Repeated randomness assumption and the projection operator formalism

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In this Brief Report we show explicitly how the repeated randomness assumption commonly used to derive irreversible transport equations in statistical mechanics can be put in the language of Zwanzig's projection operator technique. Some consequences of the results are also discussed. [S1063-651X(96)05406-2]

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We present the form that the repeated randomness assumption takes when cast in the language of Zwanzig's approach to nonequilibrium statistical mechanics, which is based on the projector operator technique. The randomness assumption is a basic postulate to understanding the form in which microscopic reversibility is connected with the irreversibility of the macroscopic processes. This work aims to establish a bridge between the powerful mathematical formalism of Zwanzig with the very clear physical description given by van Kampen. Thus we attempt to express van Kampen's ideas about the randomness assumption [1–3] in a simple mathematical formalism.

We consider the ensemble associated with the system under study, and denote by $N(\vec{a},t)\Delta\vec{a}$ the number of the systems that at time t are in the a cell, i.e., in the region defined by $\vec{a}\leqslant\vec{A}(\Gamma)\leqslant\vec{a}+\Delta\vec{a}$. Thus

$$N(\vec{a},t)\Delta\vec{a}=\int_{\vec{a}\leqslant A(\Gamma)\leqslant\vec{a}+\Delta\vec{a}} N\rho(\Gamma,t)d\Gamma = N\int \rho(\Gamma,t)D\left(\frac{\vec{A}(\Gamma)-\vec{a}}{\Delta\vec{a}}\right)d\Gamma, \tag{1}$$

where $D\{[\vec{A}(\Gamma)-\vec{a}]/\Delta\vec{a}\}$ is the characteristic function of the $\vec{a}$ cell. In the limit of exact measure [4,5] we have that

$$N(\vec{a},t)=N\lim_{\Delta\vec{a}\to 0}\int \rho(\Gamma,t)\,\frac{1}{\Delta\vec{a}}\,D\left(\frac{\vec{A}(\Gamma)-\vec{a}}{\Delta\vec{a}}\right)d\Gamma = N\int \rho(\Gamma,t)\,\delta(\vec{A}(\Gamma)-\vec{a})d\Gamma. \tag{2}$$

Thus $N(\vec{a},t)$ is the number of systems that satisfies the condition that $\vec{A}(\Gamma_t)=\vec{a}$.

When we perform a measurement on the ensemble at time t_1, we determine the number occupation set $\{N(\vec{a}_1,t_1)\}$ for all possible values of the $\vec{a}$'s. In order to determine the occupation number's time evolution we introduce the randomness assumption: *The future values $\vec{A}(\Gamma_t)$ do not depend on the precise position of Γ_t within the phase cells* [2]. This assumption implies that $\{N(\vec{a},t)\}$ is only a time independent functional of the occupation numbers at t_1, namely,

$$\{N(\vec{a},t)\}=F(\{N(\vec{a}_1,t_1)\}), \tag{3}$$

where clearly $t>t_1$. This functional restriction implies that a certain constraint has been made regarding the form of the initial distribution function. Indeed, it can be seen from the expression for $N(\vec{a},t)$, which is given by Eq. (2), that the randomness assumption implies that we do not need the precise form of the distribution function at the initial time to evaluate the future values of the cell's occupation number, we only require the dependence through the initial cell's occupation numbers $\{N(\vec{a}_1,t_1)\}$. As we shall see below, this dependence is given by the projected part of $\rho(\Gamma,t_1)$.

To pursue the argument, assume that at a certain time t_1 we determine by direct observation the occupation numbers $\{N(\vec{a}_1,t_1)\}$. From the microscopic point of view, knowledge of these quantities does not determine $\rho(\Gamma,t_1)$. Indeed, there is a whole set of functions, call it $\mathscr{R}(t_1)$, such that

$$\mathscr{R}(t_1)=\left\{\rho(\Gamma,t_1)\,\middle|\,N(\vec{a}_1,t_1)=N\int d\Gamma\ \rho(\Gamma,t_1)G(\vec{a}_1,0)\right\}, \tag{4}$$

where $G(\vec{a}_1,0)=\delta(\vec{A}(\Gamma,0)-\vec{a}_1)$. Nevertheless, the set $\{N(\vec{a}_1,t_1)\}$ does have the property of uniquely determining one part of any member of this family. Indeed, take Eq. (2), which defines according to Eq. (4) the members of the family $\mathscr{R}(t_1)$, multiply it by $G(\vec{a}_1,0)/W(\vec{a}_1)$ on both sides, and integrate over the whole $\vec{a}$ space. Here $W(\vec{a}_1)=\int d\Gamma\ \delta(\vec{A}_1(\Gamma)-\vec{a}_1)$ is the volume of the $\vec{a}_1$ cell in the phase space. After the $\vec{a}$ integration is performed on the right-hand side, we get;

$$\int N(\vec{a}_1,t_1)\,\frac{\delta(\vec{A}(\Gamma,0)-\vec{a}_1)}{W(\vec{a}_1)}\,d\vec{a} = N\int d\Gamma'\rho(\Gamma',t_1)\,\frac{\delta(\vec{A}(\Gamma',0)-\vec{A}(\Gamma,0))}{W(\vec{A}(\Gamma,0))}. \tag{5}$$

But according to Zwanzig [6–7] the right-hand side of Eq. (5) is precisely the ''projected'' part of the $\rho(\Gamma,t_1)$ over the microcanonical cell whose volume is $W(\vec{a})$, so that, in fact,

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$$\hat{\rho}(\Gamma,t_1)\equiv P_z\rho(\Gamma,t_1)=\int \frac{N(\vec{a},t_1)}{N}\frac{G(\vec{a},0)}{W(\vec{a})}\,d\vec{a}, \qquad (6)$$

where P_z is Zwanzig's projection operator [6,7].

In other words, of the family $\mathscr{R}(t_1)$, the set $\{N(\vec{a}_1,t_1)\}$ uniquely determines the projected part of the distribution function of the members of such a family, namely, $P_z\rho(\Gamma,t_1)$ defined by Eq. (6). Therefore, with the knowledge of $\{N(\vec{a}_1,t_1)\}$ we describe the system's state by an ensemble formed by a superposition of microcanonical ensembles in each cell. This is the more logical selection from the probabilistic point of view because we do not have more detailed information that allows us to know the precise position of the phase point within the cell for each ensemble's member. This latter information is contained in the irrelevant projected part of the distribution function, and the randomness assumption tells us that it is irrelevant for the future description of the phase functions $\vec{A}(\Gamma,t)$. Thus, for macroscopic purposes, we consider that $(1-P_z)\rho(\Gamma,t_1)=0$, which implies that $\rho(\Gamma,t_1)=P_z\rho(\Gamma,t_1)$. This assumption is compatible with Eq. (3), as seen when we separate the distribution function in both its parts. Indeed, Eq. (2) takes the form

$$N(\vec{a},t)=\int d\vec{a}_1 N(\vec{a}_1,t_1)\frac{(G(\vec{a},t),G(\vec{a}_1,t_1))}{W(\vec{a}_1)} + \int d\Gamma\{N(1-P_z)\rho(\Gamma,t_1)\}G(\vec{a},t-t_1),$$

which after use is made of the condition $(1-P_z)\rho(\Gamma,t_1)=0$ simply reduces to

$$N(\vec{a},t)=\int d\vec{a}_1 N(\vec{a}_1,t_1)\frac{(G(\vec{a},t),G(\vec{a}_1,t_1))}{W(\vec{a}_1)}. \qquad (7)$$

Equation (7) shows that applying the randomness assumption guarantees the functional relationship given by Eq. (3). Thus the functional form of this equation is entirely equivalent to the randomness assumption given by Eq. (6).

We now proceed to give a physical interpretation for the inner product

$$(G(\vec{a},t),G(\vec{a}_1,t_1))=\int d\Gamma\,\delta(\vec{A}(\Gamma,t)-\vec{a})\delta(\vec{A}(\Gamma,t_1)-\vec{a}_1), \qquad (8)$$

which can be expressed in the following form:

$$(G(\vec{a},t),G(\vec{a}_1,t_1))=\lim_{\substack{\Delta\vec{a}\to 0\\ \Delta\vec{a}_1\to 0}}\int d\Gamma\,\frac{1}{\Delta\vec{a}}D\left(\frac{\vec{A}(\Gamma,t)-\vec{a}}{\Delta\vec{a}}\right)\times\frac{1}{\Delta\vec{a}_1}D\left(\frac{\vec{A}(\Gamma,t_1)-\vec{a}_1}{\Delta\vec{a}_1}\right).$$

Therefore,

$$(G(a,t),G(a_1,t_1))d\vec{a}\;d\vec{a}_1=\int_{\substack{\vec{a}_1\leqslant\vec{A}(\Gamma,t_1)\leqslant\vec{a}_1+d\vec{a}_1\\ \vec{a}\leqslant\vec{A}(\Gamma,t)\leqslant\vec{a}+d\vec{a}}}d\Gamma, \qquad (9)$$

thus $(G(\vec{a},t),G(\vec{a}_1,t_1))$ is the phase volume occupied by the system's ensemble such that at time t_1 the representative points are in the $\vec{a}_1$ cell, and at time t they are in $\vec{a}$ cell. We denote by $N(\vec{a},t;\vec{a}_1,t_1)$ the number of these systems, so that we have

$$N(\vec{a},t)=\int d\vec{a}_1 N(\vec{a},t;\vec{a}_1,t_1). \qquad (10)$$

When we compare this expression with Eq. (7), we obtain that the randomness assumption implies that

$$\frac{N(\vec{a},t;\vec{a}_1,t_1)}{(G(\vec{a},t),G(\vec{a}_1,t_1))}=\frac{N(\vec{a}_1,t_1)}{W(a_1)}. \qquad (11)$$

Thus Eq. (11) means that the ensemble's number density is constant in the course of macroscopic times. In some sense Eq. (11) is similar to a macroscopic Liouville theorem, because the local number density $N(\vec{a}_1,t_1)/W(\vec{a}_1)$ does not change in macroscopic times, although the phase volume is not an arbitrary small $d\Gamma$, but the volume associated with the system's macroscopic observables.

We now proceed to apply the repeated randomness assumption when we consider the time evolution of the ensemble for three times $t_3>t_2>t_1$ such that the time intervals are macroscopic intervals, namely, those in which we make a macroscopic measurement on the system. In this case, the randomness assumption can be applied separately to times t_3 and t_2, a condition that according to Eq. (3), may be expressed as

$$\{N(a_3,t_3)\}=F_{\Delta t''}(\{N(a_1,t_1)\}) \quad \text{with} \quad \Delta t''=t_3-t_1, \qquad (12a)$$

$$\{N(a_2,t_2)\}=F_{\Delta t}(\{N(a_1,t_1)\}) \quad \text{with} \quad \Delta t=t_2-t_1. \qquad (12b)$$

However, the interval $t_3-t_2=\Delta t'$ is also a macroscopic time interval, so that the repeated randomness assumption allows us to treat the evolution during this interval in the same manner as we do with the first interval $t_2-t_1=\Delta t$. Then, we also have that

$$\{N(a_3,t_3)\}=F\Delta t'(\{N(a_2,t_2)\}). \qquad (13)$$

This last expression implies that the system goes from t_1 to t_2 in such a form that (12b) is satisfied, and the occupation numbers at t_2 are given by Eq. (7). Thus we redistribute the systems inside each cell to obtain a distribution with constant density, so that according to Eq. (7),

$$\frac{N(\vec{a}_2,t_2)}{W(\vec{a}_2)}=\int d\vec{a}_1 N(\vec{a}_1,t_1)\frac{(G(\vec{a}_1,t_2),G(\vec{a}_1,t_1))}{W(\vec{a}_2)W(\vec{a}_1)}. \qquad (14)$$

Notice that we repeat here the same procedure that is followed to select the distribution function at the initial time after the system evolves to t_3, and due to the fact that the time interval $t_3-t_2=\Delta t'$ is a macroscopic one, Eq. (11) is satisfied, so we have that

$$\frac{N(\vec{a}_3,t_3;\vec{a}_2,t_2)}{(G(\vec{a}_3,t_3),G(\vec{a}_2,t_2))}=\frac{N(\vec{a}_2,t_2)}{W(\vec{a}_2)}, \qquad (15)$$

and the cell's occupation numbers are given by

$$N(\vec{a}_3,t_3)=\int d\vec{a}_2 N(\vec{a}_2,t_2)\,\frac{(G(\vec{a}_3,t_3),G(\vec{a}_2,t_2))}{W(\vec{a}_2)}. \tag{16}$$

Of course the procedure can be repeated for all future times, with the condition that the corresponding time intervals involved be macroscopic. This is precisely the significance of the repeated randomness assumption.

Now we draw the conclusion arising from the requirement that Eqs. (12) and (13) must be compatible. The repeated randomness assumption implies that

$$F_{\Delta t'+\Delta t}(\{N(a_1,t_1)\})=F_{\Delta t'}(F_{\Delta t}(\{N(a_1,t_1)\})). \tag{17}$$

The right hand side of this functional equation is obtained when we substitute Eq. (14) into Eq. (16), so that we get

$$\begin{aligned} N(\vec{a}_3,t_3)&=\int d\vec{a}_2\left\{\int d\vec{a}_1 N(\vec{a}_1,t_1)\,\frac{(G(\vec{a}_2,t_2),G(\vec{a}_1,t_1))}{W(\vec{a}_1)}\right\}\frac{(G(\vec{a}_3,t_3),G(\vec{a}_2,t_2))}{W(\vec{a}_2)}\\ &=\int d\vec{a}_1\,\frac{N(\vec{a}_1,t_1)}{W(\vec{a}_1)}\left\{\int d\vec{a}_2\frac{(G(\vec{a}_3,t_3),G(\vec{a}_2,t_2)}{W(\vec{a}_2)}(G(\vec{a}_2,t_2),G(\vec{a}_1,t_1))\right\} \end{aligned} \tag{18}$$

and the left hand side of Eq. (17) referred to the initial time t_1 is

$$N(\vec{a}_3,t_3)=\int d\vec{a}_1\,\frac{N(\vec{a}_1,t_1)}{W(\vec{a}_1)}\,(G(\vec{a}_3,t_3),G(\vec{a}_1,t_1)). \tag{19}$$

Therefore, Eq. (17) implies that

$$\begin{aligned}(G(\vec{a}_3,t_3),G(\vec{a}_1,t_1))&=\int d\vec{a}_2\,\frac{(G(\vec{a}_3,t_3),G(\vec{a}_2,t_2))}{W(\vec{a}_2)}\\ &\times(G(\vec{a}_2,t_2),G(\vec{a}_1,t_1)).\end{aligned} \tag{20}$$

Thus the repeated randomness assumption implies this relationship between the phase volume. Using now the fact that the macroscopic phase density is constant in a macroscopic time interval, Eq. (20) can be expressed in a more familiar form, by dividing both sides by $W(\vec{a}_1)$ and using Eq. (11). This leads to the expression.

$$\frac{N(\vec{a}_3,t_3;\vec{a}_1,t_1)}{N(\vec{a}_1,t_1)}=\int d\vec{a}_2\,\frac{N(\vec{a}_3,t_3;\vec{a}_2,t_2)}{N(\vec{a}_2,t_2)}\,\frac{N(\vec{a}_2,t_2;\vec{a}_1,t_1)}{N(\vec{a}_1,t_1)}. \tag{21}$$

Finally, using the fact that the conditional probability is given by

$$P(\vec{a},t|\vec{a}_1,t_1)=\frac{N(\vec{a},t;\vec{a}_1,t_1)}{N(\vec{a}_1,t_1)}, \tag{22}$$

Eq. (21) takes the form

$$P(\vec{a}_3,t_3|\vec{a}_1,t_1)=\int d\vec{a}_2 P(\vec{a}_3,t_3|\vec{a}_2,t_2)P(\vec{a}_2,t_2|\vec{a}_1,t_1), \tag{23}$$

which is the Chapman-Kolmogorov equation. In other words, the fact that the randomness assumption implies the conservation of the number density of the members of the representative ensemble, provided macroscopic time intervals are taken to measure, is equivalent to asserting that the conditional probability is governed by a Markovian random process. This result is *per se* not new, it was obtained by van Kampen over 30 years ago [3]. The novel aspect of this derivation is the fact that successive applications of the randomness assumption in macroscopic time intervals is equivalent to the operation behind Zwanzig's projection operator.

We now briefly analyze Zwanzig's formulation and discuss the form in which the randomness assumption is used in this formalism. The central quantity in his formulation is the distribution function

$$g(a,t)=\int \rho(\Gamma,t)G(a,0)d\Gamma, \tag{24}$$

which is proportional to $N(\vec{a},t)$, as follows from Eq. (2). Thus we discuss Zwanzig's approach in terms of the cell's occupation numbers. He begins deriving the exact time evolution equation for $N(\vec{a},t)$, which has the following form:

$$\begin{aligned}\frac{\partial N(\vec{a},t)}{\partial t}&=\int d\vec{b}\; i\Omega(\vec{a},\vec{b})N(\vec{b},t)\\ &-\int_0^t ds\int d\vec{b}\; K(\vec{a},\vec{b},t-s)N(\vec{b},s)\\ &+((1-P_z)\rho(\Gamma,0),F(\vec{a},t)).\end{aligned} \tag{25}$$

The explicit forms for the quantities $i\Omega$, K, and F are irrelevant in this work, but are explicitly given in Eqs. (33) and (34) in Ref. [8]. To proceed, one requires some information about the initial distribution function, which indeed implies the randomness assumption when the requirement is made that

$$\rho(\Gamma,0)=P_z\rho(\Gamma,0). \tag{26}$$

Use of Eq. (26) leads to a closed equation for the occupation number, due to the fact that the last term of the right hand side in Eq. (25) is zero. However, the resulting equation is very complicated because there appears a memory term $K(\vec{a},\vec{b},t-s)$ and it is necessary to introduce another simplification, the so called slow approximation. For

this purpose, one assumes that the times in which we are observing the system are sufficiently long compared with the correlation time of the kernel K, in such a way that for such time scales $K(\vec{a},\vec{b},t)=2K(\vec{a},\vec{b})\delta(t)$, the kinetic equation takes the form

$$\frac{\partial N(\vec{a},t)}{\partial t}=\int d\vec{b}\{i\Omega(\vec{a},\vec{b})-K(\vec{a},\vec{b})\}N(\vec{b},t). \qquad (27)$$

It is also possible to show that the slow approximation [9] is equivalent to the statement that the conditional probability satisfies the Chapman-Kolmogorov equation.

Therefore, to obtain the Chapman-Kolmogorov equation from Liouville's equation it is necessary to make three assumptions. First, imposing the condition that the initial phase distribution function satisfy Eq. (26), which means that the randommness assumption is used; second, that the stochastic process $\vec{A}(\Gamma,t)=\vec{a}(t)$ is a slow one, which is valid only within certain time scales; and third, that the dynamic process is stationary for such time scales. These last conditions may be seen to be equivalent to the repeated randomness assumption.

As a final remark we wish to state that the results presented here may be used to establish a bridge between the usual repeated randomness assumption and the information theory. This is accomplished in terms of a principle called the principle of operational compatibility [10], relying upon Mackey's formalism of the dynamical origin of increasing entropy [11]. Also, it is possible to establish the relationship between van Kampen's point of view for nonequilibrium statistical mechanics with a Nicolis's theory for conservative dynamical systems [12]. This will be discussed elsewhere.

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