STP Resources for Statistical & Thermal Physics:

STP Boltzmann Distribution

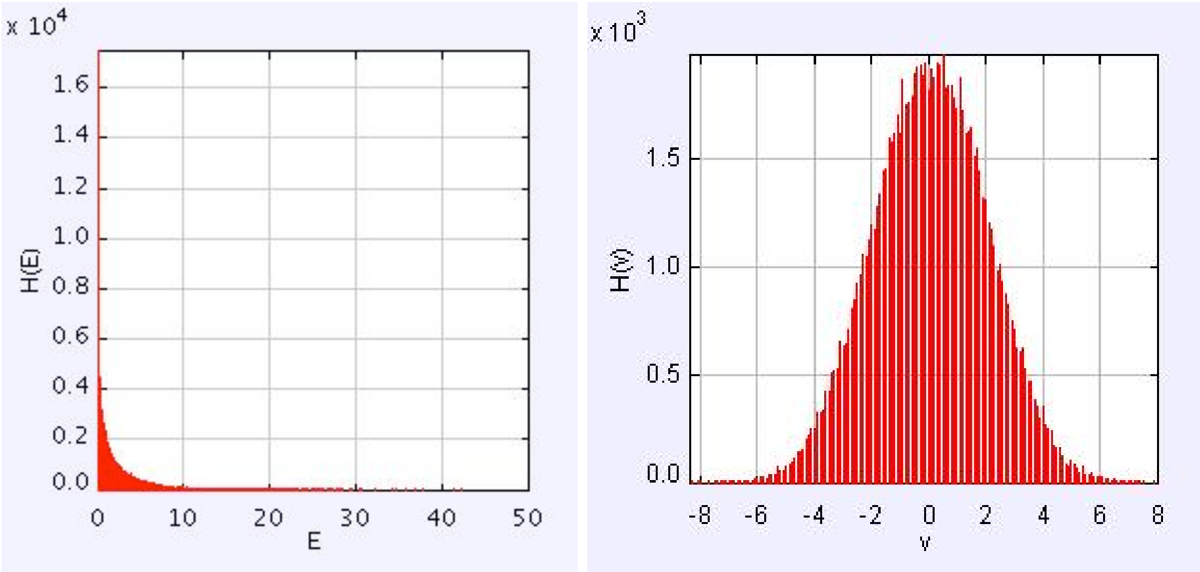

FIG. 1: Output of `stp_boltzmann.jar` showing the histograms of the energy and velocity of a particle in equilibrium with a heat bath.

I. INTRODUCTION

The STP `Boltzmann` program displays histograms of the velocity and energy of a classical particle in contact with a heat bath at temperature T. The default temperature of the heat bath is 4.0. Additional states and parameters can be specified using the `Display|Switch` GUI menu item.

STP `DemonIdealGas` is part of a suite of Open Source Physics programs that model aspects of Statistical and Thermal Physics (STP). The program is distributed as a ready-to-run (compiled) Java archive. Double-clicking the `stp_boltzmann.jar` file will run the program if Java is installed on your computer. Additional programs can be found by searching ComPADRE for Open Source Physics, STP, or Statistical and Thermal Physics.

II. DESCRIPTION

Consider a system of many particles in equilibrium with a heat bath at temperature T. What is the probability that the system is in a particular microstate with energy E? What is the probability that the system has energy between E and $E + \Delta E$? The form of the probability distributions is independent of whether the system is described by classical or quantum mechanics, and whether the system is a gas, liquid, solid, or a system of spins.

The program implements a Monte Carlo simulation of a classical particle in one dimension in equilibrium with a heat bath. The microstate of the particle is characterized by its velocity. Because the latter is a continuous variable, we have to bin the velocities.

Double-click on the `stp_boltzmann.jar` file to open the program, and click the `Run/Calculate` button to begin the simulation. The program computes the histograms $H(v)$ and $H(E)$, where $H(v)\Delta v$ is the number of times that the particle has a velocity between v and $v + \Delta v$ and $H(E)\Delta E$ is the number of times that the particle has energy between E and $E+\Delta E$ during the simulation. The message window gives the mean velocity, the mean energy, and the fraction of times a trial change is accepted.

The input parameter is the temperature of the heat bath. You can change the temperature by typing in a new number. (After you type in a value, the box remains yellow, which signifies that the program has not incorporated the new value until you press Enter).

III. ALGORITHM

The Metropolis algorithm for sampling the states of the system in equilibrium with a heat bath can be summarized by the following steps:

1. Make a random trial change in the velocity of the particle according to

$$v \to v + (2r - 1)\delta, \tag{1}$$

   where δ is the maximum change in the velocity, and the random number r is uniformly distributed in the interval $0 \leq r < 1$.

2. Compute the change in energy ΔE. For a single particle $E = mv^2/2$.

3. If $E < 0$, accept the change. If $\Delta E > 0$, then compute $e^{-\Delta E/kT}$, where k is Boltzmann's constant. If $r < e^{-\Delta E/kT}$, where r is another random number between 0 and 1, the trial change is accepted. Otherwise, the trial change is not accepted and the original velocity is retained and counted in the various averages. We choose units such that Boltzmann's constant $k = 1$ and the mass $m = 1$.

4. Compute the various quantities of interest.

5. Repeat for many trial changes (Monte Carlo steps).

IV. QUESTIONS

You can change more parameters such as the initial speed of the particle and, δ, the maximum change in the velocity, by selecting the `Display` menu in the window with the `Run/Calculate` and `Reset` buttons, and choosing `Switch GUI`. A complete description of the parameters is given in the next section.

1. Show that the results for the mean energy $<E>$ and the mean velocity $<v>$ of the particle are insensitive to the values of the initial speed and δ.

2. What is the form of the probability distribution of the velocity? Show that the width of the distribution is proportional to the temperature by doing simulations at different temperatures.

3. Describe the shape of the probability distribution of the energy. Confirm that the form is an exponential and show that the energy distribution is proportional to $e^{-E/T}$. (Units have been chosen such that Boltzmann's constant is equal to unity.)

V. INPUT AND OUTPUT PARAMETERS

Parameter	Description
Temperature	temperature of the heat bath
Number of MC steps	total number of trial changes
Initial speed	initial speed of the particle
δ	maximum change in velocity

TABLE I: Control parameters.

Parameter	Description
$<v>$	mean value of the velocity
$<E>$	average energy of the particle (in units where $k = 1$)
acceptance probability	percentage of trials for which the change of velocity is accepted

TABLE II: Output parameters.

VI. RELATED CURRICULAR PACKAGES

This model is described in Chapter 15 of *An Introduction to Computer Simulation Methods* by Gould, Tobochnik and Christian (NY: Addison-Wesley, 2006) and Chapter 4 of *Statistical and Thermal Physics* by Gould and Tobochnik available on ComPADRE. Other resources are available for Statistical and Thermal Physics from `osp_stp.jar` or searching ComPADRE for STP, OSP, or Statistical and Thermal Physics.

15 May 2008.