Proof a a stratification of temperature in a heavy column of gas by Liouville's theorem

1. Liouville's theorem

Liouville's theorem shall be elaborated.

a) Let us define a parameter H (called Hamiltonian) in the following way (U is the potential energy of a particle, m its mass, p its momentum):
(1)

$$H = \sum_{i} \left(\frac{1}{2}mv_{i}^{2} + U_{i}(x_{i})\right) = \sum_{i} \left(\frac{1}{2}m\dot{x}^{2} + U_{i}(x_{i})\right) = \sum_{i} \left(\frac{p_{i}^{2}}{2m} + U_{i}(x_{i})\right)$$

Partially differentiating **H** with respect to a single **p**, that is, with respect to the momentum component in one direction of a single particle of mass **m**, gives: (2)

$$\frac{\delta H}{\delta p_i} = \frac{p_i}{m} = v_i = \dot{x}_i$$

Partially differentiating **H** with respect to a single \mathbf{x} , that is, with respect to the spatial position of a single particle, gives (**F** is force on a particle): (3)

$$\frac{\delta H}{\delta x_i} = \frac{\delta U_i}{d x_i} = -F_i = -\dot{P}_i$$

One should also note that, even if **dH** (the total differential of **H**) is exactly zero (which is the case if the total energy of the system, kinetic and potential, stays fixed), **partial delta H** may nevertheless be different from zero.

We shall now imagine that each of the many particles is moving in a six-dimensional phase space. That is to say: Each particle has, at any moment in time, six coordinates, which are \mathbf{x} , \mathbf{y} , \mathbf{z} , $\mathbf{p}_{\mathbf{x}}$, $\mathbf{p}_{\mathbf{y}}$, $\mathbf{p}_{\mathbf{z}}$.

At a later moment in time, the single point that represents that particle in six-dimensional phase space may have shifted. If there are many neighbouring points (in six-dimensional phase space) which each represent a particle, we are confronted with what we may call a "flow of stuff" in the six-dimensional phase space. We would like to find out whether or not the number of points in a stationary (six-dimensional) volume element (of constant volume, shape and position) stays constant over time.

If, for a better illustration, we reduce the dimensions from six to merely two (this is for a

short while only), that is **x** and \mathbf{p}_x , we would get for $\mathbf{dZ/dt}$, that is, for the increase or decrease in the number **Z** of particles in the two-dimensional "volume" element over an interval of time (**A** is a factor that is an expression of the particle density in phase space; without any further knowledge, all parameters could depend on position in phase space and on time): (4)

$$-\frac{dZ}{dt}(x,p_{x},t) = A(x,p_{x},t) \left[\frac{v_{horiz_{2}}-v_{horiz_{1}}}{x_{2}-x_{1}}(x,p_{x},t) + \frac{v_{vertic_{2}}-v_{vertic_{1}}}{p_{x_{2}}-p_{x_{1}}}(x,p_{x},t)\right]$$

$$= A(x_{x_{x}}p_{x},t) \left[\frac{\delta \dot{x}}{\delta x}(x_{x}p_{x},t) + \frac{\delta \dot{p}_{x}}{\delta p_{x}}(x_{y}p_{x},t)\right]$$

The equation is based on the assumption that a large number of particles find themselves within the volume element and nearby. Horizontal velocities \mathbf{v}_{horiz} and vertical velocities \mathbf{v}_{vertic} refer to velocities of particle points in the two-dimensional diagram in which the horizontal axis stands for the direction \mathbf{x} , and the vertical axis stands for the \mathbf{x} -component of momentum \mathbf{p} . The subscript 1 refers to the location where particle-points enter the fixed volume element. The subscript 2 refers to the location where particle points-leave the volume element. We assume that the changes in velocities from particle to particle at a frozen moment in time apply to a great number of particles which behave the same way.

b) When returning to six dimensions (instead of just two), we have:(5)

$$-\frac{dZ}{dt} = A \left(\frac{\delta \dot{x}}{\delta x} + \frac{\delta \dot{y}}{\delta y} + \frac{\delta \dot{z}}{\delta z} + \frac{\delta \dot{p}_x}{\delta p_x} + \frac{\delta \dot{p}_y}{\delta p_y} + \frac{\delta \dot{p}_z}{\delta p_z}\right)$$

When making use of (2) and (3), (5) turns into: (6)

$$-\frac{dZ}{dt} = A \left(\frac{\delta}{\delta x} \frac{\delta H}{\delta p_x} + \frac{\delta}{\delta y} \frac{\delta H}{\delta p_y} + \frac{\delta}{\delta z} \frac{\delta H}{\delta p_z} - \frac{\delta}{\delta p_x} \frac{\delta H}{\delta x} - \frac{\delta}{\delta p_y} \frac{\delta H}{\delta y} - \frac{\delta}{\delta p_z} \frac{\delta H}{\delta z}\right)$$

Or, after re-arranging the order of summands: (7)

$$-\frac{dZ}{dt} = A(x_x y_z z_y p_x p_y p_z) \left[\left(\frac{\delta}{\delta x} \frac{\delta H}{\delta p_x} - \frac{\delta}{\delta p_x} \frac{\delta H}{\delta x} \right) + \left(\frac{\delta}{\delta y} \frac{\delta H}{\delta p_y} - \frac{\delta}{\delta p_y} \frac{\delta H}{\delta y} \right)$$

+
$$\left(\frac{\delta}{\delta z} \frac{\delta H}{\delta p_z} - \frac{\delta}{\delta p_z} \frac{\delta H}{\delta z}\right) = 0$$

Since the order of two partial differentiations can be reversed without affecting the result, each of the three brackets in (7) is zero, and so is the whole sum. Given the number of particle-points in a fixed six-dimensional volume element of phase space does not change with time, \mathbf{A} (which is an expression of particle density in phase space) does not depend on time.

c) With the density of particle-points in the fixed six-dimensional volume element of phase space being constant over time (which is true as long as the moving lump of particle-points has not left that volume element), the ensemble of particle-points in six-dimensional phase space behaves like an incompressible liquid in real space that has a homogeneous density.

Note that (7) is valid in the interior of a "lump" of particle points only, and is not applicable right at the surface of the lump, where \mathbf{H} is not differentiable. Also note that there may be different "lumps" of particle points at the same time that have different homogenous densities in phase space (similar to incompressible liquids in real space, which, too, come in different densities).

2) Inhomogeneity of temperature in a gas subject to gravity

a) Imagine all **N** particles of a gas are evenly, that is, equidistantly arranged so that they form a cube in real space with homogeneous density. The edges of the cube run parallel to the three axes of a Cartesian system of coordinates.

In six-dimensional phase space, the center of the cube shall coincide with the origin of coordinates. Let us concentrate on just two dimensions of the six-dimensional phase space. Let the spatial **x**-axis (one of three spatial directions) be the horizontal axis, and let the $\mathbf{p_x}$ -momentum axis (one of three momentum components) be the vertical axis of the diagram. In that partial phase space, the gas particles (in the initial moment) form a two-dimensional area. Due to the arrangements put in place, the particle-point density (that is, the density of points in phase space) shall be homogeneous throughout the whole six-dimensional volume, and hence also throughout the two-dimensional area, no matter what distribution of momenta is necessary to achieve such a state in phase space.

For reason of symmetry, the situation must look alike when considering the partial, twodimensional phase space which consists of the spatial **y**-axis as the horizontal axis and the \mathbf{p}_{y} axis as the vertical axis, or when considering the partial, two-dimensional phase space which consists of the spatial **z**-axis as the horizontal axis and the \mathbf{p}_{z} -axis as the vertical axis.

b) Let us now imagine that the particles give in to the forces of mutual gravitational attraction they are subject to. Let us wait for a while, until a stationary state of motion of the particles

has been achieved. We know from Liouville's theorem that the six-dimensional volume of the lump of particle-points in phase space has not changed. We also know that the particlepoint density in each of the three partial, two-dimensional phase spaces (formed by **x** and **p**_x, or by **y** and **p**_y, or by **z** and **p**_z), has not changed either. But it can be considered as an empirical fact that, in the stationary, radially symmetrical state which has formed, the density of the gas in real space (particles per spatial unit volume) decreases with distance from the origin of coordinates. For our two-dimensional, partial phase space, this results in the following: When sliding the edge of a ruler horizontally from far left to right over the surface of the diagram, the number of particle-points passed per unit distance of horizontal displacement of the edge of the ruler would not be constant, but would increase until we reach the origin of coordinates. This property of the two-dimensional lump of particle-points in phase space shall be called property number one.

If assuming that the temperature of the gas is homogeneous regardless of distance from the center of origin, the vertical extension (height) of our two-dimensional lump of particle-points in two-dimensional phase space (that is, the range of momenta of particles) would have to be the same everywhere. This property of the two-dimensional lump of particle-points in phase space shall be called property number two. But with these two properties (of our two-dimensional lump of particle points) combined, it is impossible for the lump of particle points to have a homogeneous density in phase space.

Moreover, in case Boltzmann's distribution of kinetic energies held true for the gas of assumed homogeneous temperature, the vertical extension of the lump of particle-points in two-dimensional phase space would be infinite, and the average density of points in two-dimensional phase space would consequently approach zero, quite different from the initial state of the gas. But this is forbidden by Liouville's theorem. Hence, in order to avoid infinitely high values of variables, we shall assume that the gas is confined to the interior of a hollow sphere with a finite radius. We also assume that the microstate of the gas we are considering is of a kind in which particles do not occur that in Boltzmann's distribution of energies belong to the upper 0.01 percent. Then, in case of a homogeneous temperature of the gas, the lump of particle-points in a partial, two-dimensional phase space would have to form a rectangle with finite extensions, but with varying densities of particle-points from place to place. But this, too, is forbidden by Liouville's theorem. A homogeneous temperature of the gas is thus excluded.

Last, not least: A volume element in the interior of a bulk of gas (whose particles attract each other because of gravity) in real space does not know whether the center of the bulk consists of other gas particles or of solid matter, instead. In other words: The impossibility of a homogeneous temperature of a gas holds true also for an atmosphere of a planet.

Thereby it is proved that a homogeneous temperature of a heavy gas cannot exist in real space. Quod erat demonstrandum.

c) Only if we assume that the heavy gas is warmer at the bottom and colder in the upper regions, there would no longer be a conflict with Liouville's theorem: The height of our lump of particle-points in two-dimensional phase space would then be larger near the origin of coordinates (center of the sphere), and smaller at regions some horizontal distance away.

Thereby a homogeneous density of particle-points in two-dimensional, partial phase space is possible, as is required by Liouville's theorem.

A stratification of temperature in a heavy gas corresponds to a steady upward and downward flow of parcels of gas, that is to a situation permanently out of static equilibrium, whereby the adiabatic lapse rate of temperature with height is being approached.

d) Our result is equivalent to the recognition that the distribution of momenta and kinetic energies among the particles cannot be that of Boltzmann. For if Boltzmann's distribution of energies were strictly valid everywhere, the temperature of the gas would have to be the at all heights (see Alan J. Walton, Archimedes' principle in gases, Contemporary Physics, Vol. 10 – 1969 –, p. 185; Claude Garrod, Statistical mechanics and thermodynamics, Oxford University Press, 1995; and also K. Zhang / Y.-J. Zhang, Principle of detailed balance and a dilute gas in gravitational field, arXiv:1607.06692v3 [cond-mat. stat-mech] 30 Nov 2016). But it isn't. In other words: The initial arrangement of particles cannot have converted into a gas that strictly obeys Boltzmann's rule of distribution of kinetic energies.

3) The general physical law implicitly contained in Liouville's theorem

But how can it be possible to derive the behaviour of a heavy gas from Liouville's theorem? In other words: What empirical physical laws are contained in it?

At first sight, one might be inclined to believe that Liouville's theorem does not contain any empirical laws at all, but only definitions (which are contingent). But this first impression is wrong. Equation (3) postulates:

$$\frac{\delta H}{\delta x_i} = \frac{\delta U_i}{dx_i} = -F_i = -\dot{P}_i$$

It presupposes that the potential energy **U** of a particle is differentiable. Moreover, in order for the particle to have a definitive potential energy, the gravitational field must be conservative (any closed-loop integral of the vector \mathbf{g} – gravitational acceleration – must vanish). The "conservativeness" of the gravitational field can thus be identified as the empirical law implicitly contained in Liouville's theorem.

Hence, the stratification of temperature in a heavy gas is derived from the empirically corroborated "conservativeness" of the gravitational field, and Liouville's theorem is merely the vehicle for performing this derivation.

4) Confirmation of L. Susskind's theorem of a permanent instability of a heavy gas

a) The above disproof of a homogeneous temperature of the heavy gas was inspired by L. Susskind, who, in his online lectures on Statistical Mechanics, Spring 2009, Lecture 10,

0:54:30 h to 1:04 h, points out that a bulk of particles under its own gravity has "negative specific heat": When thermal energy is added, it expands against its own gravity, and does mechanical work. Thereby it is getting cooler than it has been before. Conversely, when thermal energy is removed, the bulk of particles contracts, and is getting warmer than it has been before. This is because of the following theorem of mechanics: Whenever one has removed an amount of kinetic energy W_0 from an orbiter, it takes on a new (lower) orbit on which the potential energy has decreased by exactly double that amount, that is by $2W_0$, and on which its kinetic energy has gone up by that amount, that is by W_0 .

A negative specific heat comes along with an unstable state. This is because of the following: When the energies of separate parts of the gas fluctuate (and are interchanged among those parts), the fluctuation tends to build up.

In Susskind's words:

"Gravity has all kinds of problems with thermodynamics, even just Newtonian gravity. Newtonian gravity does not have a good thermal equilibrium. ... Gravity itself is a disastrous thing when you are thinking about thermal equilibrium." It "cannot correspond to a genuine equilibrium situation. ... Systems with negative specific heats cannot be in equilibrium with their environment. ... Thermodynamics breaks down eventually for systems with gravity."

b) As has been shown above, Susskind's theorem is confirmed by an application of Liouville's theorem. Both in the proof based on Liouville's theorem and in Susskind's theorem (of gas under gravity being out of equilibrium all the time), the only general physical law applied is that of the "conservativeness" of gravity, and nothing else.

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