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Modelling thermionic emission by using a two-level mechanical system

(A pedagogical approach to the Boltzmann factor)

Onofrio R. Battaglia
UoP_PERG (University of Palermo Physics Education Research Group)
Dipartimento di Fisica e Tecnologie Relative, Università di Palermo - Palermo, Italy

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Summary. — The Boltzmann factor is at the basis of a great amount of thermodynamic and statistical physics, both classical and quantum. It describes the behaviour of natural systems that exchange energy with the environment. However, why does the expression have that specific form? *The Feynman Lectures on Physics* justifies it heuristically by referencing to the "exponential atmosphere" example. Thermodynamics textbooks usually give a more or less complete explanation that mainly involves a mathematical analysis, where it is hard to see the logic flow. Moreover, the necessary mathematics is not at the level of high school or college students' preparation. Here we present an experiment and a simulation aimed at deriving the Boltzmann factor expression and illustrating the fundamental concepts and principles of statistical mechanics. Experiments and simulations are used in order to visualise the mechanisms involved; the experiments use easily available laboratory equipment, and simulations are developed in NetLogo, a software environment that, besides having a really friendly interface, allows the user to easily interact with the algorithm, as well as to modify it.

PACS `01.40.-d` – Education.
PACS `01.40.gb` – Teaching methods and strategies.
PACS `01.50.H-` – Computers in education.
PACS `01.50.Pa` – Laboratory experiments and apparatus.

1. – Introduction

In this paper we present an example of a more general project aimed at developing methods for the introduction of the basic concepts of statistical mechanics at high school, as well as at scientific undergraduate level. The approach uses some unifying concepts and ideas of different areas of physics (mechanics, thermodynamics, electromagnetism) and modern information and communication technology tools in order to stimulate a meaningful learning.

The Boltzmann factor is actually one of these unifying concepts and it is easy to find it in many physics topics, as well as in other scientific fields such as chemistry and biology. For its characteristics of great generality and simplicity, the Boltzmann factor can be successfully used for the pedagogical introduction to statistical mechanics, in particular for the introduction of the statistical distribution concept at high school, as well as at undergraduate level.

Conventional approaches to its formalization are essentially two. The first, less general and easier, makes use of techniques of combinatory calculus and has been used by Maxwell and Boltzmann to obtain their famous distribution functions. The second approach, mainly due to Gibbs, is more general and refers to the theory of "Statistical Ensembles". A heuristics justification due to Feynman (the exponential atmosphere example [1]), is usually reported in many textbooks in order to derive the mathematical expression of the Boltzmann factor.

All these methods show some problems. The deduction achieved by combinatory calculus techniques applied to the microstates associated to a thermodynamic macrostate makes use, in the core part, of the so-called Stirling factorial logarithm approximation. The limit of this approximation is that the occupation number of cells corresponding to a great energy is small, in contrast to the assumptions of strict validity of the approximation itself. The Gibbs approach to statistical ensembles is based on the so-called "ergodic hypothesis". This last hypothesis, although valid for many systems and accepted for reasons of physical plausibility (Landau, see [2]), needs to be demonstrated. A classic example is the system of coupled oscillators of the famous FPU experiment-simulation, due to Fermi, Pasta and Ulam [3]. This system, for which the ergodicity property was considered obvious, revealed its nonergodicity, in a very broad range of initial conditions. The Feynman approch, while proposing a simple and intuitive conceptual visualization, certainly suffers from some logical drawbacks. Moreover, the previously described approaches to statistical distributions offer some mathematical and conceptual difficulties as well as the need of a theoretical knowledge that is not always well mastered by the student target of our study.

Here, we propose an approach involving some experiments of simple two-level physical systems, in which the Boltzmann factor appears in the proper interpretation of their time evolution. Moreover, some computer simulations make evident the role of the physical variables involved through visualization and easy calculations. The experiments, that can be easily performed in a high school or undergraduate context, include some chemical reactions, the study of the vapour pressure in liquid systems, the thermionic effect and the analysis of semiconductor resistance (thermistors). In this paper we will concentrate on the experiments dealing with the thermionic effect and on some simulations.

2. – Experimental set-up

A vacuum tube (diode) can be used in order to introduce pupils to the role of the Boltzmann factor in modelling simple two-level systems. In particular, the calculation of the electron concentration outside a cathode (led to an appropriate temperature) can be performed. This population is in thermodynamic equilibrium with the remaining free electrons within the metal. The experiment is aimed at obtaining an estimate of such electron concentration, which depends on the temperature of the cathode according to the Boltzmann factor.

The experimental set-up makes use of instruments readily available in school laboratories and the measurements to perform are very easy: the diode filament voltage

(a) (b)

Fig. 1. – (a) The experimental apparatus: vacuum tube, voltage generator, digital multimeters and accessories. (b) Diode equivalent circuit and measurement set-up.

and current, the anode current and the cathode temperature (measured indirectly, as described in subsect. **2**˙2). In order to perform this experiment, pupils only need to know the basic laws of fundamental electrical phenomena.

Since calculations require the values of some diode parameters, related to the geometrical form and size of its internal parts, a diode identical to the one used for measurements has been opened and closely inspected.

2˙1. *Voltage and current measurements.* – The values of voltages and currents, involved in the vacuum tube normal operation, have been measured by using the simple circuit [4] shown in fig. 1. We used a voltage generator capable of giving a continuously adjustable signal sweeping from 0 to 6 V, three digital multimeters, including one with at least 200 μA full scale and with 1 μA sensitivity, a vacuum tube (diode) with indirectly heated cathode.

By using the measurement set-up sketched in fig. 1 it is possible to carry out measures as follows: the voltage generator signal is swept, according to the diode characteristics, and filament voltage and current are recorded, as well as the current output from the diode. For our specific vacuum tube (an $EZ81$ one, with a tungsten filament [5]), the filament current was varied in the range 0.75 A–1.08 A and three sets of nine well-spaced experimental points were taken.

2˙2. *Temperature measurament.* – In order to obtain estimates of the cathode temperature one can, as a first approximation, consider that it has to be equal to the filament one. This last value can be found by using filament voltage and current measurements. We take into account a phenomenological law relating the filament temperature, T, to the ratio between its resistance at temperature T, $R(T)$ and the resistance value at 300 K, $R_{\rm env}$. In the case of tungsten filament tubes, this law can be written as follows [6]:

$$T = a_0 + a_1 \frac{R(T)}{R_{\rm env}} + a_2 \left(\frac{R(T)}{R_{\rm env}}\right)^2 + a_3 \left(\frac{R(T)}{R_{\rm env}}\right)^3, \tag{1}$$

where the coefficients a_i are well-known parameters. As shown in fig. 2, eq.(1) can be resonably approximated to a linear function in the range of our interest. On the other

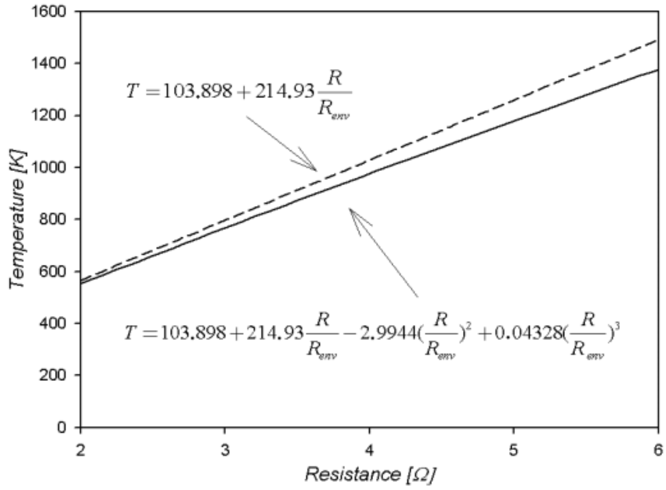

Fig. 2. – Temperature *vs.* resistance for tungsten. The lower, continuous curve shows data of T *vs.* R obtained by using (1). The upper, dashed line represents the linear approximation of (1).

hand, one has to consider that this method to obtain the cathode temperature considers it equal to the filament temperature and actually approximates its value.

2˙3. *Room temperature resistance measurament*. – The circuit in fig. 3 is used for the resistance measurements. The value of resistance R is obtained by the relation

$$R = R_0 \frac{V_1}{V_2}\,, \tag{2}$$

where R_0 is a known resistance.

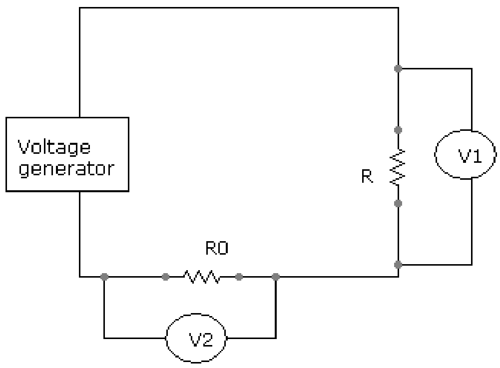

Fig. 3. – Equivalent circuit for R environment measurement.

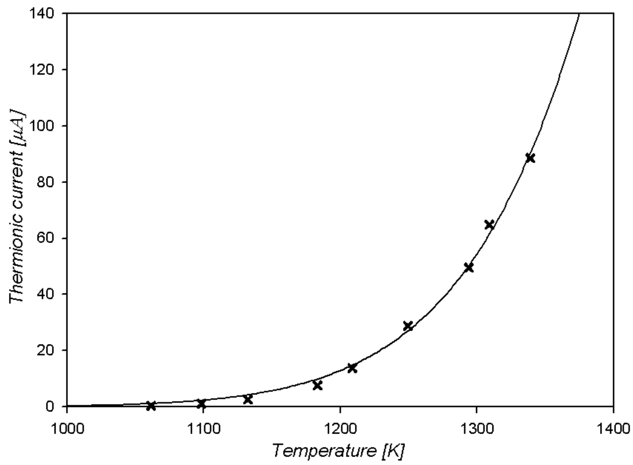

Fig. 4. – Data points experimental results (crosses) and Richardson law (line) data fitting.

3. – Experimental results and analisys

Figure 4 shows the experimental data of current as a function of temperature. In order to have experimental evidence of the actual cathode material, data were fitted by using the well-known mathematical function of the Richardson theory of thermionic effect

$$I_{\rm th} = AT^2 e^{-\frac{w_e}{kT}}, \tag{3}$$

where w_e is the extraction work for the cathode material and k is the Boltzmann constant.

From data fitting an estimate of parameters w_e and A can be obtained. In particular, the values of $w_e = (1.7 \pm 0.1)\,\text{eV}$ and $A = (150 \pm 100)\,\mu\text{A/K}^2$ are found. The value of w_e can be confronted with the accepted values of (1.0–1.9) eV in metal oxide [7]. The wide inaccuracy in the A value can be ascribed to the small range of analysed temperatures (a choice partially imposed by the need to consider constant the extraction work for all our measures).

The calculation of the electron concentration in equilibrium with the heated cathode can be carried out by taking into account thermionic current $I_{\rm th}$ and cathode temperature T measurements and using the relation

$$n = \frac{I_{\rm th}}{Sq}\sqrt{\frac{2\pi m}{kT}}, \tag{4}$$

where S is the anode area, q and m are the electron charge and mass, respectively. Expression (4) is obtained from the classical relation between the thermionic current density, j, the electron charge density in vacuum, ρ, and the mean value of electron speed, $\langle v \rangle$, between anode and cathode

$$j = \rho \langle v \rangle, \tag{5}$$

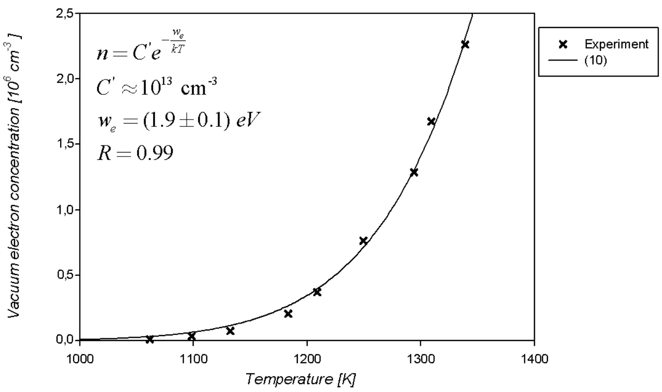

Fig. 5. – Vacuum electron concentration *vs.* temperature and fitting curves given by eq. (10).

where

$$\langle v \rangle = \left(\frac{m}{2\pi kT}\right)^{1/2} \int_0^\infty v e^{-\frac{mv^2}{2kT}} \mathrm{d}v. \tag{6}$$

We note that electrons in vacuum are here treated as classical particles. This can be justified by the particle low density and the values of the involved temperatures. In fact, an estimate of the Fermi temperature, for the concentration of our interest, gives a value lower than the operating temperature of the diode. From relations (3) and (4) we obtain

$$n = CT^{3/2} e^{-\frac{w_e}{kT}}. \tag{7}$$

By taking the natural logarithm of relation (7) we obtain

$$Y = C^* - \frac{3}{2}\ln(X) - BX \tag{8}$$

with

$$Y = \ln(n), \qquad C^* = \ln(C), \qquad X = \frac{1}{T}, \qquad B = \frac{w_e}{k}. \tag{9}$$

In relation (8) the term $\frac{3}{2}\ln(X)$ changes very slowly with respect to X, at least in the temperature range of our interest, and it can be substituted with a costant without sensibly modifing the term w_e/k. As a consequence an approximation of eq. (7) is

$$n = C' e^{-\frac{w_e}{kT}}. \tag{10}$$

As a result, the obtained values of the density of electron in equilibrium outside the cathode can be fitted, with respect to temperature, by using the simple expression of the Boltzmann factor, as reported in fig. 5. The extraction work value w_e, obtained by the data fitting, is consistent with the accepted values, althought it appears to be overestimated. This is an expected result for indirect heating tubes, since experimental values of

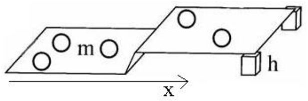

Fig. 6. – A mechanical model for a two-level system.

extraction work are affected by both the error in cathode temperature measurement and the lack of external tension between anode and cathode, that makes not all the electrons emitted by the cathode being collected by the anode.

4. – A mechanical model and simulations

The described experiment exhibits a clear pedagogical problem: it does not allow pupils to easily understand what is actually happening during the time evolution of the thermionic emission. For this reason, we found it useful to develop a simulation representig a mechanical model (fig. 6), that can supply a clear view of the two-level system dynamic and work by analogy with respect to the performed experiment. Such a system consists of a box within which some elastic balls are supposed to move [8]. This box is divided into two separate floors, with a height difference, h, through a slope. The balls are distributed over one of the floors with random positions and velocities. Molecular dynamics can be used for the numerical resolution of the equations of motion. The mutual collisions between balls and the collisions between balls and the box walls are considered perfectly elastic and they are the only interactions taken into account. After each collision, the new components of each ball velocity can be found by applying the law of energy and momentum conservation. Any ball, moving on the lower plane, can move to the upper plane if the velocity component along x is such that

$$v_x \geq \sqrt{2gh}. \tag{11}$$

This model can be easily implemented on NetLogo [9] by using 2D or 3D views. The first is used to get results reliable and comparable with actual experimental results, while the second one can be used to obtain a more realistic view of the model evolution. Both allow an easy interaction with the user. Figure 7 shows some screenshots resulting from the 3D version of the simulation. Figure 8 shows some results obtained by the 2D simulation obtained by varying the average kinetic energy of particles and taking into account the time evolution of the population ratio between the two levels.

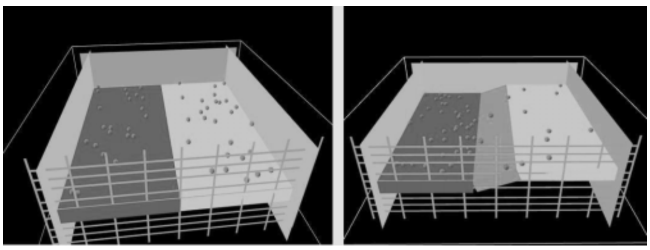

Fig. 7. – Simulation of a two-level mechanical system a NetLogo 3D enviroiment.

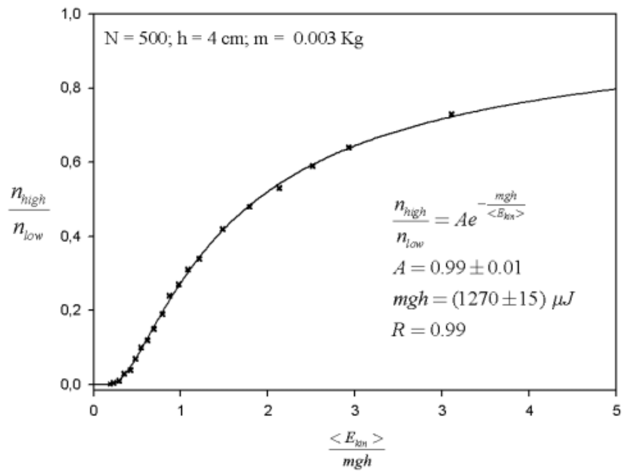

Fig. 8. – NetLogo simulation results: higher/lower level population as a function of the average kinetic energy.

In order to best represent what is happening inside the two-level diode system, we must choose to analyse into details the system behaviour for great values of the ratio w_e/kT. We obtain the graph of fig. 9, that, when confronted with fig. 5 (reporting the vacuum electron concentration as a function of temperature in diode) exhibits a very similar behaviour. Figure 9 shows enlargement of the initial part of fig. 8; the dependence of particle concentration on the Boltzmann factor is evident.

5. – Conclusion

This pedagogical approach has been experimented with a group of trainee teachers of the Italian graduate school for physics teacher education, at the University of Palermo.

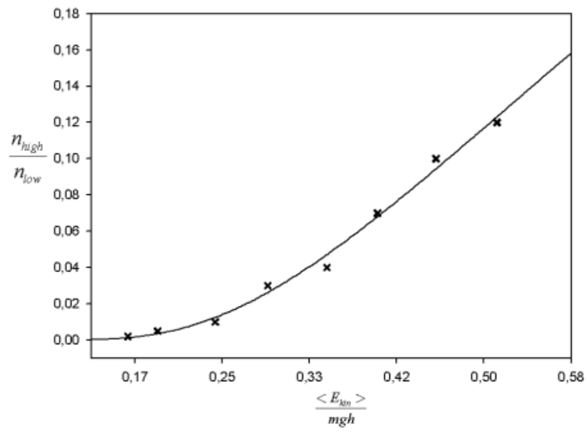

Fig. 9. – NetLogo simulation results: higher/lower level population as a function of the average kinetic energy. Enlargement of the initial part of fig. 8.

From a preliminary analysis of the trainee teachers logbooks and worksheets, we can infer that lab work and simulations helped students to better understand the physical meaning of the Boltzmann factor and the way a two-level system actually works. Moreover, our approach gives a confirmation of the relevance for a meaningful understanding of teaching strategies integrating lab-work and simulations, well experimented in other physics fields [10]. A broader study is in progress, in order to obtain a more complete and formal deduction of the Boltzmann factor, through an elementary analysis of the transition probabilities of a two-level system, aimed at the canonical ensemble introduction at high school, as well as at undergraduate levels.

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