

# **A Pedagogical Approach to Modelling Electric Conduction in Solids.**

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## **Abstract**

We present a pedagogic approach aimed at modelling electric conduction in metals, built by using the modelling environment Net Logo, and describe some related activities. The reported examples have been experimented during the laboratory courses of the Italian Pre-Service School for Physics Teacher Education (S.S.I.S.).

## **Introduction**

Computer modelling and simulation tools can help physics teachers to focus on relationships between macroscopic and microscopic properties of matter, enabling students to model systems directly at the level of their individual constituent elements and their interactions, in order to understand emergent macroscopic properties.

The benefits of multi-agent simulations for understanding how a variety of complex behaviours derive from simple interactions of local agents are today well known [1]. A core feature of multi-agent simulation environments is that students can apply a small number of rules to capture fundamental causality structures underlying behaviours in a range of apparently disparate phenomena.

Building a model by thinking in terms of individual agents appears to be intuitive, particularly for the mathematically uninitiated [2, 3]: the related pedagogic activities may be centred on an approach to learning physics that follows the same steps than learning a new language [4].

Here we present some pedagogic procedures aimed at relating measurements of electric properties of conductors with “virtual experiments” built by using NetLogo [5]. Models of both classic and quantum electric conduction in metals, such as the Drude-Lorentz and Sommerfeld ones, have been implemented. The different model predictions about the resistivity vs. temperature dependence and some related parameters have been related to experimental results.

The reported activities have been experimented during the laboratory courses of the Italian Graduate School for Physics Teacher Education (S.S.I.S.).

## **Experimental results**

Resistivity vs. temperature measurements have been performed in the context of an education project aimed at studying electric conduction properties of solid conductors, semiconductors and superconductors [6].

Measurements have been performed by using an electronic board allowing to take data of the electric current circulating in a sample when it is subject to a given voltage, as a function of the sample temperature. The board is designed to study the resistance of high  $T_c$  superconductor samples but we have modified it to take also measurements with conductors and semiconductors. Here we report only the data taken in conductors.

The resistance data at low temperature values are taken by suspending the metallic sample in a thermally insulated container and letting it cool under the action of liquid nitrogen vapours placed in the container. Current and voltage, as well as temperature data have been collected by using digital multimeters connected to the electronic board, as shown in figure 1.

Fig. 1. The experimental apparatus.

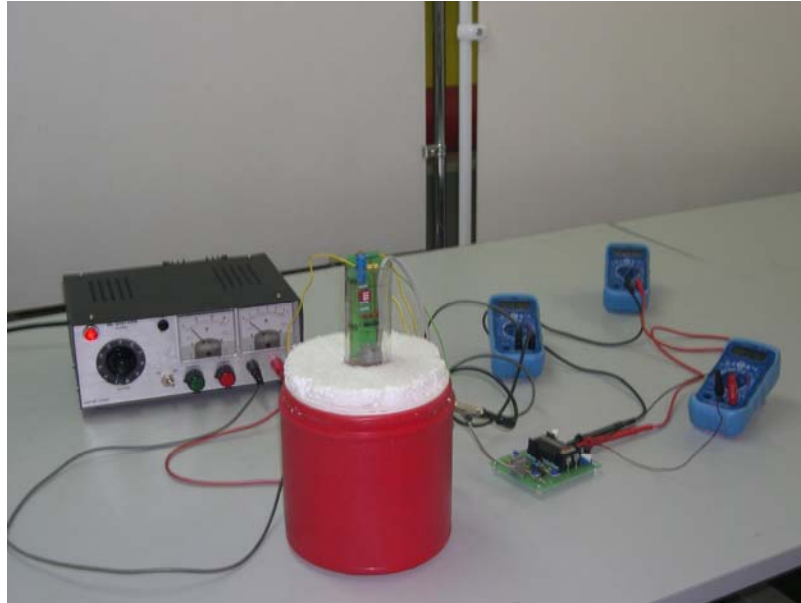
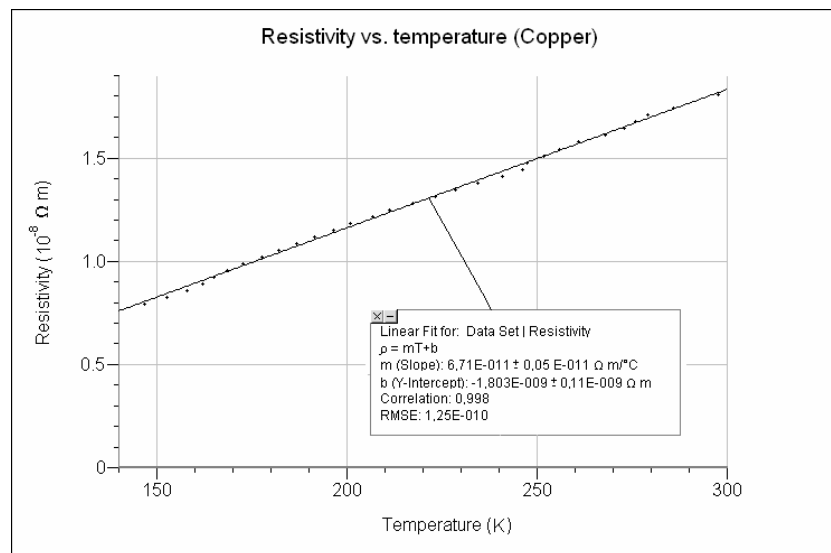


Figure 2 shows data taken by using a thin copper wire, of length  $L = 0.5$  m and cross sectional diameter  $d = 2 \times 10^{-4}$  m.

Fig. 2. Resistivity vs. temperature in a copper wire.



A linear dependence of resistivity from temperature is evident, as expected for a conductor in the range of analysed temperatures.

From the well known resistivity vs. temperature formula

$$\rho = \rho_0 [1 + \alpha(T - T_0)]$$

and from the linear fit parameters reported in figure 2, it is easy to obtain an estimate of the temperature coefficient  $\alpha$  in copper.  $\rho_0$  is the resistivity at  $T_0 = 273$ K.

$$\alpha = (4.07 \pm 0.04) \times 10^{-3} \frac{1}{K}$$

This value is in accordance with the expected value for  $\alpha$  in copper [7].

These results are in good agreement with other measurements [8] aimed at help students to better understand the electrical behaviour of conductors and semiconductors.

## Modelling

Microscopic models describing and explaining the experimental results have been implemented by using classical and semi-classical models implemented in NetLogo.

The main pedagogical purposes of such simulations can be summarized as follows:

- to emphasize the fundamental concepts related to electron motion and electron-crystal lattice interactions as key concepts to understand the electron transport phenomena and the effects of temperature variation;
- to supply a deep understanding of microscopic conduction mechanisms and their modifications due to the temperature, emerging from different and more refined microscopic models of metals.

The implemented models share some characteristics with well known historical models and will be described in the following.

The first and simplest model, fitting some of the conduction properties of metals, is the ‘Drude-Lorentz model’. It considers the electrical conduction as due to a “gas of free electrons” moving through a lattice of fixed ions, against which they collide. If an electric field is applied, electrons, of charge  $e$  and mass  $m_e$ , are subject to an acceleration  $eE/m_e$ . The whole effect of collisions is viewed as a viscous force, counterbalancing the electrical force and maintaining constant the velocity of electrons.

If  $n_e$  represents the number of free electrons in a unitary volume and  $v_d$  is the drift velocity of the electrons, i.e. the mean velocity of the electrons in the field direction, the metal resistivity can be written as:

$$\rho = \frac{E}{n_e e v_d} \quad (1)$$

The mean time  $\tau$  between collisions is expressed in term of the electrons’ mean thermal velocity  $v_m$  and of the total cross-sectional area  $A$  for the electron-ion scattering.

$$\tau = \frac{1}{n_e v_m A} \quad (2)$$

The drift velocity and the metal resistivity can be related to  $\tau$  by the formulas:

$$v_d = \frac{eE}{m_e} \tau, \quad \rho = \frac{m_e}{n_e e^2 \tau} \quad (3)$$

The crucial point in this microscopic representation (“relaxation time approximation”) lies in the interpretation of  $v_m$  and  $A$ . Our simulations use three different interpretations or ‘pictures’: the ‘Drude-Lorentz’ one, the ‘Full classic’ picture and the ‘Semi classic Sommerfeld’ picture, described in the next section.

## Model implementations

The models have been implemented by using NetLogo 3.0.2 and NetLogo 3D preview 1 [5]. We consider a small volume of copper containing the same numbers (about 100) of free electrons and ions arranged in a regular three-dimensional crystal lattice. Electron and ions are modelled as small elastic spheres of given mass and dimension. Electron-electron and ion-electron Coulomb interactions are not considered. Consequently, the trajectory of an electron is a straight line/an arc of parabola, in the absence/presence of electric field  $E$ .

Although the simulation runs in a three dimensional space, the system can be visualised both in three dimensions (figure 5) and in a two-dimensional projection (figure 6).

Fig. 5. NetLogo 3-D visualisation of electrons moving in the ion lattice.

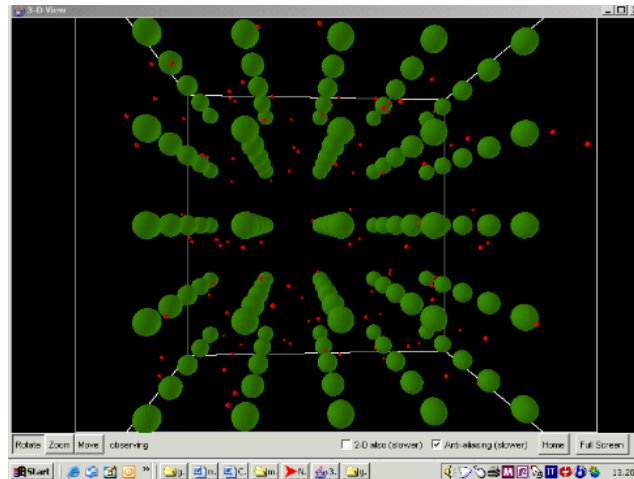
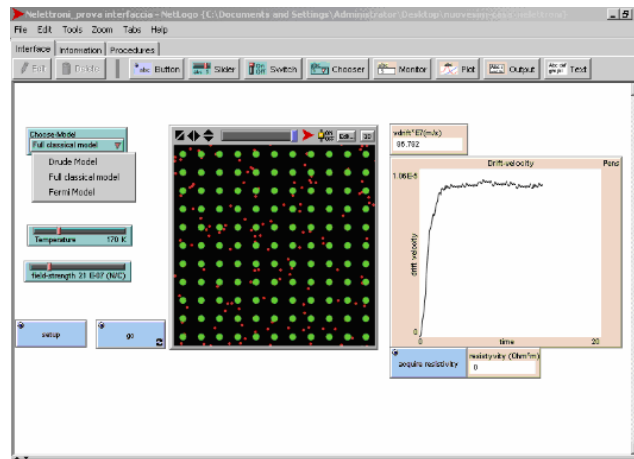


Fig. 6. A two-dimensional projection of the 3-D space and the simulation result: the graph of electron drift velocity as a function of time.



The user can choose one of the three models previously described, set the temperature and the electric field strength and perform two different types of ‘virtual experiments’: a) by varying the field strength at a constant temperature; b) by varying the temperature at a constant field strength. The program output is the electron drift velocity as a function of time. When the drift velocity reaches its steady value it can be acquired and the resistivity value is calculated (1). With several values of resistivity corresponding to different temperatures a graph of  $\rho$  as a function of  $T$  is built.

The detailed implementation of the three models presents some differences, both statistical and dynamical, reflecting the different characteristics of these models.

### ***Drude-Lorentz model***

Here the electrons have a velocity distribution in accordance with Maxwell-Boltzmann statistics. Then, to a given temperature  $T$ ,  $v_m$  corresponds to the mean square root velocity  $v_{rms}$

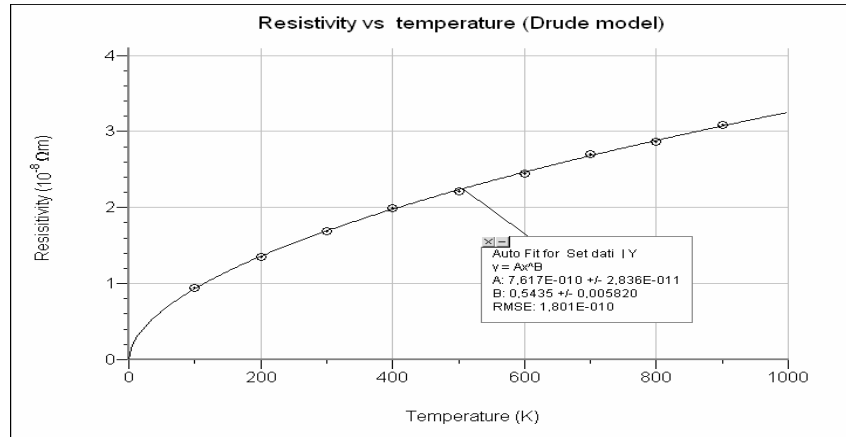
$$v_m = v_{rms} = \sqrt{\frac{3kT}{m_e}}$$

The lattice ions are considered at rest with a radius equal to ion radius (for copper,  $r_0 = 0.361 \text{ \AA}$ ).

The electron-ion collisions are treated as perfectly elastic and no dissipation mechanisms are considered. For not too high electric field strengths (below 100 V/m), the system reaches a steady state condition in which the dynamical quantities, such as drift velocity

and mean relaxation time, are constant (figure 6). By changing the system temperature (i.e. the value of  $v_{rms}$ ), a plot of resistivity as a function of  $T$  can be obtained, as shown in figure 7 .

Fig. 7. Resistivity vs. temperature graph obtained by implementing in the simulation the Drude-Lorentz model.



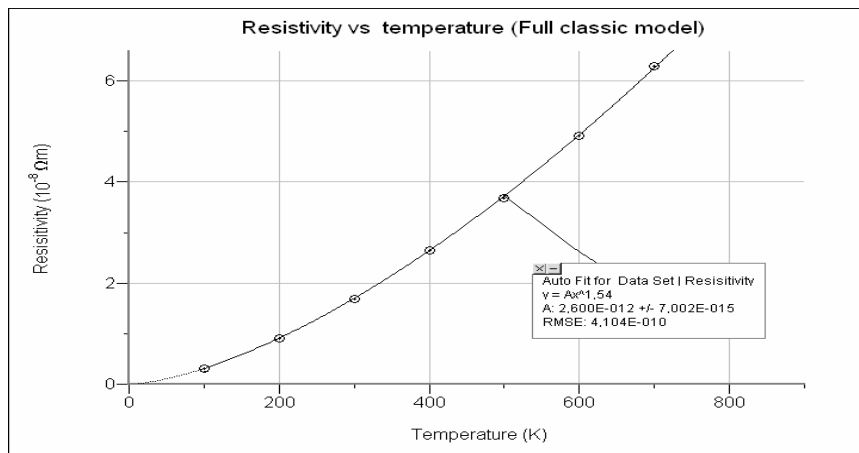
### ***'Full classical' model***

In this model we take into account the ion oscillations by assuming that they depend on the temperature. From theoretical considerations it is possible to assume that the effective maximum oscillation amplitude is proportional to  $T^{1/2}$ .

The effective ionic radius  $r$  is assumed to be equal to the maximum oscillation amplitude. Electron-ion collision is assumed to be elastic, with exchanges of energy and momentum. We also consider a dissipation mechanism in the model, by keeping ions in equilibrium with a thermal bath at constant temperature.

Figure 8 shows the resistivity vs. temperature data obtained in the temperature range 100K – 700K. As expected, results of this classical model are in discordance with the experimental results (see figure 2).

Fig. 8. Resistivity vs. temperature graph obtained by implementing the full classical conduction model within the simulation.

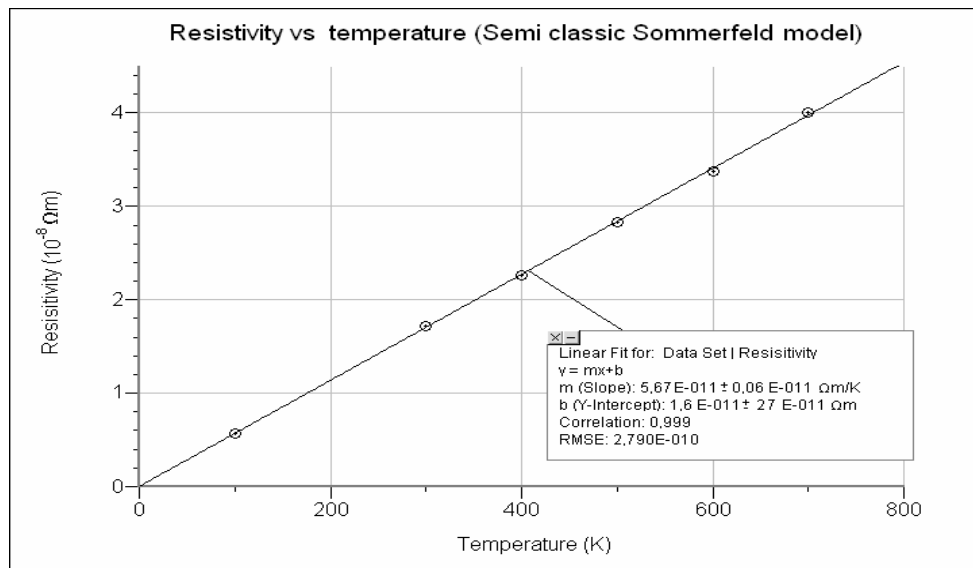


### ***Semi-classical Sommerfeld model***

The implementation of this model differs from the previous ones since here the quantum nature of electrons is taken into account by considering the Fermi-Dirac statistic. Then, in the temperature range of interest, the distribution of electrons velocity is almost independent from

the temperature. As in the previous models, the electron-ion interactions are considered perfectly elastic.

Fig. 9. Resistivity vs. temperature graph obtained by implementing the semi-classic Sommerfeld model within the simulation.



The result obtained with the semi classical Sommerfeld model (figure 9) are in good agreement with the experimental data, reported in figure 2 : the linear dependence of  $\rho$  from temperature is found and physical parameters, like the temperature coefficient and the resistivity values at  $T = 273K$ , are close to the ones obtained from the real experimental data.

### Discussion and conclusion

Our models are based on a few fundamental rules of atomic interactions that exhibit emergent behaviours reproducing important aspects of the properties of materials, as electric conductivity.

There are several features of our pedagogical approach that may contribute to student learning. In our simulations, the same underlying computational model appears in different contexts and gradual modifications of the model are outlined. This provides several advantages:

- students gain familiarity with different representations and ways in which electrons behave and interact with nuclei;
- the model parameters can be set by the student, in the same way in which they interact and control the experimental parameters;
- the macroscopic properties of the model emerge from the details of the atomic-scale interactions in just the way that the corresponding properties emerge in real atoms.

A preliminary analysis of prospective teachers worksheets allows us to infer that laboratory activities, scaffolded by modelling, can improve students' learning about actions and interactions of individual objects resulting in emergent system properties.

Prospective teachers showed a better understanding of the difference between simply describing a situation in terms of equations and interpreting it on the basis of mechanisms of functioning. After the lab part of the workshop, prospective teachers showed a renewed attitude to search for interpretative models, even involving microscopic interactions, explaining why a phenomenon develops in a given way or some specific experimental results are obtained.

### Acknowledgements

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