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1990 J. Phys. A: Math. Gen. 23 L427

(http://iopscience.iop.org/0305-4470/23/9/005)

J. Phys. A: Math. Gen. 23 (1990) L427-L432. Printed in the UK

LETTER TO THE EDITOR

The Boltzmann function as an embedded property of Liouville's equation

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Received 23 November 1989, in final form 22 January 1990

Abstract. A classical system of indistinguishable interacting point-particles is considered whose probability density function satisfies Liouville's equation. It is shown that, for a general Hamiltonian system, the Boltzmann function is the only single-particle measure on the phase space which can be interpreted as information content out of equilibrium. There is no connection between entropy flow and the arrow of time for the exact dynamics.

The concept of entropy and its meaning has always been a fascinating subject. As pointed out by Andrew (1984), however, entropy does not appear in any of the equations of motion, and so its meaning, apparently, remains open to interpretation. Much of the argument stems from problems concerning the connection between time-reversible dynamics and irreversibility in the real world. Further difficulties are encountered when one attempts to establish links between irreversibility and the measure function $-x \ln x$. Fox (1982) has apparently shown that the exact time-reversible dynamics of a system of non-interacting particles can give rise to a monotonic increasing entropy function. This has been refuted by Mandel (1984) who claims that, essentially, the initial conditions are not consistent in the analysis. The underlying problem appears to be that many extra assumption are made often leading to different definitions of reversibility (Illner and Neunzert 1987) so that different writers are talking different languages with no possibility of agreement.

Prigogine (1979a) has stated that the Liouville equation does not define a unique entropy type function primarily because

$$\int F(D)\, \mathrm{d}\Omega \tag{1}$$

is a constant of the motion for any function F of the evolving probability density D. In (1) $\mathrm{d}\Omega$ represents the elemental phase-space volume of a system described by Hamiltonian dynamics. Indeed, the Poincaré–Misra theorem (Prigogine 1979b) states that there cannot be a Lyapounov function defined on the phase space for the exact dynamics. This letter offers a different approach to the problem by answering the question: what is it about the Boltzmann H-function that makes it qualitatively different from any other phase-space measure for the exact dynamics? Later this question is answered by showing that functions of the form $\pm x \ln x$ transform the time derivatives of the measure function into a structure-preserving form subject only to a symmetry condition on the Hamiltonian. Some concluding remarks are made at the end of this letter.

0305-4470/90/090427+06\$03.50

Since the results that follow rely heavily on the correlation equations of Balescu (1975a) his notation is adopted in this letter. The Hamiltonian is written in the following form:

$$H = H^0 + H^F + H^1$$
$$= \sum_{j=1}^{N} \frac{p_j^2}{2m} + \sum_{j=1}^{N} \Phi_j^F + \sum_{j<k=1}^{N} \Phi_{jk} \tag{2}$$

where $\Phi_j^F = \Phi^F(q_j, p_j, t)$ is the external field potential, m is the particle mass, N the number of interacting particles and Φ_{jk} represents the particle interaction potential satisfying the property

$$\Phi_{jk} = \Phi_{kj} = \Phi(\boldsymbol{q}_j, \boldsymbol{p}_j, \boldsymbol{q}_k, \boldsymbol{p}_k, t). \tag{3}$$

$\boldsymbol{q}_j, \boldsymbol{p}_j$ represent the coordinates and the conjugate momenta for the system under discussion. Property (3) covers all classical forms of particle interaction with no assumption about time symmetry being necessary. Equation (3) represents a generalisation of the more usual form considered in classical statistical mechanics, namely $\Phi_{jk} = \Phi(|\boldsymbol{q}_j - \boldsymbol{q}_k|)$.

Corresponding to the breakup of H in (2) it is necessary to construct phase-space operators from the Poisson bracket according to the rules

$$L_j^0 = [H_j^0, \ldots]_p = -\frac{p_j}{m} \cdot \nabla_{q_j} \tag{4a}$$

$$L_j^F = [\Phi_j^F, \ldots]_p = \nabla_{q_j}\Phi_j^F \cdot \nabla_{p_j} - \nabla_{p_j}\Phi_j^F \cdot \nabla_{q_j} \tag{4b}$$

$$L_{jk} = [\Phi_{jk}, \ldots]_p = \nabla_{q_j}\Phi_{jk} \cdot \nabla_{p_j} - \nabla_{p_j}\Phi_{jk} \cdot \nabla_{q_j} + \nabla_{q_k}\Phi_{jk} \cdot \nabla_{p_k} - \nabla_{p_k}\Phi_{jk} \cdot \nabla_{q_k}. \tag{4c}$$

L_j^F and L_{jk} are time dependent operators and $L_{jk} = L_{kj}$ because of (3). Equation (4c) has the alternative useful form (when integrating over phase space)

$$L_{jk} \ldots = \nabla_{p_j} \cdot (\ldots \nabla_{q_j}\Phi_{jk}) - \nabla_{q_j} \cdot (\ldots \nabla_{p_j}\Phi_{jk}) + \nabla_{p_k} \cdot (\ldots \nabla_{q_k}\Phi_{jk}) - \nabla_{q_k} \cdot (\ldots \nabla_{p_k}\Phi_{jk})$$

and similarly for L_j^F. The $\ldots$ indicate any scalar function on which the various operators act. Since the particles are indistinguishable, the Liouville function is assumed invariant under particle relabelling. Hence (4a–c) can be specialised with $j = 1$ and $k = 2$.

Explicit time equations are required for the univariate distribution $f_1 = f_1(\boldsymbol{q}_1, \boldsymbol{p}_1, t)$ and the pair correlation $g_{12} = g_{12}(\boldsymbol{q}_1, \boldsymbol{p}_1, \boldsymbol{q}_2, \boldsymbol{p}_2, t)$ in the form (Balescu 1975a)

$$\partial_t f_1 = (L_1^0 + L_1^F) f_1 + \int L_{12} f_1 f_2 \, \mathrm{d}x_2 + \int L_{12} g_{12} \, \mathrm{d}x_2 \tag{5a}$$

$$\partial_t g_{12} = (L_1^0 + L_1^F + L_2^0 + L_2^F) g_{12} + L_{12} f_1 f_2 + L_{12} g_{12} + M_{12} \tag{5b}$$

where

$$M_{12} = \int [L_{13} f_1 g_{23} + L_{23} f_2 g_{13} + (L_{13} + L_{23})(f_3 g_{12} + g_{123})] \, \mathrm{d}x_3.$$

In (5b) g_{123} is the triple correlation function for the evolution.

Finally, it is assumed that the Liouville function D together with a sufficient number of its derivatives vanish on the boundaries of the system in phase space (Balescu 1975b). Clearly all derived functions from D will have similar properties.

A measure function on phase space, $H(t)$, can be defined as

$$H(t) = \int F(f_1) \, \mathrm{d}x_1 \tag{6}$$

where dx_1 is the elemental volume in μ-space and the form of F is to be determined from the phase-space flow. Although (6) is overly general, the time derivatives of H can be evaluated for the general case. It is a requirement that H is a sensible measurement in that it presumably measures something useful and so varies with time.

Differentiating (6), using (5a) and the definitions (4a–c) yields

$$\dot{H}(t) = \int \frac{\partial F}{\partial f_1} L_{12} g_{12}\, dx_1\, dx_2 \tag{7}$$

where the other terms can easily be shown to vanish on the phase-space boundaries, providing the measure function F and its derivatives vanish there also. (7) is valid $\forall t$, but since $\dot{H}$ can have any value, (6) does not define a Lyapounov function.

Putting $Q(f_1) = \partial F / \partial f_1$ and noting by symmetry that

$$\dot{H}(t) = \int Q(f_2) L_{12} g_{12}\, dx_1\, dx_2$$

it follows that

$$\dot{H}(t) = \frac{1}{2} \int \{Q(f_1) + Q(f_2)\} L_{12} g_{12}\, dx_1\, dx_2. \tag{8}$$

Equation (8) is valid for any Hamiltonian system satisfying (2), (3) and shows that $\dot{H}(t)$ depends only on the interaction operator L_{12}. In order to preserve this dynamical interaction picture in relation to evolution equations like (5a, b) only the correlation patterns, defined by Balescu (1975a) as

$$\pi(1/2) = f_1 f_2 \qquad \text{and} \qquad \pi(12) = g_{12} \tag{9}$$

are admissible in (8). This simply requires that

$$Q(f_1) + Q(f_2) = Q_1(f_1 f_2)$$

with the unique solution (Rasetti 1986)

$$Q(f_1) = k \ln f_1,\ Q_1 = Q$$

where k is an arbitrary constant. Hence the non-trivial measure F is given by

$$F(f_1) = k f_1 \ln f_1 .$$

Equation (8) then becomes expressible in terms of correlation patterns only. Specifically

$$\begin{aligned} \dot{H}(t) &= \frac{k}{2} \int \ln \pi(1/2) L_{12} \pi(12)\, dx_1\, dx_2 \\ &= -\frac{k}{2} \int \frac{L_{12}\pi(1/2)}{\pi(1/2)} \pi(12)\, dx_1\, dx_2. \end{aligned} \tag{10}$$

Unless (7) can be mapped onto the π correlation patterns (9), the measure function is not structure preserving with respect to the property of pairwise interaction via L_{12}.

The above proof of the Boltzmann function out of equilibrium for the exact dynamics appears, superficially, to be deceptive. Certainly its brevity is, perhaps, a cause for concern. If the simple mapping (9) is correct, other interesting properties should result from it. This can be demonstrated by evaluating $\dot{H}$ from (10). Omitting k yields the following result from (10):

$$\ddot{H}(t)=\frac{1}{2}\frac{\partial}{\partial t}\int \ln \pi(1/2)L_{12}\pi(12)\,\mathrm{d}x_1\,\mathrm{d}x_2$$
$$=\frac{1}{2}\int\left(\frac{\partial}{\partial t}-L_1^0-L_1^F-L_2^0-L_2^F\right)\ln \pi(1/2)L_{12}\pi(12)\,\mathrm{d}x_1\,\mathrm{d}x_2$$
$$=\frac{1}{2}\int \partial_t^{(2)}\ln \pi(1/2)L_{12}\pi(12)\,\mathrm{d}x_1\,\mathrm{d}x_2$$
$$=\frac{1}{2}\int\left\{\frac{\partial_t^{(2)}\pi(1/2)}{\pi(1/2)}L_{12}\pi(12)+\ln \pi(1/2)\partial_t^{(2)}L_{12}\pi(12)\right\}\mathrm{d}x_1\,\mathrm{d}x_2. \qquad (11)$$

The operators $\partial_t^{(2)}$ and L_{12} do not, in general, commute but satisfy the relation

$$\partial_t^{(2)}L_{12}=L_{12}\partial_t^{(2)}+L_{12}^{(2)}$$

where

$$L_{12}^{(2)}=[\partial_t^{(2)}\Phi_{12},\ldots]_p.$$

Balescu (1975a) has given the equations for $\dot{\pi}(1/2)$ and $\dot{\pi}(12)$ in the form:

$$\partial_t^{(2)}\pi(1/2)=\int (L_{13}+L_{23})\pi(1/2/3)\,\mathrm{d}x_3+\int L_{13}\pi(2/13)\,\mathrm{d}x_3+\int L_{23}\pi(1/23)\,\mathrm{d}x_3$$

$$\partial_t^{(2)}\pi(12)=\int [L_{13}\pi(1/23)+L_{23}\pi(2/13)$$
$$+(L_{13}+L_{23})(\pi(3/12)+\pi(123))]\,\mathrm{d}x_3+L_{12}\pi(1/2)+L_{12}\pi(12).$$

Substituing into (11) yields the following representation of $\ddot{H}(t)$ as

$$\ddot{H}(t)=\frac{1}{2}\int \ln \pi(1/2)L_{12}(L_{12}\pi(1/2))\,\mathrm{d}x_1\,\mathrm{d}x_2$$
$$+\frac{1}{2}\int \ln \pi(1/2)[L_{12}^{(2)}\pi(12)+L_{12}(L_{12}\pi(12))+L_{12}M_{12}]\,\mathrm{d}x_1\,\mathrm{d}x_2$$
$$+\frac{1}{2}\int \frac{L_{12}\pi(3/12)}{\pi(1/2/3)}[(L_{13}+L_{23})\pi(1/2/3)+L_{13}\pi(2/13)$$
$$+L_{23}\pi(1/23)]\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3. \qquad (12)$$

M_{12} has the representation (Balescu 1975a)

$$\int [L_{13}\pi(1/23)+L_{23}\pi(2/13)+(L_{13}+L_{23})(\pi(3/12)+\pi(123))]\,\mathrm{d}x_3.$$

The second time derivative of the Boltzmann function (12) is a function of the correlation patterns (π) up to order 3. The leading term of (12) can be rewritten as the sink term

$$\ddot{H}_{\mathrm{SINK}}(t)=-\frac{1}{2}\int \frac{[L_{12}\pi(1/2)]^2}{\pi(1/2)}\,\mathrm{d}x_1\,\mathrm{d}x_2\leqslant 0$$

$\forall t \in R$. The action of L_{12} on the uncorrelated part of the distribution function contributes a continual loss to the H-function in any time direction. This result is independent of the initial conditions. Since

$$\ddot{H}_{\mathrm{SINK}}(t)=0 \qquad \text{only if } L_{12}\pi(1/2)=0 \text{ everywhere}$$

the Boltzmann function is a true measure out of equilibrium (i.e. $\forall t$). $H(t)$ then satisfies the evolution condition

$$\ddot{H}(t)=\ddot{H}_{\mathrm{SINK}}(t)+G(t)$$

where the sign of $G(t)$ is dependent on the dynamics (the correlated part of the probability distribution). The leading term in (12) becomes a source term for the measure $-f_1 \ln f_1$.

From (10) and (12) the following correspondence can be noted:

$$\begin{aligned}
&\dot{H}(t) \leftrightarrow \pi(1/2),\ \pi(12)\\
&\ddot{H}(t) \leftrightarrow \pi(1/2),\ \pi(12),\ \pi(1/2/3)\\
&\qquad\quad \pi(1/23),\ \pi(2/13),\ \pi(3/12)\\
&\qquad\quad \pi(123).
\end{aligned}$$

This leads to the conjecture that $\partial_t^n H(t)$ depends only on the correlation patterns for orders $\leqslant n+1$, which trivially follows using induction and noting that for a pattern of order l, $\pi^{(l)}$, $\dot{\pi}^{(l)}$ depends on patterns of order $\leqslant l+1$ as is evident from Balescu's (1975a) hierarchy. Successive time derivatives of $H(t)$ also yield measure functions on the phase space corresponding to more complicated correlation patterns. It is apparent that the requirement of the mapping (9) is necessary and sufficient to ensure $\partial_t^n H$ depends only on the action of L_{12} on the correlation patterns. This neatly fits in with Balescu's (1975c) theory representing classical dynamics purely as a dynamics of correlations. Any other measure function produces new operators in phase space which do not appear in the original Liouville equation and therefore do not model the interaction process.

Since there exist only two measures on the phase space (differing in sign), then the mapping onto the names 'information' and 'entropy' is uniquely defined by

$$\begin{aligned}
f_1 \ln f_1 &\leftrightarrow \text{information}, \ (\ddot{H}_{\mathrm{SINK}}(t))\\
-f_1 \ln f_1 &\leftrightarrow \text{entropy}, \ (\ddot{H}_{\mathrm{SOURCE}}(t))
\end{aligned}$$

up to an arbitrary positive constant.

This letter has shown that although the function $kx \ln x$ does not appear in any equation of motion explicitly, it appears as an embedded property of the Liouville equation in a natural and meaningful way. This answers some of the points raised by Andrew (1984).

Contentious points like time asymmetry and a link between entropy and time have not been discussed primarily because it is believed that these results have actually broken that link. Indeed, in the theory presented here, t is merely an independent parameter and has no future or past interpretation built into the equations. Curiously, also, these results do not contradict any theorems concerning the existence of Lyapounov functions on the phase space simply because $f_1 \ln f_1$ is a unique measure of information for the exact dynamics but is not Lyapounov (e.g. the Poincaré-Misra theorem, Prigogine 1979b). It is emphasised that the only assumptions made here concern the existence of Liouville's equation, property (3) and the usual boundary conditions over phase space assumed by other authors. Further, no appeal to coarse graining is required in the theory with the unique existence of the Boltzmann function being solely a property of Liouville's exact equation for the microscopic flow. In particular, this letter has widened the discussion to any interaction potential, satisfying condition (3), which now includes magnetic phenomena.

The results here strongly suggest that the Liouville equation itself defines, implicitly, the sort of entropy function that should be used. Thus the concepts of 'information' and 'entropy' should, in principle, be deducible from the governing (Liouville) equation. The constancy of (1) for an arbitrary function F, can only be interpreted as $F = \pm D \ln D$ because of the results achieved earlier.

References

Andrew K 1984 *Am. J. Phys.* **52** 492-6
Balescu R 1975a *Equilibrium and non-Equilibrium Statistical Mechanics* (New York: Wiley) pp 479-81
—— 1975b *Equilibrium and non-Equilibrium Statistical Mechanics* (New York: Wiley) p 79
—— 1975c *Equilibrium and non-Equilibrium Statistical Mechanics* (New York: Wiley) pp 484-9
Fox R F 1982 *Am. J. Phys.* **50** 804-5
Illner R and Neunzert H 1987 *Trans. Theor. Stat. Phys.* **16** 89-112
Mandal G 1984 *Am. J. Phys.* **52** 462-3
Prigogine I 1979a *From Being to Becoming* (San Francisco: Freeman) p 170
—— 1979b *From Being to Becoming* (San Francisco: Freeman) pp 171-3
Rasetti M 1986 *Modern Methods in Equilibrium Statistical Mechanics* (Singapore: World Scientific) p 199