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On the nature of irreversibility in soluble classical systems

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Abstract. We investigate a restricted type of classical Hamiltonian system which includes all exactly soluble ones. The Liouville equation is solved exactly and an unambiguous expression obtained for a reduced distribution function in the thermodynamic limit. It is found that this reduced function cannot show irreversible behaviour due to the dynamics, although the boundary of the system or its initial condition may produce this behaviour. We conclude that approximate methods must be used to study dynamical irreversibility in Hamiltonian systems.

1. Introduction

The main purpose of the theory of non-equilibrium statistical mechanics as developed by Prigogine and his co-workers (Prigogine 1962, Resibois 1966) is to look for irreversibility, that is, an evolution to a time-independent distribution, coming from the purely mechanical basis of the theory. Thus one looks for the source of irreversibility in particle interactions and not in the containing walls of the system or some other stochastic element in the theory. The formalism as applied to either classical or quantum systems is rather complex and normally involves several approximate expansions whose range of accuracy is difficult to establish in any general way. It is therefore of great interest to apply the methods to problems involving exactly soluble models.

The problems in classical mechanics which can be solved in closed form are those for which the Hamilton–Jacobi equation is separable (Goldstein 1950), and thus for which some new coordinates may be found in terms of which there is no longer any interaction. It might be conjectured that such systems cannot show irreversibility in the above sense even in the limit of a large system and, indeed, it has been shown, at least in a formal way (Leaf and Schieve 1967) by operating on the full distribution function, which is not strictly defined in this limit, that this is the case. It is possible, however, for such systems to exhibit other sorts of irreversibility: for example, an infinite chain of linked harmonic oscillators may relax in the sense that the initial configuration may disappear and never recur.

In this paper we start from this class of soluble problems and, after emphasizing the essential role of boundary conditions, show that when suitable eigenfunctions of the Liouville operator exist, the solution to the Liouville equation can be obtained exactly. In order to discuss rigorously the thermodynamic limit, it is necessary to introduce reduced distribution functions and examine with some care the interchanges of the various limiting processes involved. The result shows that ‘Hamiltonian irreversibility’ is indeed impossible for these systems, while the possibility for ‘initial condition irreversibility’ remains.

2. Specification of the problem

We consider Hamiltonians $H(\mathbf{q}, \mathbf{P})$ describing a system of N degrees of freedom:

$$\dot{\mathbf{P}} = - \frac{\partial H}{\partial \mathbf{q}}, \quad \dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{P}}$$

(\mathbf{P} and \mathbf{q} are N -component vectors) for which there exist N first integrals in involution, i.e. the Poisson bracket of any pair of the integrals vanishes identically. This includes those systems for which the Hamilton–Jacobi equation

$$H\left(\mathbf{q}, \frac{\partial W}{\partial \mathbf{q}}\right) = \alpha$$

for the characteristic function W is separable in the sense that a W of the form

$$W = \sum_{i=1}^N W_i$$

splits the equation into N first-order ordinary differential equations. For such systems there exist (Arnold and Avez 1968) canonical variables \mathbf{p} , \mathbf{x} and Hamiltonian K which satisfy the equations of motion:

$$\dot{\mathbf{p}} = 0, \quad \dot{\mathbf{x}} = \boldsymbol{\omega}(\mathbf{p}), \quad \boldsymbol{\omega}(\mathbf{p}) = \frac{\partial K}{\partial \mathbf{p}}$$

with $\boldsymbol{\omega}(\mathbf{p}) = \mathbf{p}/m$. These equations hold for all times.

We describe the system by a distribution function $\rho(\mathbf{x}, \mathbf{p}, t)$ whose equation of evolution is Liouville's equation:

$$\frac{\partial \rho}{\partial t} + \{\rho, K\} = 0$$

where $\{\dots, \dots\}$ is the Poisson bracket. In the coordinates \mathbf{x} , \mathbf{p} , this takes the form

$$i \frac{\partial \rho}{\partial t} = L\rho \tag{1}$$

where L is the Liouville operator:

$$L = -im^{-1}\mathbf{p} \cdot \frac{\partial}{\partial \mathbf{x}} \tag{2}$$

The solution of (1) can be written (Prigogine 1962)

$$\rho(t) = \exp(iLt)\rho(0) = \frac{1}{2\pi i} \int_{\gamma} dz \exp(-izt) \frac{1}{z-L} \rho(0) \tag{3}$$

where γ is a contour in the z plane parallel to the real axis and above all singularities of the integrand. The operator L must be self-adjoint on the space of distribution functions and hence the resolvent operator $(z-L)^{-1}$ is a bounded operator on this space for z not on the real axis (Hille and Phillips 1957). The time development operator $\exp(iLt)$ is unitary and therefore also bounded.

The possible solutions of the eigenvalue equation

$$L\phi_{\mathbf{k}, \mathbf{p}^0} = \lambda_{\mathbf{k}, \mathbf{p}^0} \phi_{\mathbf{k}, \mathbf{p}^0} \tag{4}$$

are

$$\phi_{\mathbf{k}, \mathbf{p}^0} = C \exp(i\mathbf{k} \cdot \mathbf{x}) \delta(\mathbf{p} - \mathbf{p}^0)$$

(δ is an N -dimensional Dirac delta function), and

$$\lambda_{\mathbf{k}, \mathbf{p}^0} = m^{-1}\mathbf{k} \cdot \mathbf{p}^0$$

In order to decide if these possible eigenfunctions are indeed eigenfunctions, it is necessary to discuss the nature of the space of distribution functions including some

account of the boundary conditions. We shall take all distribution functions to lie in the Hilbert space of square integrable functions of $2N$ variables, this being the smallest space which contains reasonable distribution functions and yet has useful mathematical properties. It is at once clear that the functions (4) cannot, strictly speaking, be eigenfunctions, since the delta functions prevent them from being square integrable. The Liouville operator has a continuous spectrum which is all of the real axis since each component of \mathbf{p}^0 , and hence $\lambda_{\mathbf{k}, \mathbf{p}^0}$, can take any real value. However, the components of \mathbf{p} are constants of the motion, and so if we choose $\rho(0)$ in a subspace defined by definite momenta \mathbf{p} , $\rho(t)$ will remain in this subspace for all time. The restriction of L to this subspace will have a much smaller spectrum depending only on the \mathbf{x} -dependent part of (4), which is square integrable over the subspace; and we can now proceed. To simplify the notation we shall retain the original L and the delta functions in the working below. The space of distribution functions is further restricted by the choice of boundary conditions. Suppose first that the system is defined in a cube \mathcal{D} (or more generally a rectangular box) in \mathbf{x} space given by

$$-\frac{1}{2}l < x_i < \frac{1}{2}l$$

for each component x_i ($i = 1 \dots N$) of \mathbf{x} .

If we consider functions of the form $\exp(i\mathbf{k} \cdot \mathbf{x})$ with \mathbf{x} lying in this box and use the self-adjointness of L , that is, with the appropriate scalar product

$$(\exp(i\mathbf{k} \cdot \mathbf{x}), L \exp(i\mathbf{k}' \cdot \mathbf{x})) = (L \exp(i\mathbf{k} \cdot \mathbf{x}), \exp(i\mathbf{k}' \cdot \mathbf{x}))$$

we obtain immediately

$$\mathbf{p} \cdot (\mathbf{k} - \mathbf{k}') \int_{\text{cube}} d\mathbf{x} \exp\{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{x}\} = 0 \quad (5)$$

that is

$$\mathbf{p} \cdot (\mathbf{k} - \mathbf{k}') \prod_{j=1}^N \frac{\sin \frac{1}{2}l(k_j - k'_j)}{k_j - k'_j} = 0$$

where the k_j are the components of \mathbf{k} . If the components of \mathbf{p} are non-zero, the result is that \mathbf{k} must have the form

$$\mathbf{k} = \frac{2\pi\mathbf{n}}{l}$$

where \mathbf{n} is a set of N integers. Conversely any \mathbf{k} of this form will suffice. For the cube (or the rectangular box) it appears that L has a complete orthonormal set of eigenfunctions which, with the provision above, may be written

$$l^{-N/2} \exp(i\mathbf{k} \cdot \mathbf{x}) \delta(\mathbf{p} - \mathbf{p}^0)$$

and eigenvalues

$$\lambda_{\mathbf{k}, \mathbf{p}^0} = m^{-1} \mathbf{k} \cdot \mathbf{p}^0 = \frac{2\pi}{lm} \mathbf{n} \cdot \mathbf{p}^0.$$

In this case L has a pure point spectrum. The choice of a cube in \mathbf{x} space will correspond in general to very complicated \mathbf{P} -dependent boundaries in the original phase space of \mathbf{P} and \mathbf{q} . It is usually assumed that since we are ultimately going to take the limit of a large system it will not matter what is taken as the boundary of the system. There is, however, another reason for making the above choice; namely, that any other choice will lead to an incomplete set of eigenfunctions for L .

To see this, let us consider a system defined on a domain \mathcal{D}' composed of two rectangles:

$$\begin{aligned} -\frac{1}{2}l < x_1 < 0, & \quad -\frac{1}{2}l < x_m < \frac{1}{2}l, & \quad m = 2, \dots, N \\ 0 < x_1 < \frac{1}{2}l, & \quad -\frac{1}{2}l' < x_2 < \frac{1}{2}l', & \quad -\frac{1}{2}l < x_n < \frac{1}{2}l, & \quad n = 3, \dots, N \end{aligned}$$

shown schematically in figure 1. The self-adjointness condition (5) becomes:

$$\mathbf{p} \cdot (\mathbf{k} - \mathbf{k}') \int d\mathbf{x} \exp\{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{x}\} = 0$$

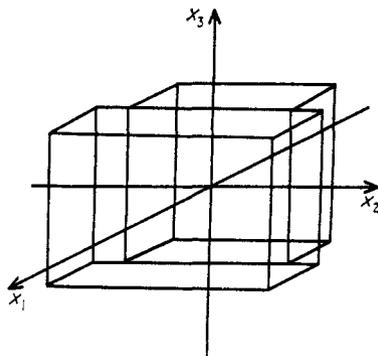


Figure 1.

where the integration is now over the domain \mathcal{D}' . This gives

$$\begin{aligned} \mathbf{p} \cdot (\mathbf{k} - \mathbf{k}') \left[\prod_{j=3}^N \frac{\sin\{\frac{1}{2}(k_j - k'_j)l\}}{k_j - k'_j} \right] \frac{\sin\{\frac{1}{4}(k_1 - k'_1)l\}}{(k_1 - k'_1)(k_2 - k'_2)} \\ \times [\exp\{\frac{1}{4}i(k_1 - k'_1)l\} \sin\{\frac{1}{2}(k_2 - k'_2)l\} + \exp\{-\frac{1}{4}i(k_1 - k'_1)l\} \sin\{\frac{1}{2}(k_2 - k'_2)l\}] = 0. \end{aligned}$$

We apply this condition to two eigenfunctions which differ only in their k_1 variables and then require

$$p_1 \sin\{\frac{1}{4}(k_1 - k'_1)l\} [\frac{1}{2}l \exp\{\frac{1}{4}i(k_1 - k'_1)l\} + \frac{1}{2}l' \exp\{-\frac{1}{4}i(k_1 - k'_1)l\}] = 0.$$

If $p_1 \neq 0$, then either

$$\sin\{\frac{1}{4}(k_1 - k'_1)l\} = 0 \quad (6)$$

or

$$l \exp\{\frac{1}{4}i(k_1 - k'_1)l\} + l' \exp\{-\frac{1}{4}i(k_1 - k'_1)l\} = 0. \quad (7)$$

The first case imposes

$$k_1 - k'_1 = \frac{4n\pi}{l} \text{ for some integer } n.$$

The second case leads to non-real values of $k_1 - k'_1$ unless $l = l'$. Since we assumed that $l \neq l'$ and since the self-adjoint operator L has only real eigenvalues, the condition (7) cannot be satisfied, and (6) must hold. This means that if $l \neq l'$ the x_1 dependence of the eigenfunctions is $\exp(4in\pi x_1/l)$, which yields an incomplete set in \mathcal{D}' .

Any more general domain \mathcal{D}'' can be approximated by a system of rectangles built up in this way, and it is clear that the system of resulting eigenfunctions can never be

complete. This incompleteness implies that the spectrum of L is no longer a pure point spectrum, and it is known (Prigogine 1962) that a continuous spectrum for L is at least a necessary condition for irreversible behaviour. This shows that there is a possibility of irreversibility due to the choice of the boundary of the system. But, since the object of this paper is to look for irreversibility directly from the system Hamiltonian, we shall not pursue this interesting line any further here.

3. The reduced distribution function

We now consider the solution (3) of the Liouville equation for a system defined on the rectangular domain \mathcal{D} for which L has a complete orthonormal set of eigenfunctions, as discussed in the preceding section. The initial distribution function $\rho(0)$ is expanded in terms of these eigenfunctions as follows

$$\rho(0) = l^{-N/2} \sum_{\mathbf{k}} \rho(\mathbf{k}, \mathbf{p}^0) \exp(i\mathbf{k} \cdot \mathbf{x}) \delta(\mathbf{p} - \mathbf{p}^0) \quad (8)$$

where \mathbf{x} has N components and \mathbf{k} is summed over the values $2\pi\mathbf{n}/l$. The action of the time development operator on any eigenfunction is

$$\exp(iLt) \exp(i\mathbf{k} \cdot \mathbf{x}) \delta(\mathbf{p} - \mathbf{p}^0) = \exp\left(\frac{i\mathbf{k} \cdot \mathbf{p}^0 t}{m} + i\mathbf{k} \cdot \mathbf{x}\right) \delta(\mathbf{p} - \mathbf{p}^0).$$

We assume throughout the remainder of the paper that $\rho(\mathbf{x}, \mathbf{p}, 0)$ is a continuous function of the \mathbf{x} . With this provision, the expansion (8) is *uniformly convergent* (Whittaker and Watson 1963) with respect to \mathbf{x} in a rectangular domain \mathcal{D}_δ with sides $-\frac{1}{2}l + \delta \leq x_i \leq \frac{1}{2}l - \delta$ where δ can be arbitrarily small. Since we are ultimately going to integrate over $N-1$ components of \mathbf{x} and take the limit of a large system, the difference between \mathcal{D} and \mathcal{D}_δ is of no consequence. As $\exp(iLt)$ is a *bounded operator* in the norm of the Hilbert space of distribution functions, we may operate term by term on the infinite series (8) and obtain a series convergent to $\exp(iLt)\rho(0)$. Thus (3) may be written

$$\rho(t) = l^{-N/2} \sum_{\mathbf{k}} \rho(\mathbf{k}, \mathbf{p}^0) \exp\left(\frac{i\mathbf{k} \cdot \mathbf{p}^0 t}{m} + i\mathbf{k} \cdot \mathbf{x}\right) \delta(\mathbf{p} - \mathbf{p}^0). \quad (9)$$

The objects of physical interest, and indeed the only entities meaningful in the thermodynamic limit, are the so-called reduced distribution functions, not $\rho(t)$ itself. For simplicity in the remainder of the paper we shall consider the reduced distribution function for one degree of freedom only, defined as

$$\begin{aligned} f(x_1, p_1, t) &= g(N) \int_{-l/2}^{l/2} dx_2 \dots \int_{-l/2}^{l/2} dx_N \int_{-\infty}^{\infty} dp_2 \dots \int_{-\infty}^{\infty} dp_N \rho(\mathbf{x}, \mathbf{p}, t) \\ &= g(N) \int_x \int_p \rho(t) \end{aligned}$$

where \int_x and \int_p are the multiple integral operators in this expression and f is normalized to a function $g(N)$, the choice of which is postponed to § 4. The analysis which follows is easily extended to reduced functions for several degrees of freedom.

From (9) we obtain an equation for $f(t)$

$$f(t) = g(N) l^{-N/2} \int_x \int_p \sum_{\mathbf{k}} \rho(\mathbf{k}, \mathbf{p}^0) \exp\left(\frac{i\mathbf{k} \cdot \mathbf{p}^0 t}{m} + i\mathbf{k} \cdot \mathbf{x}\right) \delta(\mathbf{p} - \mathbf{p}^0). \quad (10)$$

In order to perform the reduction explicitly it is necessary to interchange the order of the integrations and summations in (10). The integrations \int_p are purely formal and

can be performed at once to give

$$f(t) = g(N)l^{-N/2}\delta(p_1 - p_1^0) \int_x \sum_{\mathbf{k}} \rho(\mathbf{k}, \mathbf{p}^0) \exp\left(\frac{i\mathbf{k} \cdot \mathbf{p}^0 t}{m} + i\mathbf{k} \cdot \mathbf{x}\right). \quad (11)$$

Now, the infinite series in (11) is, apart from the delta function, the Fourier expansion of $\rho(t)$, and is essentially the same series discussed above and found to be uniformly convergent with respect to \mathbf{x} in \mathcal{D}_δ . Since \int_x is over a finite range, it follows (Whittaker and Watson 1963) that we may interchange \int_x with the summation in (11) to obtain

$$f(t) = g(N)l^{-N/2}\delta(p_1 - p_1^0) \sum_{\mathbf{k}} \rho(\mathbf{k}, \mathbf{p}^0) \exp\left(\frac{i\mathbf{k} \cdot \mathbf{p}^0 t}{m}\right) \int_x \exp(i\mathbf{k} \cdot \mathbf{x}). \quad (12)$$

The x integrals are now very simple to perform: for example,

$$\int_{-l/2}^{l/2} \exp(ik_2 x_2) dx_2 = \frac{\exp(\frac{1}{2}ik_2 l) - \exp(-\frac{1}{2}ik_2 l)}{ik_2} = \begin{cases} 0 & \text{if } k_2 \neq 0 \\ l & \text{if } k_2 = 0 \end{cases}$$

where we use $k_2 = 2\pi n_2/l$. Thus each $\int dx_j$ gives a factor $l\delta_{k_j, 0}$, which takes out most of the terms in the summation over \mathbf{k} , leaving

$$f(t) = g(N)l^{N/2-1}\delta(p_1 - p_1^0) \sum_{k_1} \rho\{k_1, \mathbf{p}^0, (k_j = 0)\} \exp\left(\frac{ik_1 p_1^0 t}{m} + ik_1 x_1\right). \quad (13)$$

4. The thermodynamic limit

We now wish to examine the behaviour of $f(t)$ in the limit of a large system, that is when $N \rightarrow \infty$ and the concentration remains a finite constant. Since the length l defined in § 2 measures the size of the system in \mathbf{x} space and not in the original physical space described by \mathbf{q} , it is not necessary that $l \rightarrow \infty$ in this limit. However, in the case when l does not tend to infinity the values of $k_1 = 2\pi n_1/l$, which appear in the summation in (13) remain discrete. Thus $f(t)$ remains a periodic function of t with period ml/p_1^0 . The analogous reduced distribution function for more than one degree of freedom will be almost periodic unless the periods associated with these degrees of freedom are commensurable. This corresponds to the remark made in § 2 that a discrete spectrum for L cannot lead to irreversible behaviour. We need consider therefore only the alternative case when $l \rightarrow \infty$ as $N \rightarrow \infty$. Here the variable k_1 becomes continuous in the limit and the summation in (13) can be written as a Riemann integral if we choose the function $g(N)$ properly as below.

The Fourier coefficients in (13) depend on N and l . Let us rewrite them

$$\rho\{k_1, \mathbf{p}^0, (k_j = 0)\} = 2\pi h(N, l)\hat{\rho}(k_1)$$

where $\hat{\rho}(k_1)$, apart from possible isolated singularities, is well-behaved as $N \rightarrow \infty$ and we have suppressed the dependence on \mathbf{p}^0 which is constant for the problem. In the limit as $N \rightarrow \infty$

$$\frac{2\pi}{l} \sum_{k_1} \hat{\rho}(k_1) \exp\left(\frac{ik_1 p_1^0 t}{m} + ik_1 x_1\right)$$

will become an integral over k_1 . Thus, if we choose a $g(N)$ such that as N (and therefore l) tends to infinity, $g(N)l^{N/2}h(N, l)$ tends to a constant c , which is usually chosen to be a suitable power of the concentration, the thermodynamic limit of $f(t)$ is well defined. For a finite system this choice of $g(N)$ is clearly just a matter of notation. Equation (13) is now

$$\lim f(t) = c\delta(p_1 - p_1^0) \int_{-\infty}^{\infty} dk_1 \hat{\rho}(k_1) \exp\left(\frac{ik_1 p_1^0 t}{m} + ik_1 x_1\right). \quad (14)$$

$\hat{\rho}$ is a function of the continuous real variable k_1 and substituting $t = 0$ in (14) identifies it as the Fourier integral transform of $\lim f(0)$, the initial reduced distribution function.

As regards the time dependence of $\lim f(t)$, it is clearly a superposition of exponential oscillations whose exact behaviour is determined by the details of the singularities of $\hat{\rho}$ in the complex plane of k_1 . Thus any apparent irreversibility depends on the choice of $\hat{\rho}$, that is on the initial distribution, and not on the dynamics of the system. For example, the presence of a simple pole of $\hat{\rho}$ can lead to transient contributions to $\lim f(t)$ which are exponentially damped (compare with Balescu 1963).

5. Conclusions

The classical systems considered in this paper form a very restricted class, namely those for which there exist as many integrals in involution as degrees of freedom. Nevertheless, this class is important as it includes all problems of classical mechanics which are exactly soluble (Goldstein 1950).

Since we have been interested in examining such systems for possible irreversible behaviour arising from the dynamics as specified by the Hamiltonian (Hamiltonian irreversibility), we have been forced in this investigation to a very particular choice of boundary conditions. The requirements that the Liouville operator L of equation (2) be self-adjoint and that it possess a complete set of eigenfunctions are sufficient to impose the rectangular boundary conditions we have used. Further, any other choice, as we have seen, does not admit such a complete set and so leads to a continuous spectrum for L and, consequently, possible irreversible behaviour due to the boundary. As remarked in § 2, our choice does not correspond to walls which might be realized in any simple physical way, but none the less it is certainly sufficient in the limit of a large system for the study of Hamiltonian irreversibility. In cases where the physical boundaries are important what we have shown therefore is that either these boundary effects must be included in the Hamiltonian, which will usually lead to an insoluble problem, or else they will coincide with those chosen for mathematical reasons. Examples of this latter case are free particles in a physical rectangular box or a bound system describable in terms of action and angle variables.

The thermodynamic limit, as we have treated it in § 4, is unambiguously defined. The procedure used is quite general and is applicable in all cases where the spectrum of L becomes continuous in the limit of a large system. The choice of the Hamiltonian K in free-particle form means that in these cases the parameter l always tends to infinity with N and cannot be maintained at some finite value as would be the case for the range of an angle variable. In particular, this will be so for a chain of coupled harmonic oscillators, although in the usual action-angle variable description the range of the angle variables is always 0 to 2π .

Our analysis seems to show three possible sources of irreversible behaviour for reduced distribution functions:

- (i) The physical boundaries or walls of the systems.
- (ii) The choice of the initial distribution which may lead to a phase mixing of transient contributions.
- (iii) The Hamiltonian of the system.

We have shown in § 4 that the third case does not arise for the class of Hamiltonians considered in this paper. Cases (i) and (iii) are linked mathematically as there is a certain amount of choice as to whether physical walls are included directly in the Hamiltonian or treated as boundary conditions, but so long as one distinguishes physically between a system and its walls the two cases can be separated. The results of this paper have been expressed in a special set of canonical coordinates \mathbf{x} , \mathbf{p} , in which the distribution function $f(t)$ does not become time independent for large t . If the calculation were performed in another set of variables obtained from \mathbf{x} , \mathbf{p} by a

time-independent canonical transformation, it is clear that the resulting reduced distribution function would also have this property. However in these new coordinates it is not evident that one may now distinguish easily between sources (ii) and (iii) of irreversible behaviour.

It appears therefore that any investigation of irreversible behaviour in classical Hamiltonian systems must employ approximate methods, as soluble models may show only the irreversibility from sources (i) and (ii). Of course, if one abandons the strictly mechanical approach starting from a deterministic Hamiltonian, it is possible to devise exactly soluble systems which contain an intrinsic stochastic element (see, for example, Sutherland 1969).

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