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Approach to equilibrium in integrable gas models

P. Kasperkovitz and Ch. Foidl
Institut für Theoretische Physik, Technische Universität Wien, Karlsplatz 13, A-1040 Wien, Austria
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The approach to equilibrium found recently by Georgallas [Phys. Rev. A **35**, 3492 (1987)] is analyzed and compared with previous work on this problem.

I. INTRODUCTION

In a recent paper Georgallas[1] considered the expansion of an ideal gas initially compressed into a corner of a rectangular box. He calculated the one-particle distribution corresponding to this initial configuration and a special velocity distribution (see item Sec. IV below) and found that it converges (weakly) to a stationary distribution. This decay, characterized by a $1/t$ law, was also found for the expectation value of the position and the velocity of the center of mass. Essentially the same problem has been considered previously by several authors[2-4] none of whom are mentioned in Ref. 1; also, these findings were not related to the decay of the velocity autocorrelation function which also has been calculated for this system some time ago.[5,6] The only two papers Georgallas cites are that of Frisch[7] on a different model (periodic boundary conditions instead of walls) and that of Ford[8] who considers, besides one single anharmonic oscillator, anharmonic chains which are nonintegrable and therefore of no relevance here.

The purpose of this comment is (i) to relate Georgallas's work to previous investigations, (ii) to clarify the meaning of "approach to equilibrium" for this and other integrable systems, and (iii) to point out that the only fundamental problem is to *motivate* the choice of the initial distribution function and to *interpret* the resulting decay of expectation values.

II. DYNAMICS

Both in the title and in the introduction of Ref. 1, Georgallas considers the expansion of a gas initially compressed into one of the corners of the container. This is a sequence of states, each characterized by the positions and the velocities of all the particles, starting from a given configuration and some set of initial velocities. One might argue that it is not possible to specify the initial "microscopic" state completely (this point will be taken up in Sec. IV below), but conceptually microscopic dynamics has to be fixed first before one can discuss the evolution of certain "macroscopic" observables. For the system at hand this dynamics is especially simple: The N particles do not interact and are confined in a rectangular box of dimension D, so the system decomposes into ND noninteracting subsystems of degree one. Although, strictly speaking, not Hamiltonian these one-dimensional subsystems are known to be integrable,[9,10] i.e., they allow a description in terms of action and angle variables (a,α),[10,11]

$$\begin{aligned}&\text{(i)}\quad p>0,\quad x\in(0,L)\Longleftrightarrow a>0,\alpha(\mathrm{mod}\ 2\pi)\in(0,\pi)\ ,\\ &\qquad pL=a\pi,\quad x/L=\alpha/\pi\\ &\text{(ii)}\quad p<0,x\in(0,L)\Longleftrightarrow a>0,\alpha(\mathrm{mod}\ 2\pi)\in(-\pi,0)\ ,\\ &\qquad -pL=a\pi,\quad -x/L=\alpha/\pi\ .\end{aligned}\tag{1}$$

In these variables the evolution of the system appears as free motion on a torus of dimension ND,

$$\alpha_t=\alpha_0+\omega t,\quad \omega=\partial H/\partial a=a\pi/mL\ .\tag{2}$$

In general, the orbit covers the whole torus uniformly (irrational tori), but if one or more relations of the form $\sum_k r_k\omega_k=0$, r_k rational, exist between the frequencies the motion is restricted to a subset of lower dimension (rational tori). Because of (1) and (2) rational and irrational tori may be obtained here by varying the sides of the box for fixed initial velocities.[1]

It should be noted that the model considered by Georgallas (and others[3-6] before) is not the only integrable model of a gas. There are a few other possible forms of the container (e.g., a regular trigonal prism for $D=3$) or the particles may interact through elastic collisions if $D=1$ and all masses are equal.[12] In all these models the

existence of action and angle variables clearly shows that the motion of the particles is almost periodic[13] so that all the particles will return again and again to one corner of the container if they were initially located there (this happens also under much weaker assumptions).[9] This recurrence may be a mathematical proposition without any practical relevance.[13] In any case, there exists nothing like an "equilibrium state" on a microscopic scale.

III. PHASE-SPACE FUNCTIONS

The evolution of the system will look more uniform if only a small subset of the information needed to specify a microscopic state is followed in time. The properties of the system one is interested in are described by phase-space functions. They change their value from $G(\mathbf{P},\mathbf{X})$ to $G(\mathbf{P}_t,\mathbf{X}_t)$ if the microscopic state changes from $(\mathbf{P},\mathbf{X})$ to $(\mathbf{P}_t,\mathbf{X}_t)$ during a period of length t; here $(\mathbf{P},\mathbf{X})=(\mathbf{x}_1,\ldots,\mathbf{p}_N)$ and $\mathbf{P}_t=\mathbf{P}_t[\mathbf{P},\mathbf{X}],\mathbf{X}_t=\mathbf{X}_t[\mathbf{P},\mathbf{X}]$ are the solutions of the equations of motion with initial data $\mathbf{P},\mathbf{X}$. Hobson and Loomis[4] considered all moments $p_k^J x_k^K (J,K\in\mathbb{N}_0, k=1,\ldots,ND)$ from which all analytical functions G and, by suitable limits, many others may be obtained. The other authors discuss one-particle observables only, i.e., functions of the form

$$G(\mathbf{P},\mathbf{X})=(1/N)\sum_i g(\mathbf{p}_i,\mathbf{x}_i)\ ; \tag{3}$$

examples are the spatial density,[1,2] the number of particles to be found in the left half of the box,[3] the velocity distribution,[1,2] or the number of particles moving from the left to the right.[3] The evolution of the functions g is especially transparent if they are expressed in terms of action and angle variables,

$$g(\mathbf{p}_t,\mathbf{x}_t)=\sum_{\mathbf{z}}\tilde{g}(\mathbf{a},\mathbf{z})\exp[i\mathbf{z}\cdot(\boldsymbol{\alpha}+\boldsymbol{\omega}t)]\ . \tag{4}$$

In this equation $\mathbf{p}_t=\mathbf{p}_t[\mathbf{p},\mathbf{x}]$, $\mathbf{x}_t=\mathbf{x}_t[\mathbf{p},\mathbf{x}]$, $\mathbf{a}=\mathbf{a}(\mathbf{p},\mathbf{x})$, $\boldsymbol{\alpha}=\boldsymbol{\alpha}(\mathbf{p},\mathbf{x})$, $\boldsymbol{\omega}=\boldsymbol{\omega}(\mathbf{a})$, and $\mathbf{z}\in\mathbb{Z}^D$. The observable g is constant in time if, and only if, it is an even function of $\mathbf{p}$ and independent of $\mathbf{x}$. All the conserved quantities can be expressed as functions of the action variables a_k or, because of (2), of the frequencies $\omega_k(k=1,\ldots,ND)$. How a one-particle function (3) fluctuates around its time average depends on the expansion coefficients $\tilde{g}(\mathbf{a},\mathbf{z})$, $\mathbf{z}\neq\mathbf{0}$, and on the frequencies ω_i. If N is large one might conjecture that the fluctuations, to be seen, e.g., in a computer simulation, are small for most of the time, so that large deviations from the time average will persist for very short times only. This would allow us to discuss the "approach to equilibrium" in terms of the evolution of observables. But whether or not such a behavior is actually found in a computer experiment depends on the initial data.

IV. INITIAL CONDITIONS

It is generally agreed that the initial state of a many-particle system cannot be fixed uniquely. In Georgallas's example the initial positions of all the particles are assumed to be known but not their velocities. Some authors[1,3] feel that these should be chosen from a Maxwellian distribution. But why? Such a distribution is found if (i) the particles interact through elastic collisions, (ii) the system is ergodic (hard disks or spheres, one-dimensional systems with different masses), and (iii) the thermodynamic limit is considered (otherwise it is a beta distribution). The Maxwellian velocity distribution then emerges as time average for one particle whose free (integrable) motion is stopped and reinitialized again and again by the interaction with the other particles. The gas models considered here have entirely different properties, so one has to look for different reasons to motivate the introduction on an initial velocity distribution and to specify its form. In their choice Hobson and Loomis[4] refer to the principle of maximum entropy, an idea especially advocated by Jaynes.[14] According to this philosophy the initial distribution is not related to the interaction of the system with its environment; it represents nothing but the observer's knowledge about the state of the system. For Hobson and Loomis this is a generalized canonical distribution since they assumed that only the expectation values of total energy, total momentum, and position of the center of mass are initially known. The initial distributions used in Ref. 1–3, 5, and 6 may also be interpreted in the sense of Jaynes.[14] For instance, the uniform velocity distributions, chosen in Refs. 1 and 3 for mathematical simplicity only, correspond to a situation where upper and lower bounds are known for all the conserved quantities but nothing more.

V. EXPECTATION VALUES

Once a distribution function $F(\mathbf{P},\mathbf{X})$ is given one can calculate the expectation value

$$\langle G\rangle_t=\int\int d\mathbf{P}\,d\mathbf{X}\,F(\mathbf{P},\mathbf{X})G(\mathbf{P}_t[\mathbf{P},\mathbf{X}],\mathbf{X}_t[\mathbf{P},\mathbf{X}]) \tag{5}$$

of the observable $G(\mathbf{P},\mathbf{X})$ as a function of time. If we consider an observable $g(p_k,x_k)$ depending on one degree only the evolution of its expectation value is determined by the reduced distribution $f(p_k,x_k)$ obtained from $F(\mathbf{P},\mathbf{X})$ by integrating over the remaining degrees. If F is of the form $U(\mathbf{P})\delta(\mathbf{X}-\mathbf{X}_0)$ and U an even function of the momentums p_k, the reduced distribution, expressed in action and angle variables, has the form $\bar{u}(a_k)[\delta(\alpha-\alpha_0)+\delta(\alpha+\alpha_0)]$. Using the corresponding representation of g, Eq. (4), and the fact that $\bar{u}(a_k)=\bar{u}(\omega_k)$ [cf. Eq. (2)] we see that the evolution of the expectation value depends on the asymptotic form of the integrals

$$I_{t,z}[u,g]=\int d\omega\bar{g}(\omega,z)\bar{u}(\omega)\exp(i\omega zt) \tag{6}$$

for $t\to\infty$. For a moment $g(p,x)=p^Jx^K$ that is not constant in time $\bar{g}(\omega,z)=\omega^J c_{JK}\neq 0$ for $z\neq 0$, so the power ω^J and the one-particle distribution $\bar{u}(\omega)$ determine how the expectation value of the moment tends to a constant value (if it converges at all). (i) For the canonical distribution[4] $\bar{u}\propto\exp(-\gamma\omega^2)$, $\gamma>0$; $I^{JK}\sim t^J\exp(-\delta t)$, $\delta>0$. (ii) For the microcanonical distribution[12] $\bar{u}\propto[1-(\omega/c)^2]^{ND}$ for $\omega<c$, $\bar{u}=0$ for $\omega>c$, $c^2=O(ND)$; $I^{JK}\sim t^{-(ND-1)/2}$. (iii) If a canonical distribution is chosen for each degree[2,3,5–7] one gets the same results as for (i). (iv) For the uniform distribution for each degree[1,3,7] $\bar{u}=\text{const}$ for $\omega\in(\omega',\omega'')$, $\bar{u}=0$ otherwise;

$I^{JK} \sim t^{-1}$. (v) For the microcanonical distribution for each degree[6,7] $\bar{u} \propto \delta(\omega - \omega_0)$; I^{JK} periodic. These different "approaches to equilibrium" can be consistently interpreted following Jaynes's argumentation;[14] like the evolution of the entropy[4] the convergence of these expectation values simply shows that our knowledge of the instantaneous state of the system decreases in the course of time if it is incomplete already in the beginning. As emphasized by Frisch,[7] it is here the spread in the initial velocities and the finite volume of the system that makes it more and more difficult, as time proceeds, to predict the positions of the particles and the direction of their velocities.

But where does our information about the initial velocities come from? Or, if we reject Jaynes's reasoning, which physical interaction of the system with its environment produces these initial data in a similar way as Maxwell's velocity distribution is generated for one particle by its collisions with the other ones?

VI. CONCLUSION

In an integrable system all observables are almost periodic functions of time. Irreversible behavior is only obtained if an observable is averaged over an infinite set of invariant tori with different frequencies.[7,8] While averaging seems to be necessary because of the great number of degrees it is by no means obvious how to do it in detail. This point has to be clarified first since the long-time behavior of expectation values varies with the way the individual tori are weighted in the average. Georgallas adds one more example to the literature without elucidating the physical reasoning behind his approach.

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