ĐẠI HỌC QUỐC GIA TP HỒ CHÍ MINH

TRƯỜNG ĐẠI HỌC BÁCH KHOA

Assignment of

GENERAL PHYSICS I

Project 10

Maxwell – Boltzmann velocity distribution

Lecturer: Phạm Tấn Thi

Nguyễn Trung Hậu

Class: CC07 BT; CC04 LT- **Group:** 03

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Sinh viên thực hiện	**Mã số sinh viên**
Nguyễn Tiến Hưng	2252280
Lê Minh Khanh	2252296
Nguyễn Võ Hoàng Khang	2252306
Phạm Đình Khang	2252309

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PREFACE

General Physics 1 is an important general subject for HCMUT students in particular and students major in the science and technology field in general. Therefore, devoting a certain amount of time into studying and practicing is essential for students to develop a solid foundation of this subject as well as other ones during the training program.

Since the term computer science was born, its development greatly supported the advancing of physics subjects. The application of computer science in the process of interpreting databases of physics, solving physics problems has shortened the time spent and brought higher efficiency. As we all know, Matlab application software has solved many problems . Therefore, learning Matlab and applying Matlab in the practice of the subject General physics 1 are very important and highly urgent.

During the process of writing the following essay, our team received much support and dedicated help from teachers, seniors and friends. In addition, the group would also like to express our sincere gratitude to Mr. Nguyen Trung Hau, who is the instructor for this topic. Thanks to his wholeheartedly instructing, the group was able to complete the essay on time and resolve the problems we encountered. His guidance had been the guideline for all the actions of the group and maximized the supportive relationship between teachers and students in the educational environment. Also, we would like to thank Mr.Pham Tan Thi for his enthusiastic teaching of the theory so that we have a solid foundation to solve this Math problem. Finally, once again, the team would like to express our deep gratitude to the teachers and everyone who took time to instruct the group. This is such a great source of motivation for the group to achieve such results.

REPORT SUMMARY

The report shows the result of the Maxwell velocity distribution and the probability of particle existence within the entered velocity range with a defined temperature T and a mass of 1 mole of a gas.

Use MATLAB software to assist in processing calculations in the process of studying and drawing the Maxwell velocity distribution and the probability of particle existence within the entered velocity range.

LIST OF TABLES AND DRAWING

REQUIREMENTS OF THE TOPIC

1.1. Content:

In physics, particularly in Thermodynamics, the Maxwell distribution, also known as the Maxwell-Boltzmann distribution, represents the distribution of speed of particle's motion in gasses, in which particles can move freely without other kinds of interaction except elastic collision causing exchanges of kinetic energy and momentum but no change of excited state.

The Maxwell distribution is expressed as a function of the temperature of the system, the mass of the particle, and the velocity of the particle in the gas.

$$f(v) = \sqrt{\left(\frac{m}{2\pi kT}\right)^3} 4\pi v^2 e^{\left(-\frac{mv^2}{2kT}\right)}$$

In this project, the student's task is to represent by MATLAB the Maxwell distribution function and find out the probability of a particle's velocity within a given velocity range.

1.2. Requirements:

1) Students should have basic programming knowledge of MATLAB.

2) Learn about symbolic calculation and graphical interpretation in MATLAB.

1.3. Task:

Write Matlab program to:

1) Enter the system temperature and velocity range needed to calculate the probability. The parameters of particle mass, Boltzmann's constant etc. are given in the program.

2) Plot the Maxwell velocity distribution.

3) Calculate the probability of particle existence within the entered velocity range. Display the area limited by this velocity range on a Maxwell distribution plot.

Note: Students can use other non-symbolic approaches.

Submitting a report has to contain text explaining the content of the program and the entire code verified to run properly in Matlab.

THEORETICAL BASIS

2.1. Introduction:

The original derivation in 1860 by James Clerk Maxwell was an argument based on molecular collisions of the Kinetic theory of gases as well as certain symmetries in the speed distribution function; Maxwell also gave an early argument that these molecular collisions entail a tendency towards equilibrium. After Maxwell, Ludwig Boltzmann in 1872 also derived the distribution on mechanical grounds and argued that gases should over time tend toward this distribution, due to collisions (see H-theorem). He later (1877) derived the distribution again under the framework of statistical thermodynamics. The derivations in this section are along the lines of Boltzmann's 1877 derivation, starting with result known as Maxwell–Boltzmann statistics (from statistical thermodynamics). Maxwell–Boltzmann statistics gives the average number of particles found in a given single-particle microstate. Under certain assumptions, the logarithm of the fraction of particles in a given microstate is proportional to the ratio of the energy of that state to the temperature of the system:

$$f(v) = \sqrt{\left(\frac{m}{2\pi kT}\right)^3} 4\pi v^2 e^{\left(-\frac{mv^2}{2kT}\right)}$$

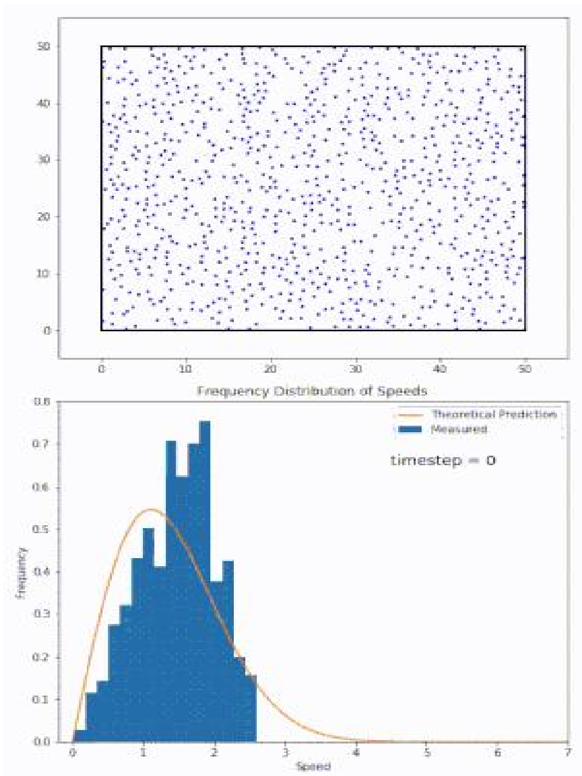

Figure 2.1: *Simulation of a 2D gas relaxing towards a Maxwell–Boltzmann speed distribution*

In physics (in particular in statistical mechanics), the Maxwell–Boltzmann distribution, or Maxwell(ian) distribution, is a particular probability distribution named after James Clerk Maxwell and Ludwig Boltzmann.

2.2. Theory:

A Maxwell-Boltzmann Distribution is a probability distribution used for describing the speeds of various particles within a stationary container at a specific temperature. The distribution is often represented with a graph, with the y-axis defined as the number of molecules and the x-axis defined as the speed. In short, the graph shows the number of molecules per unit speed. Derivations of the distribution have been conceptualized as well, including Maxwell-Boltzmann statistics, which emphasizes statistical thermodynamics.

The Maxwell-Boltzmann distribution is more concerned with molecular speeds than with their component velocities, which take the form:

$$f(v) = \sqrt{\left(\frac{m}{2\pi k_B T}\right)^3} 4\pi v^2 e^{\frac{-m(v_x^2+v_y^2+v_z^2)}{2k_B T}}$$

Or we can also use this formula :

$$f(v) = \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{m}{kT}\right)^{3/2} v^2 \exp\left[-\frac{mv^2}{2kT}\right].$$

Since the speed v in our three-dimensional (Euclidean dimension) formula:

$$v^2 = v_x^2 + v_y^2 + v_z^2$$

$$\rightarrow v = \sqrt{v_x^2 + v_y^2 + v_z^2} \text{ (m/s)}$$

Therefore, the distribution function f(v) is given by:

$$f(v) = \sqrt{\left(\frac{m}{2\pi k_B T}\right)^3} 4\pi v^2 e^{\frac{-mv^2}{2k_B T}}$$

m: mass of the molecule (kg)

T: thermodynamic temperature (Kelvin)

k_B: Boltzmann constant **(k_B= 1.38 * 10^(-23))**

We can also place three speeds on our distribution function.

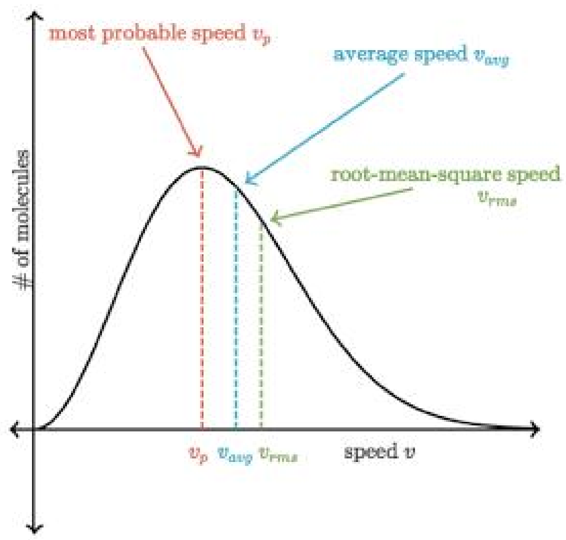

***Figure 2.2**: Graph of Maxwell-Boltzmann molecular distribution function*

The most probable speed, is the speed most likely by any molecule (of the same mass m) in the system and corresponds to the maximum value or mode of f(v):

$$Vp = \sqrt{\frac{2KT}{m}}$$

The mean speed v_{av} is the weighted average velocity, which is :

Vavg = $\sqrt{\frac{8KT}{\pi m}}$

The root-mean-square speed, v_{rms} is the square root of the average squared speed:

Vrms = $\sqrt{\frac{3KT}{m}}$

Besides, the probability that a particle has a velocity between v1 and v2

$$P(v1\ldots v2) = \int_{v1}^{v2} f(v)dv$$

It's a long and winding road to get there. It's worth noting that the front-end factor is a normalization factor that ensures the overall area under the curve (i.e., the chance of the particle having any velocity) is equal to 1. To put it another way

$$P(0...v\max) = \int_{0}^{v\max} f(v)dv = 1$$

MATLAB

3.1. Introduction to Matlab:

3.1.1. Overview of Matlab:

Matlab (short for matrix labor) is a four-level high-level programming language generation environment for arithmetic calculations, visualization and programming. Developed by MathWorks. Matlab allows manipulating matrices, drawing graphs with functions and data, displaying implementing algorithms, creating user interfaces, including C, C++, Java and Fortran; data analysis, algorithm development, prototyping and applications. Matlab has a lot of math commands and functions to help you in doing calculations, drawing common figures and diagrams, and implementing methods to calculate.

3.1.2. Commonly used functions in Matlab:

Command	*Syntax*	*Meaning*
Disp	*disp(x)* *disp('chuoi tu')*	*Display the contents of the array or chain*
Syms	*syms x*	*Declare the variable x as a symbol variable*
Input	*x=input('ten bien')*	*Show command prompt and wait for input*
Plot	*plot(x,y)*	*Generate xy . graph*
Title	*title('ten do thi')*	*Graph title*
Legend	*legend('vi tri')*	*Add a note to the graph*
Label	*xlabel('ten)* *yabel('ten)*	*Add labels to the x-axis* *Add labels to the y-axis*

***Table 3.1.2:** Some common used command in Matlab*

3.2 Matlab Code and Explanation:

In this project, we choose Oxygen molecule to study. And the Scientific format displays a number as an exponential, replacing part of the number with e+n, where e (exponential) multiplies the preceding number by 10 to the power of n. For example, a scientific format of 2 decimal places would show 12345678901 as 1.23e+10, which is 1.23 times 10 to the 10th power.

```
% Compute probabilities from Maxwell distribution
```

```
clear all; % Clear memory
help maxdist; % Print header

%@ Initialize variables
m = 5.314e-26; % Mass of oxygen molecule (32/100/6.022/10^23)
k = 1.38e-23; % Boltzmann's constant
T = input('Enter temperature (Kelvin): ');
% Compute two frequently used constants
Constant1 = 4*pi*(m/(2*pi*k*T))^(3/2);
Constant2 = m/(2*k*T);
% Enter the lower and upper bounds for integration
vLow = input('Enter lower bound speed (m/s): ');
vHigh = input('Enter upper bound speed (m/s): ');

%@ Perform running sum to estimate the integral
NSum = 300; % Number of elements in the sum
DeltaV = (vHigh - vLow)/(NSum - 1); % Delta v
Probability = 0.0; % Set running sum to zero
for iSum=1:NSum % Loop until hitting the break
%@ Compute probability density for speed v
v = vLow + (iSum-1)*DeltaV;
ProbDensity = Constant1* v^2 *exp(-Constant2*v^2);
%@ Accumulate running sum
Probability = Probability + ProbDensity*DeltaV;
end

%@ Set up the plotting variables
```

```
vPlotMax = 5*sqrt(k*T/m); % Maximum speed to plot
NPoints = 100; % Number of points used in plot
for iPoint=1:NPoints
% Compute x-axis values for the plot
vPlot(iPoint) = (iPoint-1)/(NPoints) * vPlotMax;
% Compute y-axis values for the plot
fPlot(iPoint) = Constant1 * vPlot(iPoint)^2 * ...
exp(-Constant2 * vPlot(iPoint)^2);
end

%@ Create the plot
clf; figure(gcf); % Clear the figure; bring window forward
plot(vPlot,fPlot,'-'); % Plot the probability density function
hold on; % Hold the graph to add vertical dashed lines
% Compute values of probability at vLow and vHigh
fLow = Constant1 * vLow^2 * exp(-Constant2 * vLow^2);
fHigh = Constant1 * vHigh^2 * exp(-Constant2*vHigh^2);
% Draw vertical dashed lines between the lower and upper
% bounds of integration
for v=vLow:(vHigh-vLow)/10000:vHigh
f = Constant1 * v^2 * exp(-Constant2*v^2);
plot([v v],[0 f],'-b');
end

plot(vLow,0,'*r',vHigh,0,'*r'); % Mark endpoints on the x-axis
xlabel('Speed (m/s)');
ylabel('Distribution function');
```

title(sprintf('Probability in dashed area = %g',Probability));

3.3 Result:

- At t = 0^0C (= 273K). (Cold temperature)

```
Command Window
  maxdist - Compute probabilities from Maxwell di

    Other functions named maxdist

Enter temperature (Kelvin): 273
Enter lower bound speed (m/s): 200
Enter upper bound speed (m/s): 700
fx >>
```

Figure input number 1

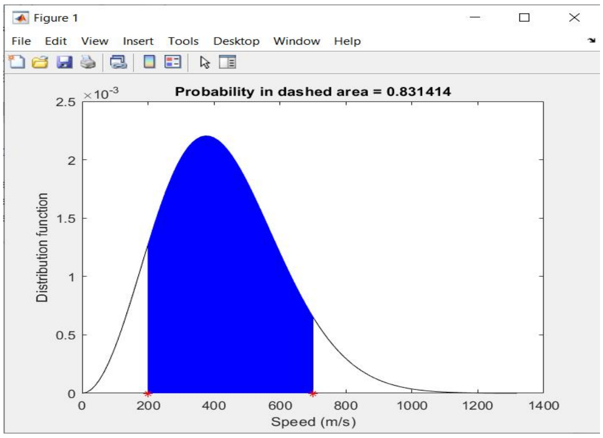

Figure result number 1

- At t = 100^0C (= 373K).

```
Command Window
  maxdist - Compute probabilities from Max

    Other functions named maxdist

Enter temperature (Kelvin): 373
Enter lower bound speed (m/s): 200
Enter upper bound speed (m/s): 700
fx >>
```

Figure input number 2

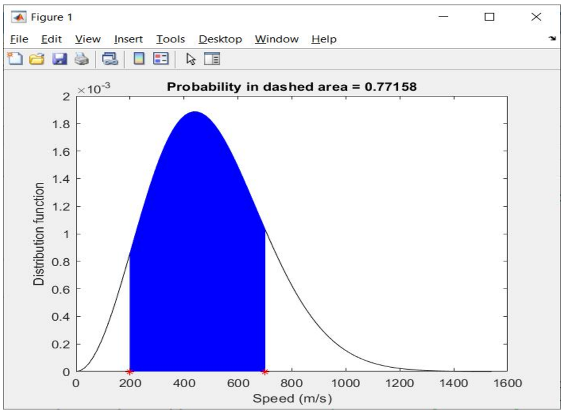

Figure result number 2

- At t = 527^{0}C (= 800K). (High temperature)

```
Command Window
  maxdist - Compute probabilities from Ma

     Other functions named maxdist

  Enter temperature (Kelvin): 800
  Enter lower bound speed (m/s): 200
  Enter upper bound speed (m/s): 700
fx >>
```

Figure input number 3

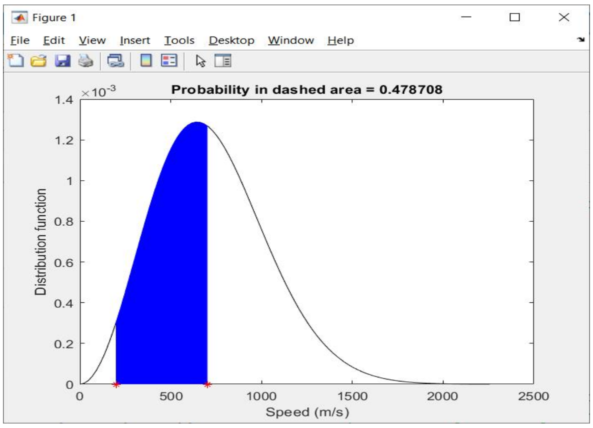

Figure result number 3

- At t = 100^{0}C (= 373K).(This time we input the interval from 0 to infinity)

```
Command Window
  maxdist - Compute probabilities from M

     Other functions named maxdist

  Enter temperature (Kelvin): 373
  Enter lower bound speed (m/s): 0
  Enter upper bound speed (m/s): 9999
fx >>
```

Figure input number 4

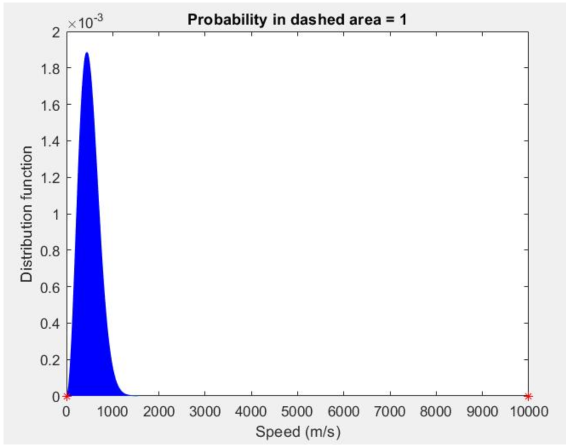

Figure result number 4

We assume that the maximum(of the infinite) velocity is 9999 m/s to show that the probability is approximately equal to 1.

3.4 Evaluate and analysis:

Because the probability of a particle is an integral: P(v1…v2) = $\int_{v1}^{v2} f(v)dv$

So the probability is also an area under the curve from v1 to v2 (the blue area).

The figure displays a curve which is created by a Maxwell-Boltzman distribution. The x-axis is the range of velocity of oxygen. The y-axis is the distribution function and also the number of molecules per unit speed.The total area under the entire curve is equal to the total number of molecules in the gas.

As the gas gets colder, the graph becomes taller and narrower. Similarly, as the gas gets hotter, the graph becomes shorter and wider. This is required for the area under the curve (i.e. total number of molecules) to stay constant.

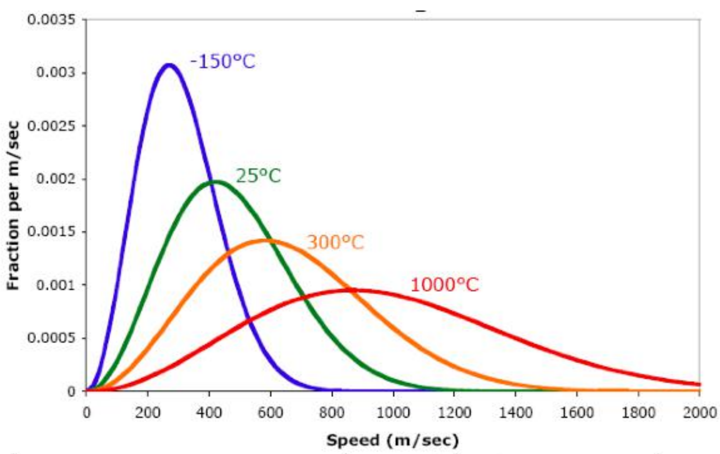

Figure 3.4.1: *Image illustrate the graph when there are many temperature*

CONCLUSION

Thus, we have gone from general problems to quite complex specific problems that require lots of computational work with problem solvers. However, with the support of the Matlab tool, solving and surveying problems becomes easy, lively and direct. We can easily use Matlab to simulate or calculate the distribution of an oxygen molecule and also the probability that a molecule has a velocity in an interval velocity given.

Advantages:

- Calculation is easy and convenient, giving accurate results like the common calculation method.

- Help to understand more about Matlab applications in technical problems.

- Save operation and calculation time compared to common calculation methods.

- Use content announcement commands that make the usage structure relatively simple, easy to understand, easy to use and suitable for everyone.

Weakness:

- Designing code takes a lot of time and effort.

- The code is cumbersome.

- Also simulated within the specified topic, not yet created to other topics other technical calculations.

THE WORK OF EACH MEMBER

-***<u>Nguyễn Tiến Hưng, Phạm Đình Khang</u>*** :Study the research and make the form of report.

-***<u>Nguyễn Võ Hoàng Khang, Lê Minh Khang</u>*** :Edit the report and find more reference.

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