An algorithm-based introduction to the evolution of physical systems

Eliana D'Ambrosio - Dipartimento di Fisica "Ettore Pancini", Università degli Studi di Napoli "Federico II" - elianadambrosio5@gmail.com
Rodolfo Figari - Dipartimento di Fisica "Ettore Pancini", Università degli Studi di Napoli "Federico II" - figari@na.infn.it
Emilio Balzano - Dipartimento di Fisica "Ettore Pancini", Università degli Studi di Napoli "Federico II" - balzano@na.infn.it

Abstract: We propose a unified introduction to evolution equations of classical and (simple) quantum physical systems. Our attempt is to circumvent the lack of mathematical knowledge with the use of simplified forms of numerical analysis. We consider a discretized space-time where the evolution equations become recurrence relations that students are first required to handle with the use of a spreadsheet. Given any initial condition, solutions at any future time are computed and graphically represented. The continuous space-time limit is then qualitatively obtained looking at the solutions on a scale where discretization become unnoticeable, avoiding all mathematical details. The aim is to allow students to autonomously examine dynamical features of complex systems whose study is generally considered too complicate to be part of a Physics course in high school as well as in the college level General Physics courses (e.g. many body gravitational systems, large amplitude pendulum oscillations, stochastic dynamical laws, quantum wave packet evolution etc.). In this way students can investigate the effectiveness of dynamical laws in modeling the evolution of real world systems.

Keywords: Physics education, dynamic laws, learning modern physics, numerical solution algorithm, secondary school.

1. Introduction

The Italian Ministry of education guidelines about Physics teaching recommend that the new generations' scientific knowledge includes some selected items of modern physics (Indire). Nevertheless, teachers meet known pedagogical difficulties in complying such recommendations. On one hand, high school students do not have the mathematical skills needed for an introduction, not simply informational of the modern theories basics. On the other hand, the educational laboratories have not available the experimental setups necessary to reproduce key experiments in modern physics. Furthermore, the experiments outcomes are massively interpreted by the use of the theory itself. Consequently, the implementation of the guidelines about new Physics teaching is highly problematic.

These difficulties insert themselves in a context that is already fragile: in fact, students seem not to be very keen on Physics and, more in general on Science. Physics is often taught as an arid list of laws or as fragments of knowledge linked only by the chronological order in which they were discovered. Some European researchers (Sjøberg 2002) are convinced that a probable cause of the lack of interest in Physics is the way in which the subject is presented: it is often overloaded with information and data and tends to provoke "a mechanical learning without a deeper comprehension" instead of focusing on "big and fundamental ideas and principles".

Most of the introductions to quantum physics trying to comply with the guidelines use a historical approach. Even though it is essential to show the incompatibility between experimental evidence and classical knowledge, such an approach cannot be adopted rigidly.

For example, high school students are generally not introduced either to the problem of equilibrium of classical radiation in a cavity or to the radiation by accelerated charges. As a consequence they cannot catch the reasons of Planck's hypothesis and the absence of stable orbits for classical point charges in mutual interaction. So it is evident that, in order to draw concretely achievable introductions in the high school, it is necessary to take into consideration students' knowledge.

Nowadays many scientific education researches indicate the importance of using technological applications as teaching support: in fact, they are important resources to comprehend the physical world with a scientific approach. Both new technological tools and common software (i.e. database, spreadsheets, graphics programs, etc.) are considered as key elements for the development of teaching and learning, as well as modeling, visualization and simulation of processes. Their effectiveness is especially evident in the presentation of physical models. In this domain, the information technology enables to explore phenomenology and theory; it also helps to understand the transition from the physical world to the abstract structure representing it. It is well known that this passage is not so straightforward in quantum physics. Several teaching strategies suggest the use of specific software and multimedia presentation to introduce basic concepts in modern physics and quantum physics in particular (Muller, Wiesner 2002; Zollman *et al*. 2002; Kohnle *et al.* 2010). The goal is to fill the gap between the abstract formalism of quantum mechanics and the qualitative understanding necessary to explain, comprehend and predict the evolution of physical systems. Other educational approaches show that computational physics, besides being an effective way to find approximate solutions to specific problems in the absence of advanced mathematical knowledge, can help students to understand the basic physics concepts (Hugdal, Berg 2015). In this last direction, in particular by using simplified forms of numerical analysis, we propose a unified introduction to the dynamical equations of physics with the aim to allow students to investigate the evolution of classic systems as well as of stochastic and quantum systems and to approach both the theoretical features and the computational aspects of the evolution equations.

2. An algorithm-based introduction to the evolution of physical systems

Our idea is to simplify the computational methods to adapt them to computer skills of high school students. So we propose an approach to numerical computation through recursive algorithms that will be implemented by a spreadsheet. We chose it as computer support because it is largely used in school contexts and because we consider it an ideal environment for an intuitive approach to numerical solutions of the differential equations governing a theory. In this way, without having previous knowledge of programming languages, students can easily implement the algorithm and focus their attention on relevant dynamical features of the solutions.

More precisely, we consider a discretized space-time where the evolution equations become recurrence relations that students are first required to handle with the use of a spreadsheet. Given any initial condition, solutions at any future time are computed and graphically represented. The continuous space-time limit is then qualitatively obtained looking at the solutions on a scale where discretization become unnoticeable, avoiding all mathematical details. However, it is clear that the student should be convinced about the fact that as long as there is no absolute minimal time interval value (as it is the case when a continuous model of time is assumed) a rigorous theory is missing until the value of t remains unspecified. In this way we suggest a unified methodology to analyze the evolution laws of classical, stochastic and (simple) quantum systems. In our opinion, there are some advantages in such a presentation that are worth mentioning:

- the dynamical laws are not simply stated, but analyzed on the basis of their effectiveness in modeling the evolution of real world systems;
- students are enabled to autonomously examine dynamical features of complex systems, whose study is generally considered too complicate to be part of a Physics course in high school as well as in the college level General Physics courses (e.g. many body gravitational systems, large amplitude pendulum oscillations, stochastic dynamical laws, quantum wave packet evolution etc.);
- students are provided with some preliminary skill for examining how solutions depend on the initial conditions and on dynamical parameters;
- the possibility to compute and analyze approximate solutions of the evolution laws allows to make a first comparison between classical, stochastic and quantum world, to highlight the distinctive role played by probability in different contexts and to appreciate to what extent classic categories lose their meaning in the quantum context.

The only prerequisite to our algorithm-based introduction to the evolution of physical systems consists in knowledge of vector algebra and of some concepts of kinematics that supply the following equalities about the variation of position and velocity:

- The total displacement is equal to sum of *N* displacements between any time *t* and its next $t + \Delta t$, and each displacement is given by the "average velocity" (in the time interval Δt):

$$\vec{r}(t_N) - \vec{r}(t_0) = \sum_{i=1}^{i=N} (\vec{r}(t_i) - \vec{r}(t_{i-1})) = \sum_{i=1}^{i=N} \frac{(\vec{r}(t_i) - \vec{r}(t_{i-1}))}{t_i - t_{i-1}} (t_i - t_{i-1}) \qquad (1.1)$$

$$\cong \sum_{i=1}^{i=N} \vec{v}_{t_{i-1},t_i} (t_i - t_{i-1})$$

with the "average velocity" between times *t* and $t' > t$ defined as

$$\vec{v}_{t,t'} \equiv \frac{\vec{r}(t') - \vec{r}(t)}{t' - t}.$$

- In the same way, the total velocity variation is

$$\vec{v}(t_N) - \vec{v}(t_0) = \sum_{i=1}^{i=N} (\vec{v}(t_i) - \vec{v}(t_{i-1})) = \sum_{i=1}^{i=N} \frac{(\vec{v}(t_i) - \vec{v}(t_{i-1}))}{t_i - t_{i-1}} (t_i - t_{i-1}) \qquad (1.2)$$

$$\cong \sum_{i=1}^{i=N} \vec{a}_{t_{i-1},t_i} (t_i - t_{i-1})$$

defining the "average acceleration" between times $t' > t$ as

$$\vec{a}_{t,t'} = \frac{\vec{v}(t') - \vec{v}(t)}{t' - t}$$

2.1. Classical dynamics

The evolution equations of classical dynamics can be presented retracing Newton's ideas about the reconstruction of the planets motion evolution. Newton's idea consisted in attributing preliminarly a cause to the motion of bodies: the "forces" acting on them. Then, in detailing quantitatively their effects. According to the laws of motion, forces, expressing the interaction between bodies, generate velocity changes. He realized that a large class of motions (the "natural ones") could be explained with the single hypothesis of the existence of the gravitational force acting between material bodies.

In this way, he was able to make available a unified explanation of the Keplerian orbits of planets, of the free fall motion of bodies close to the earth surface, of the small oscillations of the pendulum etc.

The "two steps" procedure conceived by Newton to compute solutions of the dynamical equations (used in particular in the analysis of the "two-body problem") consists in solving for "short *Δt*" the following pair of recurrence equations:

$$\begin{cases} \mathbf{x}(t+\Delta t) - \mathbf{x}(t) = \mathbf{v}(t)\cdot\Delta t \\ \mathbf{v}(t+\Delta t) - \mathbf{v}(t) = \mathbf{F}(\mathbf{x}(t),t)/m\cdot\Delta t \end{cases} \tag{1.3}$$

where the a-priori known *F(x(t), t)* is the force acting on the pointlike body at instant *t* (when it is in the position *x(t)).*

When position and velocity (and, in turn, the force) are known at the initial time, the recurrence equations return position and velocity at any time *nΔt*. The Newton procedure (1.3) can be implemented in the spreadsheet. Each computational step consists in fact in the copy and paste of the previous line, where the recursion formulas are written via relative references (apart from fixed parameters appearing as absolute references).

The algorithmic calculation is easily approachable by new generations of students (born with the computer) and put into their hands the great predictive power of the dynamics laws. The procedure outlined above can be applied to few examples of classical systems, which are considered, in general, too complicate to be presented in an elementary physics course. The aim is to show that the acquisition of qualitative and quantitative understanding of relevant features of the evolution of complex system is surely within high school students' reach.

In the following we desire to mention all the paradigmatic cases we examined via numerical computation implemented in a spreadsheet.[1]

It is possible to apply the numerical computation procedure of the solution to (1.3) to the case of the *oscillatory motion of a pendulum*, for generic initial conditions, in presence of viscous friction. It is well known that the outing by the condition of small-amplitude oscillations, the equations become strongly non-linear and their analytical solution is highly problematic. On the contrary the computational procedure, does not present any difficulty: more precisely it does not change in any way.

Another paradigmatic case the computational scheme allows to cope with is the *gravitational many-body problem.* It is in fact possible to investigate numerically the evolution of a simplified circular restricted three body planetary system which allowed Euler as the first (and then Lagrange and Poincaré as the last) to understand and compute the secular variations of planet orbits. It was the starting point of the investigations about the stability of the solar system, undoubtedly, the greatest success of Newtonian mechanics.

With the same procedure, also the dynamics of classical fields can be investigated. The numerical analysis of the evolution equations of a spatially continuous system requires discretization also of the spatial coordinates. Classical fields become functions

[1] All the simulations carried out by us and presented in this paper, along with other supporting materials, will be available on the website managed by the scientific education research group based in [Università degli studi di Napoli Federico II, Dipartimento di Fisica "Ettore Pancini"], URL: <http://llp.fisica.unina.it/index.php/it> [data di accesso: 12/09/2017].

on a discrete space-time lattice. The *longitudinal vibrations of an elastic string* represent the simplest example.

2.2. Stochastic dynamics

The term stochastic dynamics refers to mathematical models. Starting from the analysis of the Brownian motion, physics begins to develop models of complex systems where it is possible to give only a probabilistic description of the evolution of the system. In same way as before it is possible to analyze stochastic processes in a discretized space-time (in particular Markov processes) where the evolution equations are equation for probability densities.

This is the case of *Brownian motion*, the random motion of particles in a fluid. The interaction between the Brownian particles and the molecules of the fluid cannot be accurately characterized dynamically, so the model supplies an evolution dynamics of the position probabilities. In particular, processes "without memory" are characteristic of these dynamics: the position at time $n + 1$ depends only on position at the previous instant n (characteristic of Markov processes). For example, we consider a particle that moves in a one-dimensional lattice. It is assumed that probability for the particle of being in i, at instant $n + 1$, is given by the sum of probabilities that particle is, at the previous instant n, in one of the points of lattice that, with one step, lead to the point i, multiplied for the respective probability of transition to i. So, the evolution of probability is governed by:

$$P_i^{(n+1)} = P_{i,i-1}P_{i-1}^{(n)} + P_{i,i+1}P_{i+1}^{(n)} - P_{i,i}P_i^{(n)} \tag{1.4}$$

If we consider equal to zero the probability for particle to remain in the point already occupied and consider equal probabilities of selecting the forward and backward transitions, the equation (1.4) becomes:

$$P_i^{(n+1)} = \frac{1}{2}P_{i-1}^{(n)} + \frac{1}{2}P_{i+1}^{(n)}. \tag{1.5}$$

When the evolution of probabilities of physics system configurations is analyzed, necessarily involves previous knowledge of some basic elements of theory and calculus of probability, of the concepts of joint and conditional probability, transition probabilities, Bayes' theorem, etc.

The equation (1.4), implemented in the spreadsheet, gives easily the position probability evolution of a Brownian particle. It is possible to visualize the spread of probability density, which, in the long run, tends to a uniform distribution.

The investigation can be generalized *analyzing Brownian motions overlaid with deterministic motion* or considering *motions in two dimensions* (in a bi-dimensional lattice). It is also possible to examine the *Langevin approach* to Brownian motion (based on forces acting on particle) without using any further technical skills.

2.3. Quantum dynamics

The same procedure can be applied to a presentation of quantum mechanics in a discretized space-time. Quantum mechanics comes from the need to justify the large amount of experimental evidence obtained on the interaction between radiation and matter. In particular, from the phenomenology of matter waves, i.e. from the two-slit experiment with electrons, come to light two fundamental aspects of quantum theory: “it is only possible a probabilistic description of the events” and “something evolves like the wave” (Bell 1987). Such statements are in respect of the fact that, in repeated tests, the impacts of electrons on a screen are distributed in different points of space, despite the identical preparation of the initial state. Additionally, the figure resulting from many electron impacts is similar to the typical interference figure of spherical waves emitted by two point sources.

Consequently, quantum mechanics can only provide calculus formulas for the probability to observe specific values of physical observables; furthermore the observations of the interference phenomena of matter waves suggest that the state of quantum particle can be associated with a vector, as the electric and magnetic fields, having values in all the points in space (a vector field).

Assuming, as previously done, the space as a large lattice (for neglecting what happens at the edges) with a very small spacing (as to confuse a discrete space with a continuous), it is possible to make *an “axiomatic” presentation* of the basic principles of quantum mechanics. The revisited postulates, concerning state and probability, assume the following form:

- The state of a particle at any time *n* is specified by the association, at each point *i* of the lattice, of a vector with two components:

$$\vec{\psi}_i(n) = \{x_i(n), y_i(n)\}$$

- The probability to find the particle at the point *i*-th of lattice, at time *n* is

$$P_i(n) = |\psi_i(n)|^2 = {x_i}^2(n) + y_i^2(n)$$

- Since the particle is necessarily somewhere, it is true that

$$\sum_i (x_i^2(n) + y_i^2(n)) = 1$$

The equations of quantum dynamics are evolution equations for the components of the vector Ψ:

$$\begin{cases} x_i(n+1) - x_i(n) = [-\frac{1}{2}y_{i+1}(n) - \frac{1}{2}y_{i-1}(n) + y_i + V_i y_i(n)]\Delta t \\ y_i(n+1) - y_i(n) = [+\frac{1}{2}x_{i+1}(n) + \frac{1}{2}x_{i-1}(n) - x_i + V_i x_i(n)]\Delta t \end{cases} \quad (1.6)$$

Also in this case, if the quantum state Ψ is known at any particular instant of time, the solution follows for any time thereafter. Now, we want to highlight two fundamental aspects emerging from a comparison between the equations of stochastic dynamics and quantum: firstly, the similarity of the equation (1.6) with the equations of position probability evolution in the case of Brownian motion (1.4) e (1.5) and secondly, that what is evolving in quantum mechanics it is not the probability but only the auxiliary vector.

In the spreadsheet, it is possible to investigate a simple model of *interference of "matter waves"*. The use of the spreadsheet allows highlighting how the evolution of a free quantum particle in a superposition state (each described by a wave packet) differs from the one of a classical particle undergoing a stochastic dynamics.

It is also possible to treat the *quantum harmonic oscillator*. It is the simplest case of the quantum system presenting *bound states* and *"almost classic" states*. The only prerequisite to computation of the equations (1.6) is the knowledge of elastic potential. Using a spreadsheet, we can prove that for initial conditions corresponding to standing waves and running waves, the evolution corresponds respectively to the two states above mentioned.

As a final remark we wont to mention that in this paper is not suggested that evolution equations are the only things that should be taught in classical and quantum mechanics. We only stress the importance of the dynamic laws in the predictive power of the theory. Moreover, allowing students to put their hands in calculation of the physics system's evolution, we think to convey them the astonishment in regard of the effectiveness of a theory.

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