Complex Systems: a Physicist's Viewpoint

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1 Introduction

In recent years physicists have been deeply interested in studying the behavior of complex systems. The result of this effort has been a conceptual revolution, a paradigmatic shift that has far reaching consequences for the very definition of physics.

In the nutshell, physics is an experimental science in which theoretical predictions are compared to experiments. It differs from other sciences of nature in the crucial role of mathematics: physicists describe the phenomena by using a mathematical model and their predictions are obtained by mathematical reasoning.

In this definition of physics the word prediction plays a crucial role. Naively one could think that the meaning of the word prediction is quite evident and no further explanation is needed. In reality its meaning has changed already in the past and it is still changing now.

Let me recall using modern language what a prediction was at the time physics was born. We assume that the state of the system at the time $t$ is represented by a vector $X(t)$ with $N$ components.

In the case of classical mechanics the state of a point-like particle is described by the three coordinates and by the three components of the velocity. The corresponding vector $X(t)$ has six components. An experiment consists in determining or imposing the position and the velocity of the particle at a given time and measuring it a later time. It is crucial that (at least in principle) the experiment can be done many times by imposing the same initial conditions. If the difference between the initial and the final time is the same, the system is always found in the same final state. When repeated, the experiment always gives the same result. The theoretical task is to predict this unique, reproducible result.

This can be done by using the equations of motion which gives the time evolution of the vector $X(t)$. In the case of classical mechanics, they have the form of Newton's second law

$$\frac{dp}{dt} = F(x), \quad \frac{dx}{dt} = \frac{p}{m} \tag{1}$$

where $F(x)$ is the force. Once that the form of the force has been established it is a well posed mathematical problem to compute the final conditions as function of the initial one.
The same perspective applies not only to simple objects but also to much more complicated situations. The description of the system may need more than one position and one velocity. The equations of motion, which are in general of the form

\[
\frac{dX}{dt} = G(X(t)),
\]

in principle allow the prediction of the final state for each initial state. The theory (which consists in assuming a particular form of the function \(G(X)\)) can be tested by measuring \(X\) at the initial time, predicting \(X\) at the final time and verifying the prediction.

In reality, the mathematical difficulties may be substantial even if the system is apparently simple. To predict the evolution of a three body system (like Sun, Earth and Moon) is a rather difficult task and it can be done only with a lot a work. At the beginning of the nineteenth century Laplace was writing that an infinitely intelligent mathematician would be able to predict with certitude the future by observing the state of the universe now and using his knowledge of the laws of motion.

In this classic, deterministic framework the word prediction has a clear meaning. Unfortunately we are not infinitely intelligent mathematicians and besides an infinitely able experimentalist is needed to measure the state of the system with extremely high accuracy. The Newton-Laplace point of view could be applied only to a restricted class of phenomena. In order to consider other phenomena which could not be studied from this point of view, it was necessary to change the general philosophy, by introducing probabilistic concepts and probabilistic predictions.

There have been three revolutions in physics which all went in this direction [1] and as a consequence they have changed the meaning of the word \(prediction\). They are:

• (1) The introduction of statistical mechanics and of the first probabilistic reasoning by Maxwell, Boltzmann and Gibbs in the second half of the last century.

• (2) The discovery of quantum mechanics at the beginning of this century.

• (3) The study of complex systems and the related techniques that have been developed in these last years.

As an effect of these revolutions, the word \(prediction\) acquired a weaker meaning. Predictions in the context of the new paradigm are not acceptable with the old one (and sometimes the supporters of the old point of view try to deny to them a scientific validity). The positive consequence of the process is that the scope of physics becomes much larger and the constructions of physics find many more applications.

My aim is to present point (3). However, it is better to start by discussing point (1) in order to understand in which way the study of complex systems forces us to use the word probability in a wider context. For our purpose we can neglect point (2), because it extends the concept of probability in a different direction.

\[1\] In quantum mechanics we have to deal with the fact that also in principle the results of a single experiment are not reproducible.
2 Introducing Probability in Physics

At the time of Boltzmann [2] and Gibbs, the main motivation for leaving the Newton-Laplace point of view was not that it was wrong, but that it was useless in many cases. Let us consider the following experiments which apparently can be repeated many times with the same result:
- We bring water to 100 centigrade: it boils.
- We bring water to 0 centigrade: it freezes.

When we study this phenomenon from a microscopic point of view, we face a serious problem. The experiment should be done by measuring the positions and the velocities of all the billions of billions of atoms and we should later use this information to compute the trajectories of all the atoms. This difficulty was bypassed by discovering that for a system composed by many many particles, practically all the initial conditions (at fixed total energy) lead to the same macroscopic behavior of the system. The task of measuring everything is not only impossible, it is also useless. If we neglect the possibility of some very special initial configuration - which happens with extremely low probability - the system always behaves in the same way.

The final predictions are the following:
- Water practically always boils at 100 degrees. The probability is so high that it is extremely likely that this kind of predictions has never failed in the whole history of the universe.
- If we measure the velocity of a single molecule of water we cannot predict anything precise. However we can compute the probability that the molecule has a velocity \( \vec{v} \) (\( P(\vec{v}) \propto \exp(-A\vec{v}^2) \) where \( A = m/(2kT) \)). Therefore if we measure the velocity of a molecule \( M \) times the observed distribution of velocity should approach the theoretical curve when \( M \) goes to infinity.

In general, we could say that for these large systems there are two kinds of quantities:
- Some quantities can be predicted with certitude and have always the same value inside a small interval (usually of order \( N^{-1/2} \) for a system with \( N \) degrees of freedom).
- Other quantities do not take always the same value. In this case a probabilistic prediction is possible.

3 Deterministic Chaos

In the previous discussion, the main motivation for introducing probability was the large number of particles present. Only in the second half of this century was it realized that there are many systems with a small number of particles, or more generally with a small number of degrees of freedom, for which it is also necessary to use probabilistic arguments [3].

In these systems (which sometimes are called chaotic) the trajectory cannot be predicted for large times, because it is too sensitive to the initial conditions. The difference in the position of the trajectories of two systems which have a very similar initial conditions increases exponentially with time. In other words, even a very small uncertainty on the initial condition leads to a total loss of knowledge after a characteristic time \( \tau \). More
precisely if

\[ X_1(0) - X_0(0) \propto \epsilon \]  

the difference \( X_1(t) - X_0(t) \) grows as function of the time \( t \) as \( \epsilon \exp(t/\tau) \) until it reaches a value of order 1.

Deterministic predictions are possible here on a time scale smaller than \( \tau \), but they become impossible at later times because we cannot measure the initial conditions with infinite precision.

A very simple example is provided by two (or more) balls on a billiard table without friction. For generic choice of the initial condition the two balls will collide from time to time, and after each collision it becomes more difficult to predict the position of the balls.

Fortunately, in many cases the probability distribution at large times for finding the system in a given configuration is independent on the initial conditions and it can be predicted. So here also we can compute only the probability distribution of some variables, not the exact evolution.

The new framework given by statistical mechanics should now be clear. We have a system, we know the equation of motion. In principle, an exact knowledge of the initial conditions allow us to compute the exact evolution of the systems. In reality this task may be impossible because we do not know the initial conditions with sufficiently high accuracy. It is also possible that the computation is terribly complicated. We can however make progress and get much more insight if we restrict ourselves to the task of predicting the probability distribution of the system at large times (in short its behavior).

Given the equation of motion \( G \) (see eq. 2) we define the probability \( P_G(X) \) [3] as

\[ \int dX f(X) P_G(X) = \lim_{T \to \infty} \frac{\int_0^T f(X(t)) dt}{T}, \]  

where \( f(x) \) is an arbitrary test function. For ergodic systems the probability \( P_G(X) \) does not depend on the choice of the initial point for almost all the choices.

The task of statistical mechanics consists in the computation for given \( G \) of the probability \( P_G(X) \) and of its properties.

4 Complex Systems

It was recently realized that this approach described in the previous section (i.e. to predict the behavior of the system from the knowledge of the equations of motion) fails in the case of complex systems for reasons that are very similar (albeit in a different contest) to those which led to the abandonment of the Newton-Laplace view-point.

There are many possible definitions of a complex system. I will use the following one. A system is complex if its behavior crucially depends on the details of the system. This dependence is often very difficult to understand \(^2\). In other words, the behavior of the

\(^2\) A single complex system may also display different types of behavior and a small perturbation is enough for switch from one behavior to another. For example an animal may: sleep, dream, run, hunt, eat, play...
system may be extremely sensitive to the form of the equations of motion and a small variation in the equations of motion leads to a large variation in the behavior of the system. More precisely for two systems with $N$ degrees of freedom with equations of motion $G_0$ and $G_1$, where

$$G_1(X) - G_0(X) = O(\epsilon), \quad (5)$$

we could have that for small $\epsilon$ but large $\epsilon N$,

$$P_{G_1}(X) - P_{G_0}(X) = O(1). \quad (6)$$

In this happens it is practically impossible to compute the asymptotic probably as function of $G$.

My aim is to show that although a system is complex, it is still possible to get predictions for its behavior, but these predictions will be now of a probabilistic nature. I will illustrate this point in a particular example. The prototype of a complex system in physics is spin glass [4]. I will choose here something more familiar to most people, a large protein.

A protein is composed by a long chain of a few hundred amino-acids and its chemical composition is specified by the sequence of aminoacids (primary structure). In physiological situations, normally a protein folds in an unique way (tertiary structure). During the folding, the protein goes to the configuration of minimal energy (more precisely, to the configuration of minimal free energy). However, there are many quite different configurations of the protein which have an energy near the minimal one. There are proteins, which are called allosteric, which have two configurations with practically the same energy. Sometimes, if we perturb the protein by a small amount, e.g. changing the pH or changing only one aminoacid in the chain, the folding changes dramatically. We can also select one of the two different configurations by the binding of a ligand.

The variations in the shape of mioglobulin in different conditions are crucial for its respiratory functions. More generally, the possibility of switching from one configuration to another is one of the fundamental mechanisms which allow proteins to work as enzymes. For example the change of configuration of allosteric proteins is used for doing useful work, e.g. for contracting muscular fibers.

The existence of allosteric proteins implies that a small variation in the form of the potential among the components of the protein changes the folding of the protein dramatically. It is thus evident that a small error in the form of the interaction among the different components of the protein or of the interaction with the solvent would lead to quite wrong results.

Natural proteins are on the borderline of what can actually be understood; we have not yet computed their folding properties, but this does not seem completely impossible, especially for the smallest ones. However, to compute the folding properties of much large proteins seems to be a hopeless task.

If an approximate knowledge of the equations of motion does not allow us to compute the behavior of a complex system, we can give up this task and restrict ourselves to compute the probability of a behavior when the equation of motions are chosen randomly inside a given class.

In other words we can study the same problem in two different ways:
In the old approach we consider a given protein (e.g. mioglobulin) and we compute the
form of the two foldings with minimal energy and their energy difference as a function
of the chemical properties of the solvent.

In the new approach we consider a class of proteins (to which mioglobulin belongs) and
we compute the probability distribution of the energy difference among the two foldings
with minimal energy [5].

Of course, this second computation will not tell us the properties of mioglobulin. It
will give us predictions that cannot be tested on a single protein (in the same way the
probability distribution of the velocities cannot be tested by measuring only one velocity);
we need to repeat the experiments on many different proteins.

Taking the new point of view, we often gain insight. The behavior of a given complex
system may be obtained only after a very long computation on a computer and often
we cannot understand the deep reasons of the final result. The study of the probability
distribution of the behavior can sometimes be done analytically and we can follow all the
steps that lead to the conclusions.

The advantage of the second point of view is that its results may be easily generalized
to other systems. For example long RNA molecules also fold in a characteristic way, in the
same way that proteins do. A general explanation which shows that some characteristic
of folding are shared by all polymers composed by different monomers may be applied to
RNA as well as to protein.

There are simple models (e.g. spin glasses [4]) in which this program works. The com-
putation of the behavior of a given system is extremely difficult and sensitive to the
minimal detail and can be done only with lengthy computer simulations. The analytic
computation of the probability distribution of the behavior for a generic system can be
done analytically and these probabilistic predictions have been successfully verified.

The extension of this program to other systems leads to two different types of difficulties.

- The generalization of the methods which allow the computation of the probability dis-
  tribution of the behavior to models which are not as simple as spin glasses, is technically
difficult and progress in this direction are rather slow.
- This point of view is quite different from the traditional one (mathematically it corre-
sponds to the use of imprecise probabilities [6]). The predictions are not made for the
properties of a given system, but for the probability distribution of those properties
which change with the system. We are not enough familiar with this new point of view
to appreciate all its potentialities.

As usual a change in the paradigm leads to a change in the questions posed. We do
not have to ask how a particular system behaves. We have to ask which are the general
features of the behavior of a system belonging to a given class.

In spite of these difficulties, this new approach seem to be absolutely necessary to get
some understanding in really complex systems. We have seen that the arguments are very
similar to those described before. In the two cases they can be summarized as follows

- The extreme sensitivity of the trajectory on the initial conditions forces us to study
  the probability distribution of the systems at large times. This must be done in spite of
  the fact that an exact knowledge of the initial condition determines the trajectory at
  all times. The behavior of the system can be computed from the equations of motion.
- The extreme sensitivity of the behavior on the detailed form of the equation of
motion forces us to study the probability distribution of the behavior of the system. This must be done in spite of the fact that an exact knowledge of the initial conditions determines the behavior. The probability distribution of the behavior of the system can be computed from the probability distribution of the equations of motion. In other terms, given a probability distribution \( \rho(G) \) we can compute the probability \( \mathcal{P}[P_G(X)] \), which of course depends on \( \rho \).

The advantage of this new point of view is to expand the range of application of physical reasoning. We shall see now how it puts the relations between physics and biology in a new perspective.

### 5 Possible Biological Applications

In biology we face a very difficult problem of how to use the immense amount of information we gather at the molecular level in order to understand the behavior of the whole organism.

Let us consider an example. One of the simplest organisms is *E. Coli*. Its genome (which is known) codes for about 3000 different proteins which interacts among themselves. Some proteins promote the production of other proteins, while other proteins have a suppressor effect.

In principle we can gather the information on the properties of the proteins, on the interaction among the proteins (for simplicity let us neglect all the other chemical elements of the cell). At the end we can use this information to construct a model of the living cell. The model may lead to a system of few thousand (or more) coupled differential equations which can be studied by lengthy computations on a computer.

If the information is accurate enough, the model will describe a living cell. However we know that in real life many mutations are lethal, and therefore it is quite likely that imprecision in the form of the interactions among proteins will lead to a non-living cell or to a living cell with a quite different behavior. It is also clear that such a gigantic computation (although welcome) will not capture the essence of life. Indeed it should be repeated nearly from scratch if instead of *E. Coli* we consider a different organism.

The previous discussion suggests that we could give up the aim of deriving the properties of a given organism from its chemical components, and ask different questions, e.g. what are the general properties of a living organism and how they do change from organism to organism.

An example of this last question has been studied by Kaufmann [7]. There is a dependence of the number different cell types on the number of genes in all kinds of living organisms.

\[
\text{# cell types } \propto (\text{# genes})^{1/2}
\]

As Kaufmann points out, this fact must have a general explanation and he proposes one based on mathematical considerations of evolution.

Another empirical law, which calls for a general explanation is

\[
\text{# species in an island } \propto (\text{# genes})^{1/4}
\]
In these two cases we can hope to compute the exponents. However in many other cases this point of view is so different from the traditional one, that it is very hard to find the right questions and also to answer to them.

A field in which this approach seems to be mandatory is the study of the origin of life. Here it is crucial to understand which are the enzymatic capabilities of the prebiotic material (maybe long randomly assembled RNA chains) before evolution starts. We would like to know which of the properties of these long chains had to be selected and which ones where already present before selection.

This approach is quite different from a reductionistic one, as far as it puts the stress on the behavior of the whole system. For the moment the largest impact of these ideas in biology has been in the field of neural networks, but in the other fields the progress is quite slow. We need to sharpen our theoretical tools in order to be able to predict the typical behavior for different classes of systems. We are seeing now only the beginning of these investigations in mathematical physics.

When the physical instruments become more robust and our theoretical command increases, the interaction with biology will become more easy. I am convinced that in the next century a much more deep understanding of life will come from this approach.

References