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Explaining Gibbsean phase space to second year students

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Abstract

A new approach to teaching introductory statistical physics is presented. We recommend making extensive use of the fact that even systems with a very few degrees of freedom may display chaotic behaviour. This permits a didactic 'bottom-up' approach, starting out with toy systems whose phase space may be depicted on a screen or blackboard, then proceeding to ever higher dimensions in Gibbsean phase space.

1. Propaedeutics for statistical physics

Teaching introductory statistical physics is a tough but rewarding exercise. Rewarding, since statistical physics is arguably one of the most beautiful achievements in our science; and there are always some students alert enough to sense this. And tough, since as a rule the necessary mathematical tools are not ready by the time StatPhys must be introduced—not later than at the beginning of the second student year.

The main didactic obstacles may be summed up as follows:

- *Classroom experiments not possible.* Except for the familiar Brownian motion demonstrations it is simply not possible to show the molecules 'at work' as they create the macroscopic effects we measure in a thermodynamics lab.
- *Subject usually presented in a purely formal way.* Due to the lack of demonstration experiments the efficient didactic double step of formal derivation–experimental corroboration is not feasible, leading to a predominance of formalism in StatPhys courses and texts.
- *Formalism rather abstract*. The didactic problems are enhanced by the fact that the said formalism refers to an abstract, high-dimensional phase space that is difficult to visualize.

These problems may be addressed by a teaching strategy combining the following elements:

- *Replace classroom experiments by simulation*. Over the last few years this has become a well-established method for the visualization and statistical analysis of the motion of model particles.

- *Support formal arguments by geometric arguments, using computer graphics.* While multidimensional space may be difficult to imagine, it is still possible to demonstrate, or at least make plausible, the relevant properties of *n*-space and simple objects such as hyperspheres.
- *Use a bottom-up approach to phase space.* Instead of starting immediately with a high-dimensional Gibbsean phase we may at first treat 'toy' systems with very few dynamical variables, then proceed to higher dimensions.

In the following sections we describe the application of these considerations in the context of a second year student course in statistical physics.

2. New didactic tools

Comparing our situation with that of our own teachers—say, 20–40 years ago—we find that there are new resources available for a serious but mathematically soft presentation of statistical physics: *live simulations* and *low-dimensional chaotic systems*.

Live simulations. Over the last decade or so PCs have become powerful enough to permit nontrivial simulation experiments in the lecture hall setting—that is, not exceeding the 'alertness span' of 1–2 min. An early attempt to use simulation in teaching is Reif's Berkeley Lectures volume on statistical physics [1]. The idea of printing snapshots of hard-disc simulations in the book appears outdated now, but there were accompanying 8 mm film clips that nicely demonstrated some essential features of molecular motion. An interesting alternative method of using computers to introduce statistical physics was suggested by Moore and Schroeder [2].

Chaos in small systems. The theory of dynamical systems has presented us with a useful side result, namely the statement that chaos may be found even in systems with very few degrees of freedom. Formerly, teachers would sometimes resort to hand-waving arguments such as 'in a phase space with zillions of dimensions we may safely assume an equidistribution of states on the energy surface'—not generally true, but not necessary either, since we can define low-dimensional yet physically relevant model systems that indeed do us the favour of being chaotic and thus allow for the application of statistical procedures. The important point here is that a phase space of just two dimensions may actually be drawn on a sheet of paper—quite a didactical advantage over the 10^{24}-dimensional Gibbsean space which is our aim but should not be our starting point.

In a second year student statistical physics course recently installed at the University of Vienna we make use of the above considerations. First the presence of chaos in a few simple model systems is demonstrated. Having thus given a reason for the use of statistical procedures we produce some predictions based on the equidistribution of states on low-dimensional energy surfaces, time and again testing our prognostics by real-time simulations. Then we gradually increase the number of degrees of freedom, always proceeding with the double step of statistical prediction and mechanical simulation. Finally we go on to very high-dimensional phase spaces, pointing out those geometrical features that are sufficient to produce the main results of statistical mechanics.

The course is completed in 7 weeks, with four weekly hours of lectures and one hour of workshop. The course material is made available to students in the format of a Web tutorial; the computer simulations shown in class are included as JAVA applets. Students may do their own online experiments with these applets, changing parameters and exploring the limits of theory.

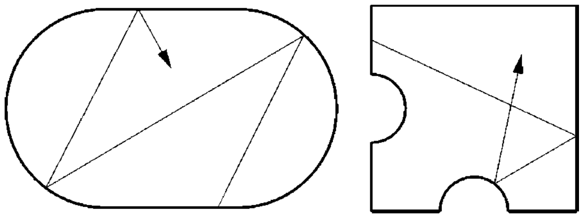

Figure 1. Left: stadium billiard according to Bunimovich; right: a variant of Sinai's billiard.

The Web tutorial, including applets, is freely accessible at the author's website. Teacher colleagues who find the material useful for their purposes are welcome to download and use it under a kind of GPL licence: full citation of source, no warranty given for codes, augmentation permitted.

3. From billiards to fluids: a bottom-up approach

Stadium billiards are the smallest chaotic systems [3]. Their phase space—at least the relevant part referring to velocity—has only two dimensions, and the energy 'surface' is in fact a line—the periphery of a circle. These features make such systems ideal objects for demonstrating the power of a statistical treatment of an intrinsically deterministic system.

Stadium billiards and the one-disc gas. For a visual demonstration of (a) instability against initial conditions and (b) equal *a priori* probability of states on the energy circle we use a simulation (applet *Stadium*) showing the following.

Two hundred rays, or point particles, are launched from the same position but with slightly varying initial directions, their tangent of ascent deviating randomly by at most one part in 10^{12}. The trajectory is drawn only for the first particle, but after each wall collision all 200 representative points on the energy circle are drawn. At first the points coincide, but after some 40 collisions they spread out and presently fill up the entire circle. Also shown is a histogram of the flight directions, ascertaining that the entire range of angles is filled up evenly.

The relevance of the said system—known as *Bunimovich's billiard*—for statistical mechanics may not be evident to students. Therefore a more physical variant of the system is studied next. Instead of a stadium with straight top and bottom sides and concave semicircular closures we take a square box with convex semicircular nobs protruding inside from its sides. In the simulation (applet *VarSinai*) one point particle (actually, a small disc) is followed as it bounces off the various parts of its cage. Theory has shown that such a system is just as chaotic as the one described before. On the other hand it may be understood to represent the simplest of all gases: a classical two-dimensional one-particle gas.

In fact, nothing keeps us from giving the moving particle a finite size, thus constructing a one-disc gas in a box with randomizers set into the walls. The respective simulation—invoking applet *Harddisks* with one particle—corroborates our expectation that the system is again chaotic, with equal probability of all flight directions.

The concept of phase space is probably new to the students. We have introduced it in connection with the simple example of the stadium billiard, where the variables v_x, v_y span the space, and the equation $v_x^2 + v_y^2 = \text{const}$ carves out the energy 'surface' pertaining to a microcanonical, or isoenergetic, ensemble of microstates. It is quite evident now that all states in that ensemble are indeed equally probable.

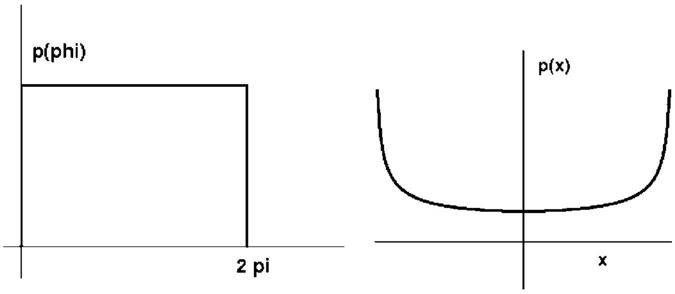

Figure 2. Projecting an equidistribution on the unit circle onto the x-axis.

Now we can begin to play. What is the probability density of some particular value of v_x? The answer is found by projecting the equidistribution along the circular periphery onto one coordinate axis.

We have found it helpful here to use a simple visualization. Handing out semi-transparent straws[1] we point out the equidistribution of colour centres on the periphery by looking along the axis of the straw. Turning the straw sideways and holding it against a light source we demonstrate that the projected density is small near the axis and high near the rim.

After this visual demonstration we derive the projected density mathematically. Let ϕ be equidistributed: $p(\phi) = 1/2\pi$ for $\phi \in [0, 2\pi]$. Using Cartesian coordinates $x = r\cos\phi$, $y = r\sin\phi$ we find for x (or y) with $x \in [\pm r]$ the density (see figure 2)

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

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

Returning to the respective simulations for the billiards and the one-hard-disc gas, and drawing attention to the histogram of $p(v_x)$, we can show that our prediction is indeed borne out by the simulation.

From 3 to N dimensions. We are now ready to go on to a three-dimensional phase space. A single hard sphere enclosed in a cubic box with elastic walls and a few randomizing dimples is described by v_x, v_y, v_z with $v_x^2 + v_y^2 + v_z^2 = \text{const}$. In other words, the microcanonical ensemble of states is restricted to a spherical surface. Moreover, the state points are again homogeneously distributed on that surface.

Using Lambert's area-preserving projection we may map the spherical surface onto a rectangle. The equidistribution of state points on the spherical surface is then demonstrated by the homogeneous filling of the rectangle.

Table 1 shows that in this case the theoretical distribution $p(v_x)$ of one velocity component is simply a constant. Starting the appropriate simulation applet (*Hspheres*) with one particle and watching the histogram of $p(v_x)$ we indeed observe that it approaches a constant.

Proceeding to systems with more degrees of freedom, such as $N = 2, 3, \ldots$ hard discs or hard spheres, we can see that the histogram $p(v_x)$—which was trough-like for $D = 2$ and flat for $D = 3$—now develops a bulge at $v_x = 0$, eventually approaching the familiar

[1] In one instance we found a sponsor who provided packs of fruit juice with attached straws to be handed out to the audience; the lecture was quite a success, didactically and otherwise.

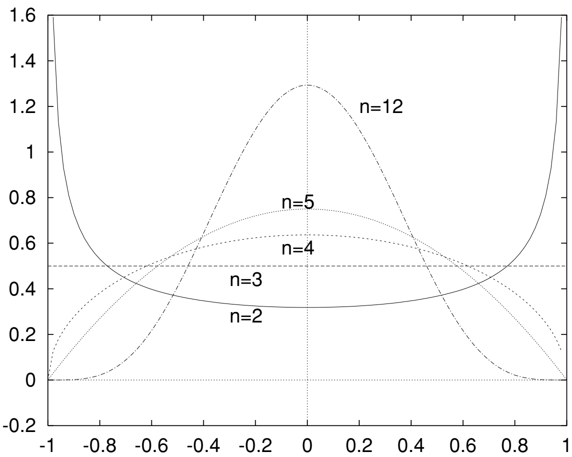

Figure 3. Distribution $p(x)$ along one axis of an n-dimensional sphere if its surface is homogeneously covered.

Table 1. Projecting constant densities on hyperspherical surfaces down onto one axis we find these marginal densities (see figure 3).

$p_2(x) = \frac{1}{\pi}(1-x^2)^{-1/2}$
$p_3(x) = \frac{1}{2}$ (constant!)
$p_4(x) = \frac{2}{\pi}(1-x^2)^{1/2}$
$p_5(x) = \frac{3}{4}(1-x^2)$
...
$p_{12}(x) = \frac{256}{63\pi}(1-x^2)^{9/2}$
...
$\longrightarrow$ eventually approaches a Gaussian!

Gaussian peak. The general expression for $p(v_x)$ for any number of d.o.f. is easily derived; a few explicit formulae are given in table 1, the respective graphs are shown in figure 3.

4. From hyperspheres to entropy

As a preparation for the discussion of entropy we now investigate the geometrical properties of high-dimensional spheres. First we derive the well-known feature that a thin (hyper-)spherical skin contains most of the sphere's volume. Once students have grasped this they are ready to explore a more challenging but physically consequential property:

> 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 runs counter to our intuition, and it is indeed valid only at high dimensionality. To help students grasp its content we have prepared a computer program that visualizes the situation. But first we have to recall the physical content of this geometrical discussion. To begin with, 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. We follow general textbook custom by suggesting this quantity as a possible entropy measure and then showing that it has indeed 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).

Now we invoke the applet (*Entropy1*) to clarify 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 $E = E_1 + E_2$, we can easily identify the entropy of the combined system as 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. Our geometrical considerations tell us 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).

Having proved that the suspected quantity has indeed the required properties, it is a simple matter now to make contact with macroscopic thermodynamics. For the classical ideal gas with energy E and volume V the exact expression $S(E, V)$ for the entropy is now completely understood, and simple manipulation of that equation (the Sackur–Tetrode formula) yields the gas law and other familiar results.

5. Application of the didactic concept

Let us consider how these ideas may be embedded in an introductory course in statistical physics.

To prepare the ground it is useful to give a quick resume of thermodynamics, putting special emphasis on those concepts and quantities that are important for an understanding of the microscopic treatment that follows—in particular, entropy and its conceptual environs such as thermal interaction, equilibrium and temperature.

Once we have arrived at a good understanding of the macroscopic view we may focus the student's attention by setting an explicit goal to be reached within the present course: we declare that we mean to find a microscopic correlate of that quantity which had been introduced in thermodynamics under the name of entropy.

Next, a number of simple but relevant model systems are introduced. These are stadium billiard/classical ideal gas/quantum ideal gas/hard discs gas/hard spheres gas/lattice of harmonic oscillators.

All these systems have the common property that their energy surfaces are hyperspherical, which makes the discussion of the microcanonical ensemble particularly simple. The stadium billiards have the additional advantage that they have only two degrees of freedom; yet they fulfil the requirement of equal *a priori* probability of states in the microcanonical ensemble.

To make good on our promise to find the microscopic correlate of entropy, we use the arguments given in the preceding section. In particular, for an ideal gas of N particles

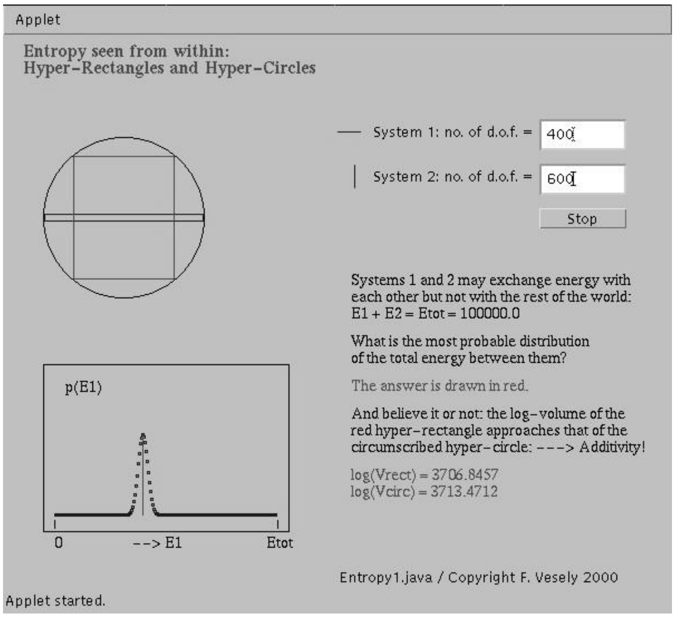

Figure 4. Applet *Entropy1*. Consider two systems (represented by the vertical and horizontal lines, respectively) in thermal contact. The total system (circle) has $n = n_1 + n_2$ degrees of freedom, and the total energy is $E = E_1 + E_2$. The log-volume in phase space is sharply peaked at the correct 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.

confined in a vessel of volume V and having a total energy E we can derive the microscopic ensemble measure (i.e. area of the energy surface)

$$\Sigma(V, E) = \left[\frac{V}{N} \left(\frac{4\pi Ee}{3Nmh^2} \right)^{3/2} \right]^N \tag{2}$$

and the entropy $S(E, V) = k \ln \Sigma(V, E)$. By inverting this equation to find the appropriate thermodynamic potential $E(S, V)$ we make contact with macroscopic thermodynamics (see the end of section 4).

From this starting point we may now set out to unfold classical thermodynamics in the usual manner: other ensembles, in addition to the microcanonical, are introduced and discussed with respect to their statistical equivalence. Ensemble measures, or partition sums, of which the above-mentioned quantity $\Sigma(E)$ is a basic example, are defined and utilized to make thermodynamic relations concise. Experience has shown that after the thorough understanding of the microcanonical ensemble achieved by the above-mentioned bottom-up approach, students have no difficulty in grasping the generalization to the canonical and grand canonical ensembles.

6. Conclusion

We have proposed a novel approach to introducing statistical physics at the second year student level. Drawing on some minor results of chaos research and—if available—using modern media we demonstrate to students the *necessity* and the *possibility* of applying statistical methods to micro-mechanical phenomena. Starting from low-dimensional systems whose phase space can be displayed on a graphics surface we proceed, step by step, to higher dimensions. Computer-aided visualization is then used to provide insight into the geometrical–physical properties of phase space.

This approach has been in use at Vienna University for several years. Experience in class as well as follow-up interviews with students indicate that the proposed method is indeed a didactically efficient way of presenting basic statistical mechanics.

Appendix. List of didactic JAVA applets

The following JAVA applets, pertaining to points discussed in this paper, may be accessed at the author's Web site (www.ap.univie.ac.at/users/ves/):

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 disc 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 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 discs in an elastic container. For $N = 1$ the behaviour 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.

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

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