diagram as a function of ΔR, assumed as the first ionization energy of the *Lithium Chua's atom*. From that we can plot, in Fig. 1, ΔR versus Z, along with the atomic first ionization energies.

At this point we must find an appropriate parametrization which gives rise to a particular ΔR. This is quite a difficult task because the circuit is chaotic. Due to the fact that C_1 and C_2 scale linearly with ΔR we obtain the necessary parametrizations. Unfortunately they are not unique because it is possible to obtain a particular ΔR from different combinations of parameters. We must impose

Table 1. Li, Be, B, C, N parametrization, $G_a(mS)$, $G_b(mS)$ and $R_0(\Omega)$ are as in Table 2. In the bifurcation diagram C_1 versus R, R_1 and R_2 are the resistances corresponding to the fixed point and the period-one orbit respectively.

Atom	$C_1(nF)$	$C_2(nF)$	$L(mH)$	$R_1(K\Omega)$	$R_2(K\Omega)$
Li	6.55	60.00	20.00	2.2587	2.2527
Be	6.90	100.00	17.00	2.2620	2.2521
B	7.28	110.00	18.00	2.2706	2.2617
C	7.34	150.00	16.00	2.2832	2.2714
N	7.38	210.00	14.00	2.2969	2.2817

Table 2. Circuit parameters for modeling Lithium atom.

Atom	$C_1(nF)$	$C_2(nF)$	$L(mH)$	$G_a(mS)$	$G_b(mS)$	$R_0(\Omega)$
Li	6.55	60.00	20.00	-0.75	-0.40	2.42

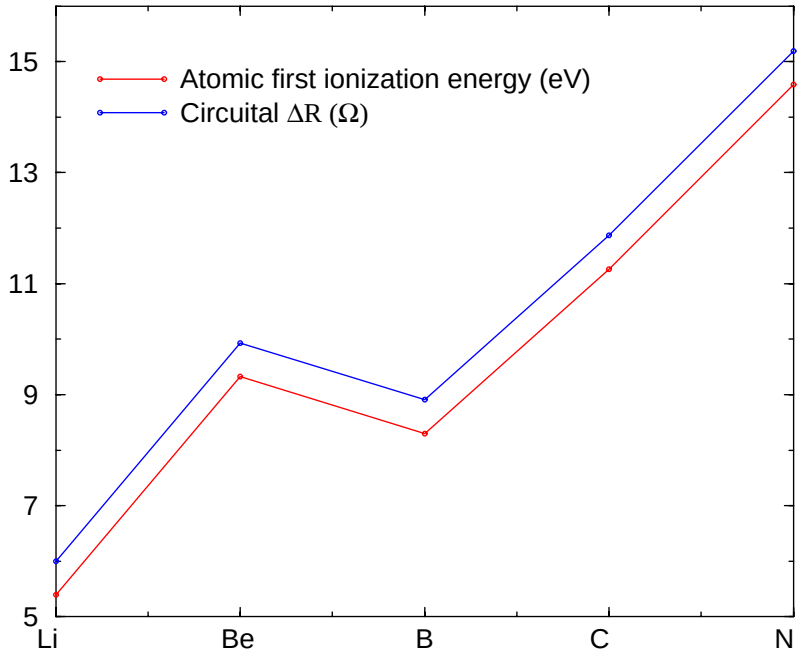

Fig. 1. Atomic first ionization energy (eV) and circuital ΔR versus atomic number Z.

some constraints on parameters variability. From the analysis of the Periodic Table it is evident the analogy between the behavior of some atomic and circuit parameters. Due to this fact we are able to estabish the following correlations:

C_1 increases as the total number of electrons Z;

C_2 represents the electronegativity which increases on going from (Li) to (N). As a consequence, the values of C_2 shall increase from one *Chua's atom* to another. We recall that the electronegativity is defined as the power of an atom to attract electrons to itself and is measured by a dimensioless number. The increase of electronegativity with Z in the first row, is due to the natural tendency of atoms to reach the nearest noble gas more stable configuration [Pauling, 1960].

L represents the atomic radius which, as shown in the Periodic Table, decreases on going from (Li) to (N) [Bransden & Joachain, 1983]. Bearing this decrease in mind we shall find the parametrization with the resulting values of Table 1.

4. Chua's Molecule

We test our atomic parametrization by studying the Li_2, Be_2, B_2, C_2, N_2 molecules.

To pass from a *Chua's atom* to a *Chua's molecule* let us recall a concept like the synchronization of two chaotic systems.

Strictly speaking, one defines synchronization of two systems as the dynamic state in which the two trajectories converge towards the same values and remain equal as time goes by [Afraimovich *et al.*, 1994]. As a consequence, the two circuits have indistinguishable behaviors when synchronization is achieved [Pecora & Carrol, 1990]. The same occurs in the covalent chemical bond in which electrons belonging to different atoms are no longer related to their original owner and form a localized molecular orbital [Pauling, 1960]. In this case too, we speak of indistinguishability. In the present study we perform a *y-coupled* Chua's configuration [Varone *et al.*, 1996].

At this point, the *chemical nature* of Chua's atoms seems reasonable. We look for a relationship between the synchronization resistance of the two circuits and the homonuclear binary molecule binding energy. To preserve coherence in our model, as before, we suggest an analogy between circuital resistances and atomic energies.

Now let us use the *Chua's atoms* previously found, with their proper parameters, and connect them in couples via a resistor. We find a different coupling-resistance, R_y, for each pair of identical circuits and report them in Table 3.

If we plot R_y versus the atomic number and compare it with that of the binding energy [1981] of a molecule, shown in Fig. 2, a great resemblance is clearly observed.

Table 3. Li_2, Be_2, B_2, C_2, N_2 Chua's *molecules* coupling resistances R_y.

Molecule	Li_2	Be_2	B_2	C_2	N_2
$R_y(k\Omega)$	563.2	563.0	565.4	567.9	570.4

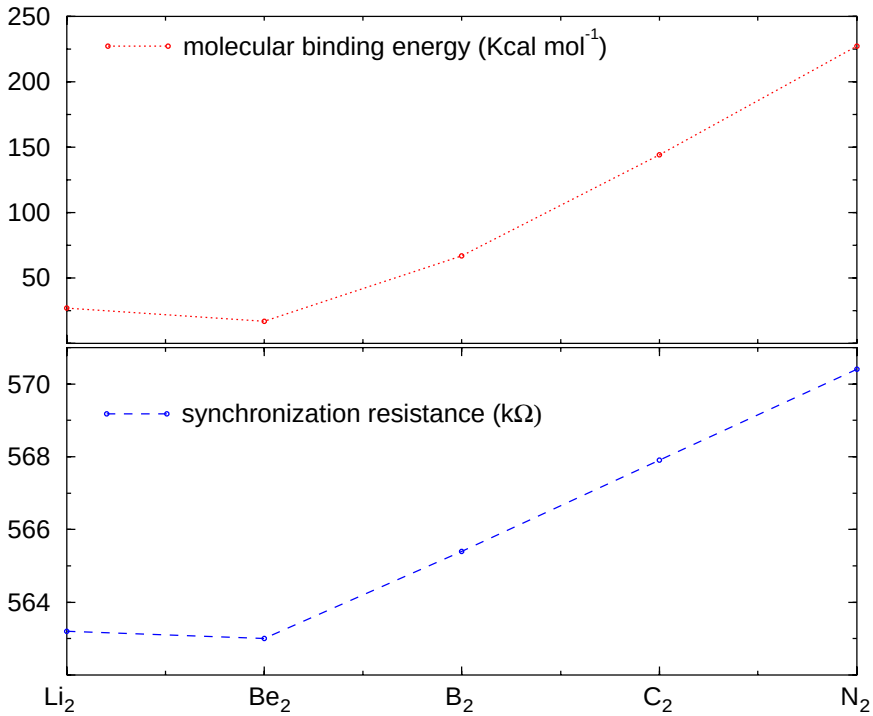

Fig. 2. Coupling resistance R_y (lower) and molecular bond energy (upper) versus atomic number Z.

5. Conclusions

In this paper we have proposed a scheme capable of correlating the electronic terms of a real Chua's circuit to some parameters to simulate an order–disorder atomic transition. Finding the proper parametrization is quite difficult due to the chaotic character of the concepts involved. Starting from a series of circuit parametrization reproducing the behavior of the first row atoms, we arrived to find an analogy between the cohesive energy of homonuclear diatomic molecules and the coupling resistance of two Chua's identical circuits. The quality of the results appears to show that the model may be extended to other atoms of the Periodic Table and to more complicated systems involving a vast range of phenomena in atomic and solid state physics.

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References

Afraimovich, V. S., Nekorkin, V. I., Osipov, G. V. & Shalfeev, V. D. [1994] *Stability, Structures and Chaos in Nonlinear Synchronization Networks* (World Scientific, Singapore).

Bransden, B. H. & Joachain, C. J. [1983] *Physics of Atoms and Molecules* (Longman Sc. & Tech., Harlow).

Fleishmann, R., Geisel, T. & Ketzmerick, R. [1992] "Magnetoresistance due to chaos and nonlinear resonances in lateral surfaces superlattices," *Phys. Rev. Lett.* **68**, 1367–1370.

Handbook of Chemistry and Physics [1981] (CRC Press Inc.).

Madan, R. N. (Guest ed.) [1993] *Chua's Circuit: A Paradigm for Chaos* (World Scientific, Singapore).

Pauling, L. [1960] *The Nature of the Chemical Bond* (Cornell University Press, Ithaca).

Pecora, L. M. & Carrol, T. L. [1990] "Synchronization in chaotic systems," *Phys. Rev. Lett.* **64**, 821–824.

Varone, A., Pegna, G. & Meloni, F. [1996] "The normality in spinels: A chaotic approach," *Crist. Res. Technol.* **31**, 857–860.