Billiards in class, entropy after hours

Statistical physics for sophomores

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1 The didactic problem

In most physics curricula statistical physics is presented for the first time around the third semester. A more or less thorough treatment of thermodynamics is usually given in the first year, meaning that we may assume a basic understanding of its concepts. In particular, the macroscopic definition and the use of entropy should be known. Entropy will later provide the bridge between the microscopic and the macroscopic – i. e. thermodynamic – description of the properties of matter.

The specific pedagogic challenges of introducing statistical physics at this stage, and suggested ways to address them, may be described as follows:

Lack of classroom experiments $\Longrightarrow$ *Simulation:* In other branches of physics teachers can make good use of an interplay of experimental demonstrations and theoretical explanations (or predictions). In statistical physics this powerful didactic double step is not possible: molecules simply cannot be watched as they cooperate in making up the macroscopically observable properties of substances.

However, with the availabilty of fast small computers it has become standard procedure to realistically simulate microscopic systems, thus creating pseudo-experiments as a replacement for real lecture hall experiments.

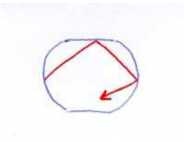
Too much formalism $\Longrightarrow$ *Visualization:* Statistical physics being an essentially theoretical field, we are back to the blackboard for weeks on end. Students, on the other hand, are only in their second year and may not yet possess the mathematical muscle and endurance to work through a long series of formal arguments and derivations.

To mend this, computer graphics may be invoked and used in many ways to point out the meaning of complex mathematical relations.

High-dimensional phase space $\Longrightarrow$ *Bottom-up approach:* To make things even more difficult, the said formal arguments take place in multidimensional geometries that are not easily depicted or visualized.

However, a minor result of chaos research may be invoked to make phase space more easily accessible: namely, it has been shown that chaos is present even in very small systems. In fact, there are systems with no more than two (relevant) degrees of freedom which nonetheless are chaotic. But such a system's phase space may actually be depicted on a screen, and the basic statistical manipulations may be demonstrated in full view. Once students have understood these fundamentals we may proceed to higher and more physically meaningful – though less intuitive – phase spaces.

In the following we show some highlights illustrating the approach. The sketches and program names refer to applets accessible via the author's website.



Chaos in small systems

Bunimovich's billiard: A point mass (or "light ray") ist started at some point along the periphery of a "corral", or stadium, comprised of two semicircular walls joined by short horizontal pieces. All wall collisions are elastic, i. e. energy is conserved. [Applet: *Stadium*]

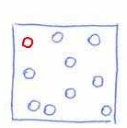
Sinai's billiard: This system may be interpreted as a 2-dimensional 1-particle gas. A small hard disc (a "gas particle") bounces about in a quadratic vessel; the vessel walls are decorated with semicircular extrusions that serve to randomize the motion. [Applet: *VarSinai*]

The statistical features of the motion are the same in both systems. Phase space – at least the relevant subspace – consists only of v_x, v_y, and energy conservation confines the state points to a circle. In the course of the simulation the state point jumps about on this circle in a chaotic manner, such that all flight directions are equally probable. However, the probability density of one velocity component, say, v_x, is quite interesting; it is peaked at large absolute values of v_x.

It is a simple exercise to derive this projected, or marginal, density mathematically. Let ϕ be equidistributed: $p(\phi) = 1/2\pi$ for $\phi \,\epsilon\, [0, 2\pi]$. Using cartesian coordinates $x = r\cos\phi$, $y = r\sin\phi$ we find for x (or y) with $x \,\epsilon\, [\pm r]$ the density

$$p(x) = p(\phi)\left|\frac{d\phi}{dx}\right| = \frac{1}{\pi}\frac{1}{\sqrt{r^2 - x^2}} \tag{1}$$

But $p(\phi)$ is just the microcanonical distribution for a system with 2 degrees of freedom. Therefore, $p(x)$ is the distribution of one d.o.f. Figure 1 shows the trough-like shape of this distribution – which is quite different from the Gaussian shape we expect for high-dimensional systems.



Adding dimensions one by one

3-dimensional 1-particle gas: One hard sphere is moving in a cubic box with semicircular scatterers mounted on some walls. [Applet: *Hspheres*]

Velocity space is now 3-dimensional, with a 2-dimensional spherical energy surface. To demonstrate the homogeneous a priory density on the energy surface we project the

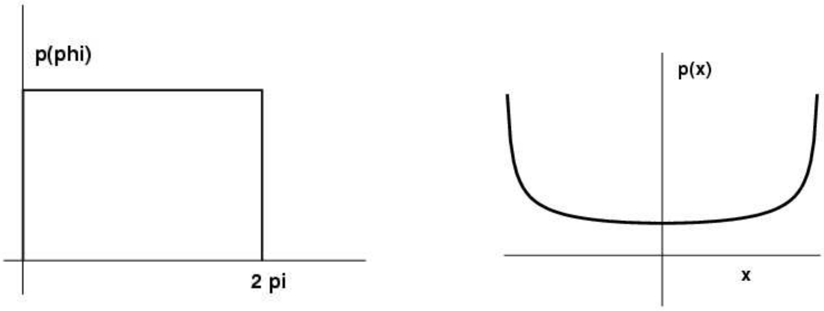


Figure 1: Projecting an equidistribution on the unit circle onto the x-axis

$$
\begin{aligned}
&p_2(x) = \tfrac{1}{\pi}(1 - x^2)^{-1/2} \\
&p_3(x) = \tfrac{1}{2} \qquad\qquad \text{constant!} \\
&p_4(x) = \tfrac{2}{\pi}(1 - x^2)^{1/2} \\
&p_5(x) = \tfrac{3}{4}(1 - x^2) \\
&\ldots \\
&p_{12}(x) = \tfrac{256}{63\pi}(1 - x^2)^{9/2} \\
&\ldots \\
&\longrightarrow \text{eventually approaches a Gaussian!}
\end{aligned}
$$

Table 1: Projecting constant densities on hyperspherical surfaces down onto one axis we find these marginal densities (see Fig. 2)

spherical surface onto a rectangle, using Lambert's area preserving (and therefore density preserving) projection. Interestingly, the velocity density $p(v_x)$ is now a constant.

N hard discs or spheres: By simulating two hard discs we arrive at 4-dimensional phase space. [Applet: *Harddisks*]

Further steps in dimensionality may be done by studying any number of spheres or discs. For example, in a gas of 4 hard spheres, velocity space has 12 dimensions. As we proceed from 3 to more dimensions the statistical distributions $p(v_x)$ and $p(|\mathbf{v}|)$approach the well-known large-N limits. In particular, the velocity density $p_{12}(v_x)$ for 4 hard spheres already resembles a Gaussian. Figure 2 shows the theoretical prediction for several dimensions: assuming an equidistribution on the "surface" of an n-sphere, what is the density $p(x)$ along one axis?

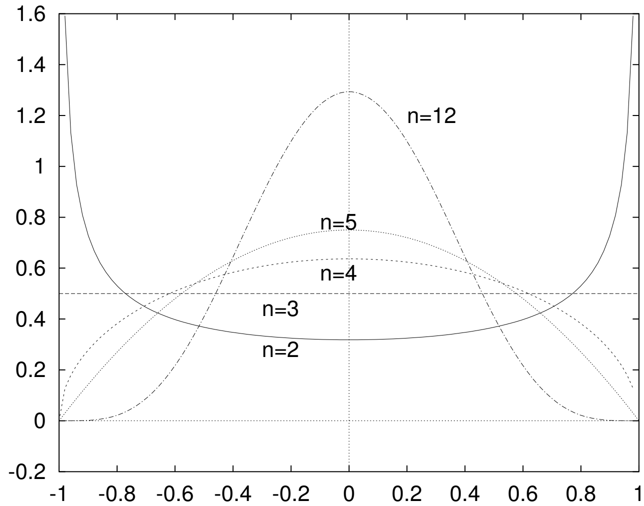
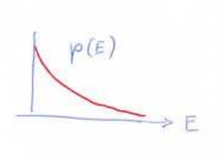


Figure 2: Distribution $p(x)$ along one axis of a n-dimensional sphere if its surface is homogeneously covered.

A sketch of kinetic theory

The kinetic transport equation is now introduced at a basic level. The meaning of the individual terms are explained, and the assumptions needed for its derivation are given. To illustrate the kind of processes Boltzmann's equation can describe, we simulate a 2-dimensional system of hard discs in a rectangular box. Starting all particles from a highly non-equilibrium configuration – their positions restricted to be in the left part of the container – we simulate their paths as they fill up the available volume and thus attain equilibrium.

[Applet: *Boltzmann*]



Boltzmann's roulette

For the hard discs system, μ-space - or rather, μ-plane - is spanned by v_x, v_y; the state of the system is represented by a swarm of N points on that plane.

To find the average (and also most probable!) distribution of particle energies Boltzmann suggested the following "game":

– Throw N particles randomly onto equal-sized cells on the μ-plane

– make sure that the sum of the particle energies equals the given system energy

– determine the mean number of particles in each cell on the μ-plane; sort the result according to the cell energies

To this date, this game has never actually been played; rather, its outcome was predicted as seen in the textbooks. The applet *LBRoulette* may be invoked to play the game.

$S = k \ln W$

Entropy seen from within

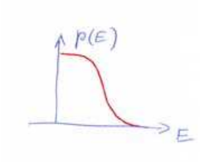
The following property of hyperspheres is discussed and linked to the defining properties of thermodynamic entropy:

> Let n_1 and $n_2 = n - n_1$ be the dimensions of two subspaces of n-space, and let us consider two hyperspheres $Sp_{1,2}$ in the respective spaces, having volumes V_1 and V_2. The combined object $Sp_1 \times Sp_2$ in n-space may be considered a hypercylinder, in analogy to a simple 3D cylinder produced by combining a 2D "sphere" (i. e. a circle) with a 1D "sphere" (namely a line). The volume of the hypercylinder is very strongly dependent on the radii $r_{1,2}$ of the subspheres.
>
> Now consider an n-sphere of given radius and inscribe a hypercylinder, varying the radii $r_{1,2}$ such that the cylinder always touches the sphere from within. It may be shown that (a) the volume of the inscribed hypercylinder passes through a very sharp maximum at a specific combination r_1, r_2; and (b) on a logarithmic scale this largest volume V_{hc} is practically equal to the volume of the circumscribed sphere.

This result is valid only at high dimensionality. To explain its physical content we introduce a likely candidate for the role of thermodynamic entropy $S(E)$, namely the log-volume $\log \Sigma(E)$ of the phase space region below the energy surface E. From the above discussion we see that this quantity has the defining properties of entropy, namely: (a) two systems in thermal contact are in equilibrium as soon as $\partial S/\partial E$ (i. e. $1/T$) is equal in both systems, and (b) $S_{1+2} = S_1 + S_2$ (additivity).

The applet (*Entropy1*) demonstrates these points. Assuming two thermally interacting samples of an ideal classical gas with a total of $N = N_1 + N_2$ particles and a given total energy $E = E_1 + E_2$, the entropy of the combined system will be given by the log-volume of the phase space hypersphere below the surface E. The inscribed hypercylinder, with varying ratio r_1/r_2, refers to different ways of distributing the available energy over the two subsystems. Playing the applet we can see that (a) there is an optimal, i. e. most probable, way of dividing up the energy E, the probability of this best partitioning overwhelming all other options; and (b) the sum of the sub-entropies (i. e. the log-volume of the largest hypercylinder, or hyper-rectangle) equals the total entropy (i. e. the log-volume of the circumscribed sphere, or circle.)

[Applet: *Entropy1*]



Fermi's quantum roulette

Having covered classical statistical mechanics we now turn to quantum systems. To obtain the most probable energy distribution in a quantum gas we return to the "game" introduced by Boltzmann. Again we define an appropriate μ-space which is now spanned by the quantum numbers $n_{i,x}, n_{i,y}, n_{i,z}$. In contrast to the classical case the states in μ-space are now discrete. In the case of Fermi particles having half-integer spin we also have to consider the Pauli principle. Allowing for these differences we may once more interpret the usual derivation of the "most probable distribution" as a kind of game of fortune. The rules of the game are, for fermions:

For non-interacting particles in a square box the μ-plane is spanned by integers n_x, n_y; each quantum state is represented by a point. A specific state of a system of N fermions is represented by a set of N inhabited points on that plane.

To find the average (and also most probable!) distribution of particles on states,

– assign N particles randomly to the states on μ-plane

– make sure that the sum of the particle energies equals the given system energy,
AND
– discard all trials in which a state is inhabited by more than one particle

– determine the mean number of particles in each state; sort the result according to the state energies

This game, as the one discussed above, has never actually been played; rather, its outcome was calculated as seen in the textbooks. In contrast, the applet *EFRoulette* reproduces the average distribution by a random process according to the rules of the game.

Appendix: List of didactic JAVA applets

The following JAVA applets may be accessed at the author's website:

Stadium: Simulates the motion of 200 mass points, in a Bunimovich corral. The initial conditions are varied ever so slightly to demonstrate the instability of the trajectories, and hence the presence of chaos. A frequency histogram of the value of one velocity component v_x is drawn, showing the trough-like probability density $p(v_x)$.

VarSinai: Simulates the motion of a very small disk in an elastic container with randomizing protuberances set into the sides. This system is quite as chaotic as the original stadium billiard but has a more physical feel about it; in fact it may be regarded as a

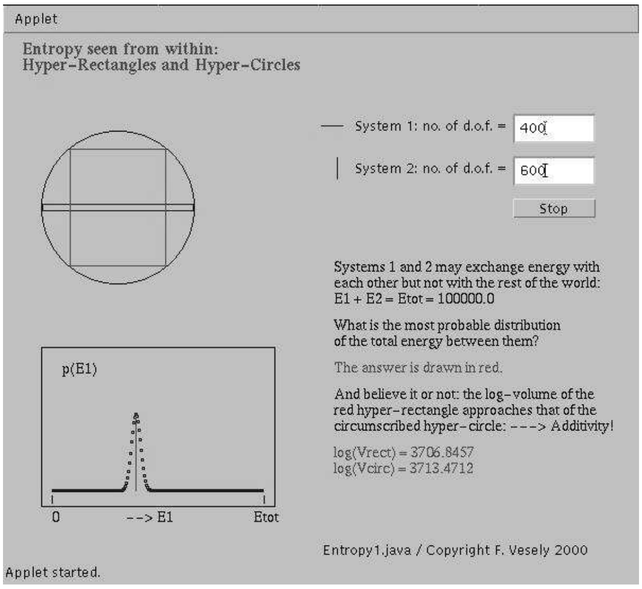


Figure 3: Applet *Entropy1*: Consider two systems (represented by the vertical and horizontal lines, respectively) in thermal contact. The total system (circle) has $n = n_1 + n_2$ degrees of freedom, and the total energy is $E = E_1 + E_2$. The log-volume in phase space is sharply peaked at the correct combination E_1, E_2 (equilibrium), and then the sum of the log-volumes of the subsystems – that is, the log-volume of the largest inscribed rectangle – equals that of the total system. The circle and rectangles shown are symbolic renderings of the actual hypersphere and hypercylinders, respectively.

2D one-particle "gas". Again, the trough-like distribution density of v_x is demonstrated.

Harddisks: Simulates the motion of up to $N = 64$ hard disks in an elastic container. For $N = 1$ the behavior is the same as in *VarSinai*, but with increasing N the distribution densities of v_x and of $|\mathbf{v}|$ approach the well-known Gaussian and Maxwell-Boltzmann shapes, respectively.

Hspheres: Simulates the motion of up to $N = 64$ hard spheres in an elastic container. For $N = 1$ we are at the limit of the graphical representability of phase space: the energy surface is two-dimensional and we invoke Lambert's projection to map the equidistribution of points on the spherical surface onto a rectangle. The distribution density of v_x turns out to be a constant. From $N = 4$ up the density $p(v_x)$ develops an ever more prominent maximum around zero, soon approaching the Gaussian limit.

LJones: Simulates a two-dimensional system of up to $N = 36$ Lennard-Jones particles. Histograms of flight directions, of $p(v_x)$ and $p(|\mathbf{v}|)$ are given.

Boltzmann: The power of Boltzmann's transport equation is discussed by simulating a non-equilibrium system: up to $N = 64$ hard disks are packed in one part of a rectangular box and are then left to expand freely into the available volume.

Entropy1: For two systems in thermal contact, the defining properties of entropy, $S(N, E) = \log \Sigma(N, E)$, are discussed: (a) S determines the equilibrium (i. e. most probable) distribution of energy between the systems; (b) in equilibrium, S is additive.

As an example, Figure 3 shows a screenshot of Applet *Entropy1*.

References

[1] F. Reif, Statistical Physics, (Vol. 5 of Berkeley Physics Course), McGraw-Hill 1967

[2] Ya. G. Sinai, Russ. Math. Surv. 25/2(1970)137; see also M. V. Berry, Eur. J. Phys. 2 (1981) 91