Relaxation times for Hamiltonian systems

A. Maiocchi*  
A. Carati§

April 8, 2009

Abstract

Usually, the relaxation times of a gas are estimated in the frame of the Boltzmann equation, which is a reduced description if compared with the microscopic Hamiltonian model, and, moreover, being a dissipative equation, already has an irreversible character. In this paper, instead, we deal with the relaxation problem in the frame of the dynamical theory of Hamiltonian systems, in which the definition itself of a relaxation time is an open question. We introduce a suitable definition of relaxation time, and give a general theorem for estimating it. Furthermore we give an application in a concrete model of a gas, providing a lower bound to the relaxation time, which turns out to be compatible with those observed in dilute gases.

1 Introduction

The definition and the estimate of relaxation times are problems of central interest when one attempts at describing macroscopic systems through microscopic Hamiltonian models.

In the case of gases, these problem are tackled, and solved, in the frame of the Boltzmann equation (see [1]). In such a frame the existence of a relaxation time is somehow obvious, due to the irreversible character of the

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*Università di Milano, Corso di laurea in Fisica, Via Celoria 12, 20133 Milano, Italy  
E-mail: alberto.maiocchi@studenti.unimi.it  
§Università di Milano, Dipartimento di Matematica, Via Saldini 50, 20133 Milano, Italy
equation, and the estimate is obtained in terms of the eigenvalues of the linearized equation, about the equilibrium solution.

There are two problems left. First, one doesn’t know how to proceed in the case of a system different from a gas. Furthermore, even in the case of a gas, the Boltzmann equation refers to a reduced description, whose relation to the original Hamiltonian system is not completely clarified.

An approach to the relaxation problem that refers to the complete system, without any reduction, was given recently (see [2]). A characteristic feature of such an approach is that the system is assumed to be non isolated, being in contact with a mechanical thermostat which makes the system dissipative albeit reversible.

In the present work we tackle the problem from the point of view of the dynamical theory of Hamiltonian systems, for systems which are isolated. In this perspective, a partial answer to the problem is given by Kubo’s linear response theory [3]. Indeed, such a theory enables one, at least in principle, to compute in microscopic terms the macroscopic transport coefficients, and then, via macroscopic equations, the relaxation time. From our point of view, however, this answer is not completely satisfactory, because it appeals to macroscopic irreversible equations, which should preliminarily be deduced from the microscopic ones.

A related but different approach is followed here, whose main scheme can be sketched as follows.

From linear response theory we take the starting point, namely, the idea of following the time evolution of the probability distribution function in phase space (and not in the reduced μ−space, as in the Boltzmann equation), when a perturbation $- \hbar A(p, q)$ to the original Hamiltonian $H_0(p, q)$ is introduced. Still following Kubo, we then choose to concentrate our attention on a particular observable, namely the one conjugated to the perturbing field, in the familiar sense in which pressure is conjugated to volume and magnetization to the magnetic field. As an example, later on in this paper we will deal with the simple case in which the perturbing field is gravity, and the conjugate observable is the height of the center of mass. However, while Kubo looks (in a heuristic way) at the asymptotic behaviour of the distribution function (and hence also at the expectation of the conjugate variable) for large times, when equilibrium has been attained, our attention is instead addressed at defining and estimating the relaxation time itself.

In the spirit of the Kubo approach it is natural to say that equilibrium is attained when the time derivative of the conjugate variable is negligible.
The main idea is then that the relaxation time should be defined as the one at which the rate of change of the conjugate variable is smaller than a certain threshold.

The aim of the present paper is indeed to give a lower bound to the relaxation time, looking at the evolution of the time–derivative of the variable conjugated to the perturbation $A$ in the Hamiltonian. It is easily seen that the time–derivative of the conjugate variable is the function $B \overset{\text{def}}{=} [H_0, A]$, so that this is the quantity on which we will concentrate in this paper. Having chosen the relevant function, namely $B$, we make use of the easily established properties that its expectation vanishes at equilibrium, and that its time–derivative is positive at the initial time. Thus a lower bound $t_{\text{relax}}$ to the relaxation time is provided by the time before which the time–derivative of the expectation of $B$ is proven to be positive.

The problem is then that one should make use of suitable a priori estimates on the dynamics, in lack of an explicit integration of the equations of motion. This can actually be implemented following the main idea introduced in paper [4], which was concerned with Hamiltonian perturbation theory in the thermodynamic limit. In such a paper, a procedure is given which, for any $L^2$ function $f$ of phase space with respect to Gibbs measure, allows one to provide an upper bound to $\|U_t f - f\|_2$, by knowing an upper bound of $\|\{f, H\}\|_2$. Here, $\{\cdot, \cdot\}$ denotes Poisson bracket, $H$ the Hamiltonian of the system, and $U_t$ the corresponding unitary evolution group.

The estimate of the lower bound $t_{\text{relax}}$ is provided by formula (9) of Theorem 1, which is stated and proved in Section 2. Such a proof is given for an ample class of Hamiltonian systems, which are the ones considered in most rigorous works in Statistical Mechanics (see [5]).

In Section 3 the general theorem is applied to the case of a gas of non–interacting point–particles enclosed in a cubic box, to which the gravity force is added as a perturbation. The relaxation time thus found turns out to be comparable with the typical relaxation times observed in dilute gases. One should actually study the model of a gas of particles interacting through a stable and temperate two–body potential. Working at a heuristic level, it is easily seen that, for a dilute gas, essentially the same estimates are obtained than in the case of a non–interacting gas. We hope to be able to give a rigorous treatment in the future.

Some further comments are given in Section 4.
2 General theorem about relaxation times

Consider a system, with phase space $\mathcal{M}$, which is in equilibrium with respect to the Gibbs measure relative to an unperturbed Hamiltonian $H_0$ at inverse temperature $\beta$, i.e., the measure with density $\rho_0$ given by

$$\rho_0 = \frac{1}{Z_0} \exp (-\beta H_0),$$

$Z_0$ being the partition function. Suppose at time 0 a perturbation $-hA(p,q)$ is introduced, where $A$ is a given function on phase space and the parameter $h > 0$ controls the size of the perturbation. So, at positive times the Hamiltonian is $H_1 = H_0 - hA$. The corresponding Gibbs density will be denoted by $\rho_1$. Our aim is to find a sensible definition and an estimate for the relaxation time $t_{relax}$ to the final equilibrium with respect to Hamiltonian $H_1$.

To this end, along the scheme sketched in the introduction, following Kubo we consider the observable $B$ defined by

$$B = [A, H_0],$$

i.e., the time derivative of the perturbation $A$ with respect to the flow generated by the total Hamiltonian $H_1$. We then consider the probability density $\rho$, solution of Liouville's equation relative to the total Hamiltonian $H_1$ with initial condition $\rho(0) = \rho_0$, and look at the evolution of the expectation of $B$, i.e., we look at the quantity

$$\overline{B}(t) = \int B \rho(t) \, dp \, dq.$$

The quantity of interest actually will be its increment

$$\Delta \overline{B}(t) \overset{\text{def}}{=} \overline{B}(t) - \overline{B}(0).$$

Writing $\rho$ in the form

$$\rho(t) \overset{\text{def}}{=} \rho_0 + \Delta \rho(t),$$

by Liouville's equations the perturbation $\Delta \rho$ satisfies the differential equation

$$\frac{\partial \Delta \rho}{\partial t} = [H_0 - hA, \Delta \rho] - h [A, \rho_0],$$
with $\Delta \rho(0) = 0$ as initial condition, and one has

$$\Delta B(t) = \int B \Delta \rho(t) \, dp \, dq . \quad (3)$$

We will show that under the familiar conditions which entail reversibility (namely, that both $H_0$ and $A$ are even in the momenta), the quantity $\Delta B$ vanishes not only (as it is obvious) at time zero, but also at equilibrium with respect to the total Hamiltonian $H_1$. This is due to the fact that the expectations of $B$ with respect to the Gibbs densities $\rho_0$ and $\rho_1$ corresponding to the Hamiltonians $H_0$ and $H_1$, both vanish by symmetry, because $\rho_0$ and $\rho_1$ are even in the momenta, whereas $B$ is odd. On the other hand, it turns out that $\Delta B$ is initially an increasing function of time, since its time–derivative is positive at time 0, as it will be shown later. Thus, the time–derivative of $\Delta B$ has to become negative if equilibrium with respect to the total Hamiltonian has to be attained, and consequently a lower bound to the relaxation time is provided by the time $t_{\text{relax}}$ up to which the time derivative of $\Delta B$ is guaranteed to be positive.

We thus define the relaxation time $t_{\text{relax}}$ by

$$t_{\text{relax}} \overset{\text{def}}{=} \sup t^* , \quad (4)$$

where $t^*$ is such that

$$\frac{d}{dt} \Delta B(t) \geq 0 \quad \text{for all} \quad 0 < t < t^* . \quad (5)$$

The problem is then to estimate the rate of growth of $\Delta B$. Now, on the one hand, following Kubo we know that $\Delta \overline{B}(t)$ is strictly related to the time–autocorrelation of $B$ (see (13) below). On the other hand, we can make use of the main result obtained in paper [4], in which it was shown how to estimate the time–autocorrelation of $B$ in terms of the Hamiltonian. Indeed, from the main result of such a paper one easily obtains the following property: an a priori estimate of the type

$$\| [B, H_0] \|_0 \leq \eta \| B \|_0 ,$$

(with the norm defined below) implies that the time–evolution of $\Delta \overline{B}$ is slow if $\eta$ is small, or, more precisely, that the relaxation time defined by (4), (5) is inversely proportional to $\eta$. 

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Here, $\| \cdot \|_0$ is the norm on $\mathcal{L}^2_0(\mathcal{M})$, the Hilbert space of square integrable complex functions on $\mathcal{M}$, with respect to $\rho_0$. We will also have to consider the Hilbert space $\mathcal{L}^2_1(\mathcal{M})$ of the square integrable complex functions with respect $\rho_1$. The corresponding $\mathcal{L}^2$–norm will be denoted by $\| \cdot \|_1$.

Under the rather natural condition (6) given below, which ensures the smallness of the “change” of the Gibbs measure induced by the perturbation $-hA$, for a large class of observables it can be proven that the two norms just introduced are asymptotically equivalent as $h \to 0$. Indeed one has the following lemma, whose proof is deferred to Appendix A.

**Lemma 1** Assume there exist $\delta > 0$ and $K > 0$ such that

\[
\int_{\mathcal{M}} dp dq e^{\delta A} \rho_0 < K \quad \text{and} \quad \int_{\mathcal{M}} dp dq e^{-\delta A} \rho_0 < K.
\]  

(6)

Then, for all real functions $f$ on $\mathcal{M}$ satisfying at least one of the conditions

\[
\| f^2 \|_0 < +\infty, \quad \| f^2 \|_1 < +\infty,
\]  

(7)

one has

\[
\| f \|_1^2 - \| f \|_0^2 = o(1), \quad \text{as } h \to 0.
\]

We are now able to give an estimate for $t_{\text{relax}}$ in terms of $\eta$, which is provided by the following Theorem 1. It will be seen that some technical hypotheses, namely those given in (8) below, are required just in order that at least one of the conditions (7) of Lemma 1 is satisfied.

**Theorem 1** Let the unperturbed Hamiltonian $H_0(p, q)$ be even in the momenta and bounded from below, and consider a perturbation $-hA(p, q)$, with $h > 0$ and $A$ even in the momenta. Suppose $A$ and $H_0$ are such that hypothesis (6) of Lemma 1 is satisfied. With $B = [A, H_0]$, suppose furthermore that the following technical conditions are satisfied:

\[
\| B^4 \|_0 < +\infty; \quad \|[B, H_0]^2\|_0 < +\infty; \quad \|[B, A]^2\|_0 < +\infty.
\]  

(8)

Then a lower bound to the relaxation time defined by (4), (5) is given by

\[
t_{\text{relax}} \geq \frac{\sqrt{2}}{\eta} + o(1), \quad \text{as } h \to 0,
\]  

(9)

where $\eta$ is such that

\[
\|[B, H_0]\|_0 \leq \eta \| B \|_0.
\]  

(10)
Remark. It may appear that some conditions are too restrictive for the Theorem to be used in the thermodynamic limit, but it turns out that such a difficulty can be overcome. For example, \( H_0 \) was required to have a finite lower bound, call it \( D \); however, the result is found not to depend on the value of \( D \). So, \( D \) can grow with the number \( N \) of degrees of freedom, without affecting the validity of the Theorem, provided \( D \) is finite for any finite \( N \). A similar way of proceeding works also as far as conditions (6) and (8) are concerned, so the Theorem holds for any system, however large it may be. This fact allows one to pass to the thermodynamic limit.

Proof of Theorem \([1]\). First of all, we notice that equation (2), which governs the time evolution of the perturbation \( \Delta \rho \), admits a unique solution in the Hilbert space \( \mathcal{L}^2_1(\mathcal{M}) \). Indeed, equation (2) is a linear inhomogeneous first-order differential equation in \( \mathcal{L}^2_1(\mathcal{M}) \) of the form

\[
\dot{x} = \hat{O} x + f ,
\]

where the operator \( \hat{O} \overset{\text{def}}{=} [H_1, \cdot] \) generates a semigroup of unitary evolution transformations (see for example \([6]\)). Thus, since the second term \( h[A, \rho_0] \) at the r.h.s. belongs to \( \mathcal{L}^2_1(\mathcal{M}) \), as will be shown below, the solution is known to exist and to be unique (see Theorem 3.3, page 104, of \([7]\)). Such a solution is given by a simple adaptation of the variation of constants formula, namely

\[
\Delta \rho(x, t) = \beta h \int_0^t ds B(\Phi^s x) \rho_0(\Phi^s x) ,
\]

where \( x \overset{\text{def}}{=} (p, q) \) denotes a point of phase space \( \mathcal{M} \), and \( \Phi^t \) the flow generated by \( H_1 \). Notice that, as the initial datum vanishes, one obviously has \( \hat{O} \Delta \rho(0) \in \mathcal{L}^2_1(\mathcal{M}) \).

We show now that \([A, \rho_0] \in \mathcal{L}^2_1(\mathcal{M}) \), too. To this end, we first notice that

\[
\|[A, \rho_0]\|_1 = \|B \rho_0\|_1 \leq \frac{e^{\beta D}}{Z_0} \|B\|_1 ,
\]

where \( D \overset{\text{def}}{=} \inf_{p,q} H_0 \). On the other hand, iterating the Schwarz inequality gives

\[
\|B\|_0 \leq \left(\|B^2\|_0\right)^{\frac{1}{2}} \leq \left(\|B^4\|_0\right)^{\frac{1}{4}} < +\infty ,
\]

in which the first hypothesis of (8) was used\(^1\). In virtue of such an hypothesis, 

\(^1\)According to the same reasoning, the square of the norm of a function will be bounded from above by the norm of the squared function.
we can also apply Lemma 1 to $B$ and observe that, for $h$ small enough, $\|B\|_1$ is finite. Thus, by (12) it is proved that $[A, \rho_0]$ belongs to $L_2^1(M)$.

We now look at the expectation $\overline{B}(t)$ and at its increment $\Delta \overline{B}(t)$. By using (11) for $\Delta \rho$ in (3), one finds for $\Delta \overline{B}(t)$ the expression

$$
\Delta \overline{B}(t) = \beta h \int_M \int_0^t ds \, B(\Phi^s x) \, B(x) \rho_0(\Phi^s x) .
$$

(13)

Using the shorthand $f(x_t) = f(\Phi^{-t} x)$, one has then:

$$
\frac{d}{dt} \Delta \overline{B}(t) = \beta h \int_M d\mathbf{x} \, B(x_t) \, B(x) \rho_0(x_t) ,
$$

or equivalently (due to preservation of Lebesgue measure),

$$
\frac{d}{dt} \Delta \overline{B}(t) = \beta h \int_M d\mathbf{x} \, B(x_t) \, B(x) \rho_0(x) .
$$

(14)

At this point we remark that the integral in (14) could be evaluated in a quite simple way, if there appeared $\rho_1$ in place of $\rho_0$. Indeed, due to the unitarity of the flow, for any $f$ in $L_2^1(M)$ one would have

$$
\int_M \int_0^t ds \, B(\Phi^s x) \, B(x) \rho_1(x) = \|f\|_1^2 - \frac{1}{2} \|f(x_t) - f(x)\|_1^2 ,
$$

(15)

and thus, on account of hypothesis (10) of the Theorem, the thesis would follow by using Theorem 1 of [4] (see below).

The rest of the proof is devoted to show that the error made by taking $\rho_0$ in place of $\rho_1$ is negligible in the limit $h \to 0$. To this end, we suitably rewrite (14) in the form

$$
\frac{d}{dt} \Delta \overline{B}(t) = \beta h \left[ \int_M d\mathbf{x} \, B(x_t) \, B(x) \rho_1(x) - \int_M d\mathbf{x} \, B(x_t) \, B(x) \rho_0(x) \right] \\
\geq \beta h \left[ \int_M d\mathbf{x} \, B(x_t) \, B(x) \rho_1(x) - \int_M d\mathbf{x} \, B(x_t) \, B(x) \left( \rho_1(x) - \rho_0(x) \right) \right] .
$$

(16)

First, we show that the second term at the r.h.s. vanishes as $h \to 0$. Indeed, by Schwarz’s inequality we have

$$
\left| \int_M d\mathbf{x} \, B(x_t) \, B(x) \left( \rho_1(x) - \rho_0(x) \right) \right| \leq \left[ \int_M d\mathbf{x} \, (B^2(x_t)) B^2(x) \rho_1(x) \right]^\frac{1}{2} \sqrt{\bar{\gamma}(h)} ,
$$

(17)
where we have defined
\[ \tilde{\gamma}(h) \overset{\text{def}}{=} \int_{M} dx \left( \frac{\rho_0(x)}{\rho_1(x)} - 1 \right)^2 \rho_1(x). \]

This function coincides with the one defined by (34) in Appendix A. As there shown, \( \tilde{\gamma}(h) \to 0 \) as \( h \to 0 \). We then make use of (15), by replacing \( B^2 \) for \( f \) and neglecting the negative term, to find an upper bound to the r.h.s. of (17): one has, in fact,
\[ \left[ \int_{M} dx \left( B^2(x_t)B^2(x) \right) \rho_1(x) \right]^{\frac{1}{2}} \leq \| B^2 \|_1. \]

In order to show that \( \| B^2 \|_1 \) is finite, we use Lemma 1, whose hypotheses are satisfied owing to the first inequality of (8). Thus, as \( \tilde{\gamma}(h) \to 0 \) for \( h \to 0 \), one gets
\[ \left| \int_{M} dx B(x_t)B(x) \left( \rho_1(x) - \rho_0(x) \right) \right| = o(1) \quad \text{as} \quad h \to 0. \quad (18) \]

We then come to the first term at the r.h.s. of (16), which, using (15) again, can be estimated as
\[ \int_{M} dx B(x_t)B(x) \rho_1(x) = \| B \|_1^2 - \frac{1}{2} \| B(x_t) - B(x) \|_1^2. \quad (19) \]

We now make use of Theorem 1 of [4], which ensures that, if
\[ \|[B, H_1]\|_1 \leq \tilde{\eta} \| B \|_1 \]
is satisfied, then one has
\[ \| B(x_t) - B(x) \|_1 \leq \tilde{\eta} t \| B \|_1. \quad (20) \]

Now, to give an estimate for \( \tilde{\eta} \), we notice that the following inequalities hold as \( h \to 0 \):
\[
\|[B, H_1]\|_1 \leq \|[B, H_0]\|_1 + h \|[B, A]\|_1 \\
\leq \left( \|[B, H_0]\|_0^2 + o(1) \right)^{\frac{1}{2}} \\
+ h \left( \|[B, A]\|_0^2 + o(1) \right)^{\frac{1}{2}}.
\]
Here, in the first line the triangle inequality was used, while the second line is a consequence of Lemma [1], the hypotheses of which are satisfied in virtue of the second and the third inequalities in (8). Hence, by hypothesis (10) we obtain

$$\| [B, H_1] \|_1 \leq \| [B, H_0] \|_0 + o(1) \| B \|_1$$

$$\leq \eta \| B \|_0 + o(1) \| B \|_1$$

$$\leq (\eta + o(1)) \| B \|_1$$ \hspace{1cm} (21)

so that $\tilde{\eta} = \eta + o(1)$.

Eventually, by replacing in (16) the estimates (18) and (19), one has

$$\frac{d}{dt} \Delta \overline{B}(t) \geq \beta h \left( 1 - \frac{\eta^2 t^2}{2} - o(1) - o(1) \cdot t^2 \right) \| B \|_1^2$$ \hspace{1cm} (22)

Therefore, in the limit as $h \to 0$, the time derivative of $\Delta \overline{B}(t)$ remains positive for

$$t < \frac{\sqrt{2}}{\eta} + o(1)$$

and this completes the proof.

Q.E.D.

3 A gas in a gravitational field

We study now a gas of $N$ non–interacting particles enclosed in a tridimensional box of side $L$. A comment on the possible extension to the case of interacting particles will be made later. Our aim is to show that Theorem 1 holds if we take as a simple example of a perturbation the force of gravity, in which case the conjugated variable will be the vertical component of the total momentum of the system.

For what concerns the interaction of the particles with the walls, due to the form of the conjugated variable it turns out that only the interaction with the horizontal walls will matter. Thus we limit ourselves to choose a particular form for the interaction potential with the horizontal walls. The unperturbed Hamiltonian $H_0$ is then

$$H_0 \overset{\text{def}}{=} \sum_{j=1}^{N} \frac{P_j^2}{2} + \sum_{j=1}^{N} \tilde{V}(z_j)$$ \hspace{1cm} (23)
where \( p_j^\alpha \in (-\infty, +\infty) \), \( q_j^\alpha \in (-L/2, L/2) \), \( \alpha = 1, 2, 3 \), \( q_j^3 = z_t \) and \( \bar{V} \) denotes the interaction potential with the horizontal walls, which we take as the repulsive part of the Lennard–Jones potential, namely as

\[
\bar{V}(z) \overset{\text{def}}{=} \delta \left[ \left( \frac{1}{z + \frac{L}{2}} \right)^{12} + \left( \frac{1}{z - \frac{L}{2}} \right)^{12} \right],
\]

where \( \delta \) is a positive parameter. According to the general scheme previously discussed, we add at time \( t = 0 \) a perturbation \( -h A \), and for the observable \( A \) we make the choice

\[
A \overset{\text{def}}{=} \sum_{j=1}^N z_j.
\]

We then have

**Theorem 2.** Let \( H_0 \) and \( A \) be given by (23) and (25) respectively. Let the parameters \( \delta \) and \( L \) in (23) be such that \( (\beta \delta)^{\frac{1}{12}} < L/3 \), where \( \beta \) is inverse temperature. Then, as \( h \to 0 \) for the relaxation time one has the estimate

\[
t_{\text{relax}} \geq t_0,
\]

with

\[
t_0 = \frac{1}{c} (\beta \delta)^{\frac{1}{12}} \sqrt{L \beta},
\]

and

\[
c \overset{\text{def}}{=} 24 \left( \int_0^{+\infty} u^{\frac{14}{13}} e^{-u} du \right)^{\frac{1}{2}} \approx 25.
\]

**Remark 1.** By inserting the proper dimension, condition \( (\beta \delta)^{\frac{1}{12}} < L/3 \) turns into \( (\beta \delta)^{\frac{1}{12}} \sigma < L/3 \), where \( \sigma \) is the characteristic parameter for the range of the Lennard-Jones potential. This just expresses the requirement that the interactions with the walls have a range which is negligible with respect to \( L \). Notice that we inserted the factor \( 1/3 \) at the r.h.s. just in order to fix a numerical value for \( c \), but any other reasonable choice would not affect the result.

**Remark 2.** The time \( t_0 \), once the correct dimensional constants have been introduced, becomes

\[
t_0 = \frac{1}{c} (\beta \delta)^{\frac{1}{12}} \sqrt{\beta m L \sigma},
\]

where \( m \) is the mass (of molecular order) of each particle. Therefore, for macroscopic systems in which \( L \) is of the order of magnitude of \( 1 \) \( m \), while
\( \sigma \approx 10^{-10} \text{ m} \), at room temperature, one gets \( t_0 \approx 10^{-8} \text{ s} \), a value which is of the order of magnitude of the typical relaxation times measured in gases. Further comments will be given in the next Section.

**Proof.** The proof consists in showing that the hypotheses of Theorem 1 hold, with

\[
\eta = \frac{\sqrt{2} c}{(\beta \delta)^{\frac{1}{2}} \sqrt{L \beta}}.
\]

In the first place, (6) is satisfied for any \( \delta \), because it involves integrals of continuous functions over a compact, and the integral over the \( p \) coordinates is equal to 1.

As far as the other hypotheses are concerned, we first notice that in the present case one has

\[
B = \sum_j p_j^z.
\]

The integral over the momenta of any power of \( B \) can be easily turned into a combination of terms of the form

\[
\int_{-\infty}^{+\infty} dp \, p^n e^{-\beta p^2},
\]

which are finite for any \( n \), thus proving the first of (8). In particular, one has

\[
\| B \|_0 = \sqrt{\frac{2N}{\beta}}.
\]

Clearly, one also has

\[
[B, A] = N,
\]

and hence the third of (8) holds. We then compute \( \| [B, H_0] \|_0 \). One has

\[
[B, H_0] = 12 \delta \sum_{j=1}^{N} \left[ \left( \frac{1}{z_j + \frac{L}{2}} \right)^{13} + \left( \frac{1}{z_j - \frac{L}{2}} \right)^{13} \right].
\]

This function, and its powers too, are actually singular at some point in phase space, but they diverge there as a power, while the density \( \rho_0 \) vanishes as an exponential, making the norm finite. So the second of (8) is proved, as well.
There finally remains the task of providing an estimate for the quantity $\eta$, which is an upper bound for the ratio $\| [B, H_0]_0 / \| B \|_0$. To this end, from (29) we get that $[B, H_0]^2$ is equal to

$$144\delta^2 \sum_{j,l} \left[ \left( \frac{1}{z_j + \frac{L}{2}} \right)^{13} + \left( \frac{1}{z_j - \frac{L}{2}} \right)^{13} \right] \left[ \left( \frac{1}{z_l + \frac{L}{2}} \right)^{13} + \left( \frac{1}{z_l - \frac{L}{2}} \right)^{13} \right],$$

and we have to estimate its $\rho_0$ norm. Now, all terms with $j \neq l$ have vanishing integral, because they are products of independent quantities with vanishing expectations (being odd functions of $z$, while the density is even). So, there remain only the $N$ terms in which $j = l$. Each of them contributes to the sum as

$$\frac{144\delta^2}{\tilde{Z}} \int_{-\frac{L}{2}}^{\frac{L}{2}} dz \left[ \left( \frac{1}{z + \frac{L}{2}} \right)^{26} + \left( \frac{1}{z - \frac{L}{2}} \right)^{26} + \frac{1}{(z + \frac{L}{2})^{13}(z - \frac{L}{2})^{13}} \right] e^{-\beta\delta \tilde{V}(z)}, \quad (30)$$

in which

$$\tilde{Z} = \int_{-\frac{L}{2}}^{\frac{L}{2}} dz e^{-\beta\delta \tilde{V}(z)}.$$

This integral cannot be computed in a closed form, so we give here an estimate: numerical computations show that $\tilde{Z}$ is larger than $L/4$ if $(\beta \delta)^{\frac{1}{12}} < L/3$. In the integral (30), the third term is always negative, while the two other ones are identical, due to symmetry. An upper bound to each of them is given by

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} dz \left( \frac{1}{z + \frac{L}{2}} \right)^{26} e^{-\beta\delta \tilde{V}(z)} \leq \int_0^L dz \frac{1}{z^{26}} \exp \left( -\frac{\beta \delta z^{12}}{z^{12}} \right) \leq \frac{1}{(\beta \delta)^{\frac{1}{12}}} \int_0^{+\infty} u^{\frac{13}{12}} e^{-u} du.$$

A quick comparison with (28) then leads to

$$\|[B, H_0]_0\|_0 \leq \frac{\sqrt{2} c}{(\beta \delta)^{\frac{1}{12}} \sqrt{L \beta}} \| B \|_0 , \quad (31)$$

with $c$ defined in (27).

This relation, on account of Theorem 1, leads to formula (26).

Q.E.D.
4 Conclusions

We have provided by Theorem 1 a lower bound to the relaxation times in Hamiltonian systems, and shown that in the case of a non–interacting gas enclosed in a box such an estimate is of the order of magnitude of the typical relaxation times measured in gases.

Obviously, the interesting case to be studied would be that of a gas of interacting particles. At the moment, we are unable to provide rigorous estimates for such a case, so we decided to limit ourselves to the non–interacting case, and we leave for future work the interacting case. The following comment is however in order. If two–body internal forces were present, it is easily seen that their contribution to $[B, H_0]$ (and to $B$ itself) would vanish. The only difference would concern the estimate of the norm of the expression (29) for $[B, H_0]$, but a heuristic argument indicates that, for sufficiently low densities, the difference with respect to the non–interacting case would be small. This argument becomes a rigorous theorem (see [8]) in the thermodynamic limit, for forces due to stable and temperate two–body potentials. So, in order to give such an estimate for finite $N$ and compute the integrals, we would need at least an estimate of the convergence rate of the Mayer–Montroll equation, in the canonical ensemble, which is not known to us. On the other hand, this fact seems to indicate that the interactions with the walls, which we have considered in the present work, might have sensible effects even when one is interested in investigating relaxations of observables related to internal interactions.

We now add some comments concerning possible further developments.

The first point concerns the hypothesis made in Theorem 1, that $H_0$ and $A$ are even in the momenta, which actually is not at all essential. Indeed, if such an hypothesis is not satisfied, it suffices to define $t_{\text{relax}}$ in a different way, namely, as the time up to which the time–derivative of $\Delta B$ remains larger than, for example, $\frac{1}{2} \frac{d}{dt} \Delta B(0)$. This way, by inequality (22) one could prove Theorem 1 except for setting $1/\eta$ in place of $\sqrt{2}/\eta$ in (9). We decided to deal with the case of reversible Hamiltonians just because it is a very important one; furthermore, in such a case the relaxation time can be defined with no reference to arbitrary features, as the factor $1/2$ introduced above.

As a more interesting fact, we are confident that our line of reasoning may be extended to the case of perturbations of a finite size $h$, because this would just entail to consider the norms in $L^1(M)$ rather than in $L^2(M)$. Indeed, if we substitute $[B, H_1]$ for $[B, H_0]$ in hypothesis (11) and use there
the norm \( \| \cdot \|_1 \) instead of \( \| \cdot \|_0 \), we can directly set \( \tilde{\eta} = \eta \) in (20) and there is no need of deducing (21), so that the second and third conditions in (8) are no more required. Moreover, the first condition in (8) can be replaced by the condition that \( \| B^2 \|_1 \) is finite, which makes trivial the proof that \([A, H_0]\) is in \( L^2_1(\mathcal{M}) \).

The really open problem that remains in order to implement an extension to the case of finite \( h \), at least for macroscopic systems, is the estimate of the difference of the two norms in (17). The estimate which appears in such a formula has the serious flaw of increasing exponentially with the number \( N \) of particles. This occurs because the upper bound provided there, which is an immediate consequence of Schwarz inequality, is valid for all functions in \( L^2 \). A way to improve such an estimate would be to restrict oneself to perturbations having some suitable characteristic feature.

In particular, the work [9] of Lanford seems to suggest a good starting point. There it is pointed out that the only observables of interest in describing a macroscopic system are the ones he calls finite range observables\(^2\), namely, observables which are sums of terms depending only on the position of a finite number of particles. The difference of the two norms in question can then be evaluated for each term and this should lead to an estimate which doesn’t increase too much with \( N \). We think that, if one limits oneself to considering a smaller class of functions, there is good chance that the problem of the number of degrees of freedom is overcome, and that some results are obtained also for the case of perturbations of finite size. These interesting investigations are left for possible future works.

\section{Appendix}

\textbf{Proof of Lemma 1.} We take as starting point the obvious equality

\[ \int_{\mathcal{M}} dp \, dq \, f^2 \rho_1 = \int_{\mathcal{M}} dp \, dq \, f^2 \rho_0 + \int_{\mathcal{M}} dp \, dq \, f^2 (\rho_1 - \rho_0) \]

which, by Schwarz inequality, gives

\[ \left| \int_{\mathcal{M}} dp \, dq \, f^2 (\rho_1 - \rho_0) \right| \leq \left( \int_{\mathcal{M}} dp \, dq \, f^4 \rho_0 \right)^{\frac{1}{2}} \sqrt{\gamma(h)} , \quad (32) \]

\(^2\)As a matter of fact, he explains that this definition is chosen to make things simpler and is too restrictive. He gives also a reference to Ruelle’s book [5] in which it is shown how to deal with a broader class of observables, which represents the class of real interest.
with
\[ \gamma(h) \overset{\text{def}}{=} \int_{\mathcal{M}} dp \, dq \left( \frac{\rho_1}{\rho_0} - 1 \right)^2 \rho_0. \]

One can also write
\[ \gamma(h) = \frac{\int_{\mathcal{M}} dp \, dq \, e^{2h\beta A} \rho_0}{\left( \int_{\mathcal{M}} dp \, dq \, e^{h\beta A} \rho_0 \right)^2} - 1, \quad (33) \]
as is seen by expanding the square and using the fact that \( \rho_0 \) and \( \rho_1 \) are the densities of the Gibbs measures corresponding to \( H_0 \) and \( H_1 \), respectively. It is also of interest to provide an upper bound to the l.h.s. of (32) in terms of \( \rho_1 \) rather than of \( \rho_0 \). Indeed, one has
\[ \left| \int_{\mathcal{M}} dp \, dq \, f^2 (\rho_1 - \rho_0) \right| \leq \left( \int_{\mathcal{M}} dp \, dq \, f^4 \rho_1 \right)^{\frac{1}{2}} \sqrt{\gamma(h)}, \]
where, in a way similar to (33), one gets
\[ \tilde{\gamma}(h) \overset{\text{def}}{=} \int_{\mathcal{M}} dp \, dq \left( \frac{\rho_0}{\rho_1} - 1 \right)^2 \rho_1 = \left( \int_{\mathcal{M}} dp \, dq \, e^{h\beta A} \rho_0 \right) \left( \int_{\mathcal{M}} dp \, dq \, e^{-h\beta A} \rho_0 \right) - 1. \]

Now, we observe that the functions \( \gamma(h) \) and \( \tilde{\gamma}(h) \) can take arbitrarily small values as \( h \) goes to 0, if (6) is satisfied. Indeed, by their definitions, they are always non-negative quantities. Thus, in order to show, for example, that \( \gamma(h) < \varepsilon \) for any fixed positive \( \varepsilon \), it will suffice that one has
\[ \frac{\int_{\mathcal{M}} dp \, dq \, e^{2h\beta A} \rho_0}{\left( \int_{\mathcal{M}} dp \, dq \, e^{h\beta A} \rho_0 \right)^2} < 1 + \varepsilon. \]

To this end, let us note that
\[ \frac{1}{\int_{\mathcal{M}} dp \, dq \, e^{h\beta A} \rho_0} \leq \int_{\mathcal{M}} dp \, dq \, e^{-h\beta A}, \]
according to Schwarz inequality. We combine this estimate with the Hölder inequality, on whose account, if \( h < \frac{\delta}{c\beta} \), one has
\[ \int_{\mathcal{M}} dp \, dq \, e^{\pm h\beta A} \rho_0 \leq \left( \int_{\mathcal{M}} dp \, dq \, e^{\pm \delta A} \rho_0 \right)^{\frac{c\beta}{\delta}} \left( \int_{\mathcal{M}} dp \, dq \, \rho_0 \right)^{\left(1 - \frac{c\beta}{\delta} \right)} \leq K^{\frac{c\beta}{\delta}}, \quad (34) \]
and we eventually obtain
\[
\frac{\int_{\mathcal{M}} dp \, dq \, e^{2h\beta A} \rho_0}{\left( \int_{\mathcal{M}} dp \, dq \, e^{h\beta A} \rho_0 \right)^2} \leq \left( \int_{\mathcal{M}} dp \, dq \, e^{2h\beta A} \rho_0 \right) \left( \int_{\mathcal{M}} dp \, dq \, e^{-h\beta A} \rho_0 \right)^2 \leq K \frac{\delta h}{\delta} \to 1 \quad \text{as} \quad h \to 0.
\]

The immediate consequence is that, if we take \( h < \min \left( \frac{\delta}{2\beta}, \frac{\delta \log(1+\varepsilon)}{4\beta \log K} \right) \), then \( \gamma(h) \) is less than \( \varepsilon \). An analogous argument, still based on inequality (34), ensures that \( \tilde{\gamma}(h) \) takes arbitrarily small values as \( h \) goes to 0, too. Hence, the difference between \( \|f\|_0^2 \) and \( \|f\|_1^2 \) vanishes with \( h \), provided \( f^2 \) belongs to \( L^2_0(\mathcal{M}) \) or \( L^2_1(\mathcal{M}) \).

Q.E.D

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