On the physical properties of memristive, memcapacitive and meminductive systems

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Abstract

We discuss the physical properties of realistic memristive, memcapacitive and meminductive systems. In particular, by employing the well-known theory of response functions and microscopic derivations, we show that resistors, capacitors and inductors with memory emerge naturally in the response of systems—especially those of nanoscale dimensions—subjected to external perturbations. As a consequence, since memristances, memcapacitances and meminductances are simply response functions, they are not necessarily finite. This means that, unlike what has always been argued in some literature, diverging and non-crossing input–output curves of all these memory elements are physically possible in both quantum and classical regimes. For similar reasons, it is not surprising to find memcapacitances and meminductances that acquire negative values at certain times during dynamics, while the passivity criterion of memristive systems imposes always a non-negative value on the resistance at any given time. We finally show that ideal memristors, namely those whose state depends only on the charge that flows through them (or on the history of the voltage), are subject to very strict physical conditions and are unable to protect their memory state against the unavoidable fluctuations, and therefore are susceptible to a stochastic catastrophe. Similar considerations apply to ideal memcapacitors and meminductors.

(Some figures may appear in colour only in the online journal)

1. Introduction

There is currently much interest in what we now call memristors, memcapacitors and meminductors, namely resistors, capacitors and inductors with memory [1–3]. This interest is not just due to the arguably catchy name these elements have. A real and obvious advantage ensues if we have two-terminal devices that store information without a power source: they may replace—at least in what concerns specific tasks regarding the manipulation and storing of information—the transistor, a hallmark of our present-day microelectronics. However, the interest does not end here. These elements, when combined in complex circuits, can perform logic [4] and non-traditional computing operations [5–10] in a massively parallel fashion and on the same physical platform where storing occurs, a striking resemblance with similar functionalities of our brain. Non-traditional computing represents an important research direction with the aim of solving the ‘von Neumann bottleneck’ that plagues our computer architectures [11]. Moreover, memcapacitors and meminductors can store energy in the electric and magnetic fields [12], respectively, in addition to information, therefore opening new avenues in the technologically important area of energy storage, distribution and manipulation [13].

Although this whole field of research has been growing at a fast pace, there is still much confusion about the fundamental physical properties that realistic systems with memory (as opposed to ideal ones) satisfy. We believe this confusion arises from the different language and background of the two schools of thought that comprise the main body of researchers in this field: electrical engineers specialized in circuit theory on one side, and, on the other, physicists, materials scientists, etc. The first group often draws
conclusions from mathematical formal analogies without much concern about the actual practical realizations of circuit elements. The second group, instead, reasons with the idea that science is, first and foremost, an experimental enterprise, and as such they place the theoretical constructs as subordinate to experimental facts. Irrespective, it is important to stress that while mathematical analogies have their value, they do not always correspond to an objective physical reality.

In this paper, due to our personal training as physicists, we take the second stance and refer to some fundamental physical theories that go way back in time, even before the year 1971 when the axiomatic definition of ‘memristors’ was first introduced [1]. These theories put on a firm ground the experimental fact that any condensed matter system—which is ultimately comprised of electrons and ions—cannot respond instantaneously to external perturbations. This is even more so in systems of nanoscale dimensions where the dynamics of a few atoms may affect the whole structure dramatically [14]. As such, some degree of memory in the response of the system to external fields is always present. This also shows that ideal resistors, capacitors and inductors are just circuit theory idealizations of actual properties of real systems, being a good representation of such properties only within a range of experimental conditions (e.g., within certain intervals of amplitudes and frequencies). It also shows that memristive, memcapacitive and meminductive systems [3, 15] are simply resistors, capacitors and inductors, respectively, whose memory is made more apparent under certain experimental conditions.

Once we realize that resistances, capacitances and inductances are simply response functions, all other constraints introduced ‘artificially’ in the mathematical (axiomatic) definition of memristors [1, 2, 16]—and still assumed in some of the literature dealing with memcapacitors and meminductors as well—have no reason to exist. Such unphysical constraints are (i) the finiteness of the responses themselves at all times, with consequent crossing of the input–output curve under a periodic drive, and (ii) in the case of memcapacitors and meminductors, positiveness of their response functions at all times.

We finally discuss some limitations of ideal memristors, memcapacitors and meminductors. By ideal memristors we mean those whose resistance depends only on the charge that flows in the system (or on the history of the voltage) [1, 3]. Ideal memcapacitors are those whose capacitance depends only on the history of the charge stored on their plates (or the history of the voltage across them) [3]. Finally, ideal meminductors are those whose inductance only depends on either the history of the current that flows through them or their flux [3]. We show that these ideal situations do not always represent the physical reality. In particular, the state of ideal memelement does not have any energetic protection against (the unavoidable) fluctuations leading to what could be named a stochastic catastrophe of the memory state.

Such a lack of protection also violates the Landauer principle of minimal energy dissipated per logic operation [17]. In addition, ideal memelement show an over-delayed switching effect not observable in actual experiments, and their modeling needs to be compatible with the symmetries of electrodynamics. In other words, the ideal memelements can only be considered as approximations of actual realizations. For instance, even the much-discussed example of memristor as put forward by Hewlett–Packard a few years back [18], and which has rekindled the interest in this field, is—in its actual material realization—not an ideal memristor. On the other hand, the model used in that publication does correspond to an ideal memristor, and is thus unable to reproduce all the experimental facts.

2. Derivation of memristive properties from Kubo response theory

In this section we show explicitly how memristive properties emerge naturally when a system is subject to an external field. In order to do this we rely on a well-known theory, that dates back to the 1950s, due to Kubo, who derived such response—both classical and quantum—using perturbation theory [19]. Although the original publication deals also with higher-order perturbations, Kubo response theory is now mainly employed in the linear response regime. In order to keep the math at a minimum, we will also focus on the linear response case, but the conclusions we draw are valid also in the non-linear case. In addition, it is not our goal here to re-derive the whole apparatus of Kubo’s theory, which can be found in the original publication or textbooks that expand on the subject (see, e.g., [14]), but just to use its salient results to make our point.

Let us then calculate the electrical current density, \( \mathbf{j}(\mathbf{r}, t) \), of a given material when subject to an external electric field, \( \mathbf{E}(\mathbf{r}, t) \). In order to do this at the microscopic level, we assume we know the many-body electron Hamiltonian, \( \hat{H}(\{\hat{\mathbf{R}}\}) \), as a function of the atomic positions, \( \{\hat{\mathbf{R}}\} \), of all the ions in the material. For simplicity, we treat here the ionic positions classically. They thus follow a classical Newton equation. For an ion with mass \( M \) this is
\[
\frac{d^2 \hat{\mathbf{R}}}{dt^2} = \frac{\hat{\mathbf{F}}(\{\hat{\mathbf{R}}\}, [d\hat{\mathbf{R}}/dt])}{M},
\]
where \( \hat{\mathbf{F}} \) is the total force acting on that particular ion.

Notice that we have explicitly included in the force \( \hat{\mathbf{F}} \) also a dependence on the velocity of the ions. The reason for this is because, even at the classical level, the electron–ion and the ion–ion interactions exert a ‘drag’ for an ion to move in the lattice under the action of an external field (a consequence of this is, e.g., the inelastic contribution to electromigration [14]). Under these assumptions, the Hamiltonian is then parametrically dependent on the ionic positions and velocities, which, in turn follow their own equations of motion. In the language of memristive systems, we can anticipate that the ionic coordinates and velocities represent state variables of the system. (Clearly, in some memory systems, some electronic degrees of freedom—such as the charges on impurity atoms—should also be considered as internal state variables.)

With this Hamiltonian in hand, we then switch on the electric field perturbation at time \( t_0 \). By applying
Kubo response theory to obtain the current–current response function [19] (whether treating the electron problem quantum-mechanically or fully classically) we then obtain (\(\mu, \nu = x, y, z\))

\[
I_{\mu}(t) = \sum_{\nu} \int \text{d}r' \int_{b_0} \text{d}r \times \sigma \left( r, r'; t, t'; \vec{R}', \frac{\text{d}\vec{R}}{\text{d}t} \right) E_{\nu}(r', t').
\]

(2)

Here, the sum is over the three spatial coordinates, and \(\sigma_{\mu\nu}(r, r'; t, t'; \vec{R}, [\text{d}\vec{R}/\text{d}t])\) is a 2-rank tensor representing the response (the electrical conductivity of the system) in the direction \(\mu\) under an electric field component in the direction \(\nu\). This response is non-local in space, as represented by the electronic coordinates \(r, r'\), but most importantly, for the discussion that follows, it is non-local in time, namely the conductivity depends on the full history of the system from the time the perturbation was switched on. We stress here that this memory is not just in the electronic degrees of freedom at fixed ionic positions, namely in the delay inherent in the effective interaction among electrons. It also originates from the dynamics of the classical ions and consequent change of the many-electron configurations, which in turn affect the current.

Assuming that the varying electric field induces a negligible magnetic field, we can now write \(\vec{E} = -\nabla V\), with \(V\) the electric potential. The total current is \(I = \int \text{d}\vec{S}, \) with \(\text{d}\vec{S}\) the infinitesimal surface vector of the surface \(S\) through which the current is measured. Then from equation (2) we find (a similar derivation can be found in [20])

\[
I(t) = G\left( \{\vec{R}\}, \left\{ \frac{\text{d}\vec{R}}{\text{d}t} \right\}, t \right) V(t),
\]

(3)

where the conductance \(G(\{\vec{R}\}, \{\text{d}\vec{R}/\text{d}t\}, t)\) for a two-terminal device along the \(x\) direction is given by

\[
G\left( \{\vec{R}\}, \left\{ \frac{\text{d}\vec{R}}{\text{d}t} \right\}, t \right) = -\int_{c_1} \text{d}r \int_{c_2} \text{d}r' \int_{b_0} \text{d}r' \times \sigma_{xx} \left( r, r'; t, t'; \{\vec{R}\}, \left\{ \frac{\text{d}\vec{R}}{\text{d}t} \right\} \right),
\]

(4)

where the integrals are over the far-left and far-right device surfaces \(c_1\) and \(c_2\).

If we now define \(\{x_1\} = \{\vec{R}\}\) and \(\{x_2\} = \{\text{d}\vec{R}/\text{d}t\}\), from the Newton equation (1) the set of equations

\[
I(t) = G(\{x_1\}, \{x_2\}, t)V(t),
\]

(5)

\[
\{\dot{x}_2\} = \left[ \begin{array}{c} \frac{\vec{E}}{M} \end{array} \right] = \frac{f(\{x_1\}, \{x_2\}, t)}{M}
\]

(6)

defines a memristive system [2], with \(\{x_1\}\) and \(\{x_2\}\) the set of internal state variables of the system (in this particular case, the positions and velocities of all ions in the material). By writing \(\{x\} = \{x_1, x_2\}\) the ensemble of all state variables, we would then write equation (5) in its most familiar form [2]

\[
I(t) = G(\{x\}, V(t))V(t).
\]

(7)

The derivation we have followed has been performed in the linear regime. A similar derivation could be carried out by including higher orders in the perturbation expansion [19]. This would lead to more complicated expressions that contain explicitly the dependence of the conductivity on the electric field (and hence potential \(V\)) making the conductance non-linear. Without writing these expressions explicitly (the reader can find, e.g., the second-order expansion in the original paper [19]) we can definitely write the current in this case as

\[
I(t) = G(\{x\}, V, t)V(t),
\]

(8)

which together with equation (6) represents a memristive system [2].

3. Derivation of memcapacitive properties from Kubo response theory

Without delving too much into the details of the calculations, one can compute the capacitive of a given system using the above response theory approach. In this case the memory may arise directly from the permittivity itself, as originating from the delayed response of dipoles in the dielectric of the capacitor, and/or in the geometrical changes of the metallic plates defining the capacitor, which again can be represented as classical equations of motion for the positions \(\{\vec{R}\}\) and velocities \(\{\text{d}\vec{R}/\text{d}t\}\) of the ions composing the metallic plates (equations (6)). The permittivity, \(\epsilon(\vec{r}, \vec{r}'; t, t'; \{\vec{R}\}, \{\text{d}\vec{R}/\text{d}t\})\), can be calculated from the density–density response function (as opposed to the current–current response function calculation of the resistivity) [19]. Performing the actual calculation of the capacitance with this permittivity would then lead to a capacitance \(C(\{x\}, t)\) that is state dependent. Going beyond linear response we would then obtain the final result

\[
q(t) = C(\{x\}, V, t)V(t),
\]

(9)

where \(q(t)\) is the total charge on the capacitor, and \(V(t)\) is the potential across it. Equation (9) represents a memcapacitive system [3].

4. Derivation of meminductive properties from microscopic theories

The calculation of meminductive properties from a microscopic theory of magnetization is trickier because of the complexity of the problem. Indeed, here quantum mechanics is necessary to explain magnetic phenomena in materials since a classical description cannot account for diamagnetism, paramagnetism, or even ferromagnetism [21]. For this reason, we generally proceed by using phenomenological equations for the magnetization dynamics [22], and then derive the magnetic flux through the inductor as response to the current flowing through it. In this case, the memory of the inductance can depend on both the magnetization history as well as the
geometrical changes of the inductor [23]. In fact, following these microscopic calculations of the inductance one can obtain relations of the type

$$\phi(t) = L(x, I, t)I(t), \quad (10)$$

where $\phi(t)$ is the flux linkage (integral of the voltage), $I(t)$ the current, and the inductance $L$ depends also on some state variables with their own equations of motion.

5. Generalized response functions

It is now a simple matter of abstraction to generalize the above definitions by invoking a general non-linear, memory-dependent response function $g$. Equations (8), (9) and (10), together with the equations of motion for the state variables, can then be lumped into a single type of expression [3]

$$y(t) = g(x, u, t)u(t), \quad (11)$$

$$\dot{x} = f(x, u, t) \quad (12)$$

with $f$ some vector function of internal state variables, and $u(t)$ and $y(t)$ the input and output signals, respectively.

At this point, due to the above derivations, we could ask the question of whether these memory elements are just a renaming of previous work, and if so what value does this have, if at all. While a case can be made regarding the renaming of certain physical features that have been studied extensively in the past, and which we should all be aware of, the definitions of memristive, memcapacitive and meminductive systems represent an economic way of describing a huge number of systems, materials and devices with memory in a unified, general framework. In fact, as we have also noted in other publications (see, e.g., our [24]), this unified description is a source of inspiration for new ideas and concepts across different disciplines. For instance, it is worth stressing that the definition embodied in equations (11) and (12) is not limited only to the input perturbations we have discussed so far, such as charge, current, voltage and flux. It represents any response of a given system to an arbitrary perturbation that induces memory in the output.

Therefore, by abstracting the general definitions from the microscopic mechanisms that lead to memory, we can study more complex situations such as, for example, the collective properties of complex networks of these elements [25], without ever specifying the particular (practical) realization of such elements. Such networks with memory are not just abstract constructs. They rather represent idealized—but nonetheless very useful—models of complex biological behavior, including possibly some features of our brain [9].

6. Some general properties of response functions

Now that we have shown that memristances, memcapacitances, and meminductances are response functions with memory, we can enumerate some of the properties that they satisfy. First of all, we need to stress that response functions are not observables: they are relations between the input and output signals, which are observables. Therefore, from a physical point of view the input and output signals have to be bound functions of time. This limitation does not translate to the response functions: at any given time the input $u(t)$ may be zero, while the output $y(t)$ remains finite. From equation (11) it is then obvious that the response function is infinite at that particular instant. An example of this is a system that is driven into a superconducting state at some moment of time from a metallic state: the conductance of the system goes from a finite value (metallic state) to an infinite value (superconducting state). Therefore, unlike what has always been assumed for memristive systems [2], we do not need to artificially enforce the response function to be finite.

This property also implies another important one. If the response function can acquire an infinite value at certain times, then it is not necessary that memristive, memcapacitive and meminductive systems—or any other system satisfying equations (11) and (12)—show ‘pinched’ hysteresis loops; namely at the time when $u$ is zero, the response $g$ may be infinite, and therefore $y$ is finite. Conversely, we may have situations in which at some time the response function is zero, the output $y$ is zero, but the input is finite. As an example, suppose that we again consider a metallic system and drive it into a superconducting state, and then revert the dynamics to the metallic state, but following a different path. This system has memory but its characteristics curve will not pass through the origin.

The existence of a pinched hysteresis curve has always been declared as a hallmark of memristive systems [2], but as we have just shown it is neither necessary nor physically important to characterize a system with memory. The pinched hysteresis curve is simply a typical feature. Similar considerations hold also for memcapacitive and meminductive systems. For example, we reported O-shaped hysteresis curves in solid state memcapacitive systems [26].

Another important property pertains to the sign of the response function $g$ at any given time. For memristive systems the condition of passivity implies that the resistance is always positive (or zero) at all times (a negative resistance can only ensue from an active element). However, such a condition does not preclude a change of sign of the capacitance and inductance at certain times. This can be physically understood quite easily. Take for instance a memcapacitive system, whose permittivity lags behind the voltage applied to the system. In that case, at the instants of time when the voltage changes sign, the dielectric cannot fully screen this field. This under-screening effect results in the ‘wrong’ sign of the voltage on the capacitor plates compared to the direction of the field, and therefore in a negative capacitance. Similar considerations can be made when the material between the plates ‘over-screens’ the field at certain instants of time. An example of negative capacitance is given in figure 1, see also [26].

Finally, these results apply also to meminductive systems, when, e.g., the permeability of the magnetic material cannot instantaneously follow the current (or flux) across the inductor. Putting all this together, we can then sketch a possible hysteresis loop for memory elements when they do not cross the origin (see figure 1).
in the presence of input noise, its internal state variable $x$ is described by

$$\frac{dx}{dt} = I(t) + \xi(t),$$

where $\xi(t)$ is, e.g., Gaussian white noise,

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2\kappa \delta(t - t').$$

Here, $\kappa$ is a positive constant characterizing the noise strength. Integrating both sides of equation (13) gives

$$x(t) - x(0) = q(t) + \int_0^t \xi(t') dt'.$$

Moving $q(t)$ to the left-hand side of equation (15), squaring both sides, and averaging over the ensemble realizations of the noise, we find

$$\langle (x(t) - x(0) - q(t))^2 \rangle = \int_0^t \int_0^{t'} \langle \xi(t')\xi(t'') \rangle dt' dt'' = 2\kappa t,$$

which shows that the characteristic deviation of the internal state variable from the deterministic trajectory $x(t) = x(0) + q(t)$ increases as the square root of time, like for a Brownian particle [27]. Similar considerations apply to all types of ideal memelements.

In particular, the (intrinsic) thermal agitation of electrons inside any voltage-controlled memristor is responsible for the well-known Johnson–Nyquist noise [28, 29] (voltage fluctuations). These fluctuations are present regardless of any applied voltage, and even in systems that are not connected to any circuit at all. The thermal voltage fluctuations thus act as an internal degradation mechanism in such devices, which, in the absence of any energy barrier to protect the state of the system, leads to a diffusive loss of information.

7.2. Violation of the Landauer principle

Moreover, the logical (and hence physical) irreversibility of any computing machine imposes a minimal heat generation condition on any memory device [17]. This minimal heat generation is of order $kT$ per machine cycle, and is known as the Landauer principle [17]. The satisfaction of this condition in memristors has indeed been questioned in a recent publication [30].

To understand the reasoning behind the conclusion in [30], let us consider the switching of a memristor at constant temperature and pressure. Under these conditions, the relevant thermodynamic potential is the Gibbs free energy, which should involve energy barriers between different information states and corresponding heat dissipation as suggested by Landauer [17]. However, the equation of memristor dynamics, such as equation (13), does not involve any restrictions on minimal switching energy, and thus violates Landauer’s principle. In fact, this is simply another consequence of not having energy barriers between different memory states in any ideal memristor model. Note that although Landauer’s principle was formulated for digital computing, the same physical constraints apply also to analog
computing, such as the one that can be performed with memory elements [7, 9].

7.3. Over-delayed switching

Another shortcoming of ideal memelements is related to the over-delayed switching effect not observable in realistic memdevices. Consider, for example, an ideal current-controlled memristor described by the resistance relation \( R = R(q) \). If the switching of this memristor occurs in the vicinity of \( q = 0 \) and the device is subsequently placed in a state with a large \( q \), then a charge \( -q \) should flow through the device for it to switch back. From experiments, however, we know that the switching actually occurs as soon as the applied voltage or current exceeds its threshold value [31, 32, 23]. Thus, in real devices, a much smaller amount of charge \( -q' \) would be enough to switch the memristor back \( (q' \ll q) \). In other words, real devices do not really ‘track’ the charge flowed through them when they are in their limiting states (e.g., ON and OFF memristance states). Indeed, this limitation of ideal models should be considered in time-dependent simulations of realistic systems.

7.4. Incompatibility with symmetries of electrodynamics

Finally, we would like to emphasize that the symmetry used to postulate the memristor [1] is not a symmetry of electrodynamics. Electrodynamics is governed by Maxwell’s equations that are invariant under charge conjugation \( (q \rightarrow -q) \), parity \((\vec{r} \rightarrow -\vec{r})\) and time reversal \((t \rightarrow -t)\) transformations [33]. Any electronic device and its models (if the device operation is based solely on microscopic electrodynamics) should satisfy these symmetries. Note, however, that resistors (as well as memristors, memristive systems, and any dissipative memelements), violate time-reversal invariance. The operation of such elements involves dissipation—the conversion of electric potential energy into heat—that cannot be reversed by changing the arrow of time. On the other hand, the other symmetries of electrodynamics—in particular, charge conjugation and parity—do need to be satisfied. For instance, for an ideal memristor, charge conjugation requires \( R(q) = R(-q) \), in such a way that equation (8) (which in this case is simply \( V(t) = R(q)I(t) \)) to be invariant, namely the resistance needs to be an even function of the charge. This is definitely not taken into account in many simple models of ideal memristors [18].

Note also that for the more realistic cases of memristive, memcapacitive, and meminductive elements, the relevant symmetries of electrodynamics are generally satisfied by the physical requirements that lead to the equations of motion of the internal state variables [23].

8. Conclusions

In conclusion, by using the modern theory of response functions (in both the quantum and classical regimes) as developed in the 1950s by Kubo [19], we have shown that memristances, memcapacitances and meminductances (that describe different devices with memory) are simply response functions. As such they have to satisfy well-defined physical properties. Consequently, any additional artificial limitation such as finiteness of these responses—introduced, for instance, in the axiomatic definition of memristive systems [1, 2, 16]—limits the range of possible physical responses.

We have also discussed several potential problems related to the axiomatic definition of ideal memory devices, such as the stochastic catastrophe, violation of the Landauer principle, over-delayed switching, and possible incompatibility with symmetries of electrodynamics. These limitations should be taken into account in circuit simulations. In fact, more realistic device models—corresponding to the more general class of memristive, memcapacitive and meminductive systems—that include the actual physics of the device operation should be used in practice. We hope this paper clarifies many misunderstandings that are still propagated in the literature.

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