

ON THE TIME AND CELL DEPENDENCE OF THE COARSE-GRAINED ENTROPY. II

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We present calculations of the coarse-grained entropy $S_{cg}(t)$ for the model of a classical point particle enclosed in a two-dimensional box with perfectly reflecting walls. We find in comparison with the one-dimensional case that the fluctuations of $S_{cg}(t)$ and of the expectation values of the position have decreased, and that $S_{cg}(t)$ does not take its asymptotic value at regular time intervals. The times after which $S_{cg}(t)$ and the expectation values have approximately reached their equilibrium values, are about equal; recurrence times are rather clearly separated from this time. Finally, we give a general estimate on the change of an expectation value due to a refinement of the cells.

1. Introduction

In a previous paper¹⁾ (referred to as I), we have discussed properties of the coarse-grained entropy in general, and we have calculated the coarse-grained entropy $S_{cg}(t)$ for a simple model system, namely a classical free particle in a one-dimensional box with perfectly reflecting walls ("PIB-1 model"). Initially, the particle is confined to a certain part of the box; this constraint is released at $t = 0$. The main results of those model calculations were:

- a) $S_{cg}(t)$ approaches its new equilibrium value nonmonotonically;
- b) $S_{cg}(t)$ depends on the number of cells very weakly from remarkably few cells on;
- c) $S_{cg}(t)$ approaches its equilibrium value faster (essentially $\sim 1/t^2$) than the expectation value of the position of the particle $\langle q \rangle(t)$ (essentially $\sim 1/t$);
- d) The stability region where the expected relaxation time¹⁾ $\langle \tau_{rel} \rangle$ is fairly stable against an increase of the number of cells, is very small, since the fluctuations of $\langle q \rangle(t)$ around the new equilibrium value are large.

The limitations of the PIB-1 model are evident: firstly the low number of dimensions of phase space Γ ($\dim. \Gamma = 2$), and secondly the highly singular interaction with the walls of the box (perfect reflection). The first defect seems even more

serious, since for one particle in one dimension, one cannot expect a clear distinction between a recurrence time and an (expected) relaxation time. A separation of these two time scales is highly desirable, however, since within which time $S_{cg}(t)$ reaches approximately its new equilibrium value, is an important question.

In this paper, we shall therefore present calculations of $S_{cg}(t)$ for a particle in a two-dimensional box with perfectly reflecting walls ("PIB-2 model"). As we shall see, some of the unpleasant properties of the one-dimensional case will be absent in the two-dimensional model. In section 2, we shall solve the Liouville equation for the model, and calculate various quantities. We shall present the results in section 3; furthermore, estimates on the change of an expectation value due to subpartitions of the phase cells will be given. The paper closes in section 4 with a discussion and summary.

2. The model

The system consists of one classical free point particle of mass m enclosed in a two-dimensional rectangular box with perfectly reflecting walls of length L and αL , $0 < \alpha \leq 1$. We describe the particle in an energy "shell" Σ , consisting of all points $(q_1, q_2, p_1, p_2) \in \mathcal{R}^4$ with

$$0 \leq q_1 \leq L, \quad 0 \leq q_2 \leq \alpha L, \quad (p_1^2 + p_2^2)/2m \leq E, \tag{2.1}$$

where E is the maximum energy of the particle. With the invariant measure $d\mu = dq_1 dq_2 dp_1 dp_2$ we have

$$\mu(\Sigma) = 2\pi m E \alpha L^2. \tag{2.2}$$

For $t \leq 0$, we shall have an equilibrium state where the particle has arbitrary energy between zero and E , and is confined to that part of the box with $0 \leq q_1 \leq q_1^{\max}$ and $0 \leq q_2 \leq q_2^{\max}$, where $0 < q_1^{\max} < L$ and $0 < q_2^{\max} < \alpha L$. We thus get for the distribution function

$$\varrho(q_1, q_2, p_1, p_2; t \leq 0) = \begin{cases} (2\pi m E q_1^{\max} q_2^{\max})^{-1} & \text{for } 0 \leq q_1 \leq q_1^{\max} \text{ and } 0 \leq q_2 \leq q_2^{\max} \\ 0 & \text{elsewhere} \end{cases} \tag{2.3}$$

which has been normalized to unity. Imposing reflecting boundary conditions for $t \geq 0$ we obtain as initial condition

$$\begin{aligned} \varrho(q_1, q_2, p_1, p_2; t = 0) &= c_1 \sum_{i_1 \in \mathcal{Z}} \theta(q_1 + q_1^{\max} - 2i_1 L) \theta(q_1^{\max} + 2i_1 L - q_1) \\ &\times \sum_{i_2 \in \mathcal{Z}} \theta(q_2 + q_2^{\max} - 2i_2 \alpha L) \theta(q_2^{\max} + 2i_2 \alpha L - q_2) \end{aligned} \tag{2.4}$$

with

$$c_1 = (2\pi m E q_1^{\max} q_2^{\max})^{-1}. \quad (2.5)$$

Since the hamiltonian consists only of the kinetic part, we get the solution of the Liouville equation for $t \geq 0$ with the initial condition (2.4) by replacing q_i by $q_i - p_i t/m$ in (2.4)². This yields

$$\begin{aligned} \varrho(q_1, q_2, p_1, p_2; t) &= c_1 \sum_{i_1 \in \mathcal{Z}} \theta(q_1/L - p_1 t/mL + q_1^{\max}/L - 2i_1) \\ &\quad \times \theta(q_1^{\max}/L + 2i_1 - q_1/L + p_1 t/mL) \\ &\quad \times \sum_{i_2 \in \mathcal{Z}} \theta(q_2/\alpha L - p_2 t/m\alpha L + q_2^{\max}/\alpha L - 2i_2) \\ &\quad \times \theta(q_2^{\max}/\alpha L + 2i_2 - q_2/\alpha L + p_2 t/m\alpha L). \end{aligned} \quad (2.6)$$

As in PIB-1, ϱ converges weakly³) to the microcanonical distribution function in Σ , that is

$$\varrho_{\text{eq}} = (4\alpha L^2)^{-1} \int_0^L dq_1 \int_0^{\alpha L} dq_2 \varrho(q_1, q_2, p_1, p_2; 0) = [\mu(\Sigma)]^{-1}. \quad (2.7)$$

The two assumptions about ϱ in paper I, section 2, are therefore fulfilled for the model.

As in I, we take as a macroscopic quantity the position of the particle, thus we have

$$A_1(q_1, q_2, p_1, p_2) = q_1 \quad \text{and} \quad A_2(q_1, q_2, p_1, p_2) = q_2. \quad (2.8)$$

The corresponding accuracies will be L/j_1^{\max} for A_1 and $\alpha L/j_2^{\max}$ for A_2 , respectively. This yields the cells⁴)

$$\begin{aligned} \Omega_{j_1 j_2} &= \{(q_1, q_2, p_1, p_2) \in \Sigma \mid (j_1 - 1)L/j_1^{\max} \leq q_1 \leq j_1 L/j_1^{\max} \\ &\quad \text{and} \quad (j_2 - 1)\alpha L/j_2^{\max} \leq q_2 \leq j_2 \alpha L/j_2^{\max}\}, \\ 1 &\leq j_1 \leq j_1^{\max}, \quad 1 \leq j_2 \leq j_2^{\max}. \end{aligned} \quad (2.9)$$

Obviously, we have cells of equal volume

$$\mu(\Omega_{j_1 j_2}) = \mu(\Sigma) / (j_1^{\max} j_2^{\max}). \quad (2.10)$$

For the calculation of the coarse-grained distribution function, we introduce the following dimensionless quantities

$$x_1 := q_1/L, \quad x_1^{\max} := q_1^{\max}/L, \tag{2.11a}$$

$$x_2 := q_2/(\alpha L), \quad x_2^{\max} := q_2^{\max}/(\alpha L), \tag{2.11b}$$

$$y_1 := p_1 t/(mL), \tag{2.11c}$$

$$y_2 := p_2 t/(m\alpha L). \tag{2.11d}$$

This yields

$$d\mu = \alpha^2 L^4 m^2 / t^2 dx_1 dx_2 dy_1 dy_2. \tag{2.12}$$

With the abbreviations

$$c_2(t) := \alpha^2 L^4 m^2 c_1 / t^2 \tag{2.13}$$

and

$$R_t := t (2E/m)^{1/2} / L \tag{2.14}$$

we get for the coarse-grained distribution function

$$\begin{aligned} P_{j_1 j_2}(t) &:= (\mu(\Omega_{j_1 j_2}))^{-1} \int_{\Omega_{j_1 j_2}} \varrho(q_1, q_2, p_1, p_2; t) d\mu \\ &= (\mu(\Omega_{j_1 j_2}))^{-1} c_2(t) \sum_{i_1 \in \mathcal{I}} \sum_{i_2 \in \mathcal{I}} \\ &\int_{(j_1-1)/j_1}^{j_1/j_1} dx_1 \int_{-R_t}^{R_t} dy_1 \theta(x_1 - y_1 + x_1^{\max} - 2i_1) \theta(x_1^{\max} + 2i_1 - x_1 + y_1) \\ &\times \int_{(j_2-1)/j_2}^{j_2/j_2} dx_2 \int_{-(R_t^2 - y_1^2)^{1/2}/\alpha}^{(R_t^2 - y_1^2)^{1/2}/\alpha} dy_2 \theta(x_2 - y_2 + x_2^{\max} - 2i_2) \\ &\times \theta(x_2^{\max} + 2i_2 - x_2 + y_2). \end{aligned} \tag{2.15}$$

The second double integral in (2.15) is a function of y_1 alone, as far as the integration variables are concerned. We thus define

$$\begin{aligned} f(y_1) &:= \int_{(j_2-1)/j_2}^{j_2/j_2} dx_2 \int_{-(R_t^2 - y_1^2)^{1/2}/\alpha}^{(R_t^2 - y_1^2)^{1/2}/\alpha} dy_2 \theta(x_2 - y_2 + x_2^{\max} - 2i_2) \\ &\times \theta(x_2^{\max} + 2i_2 - x_2 + y_2). \end{aligned} \tag{2.16}$$

$f(y_1)$ may be calculated exactly, since it is just the area of the intersection of the rectangle defined by the integration boundaries with the strip defined by the θ -functions in the x_2 - y_2 plane. The remaining two integrations in (2.15) then integrate $f(y_1)$ over an area of the same structure as that in (2.16) in the x_1 - y_1 plane. Since f does not depend on x_1 we may write for (2.15)

$$P_{j_1 j_2}(t) = [\mu(\Omega_{j_1 j_2})]^{-1} c_2(t) \sum_{i_1 \in \mathcal{Z}} \sum_{i_2 \in \mathcal{Z}} \int_{-R_t}^{R_t} h(y_1) f(y_1) dy_1, \quad (2.17)$$

where $h(y_1)$ measures the extension of the integration domain in x_1 -direction and may be calculated exactly. We have thus reduced the four-dimensional integration in (2.15) to a one-dimensional one which must be done numerically.

Finally, we note that the sums in (2.15) [and (2.17)] consist only of a finite number of terms. One may show that only those terms contribute inside Σ for which the following inequalities hold:

$$-(x_1^{\max} + R_t) < 2i_1 < (1 + x_1^{\max} + R_t) \quad (2.18)$$

and

$$-(x_2^{\max} + R_t/\alpha) < 2i_2 < (1 + x_2^{\max} + R_t/\alpha). \quad (2.19)$$

Having calculated the $P_{j_1 j_2}(t)$ we get for the coarse-grained entropy

$$S_{\text{cg}}(t) = -k \sum_{j_1=1}^{j_1^{\max}} \sum_{j_2=1}^{j_2^{\max}} \mu(\Omega_{j_1 j_2}) P_{j_1 j_2}(t) \ln P_{j_1 j_2}(t) \quad (2.20)$$

according to formula (I.3.9). Following the definition of the expectation value (I.3.8) we calculate

$$\int_{\Omega_{j_1 j_2}} q_1 d\mu = 2\pi m E \alpha L^3 (j_1 - 0.5) / ((j_1^{\max})^2 j_2^{\max}) \quad (2.21)$$

and

$$\int_{\Omega_{j_1 j_2}} q_2 d\mu = 2\pi m E \alpha^2 L^3 (j_2 - 0.5) / (j_1^{\max} (j_2^{\max})^2) \quad (2.22)$$

to be inserted into the formula

$$\langle q_i \rangle (t) = \sum_{j_1=1}^{j_1^{\max}} \sum_{j_2=1}^{j_2^{\max}} P_{j_1 j_2}(t) \int_{\Omega_{j_1 j_2}} q_i d\mu, \quad i = 1, 2. \quad (2.23)$$

Now we calculate $P^{(\infty)}(q_1, q_2; t)$ according to (I.4.28). With the substitutions (2.11) we obtain

$$\begin{aligned}
 P^{(\infty)}(q_1, q_2; t) &= (4\pi^2 E^2 x_1^{\max} x_2^{\max} t^2)^{-1} \sum_{i_1 \in \mathcal{I}} \sum_{i_2 \in \mathcal{I}} \\
 &\int_{-R_t}^{R_t} dy_1 \theta(y_1 - x_1 + x_1^{\max} + 2i_1) \theta(x_1 + x_1^{\max} - 2i_1 - y_1) \\
 &\int_{-(R_t^2 - y_1^2)^{1/2}/\alpha}^{(R_t^2 - y_1^2)^{1/2}/\alpha} dy_2 \theta(y_2 - x_2 + x_2^{\max} + 2i_2) \theta(x_2 + x_2^{\max} - 2i_2 - y_2),
 \end{aligned}$$

where the y_2 -integration can be done exactly; in the sum, only those terms contribute, for which (2.18) and (2.19) hold. Inserting the result into (I.4.30) yields $S_{cg}^{(\infty)}(t)$; the two integrations have to be done numerically.

3. Results

For the actual computation we put

$$L = 1, \quad E = 1, \quad m = 2; \tag{3.1}$$

this normalizes the time scale so that it takes the particle with maximum momentum $(2mE)^{\frac{1}{2}}$ the unit time to pass the distance L . The accuracy in the numerical integration of (2.17) has been such that the deviation of the norm of P from 1 has been less than 0.7 permille. A typical result for $S_{cg}(t)$ and $S_{cg}^{(\infty)}(t)$ (with the parameters $\alpha = \frac{2}{3}$, $x_1^{\max} = \frac{1}{2}$, $x_2^{\max} = \frac{1}{2}$) is given in fig. 1; the curves are results of interpolation of calculated points of distance $\Delta t = \frac{1}{16}$.

As in the one-dimensional case the approach to the asymptotic value is non-monotonic, but due to the more complicated geometry of the energy shell, $S_{cg}(t)$ does not take its asymptotic value in the time interval $[0, 3]$. The relative height of the first fluctuation of $S_{cg}^{(\infty)}(t)$ (relative to the change of $S_{cg}^{(\infty)}(t)$ due to the change of state) is here about 1/170, whereas in PIB-1 it has been about 1/35, thus the fluctuation amplitude has decreased. The same effect is seen in the plots of $\langle q_1 \rangle(t)$ and $\langle q_2 \rangle(t)$ in fig. 2 for the same choice of parameters as in fig. 1.

The relative height of the first fluctuation has decreased from about 1/5.8 in PIB-1 to 1/9.5 in PIB-2. As seen in fig. 3, this leads to a larger region of stability of the expected relaxation time [see (I.5.23)], since it takes higher accuracy than in the one-dimensional case to detect the fluctuations.

We note here one further general property of the coarse-graining process that has not been included in I which concerns the following requirement. Suppose we change the accuracy of the measurement of a macroscopic quantity. This

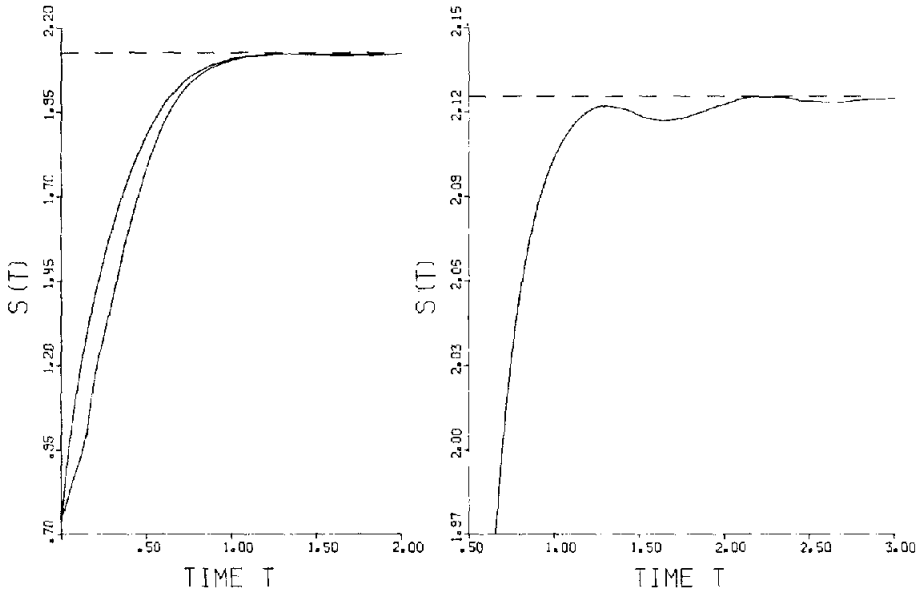


Fig. 1. The coarse-grained entropy for $j_1^{\max} = j_2^{\max} = 2$ and $j_1^{\max} = j_2^{\max} = \infty$ (below); the other parameters are $\alpha = \frac{2}{3}$, $x_1^{\max} = x_2^{\max} = \frac{1}{2}$. In b), the plot for $j_1^{\max} = j_2^{\max} = 2$ has been omitted; it would be just slightly above the given one for infinitely many cells.

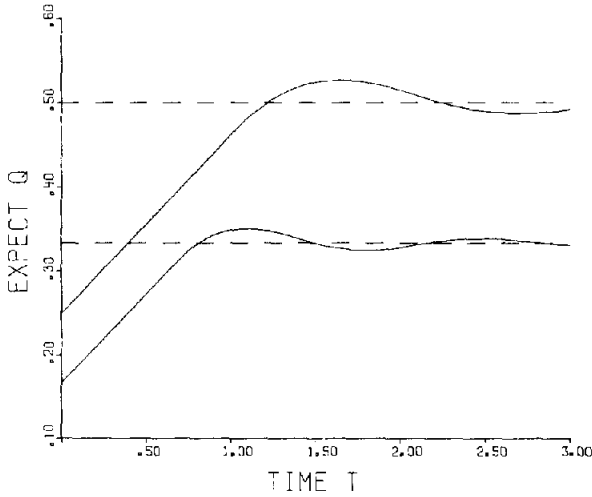


Fig. 2. The expectation values $\langle q_1 \rangle(t)$ and $\langle q_2 \rangle(t)$ (below) for $j_1^{\max} = j_2^{\max} = 2$, $\alpha = \frac{2}{3}$, $x_1^{\max} = x_2^{\max} = \frac{1}{2}$. The dashed lines represent the asymptotic values.

changes the set of phase cells, and thus the coarse-grained distribution function. One may therefore suspect that the time behavior of the expectation value of another macroscopic quantity is essentially affected by this change which should not be the case. We give now an estimate on the induced change of the expectation values.

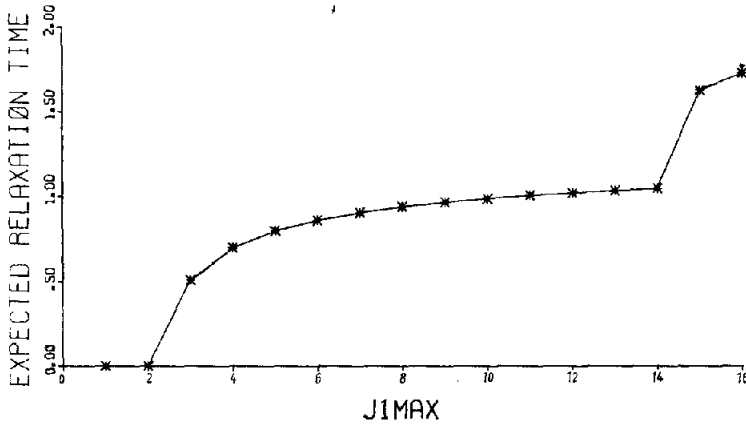


Fig. 3. Expected relaxation time $\langle \tau_{rel} \rangle$ as a function of j_1^{max} with $j_2^{max} = 2$, other parameters as before. $j_2^{max} = 3$ yields the same result, see end of section 3.

Suppose we have a subpartition $\{\Omega_j^m\}$ of $\{\Omega_j\}$ (as in section 4.5 of I), and the subpartition shall be induced by an increase of the accuracy for the measurement of an A_k^{exp} . With the original $P(x; t)$ we get

$$\langle A_i \rangle (t) := \sum_j P_j(t) \int_{\Omega_j} A_i(x) d\mu = \sum_j P_j(t) \mu(\Omega_j) A_i^{(j)}, \tag{3.2}$$

where $A_i^{(j)}$ is the mean value of $A_i(x)$ in Ω_j with

$$a_i^{(v_j)} \leq A_i^{(j)} \leq a_i^{(v_j+1)} \tag{3.3}$$

according to the definition of the cells (I.3.7). For the refined set of phase cells we get

$$\overline{\langle A_i \rangle} (t) := \sum_{j,m} P_j^m(t) \int_{\Omega_j^m} A_i(x) d\mu = \sum_{j,m} P_j^m(t) \mu(\Omega_j^m) A_i^{(jm)}. \tag{3.4}$$

Now since the Ω_j^m are subsets of Ω_j we have again

$$a_i^{(v_j)} \leq A_i^{(jm)} \leq a_i^{(v_j+1)}. \tag{3.5}$$

Putting

$$\eta_i^{jm} := A_i^{\langle j \rangle} - \overline{A_i^{\langle jm \rangle}}, \tag{3.6}$$

we get from (3.3) and (3.5)

$$|\eta_i^{jm}| \leq \max_{v_j} (a_i^{(v_j+1)} - a_i^{(v_j)}) =: \eta_i. \tag{3.7}$$

This implies

$$|\langle A_i \rangle (t) - \overline{\langle A_i \rangle} (t)| = \left| \sum_{j,m} P_j^m(t) \mu(\Omega_j^m) \eta_i^{jm} \right| \leq \eta_i, \tag{3.8}$$

where we have used (3.6), (I.4.16), the normalization of the $P_j^m(t)$ to unity, and finally (3.7). We have thus the result that the maximum change of an expectation value due to a subpartition of the original cells (introduced by higher accuracy for the same or another macroscopic quantity), is less than its maximum inaccuracy. Noticing that both estimates (3.7) and (3.8) are fairly rough we may expect an even smaller change.

For the PIB-2 model we may even show that a change of j_2^{\max} leaves $\langle q_1 \rangle (t)$ invariant (and *vice versa*) which is a consequence of the particularly simple “macroscopic” variables. Defining the coarse-grained distribution function

$$P(q_1, q_2; t) |_{(q_1, q_2) \in \Omega_{j_1 j_2}} := P_{j_1 j_2}(t) \tag{3.9}$$

which implies a correspondence of the q_i to the j_i , we have

$$\langle q_1 \rangle = \int_{\underline{z}} d\mu P(q_1, q_2; t) q_1 = 2\pi m E \int_0^L dq_1 q_1 \int_0^{\alpha L} dq_2 P(q_1, q_2; t). \tag{3.10}$$

Now we show that the function $\int_0^{\alpha L} dq_2 P(q_1, q_2, t)$ does not depend on the particular choice of j_2^{\max} . Calculating

$$\begin{aligned} \int_0^{\alpha L} P(q_1, q_2; t) dq_2 &= \sum_{j_2=1}^{j_2^{\max}} P_{j_1 j_2}(t) \alpha L / j_2^{\max} \\ &= j_1^{\max} (2\pi m E L) \sum_{j_2=1}^{j_2^{\max}} P_{j_1 j_2}(t) \mu(\Omega_{j_1 j_2}) \end{aligned} \tag{3.11}$$

according to (3.9) and (2.10), we see from (I.4.16) that the last sum in (3.11) is independent of the cell structure in q_2 direction.

4. Discussion and summary

It is instructive to summarize now the main results and differences of PIB-1 and PIB-2.

a) Both models show a very weak dependence of $S_{cg}(t)$ on the number of cells, especially after a time of the order of the expected relaxation time has elapsed.

b) In PIB-1, $S_{cg}(t)$ takes its asymptotic value at regular time intervals. This is not the case in PIB-2 (at least not in the time interval considered). Here PIB-1 should be the exception to that general behavior.

c) The fluctuations both of $S_{cg}(t)$ and of the expectation values around their asymptotic values have decreased in PIB-2 in comparison to PIB-1. This leads to a larger (approximate) plateau in a plot of $\langle \tau_{rel} \rangle$ vs. the accuracy of the measurement. We expect this trend continues for higher dimensionality of Σ .

d) Another difference between PIB-1 and PIB-2 concerns the separation of time scales. For accuracies that do not detect the fluctuations, the expected relaxation time is about unity in both models; $S_{cg}(t)$ has reached its equilibrium value after this time with even better relative accuracy than the expectation values. For a qualitative investigation of the recurrence times take a particle with maximum energy E . In PIB-1, the particle will have reached again its precise initial condition after a time $= 2$. For the particle with maximum energy E in PIB-2, however, recurrence times vary from 2α (e.g. $\alpha = \frac{2}{3}$) to infinity, depending mainly on the angle between p_1 and p_2 , and the accuracy within which the particle shall reach its initial condition again. We may therefore expect that an average recurrence time (however the averaging is done) is better separated from the expected relaxation time, than in PIB-1. It is now important to note that in both models the time after which $S_{cg}(t)$ has approximately reached its equilibrium value, is by far closer to $\langle \tau_{rel} \rangle$ than to an (average) recurrence time; because of the better separation of these times in PIB-2, the present results have more weight. Therefore, in the old controversy about the time after which $S_{cg}(t)$ has reached approximately stationary values^{5,6,7}), the assertion is supported that this time is much shorter than the recurrence time.

We may conclude that the results presented in this paper give further support to the opinion that the coarse-grained entropy is a proper microscopic expression for the entropy for both equilibrium and nonequilibrium.

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References

- 1) P. Hoyningen-Huene, *Physica* **82A** (1976) 417; a preliminary account of this work has been given in *Helv. Phys. Acta* **48** (1975) 39.
- 2) I. Prigogine, *Nonequilibrium Statistical Mechanics* (Interscience, New York, 1962).
- 3) H. Grad, *Comm. Pure Appl. Math.* **14** (1961) 323.
- 4) N.G. van Kampen, in *Fundamental Problems in Statistical Mechanics*, E.G.D.Cohen, ed. (North-Holland, Amsterdam, 1962).
- 5) P. and T.Ehrenfest, *Encykl. math. Wiss.* **IV4** (1911).
- 6) R.C.Tolman, *The Principles of Statistical Mechanics* (Oxford Univ. Press, London, 1938).
- 7) D. ter Haar, *Rev. Mod. Phys.* **27** (1955) 289.