保存的マップにおける発展方程式の固有値問題と散逸

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アブストラクト
保存系でどのように散逸が生じるかという問題は統計力学の基礎的問題の一つである。この点については通常は以下のように考えられている：まず、考えている系の自由度には制御できない部分（相空間の微細部分や環境系）があることが仮定される。つまり、「力学的情報」が流れ込むと実際上それを回復できないような自由度が存在することが仮定されるのである。このとき制御不可能部分に「力学的情報」を流すような時間発展は散逸的になる。この拡張はこれまで様々な式が定式化され、応用上も重要な役割を演じる散逸的時間発展方程式が導かれてきた。しかし、これらのアプローチは全ての自由度を考慮していないので完全に満足のいくものではない。さらに、近年の力学系理論の発達により非線形力学系が多様なあるまいを示すことが明らかにされ、そのため系の個性を考慮できる不可逆性の理論の構築が必要になってきていると考えられる。

以下では保存的混合系に論論を限定する。このような系では与えられた可観測量の任意の初期分布に関する期待値はエルゴード則的測度についての期待値に漸近的に収束する。この収束は初期分布の「平衡分布」への緩和、つまり散逸過程と見なすことができる。この弱緩和のメカニズムは次のように考えられる：まず、混合性の条件が満たされるためには分布の長時間極限は相空間の任意の領域に拡がっていなければならない。他方、相空間体積は保存される。これらが両立することは、時間発展に流れ分布の空間変動がより細かくなることを意味する。従って、初期分布の持っていた「情報」は時間発展に流れ相空間のより小さな領域に移動し、可観測量の平均をとる操作により失われていくのである。

公理A系と拡大写像という混合系に関しては、PollicottとRuelleにより、弱緩和率が相関関数のパワースペクトルの複素平面内の極（Pollicott-Ruelleの共鳴）として特徴付けられがすることが示されている。さらに、これらの複素極が分布関数の運動のジェネレーターの固有値であることが容易に分かる。ただし、これは一般化された固有値
問題と考えなくてはならない。なぜなら、通常のHilbert空間の枠で考えると運動のジェネレーターはエルミート的で実固有値しか持たないからである。

このように緩和過程を時間発展演算子の（一般化された）固有値問題によって特徴付けることが可能で、かつ一般的であることとは、1960年代後半からPrigogineらによって主張されてきた。このアプローチの著しい特徴は、運動法則を変更することなく緩和過程を相空間におけるミクロなダイナミックスのレベルで記述できる点にある。

ここでは、保存的写像について（弱）緩和過程と関連した（一般化された）固有値問題をレビューする。第2節ではバイコネ変換について緩和モードを構成し、その性質を論じる。第3節では保存的な決定論的拡散モデル（多重バイコネ変換）において緩和モードを求め、現象論的な拡散の減衰モードと比較する。第4節では同じ拡散のモデルにおいて非平衡定常状態を導き、可逆力学系における不可逆性の問題を論じる。以下で見るように、緩和モードや非平衡定常状態は相空間で定義されるフラクタル関数で表わされる。この結果は、保存系で散逸が出現する際に重要な役割を演じるフラクタル構造が存在することを示唆している。この点については最後の節で論じる。
Eigenvalue Problem of Evolution Operators and Dissipation in Conservative Maps

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Abstract

We derive, for the baker and multibaker maps, the eigendistributions of the evolution operator of distribution functions, which characterize the weak relaxation to the ‘equilibrium’ state. Non-equilibrium stationary states are also constructed for the multibaker map. We show an important role of fractal functions in the realization of dissipative eigenmodes as well as non-equilibrium stationary states.

§1. Problem of Dissipation in Conservative Systems

Understanding of dissipation in conservative systems is a long standing problem in statistical mechanics. The widely accepted picture is as follows: Firstly, one assumes that there exists a part of the system’s degrees of freedom (such as very small regions in the phase space or ‘environments’) which is uncontrollable in the sense that dynamical ‘information’ flowed there cannot be restored practically. Then the dynamical evolution, which promotes the flow of ‘information’ to the uncontrollable part, appears as dissipative. In order to formulate this picture, various approaches have been proposed so far(1). Although the conventional approaches can derive dissipative time evolutions, they are not fully satisfactory since they usually neglect parts of the dynamical information. Moreover, recent progress of the dynamical system theory reveals the variety of behaviors of nonlinear dynamical systems, and suggests a necessity of formulating a theory of irreversibility which could take into account specific features of systems in question.

Hereafter, we concentrate on conservative mixing systems, where expectation value of a given observable with respect to any initial distribution asymptotically tends to the one
with respect to the ergodic measure. This convergence could be regarded as a relaxation of the initial distribution to the 'equilibrium' one and thus as a dissipative process. The mechanism of such a weak relaxation is simple: The long time limit of the distribution should spread over an arbitrary domain of the phase space in order to satisfy the mixing condition, while the phase space volume is conserved. This is possible only when the distribution evolves into the one with finer structures as time goes on. Hence, the 'information' carried by the initial distribution moves into smaller phase-space regions in the course of the time evolution and will be lost through the averaging of a given observable.

For two classes of mixing systems, namely axiom-A systems and expanding maps, Pollicott\(^{(2)}\) and Ruelle\(^{(3)}\) have shown that the rates of the weak relaxations can be characterized by the complex poles of the power spectra of the correlation functions, known as Pollicott-Ruelle resonances. Moreover, it is easy to see that those complex poles are eigenvalues of the generator of motion for the distributions. Note that the aforementioned eigenvalue problem associated with the weak relaxation should be understood in a generalized sense, because, in the conventional Hilbert space setting, the generator of motion is Hermitian and possesses only real eigenvalues.

The possibility and the generality of such a characterization of the relaxation rates in terms of the (generalized) eigenvalue problem of the evolution operator have been emphasized and discussed by Prigogine and coworkers\(^{(4,5)}\) over the last thirty years in the field of non-equilibrium statistical mechanics. The novelty of this approach is that the relaxation is described at the level of the microscopic phase-space dynamics without any modification of the laws of motion.

In the present article, we review the (generalized) eigenvalue problem associated with the (weak) relaxation processes for conservative maps. In the next section, the relaxation modes in the baker map are constructed and their properties are discussed. In §3, for a conservative model of deterministic diffusion, called the multibaker map, the relaxation modes are obtained and compared with the phenomenological decay modes of diffusion. Non-equilibrium stationary states for the same model are derived in §4 and the problem of irreversibility in reversible systems is investigated. We found that these relaxation modes and non-equilibrium stationary states are described by fractal phase-space functions. The
result suggests that there exist fractal structures which play an important role in the appearance of dissipation in conservative systems. This point is discussed in the last section.

§2. Dissipative eigenvalue problem of evolution operator I

- weak relaxation to 'equilibrium' in the baker map -

The baker map is a textbook example of the mixing systems\(^{(1)}\) admitting the Lebesgue measure as an invariant measure, where the expectation value of a given observable with respect to any initial distribution converges, in an infinitely long time, to the one with respect to the Lebesgue measure. As mentioned in the previous section, these relaxation processes are characterized by the Pollicott-Ruelle resonances, which correspond to (generalized) eigenvalues of the evolution operator of the distribution functions. Hasegawa and Saphir\(^{(6)}\) solved the generalized eigenvalue problem for the dyadic baker map and, then, Antoniou and Tasaki\(^{(7)}\) solved the corresponding problem for the \(\beta\)-adic baker map. For the \(\beta\)-adic baker map, the evolution operator is found to have generalized eigenvalues \(1/\beta^m\) \((m = 0, 1, \ldots)\), each of which is \(m\)-fold degenerate and associated with a Jordan block of size \(m + 1\), and a procedure of calculating the corresponding principal vectors is shown. Here, we reproduce the results for the dyadic baker map, but in a more explicit manner.

The dyadic baker map is defined on a unit square \([0, 1)^2\) by two step operations:

![Baker map diagram](image-url)
1) the square is stretched by a factor 2 in x-direction and squeezed by a factor 1/2 in the perpendicular y-direction and 2) the so-obtained 2x1/2 rectangle is cut into two 1x1/2 rectangles and the right part is piled up onto the left one (cf. Fig.1):

\[ B(x, y) = \begin{cases} 
(2x, \frac{y}{2}), & 0 \leq x < 1/2 \\
(2x - 1, \frac{y+1}{2}), & 1/2 \leq x < 1
\end{cases} \]  

(2.1)

The map is uniformly hyperbolic with the maximum Lyapunov exponent \( \log 2 \). The evolution operator \( U \) of distribution functions is given by

\[ U \rho(x, y) \equiv \rho(B^{-1}(x, y)) = \begin{cases} 
\rho\left(\frac{x}{2}, 2y\right), & 0 \leq y < 1/2 \\
\rho\left(\frac{x+1}{2}, 2y - 1\right), & 1/2 \leq y < 1
\end{cases} \]  

(2.2)

The operator is unitary in the Hilbert space of square integrable functions on the unit square \([0,1)^2\) and satisfies, for any observable \( A \) and normalized initial distribution \( \rho \),

\[ \langle A \rangle_t \equiv \int_{[0,1)^2} dx dy A(x, y)U^t \rho(x, y) \to \int_{[0,1)^2} dx dy A(x, y), \quad (t \to +\infty) \]  

(2.3)

as a consequence of the mixing property of \( B \).

Once observables are restricted to functions smooth in \( y \) and initial densities to the ones smooth in \( x \), the relaxation (2.3) can be represented as a sum of exponentially decaying terms. Terms up to \( O(t/2^t) \) are given by

\[ \langle A \rangle_t = \langle A, F_0 \rangle \langle \tilde{F}_0, \rho \rangle + \left(\frac{1}{2}\right)^t \left[ \langle A, F_1^a \rangle \langle \tilde{F}_1^a, \rho \rangle + \langle A, F_1^b \rangle \langle \tilde{F}_1^b, \rho \rangle + \frac{t}{8} \langle A, F_1^b \rangle \langle \tilde{F}_1^a, \rho \rangle \right] + O\left(\frac{t^3}{4^t}\right), \]  

(2.4)

where linear functionals \( \tilde{F}_j \)'s are given by

\[ \langle \tilde{F}_0, \rho \rangle \equiv \int_{[0,1)^2} dx dy \rho(x, y), \]  

(2.5a)

\[ \langle \tilde{F}_1^a, \rho \rangle \equiv \int_{[0,1)^2} dx dy \partial_x \rho(x, y), \]  

(2.5b)

\[ \langle \tilde{F}_1^b, \rho \rangle \equiv \int_{[0,1)^2} dx dy \left( y - \frac{1}{2} \right) \rho(x, y) \\
- \int_0^1 dy \int_0^1 d\left( \frac{x^2}{4} - \frac{x}{2} - \frac{1}{2} S(x) + \frac{1}{8} T(x) \right) \partial_x \rho(x, y), \]  

(2.5c)
and $F_j$'s by
\[
(A, F_0) = \int_{[0,1]^2} dx dy A(x, y), \quad (2.6a)
\]
\[
(A, F_1^a) = \int_{[0,1]^2} dx dy \left( x - \frac{1}{2} \right) A(x, y)
- \int_0^1 dx \int_0^1 d\left\{ \frac{y^2}{4} - \frac{y}{4} - \frac{1}{2} S(y) + \frac{1}{8} T(y) \right\} \partial_y A(x, y), \quad (2.6b)
\]
\[
(A, F_1^b) = \int_{[0,1]^2} dx dy \partial_y A(x, y). \quad (2.6c)
\]

In (2.5c) and (2.6b), $T$ is the Takagi function$^{(8,9)}$ and $S$ is a related function, defined respectively as unique solutions of functional equations:
\[
T(x) = \begin{cases} 
\frac{1}{8} T(2x) + x, & 0 \leq x \leq 1/2 \\
\frac{1}{2} T(2x - 1) + 1 - x, & 1/2 \leq x \leq 1 
\end{cases} \quad (2.7)
\]
and
\[
S(x) = \begin{cases} 
\frac{1}{8} S(2x), & 0 \leq x \leq 1/2 \\
\frac{1}{2} S(2x - 1) + (1 - x)(x - \frac{1}{2}), & 1/2 \leq x \leq 1 
\end{cases} \quad (2.8)
\]

Time dependence of each term of (2.4) indicates that the functional $F_0$ is the eigendistribution of evolution operator $U$ with eigenvalue 1 and $F_1^j (j = a, b)$ the eigendistributions of $U$ with eigenvalue $1/2$, and that $\tilde{F}_0$ and $\tilde{F}_1^j (j = a, b)$ are the eigendistributions of the adjoint operator $U^\dagger$ with eigenvalue 1 and $1/2$ respectively. Indeed, we have, for an arbitrary $A,$
\[
(A, UF_0) = (A, F_0), \quad (2.9a)
\]
\[
(A, UF_1^a) = \frac{1}{2} (A, F_1^a) + \frac{1}{8} (A, F_1^b), \quad (2.9b)
\]
\[
(A, UF_1^b) = \frac{1}{2} (A, F_1^b), \quad (2.9c)
\]
and, for an arbitrary $\rho$,
\[
(U^\dagger \tilde{F}_0, \rho) = (\tilde{F}_0, U \rho) = (\tilde{F}_0, \rho), \quad (2.10a)
\]
\[
(U^\dagger \tilde{F}_1^a, \rho) = \frac{1}{2} (\tilde{F}_1^a, \rho), \quad (2.10b)
\]
\[
(U^\dagger \tilde{F}_1^b, \rho) = \frac{1}{2} (\tilde{F}_1^b, \rho) + \frac{1}{8} (\tilde{F}_1^a, \rho). \quad (2.10c)
\]
Fig. 2 Takagi function $T(x)$ (left) and function $S(x)$ defined by (2.8) (right).

We have shown that the weak convergence of the expectation value (2.3) is characterized by eigendistributions of the evolution operator and its adjoint. Remarkable feature is that parts of the decaying eigendistributions $\tilde{F}_1^b$ and $F_1^a$ are given as functionals represented by Stieltjes integrals with respect to $T$ and $S$. The Takagi function $T$ was firstly proposed by Takagi as a simple example of a continuous function without finite derivatives everywhere\(^{8,9}\). The function $S$ has the similar properties. Their singular properties can be seen in their graphs, which are typical fractals (Fig. 2). Note that the eigendistribution $F_1^a$ of the forward evolution operator $U$ and the eigendistribution $\tilde{F}_1^b$ of the ‘backward’ evolution operator $U^\dagger = U^{-1}$ are singular along their respective contracting directions (the expanding direction of the forward evolution is the contracting direction of the backward evolution!). Hence, one can consider that the singularity of eigendistributions reflects the fragmentation of the distribution resulting from the folding along the contracting direction.

§3. Dissipative eigenvalue problem of evolution operator II
- diffusive relaxation in the multibaker map -

In this and the next sections, we consider a reversible model of deterministic diffusion, called the multibaker map, which is as simple as the baker map, but is more “physical”.

- 28 -
The multibaker map is defined on a periodic array of countably many unit squares and exhibits diffusion processes. A 4-adic multibaker map has been proposed by one of us\textsuperscript{(10)} and the properties of diffusion and nonequilibrium states have been rigorously studied with the aid of zeta functions and of the "thermodynamic formalism". Multibaker maps admit the Lebesgue measure as an invariant measure and the relaxation of the deviations from this equilibrium state is described by the corresponding Frobenius–Perron operator. The spectral properties of the Frobenius–Perron operator are recently studied by Gaspard\textsuperscript{(11)}, Hasegawa and Driebe\textsuperscript{(12)} and Tasaki, Hakmi and Antoniou\textsuperscript{(13)}. The logarithms of the eigenvalues of the Frobenius–Perron operator give the decay rates of the correlation functions\textsuperscript{(11–13)}, which are known as Pollicott–Ruelle resonances\textsuperscript{(2,3)}. In this section, we discuss the spectral properties of the Frobenius-Perron operator.

3.1 Diffusive relaxation modes

The multibaker map discussed in this article is the simplest one defined on a one-dimensional array of unit squares:

$$B(n, x, y) = \begin{cases} 
(n - 1, 2x, \frac{y}{2}) , & 0 \leq x < \frac{1}{2} , \\
(n + 1, 2x - 1, \frac{y+1}{2}) , & \frac{1}{2} \leq x < 1 , 
\end{cases}$$

(3.1)
where an integer \( n \) labels the unit squares and a pair \((x, y)\) of real numbers \((0 \leq x < 1, 0 \leq y < 1)\) stands for the coordinates in each unit square. The map \( \tilde{B} \) is schematically depicted in Fig. 3. This map is area-preserving so that it admits the Lebesgue measure, \( dx dy \), as an invariant measure. As the baker map, the multibaker map \( \tilde{B} \) is uniformly hyperbolic with a stretching factor 2 and, thus, possesses a positive Lyapunov exponent equal to \( \log 2 \).

The map \( \tilde{B} \) is time-reversal invariant, i.e., there exists an involution \( I \) satisfying

\[
\tilde{B}^{-1} = I \tilde{B} I ,
\]

which corresponds to the velocity inversion in the particle system

\[
I(n, x, y) \equiv (n, 1 - y, 1 - x) .
\]

The evolution operator of the distribution functions (i.e., the Frobenius–Perron operator) \( \tilde{U} \) is then given by

\[
\tilde{U} \rho(n, x, y) \equiv \rho(\tilde{B}^{-1}(n, x, y)) = \begin{cases} 
\rho(n + 1, \frac{x}{2}, 2y), & 0 \leq y < \frac{1}{2} , \\
\rho(n - 1, \frac{x+1}{2}, 2y - 1), & \frac{1}{2} \leq y < 1 .
\end{cases}
\]

Because of the periodicity of the system, it is convenient to introduce the Fourier representation:

\[
\hat{\rho}_q(x, y) \equiv \sum_{n=-\infty}^{+\infty} e^{-inx} \rho(n, x, y) ,
\]

where the quasi-momentum \( q \) runs from \(-\pi\) to \(\pi\). Then, the expectation value of a given observable \( A \) at time \( t \) with respect to the initial distribution \( \rho \) can be rewritten as

\[
\langle A \rangle_t \equiv \int_{[0,1)^2} dx dy A(n, x, y) \tilde{U}^t \rho(n, x, y) = \int_{-\pi}^{\pi} \frac{dq}{2\pi} \int_{[0,1)^2} dx dy \hat{A}_q^* (x, y) U_q^t \hat{\rho}_q (x, y) ,
\]

where \( U_q \) is the Fourier component of the Frobenius-Perron operator given by

\[
U_q \hat{\rho}(x, y) \equiv \begin{cases} 
\hat{\rho}_q \left( \frac{x}{2}, 2y \right), & 0 \leq y < \frac{1}{2} , \\
\hat{\rho}_q \left( \frac{x+1}{2}, 2y - 1 \right), & \frac{1}{2} \leq y < 1 .
\end{cases}
\]
The operator $U_q$ is unitary in the Hilbert space of square integrable functions on the unit square $[0,1)^2$. Notice that the operator $U_q$ for $q = 0$ is equal to the Frobenius–Perron operator $U$ for the baker map.

As in the case of the baker map, once observables are restricted to functions which are smooth in $y$ and initial densities to other functions which are smooth in $x$, the integrand in (3.6) with respect to $q$-integration can be represented as a sum of exponentially decaying terms. When $\hat{A}_q$ and $\hat{\rho}_q$ are two times continuously differentiable with respect to $y$ and $x$ respectively, we have

$$
\langle A \rangle_t = \int_{|\cos q|>1/4} \frac{dq}{2\pi} \cos^t q \langle A, F_{0q} \rangle \langle \hat{F}_{0q}, \rho \rangle
+ \int_{|\cos q|>1/2} \frac{dq}{2\pi} \left( \frac{\cos q}{2} \right)^t \left[ \langle A, F_{1q}^a \rangle \langle \hat{F}_{1q}^a, \rho \rangle + \langle A, F_{1q}^b \rangle \langle \hat{F}_{1q}^b, \rho \rangle + \frac{t}{8\cos q} \langle A, F_{1q}^b \rangle \langle \hat{F}_{1q}^a, \rho \rangle \right]
+ O\left(\frac{t^3}{4^t}\right),
$$

(3.8)

where linear functionals $\hat{F}_j$'s are given by

$$
\langle \hat{F}_{0q}, \rho \rangle \equiv \begin{cases}
\int_{[0,1)^2} dG_q(x)dy\hat{\rho}_q(x,y) & \text{(for } |\cos q|>1/2) \\
\int_0^1 dy\hat{\rho}_q(1,y) - \int_{[0,1)^2} d\tilde{G}_q(x)dy\partial_x \hat{\rho}_q(x,y) & \text{(for } 1/2>|\cos q|>1/4)
\end{cases},
$$

(3.9a)

$$
\langle \hat{F}_{1q}^a, \rho \rangle \equiv \int_{[0,1)^2} dG_q(x)dy\partial_x \hat{\rho}_q(x,y),
$$

(3.9b)

$$
\langle \hat{F}_{1q}^b, \rho \rangle \equiv \int_{[0,1)^2} dG_q(x)dy \left( y - \frac{e^{-iq}}{2\cos q} \right) \hat{\rho}_q(x,y) - \int_{[0,1)^2} dG_q^1(x)dy\partial_x \hat{\rho}_q(x,y),
$$

(3.9c)

and antilinear functionals $F_j$'s by

$$
\langle A, F_{0q} \rangle \equiv \begin{cases}
\int_{[0,1)^2} dx dG_q(y)\hat{A}^*_q(x,y) & \text{(for } |\cos q|>1/2) \\
\int_0^1 dx \hat{A}^*_q(x,1) - \int_{[0,1)^2} dx d\tilde{G}_q(y)\partial_y \hat{A}^*_q(x,y) & \text{(for } 1/2>|\cos q|>1/4)
\end{cases},
$$

(3.10a)
with $\tilde{\rho}(x,y)$ and $\tilde{A}(x,y)$ being the Fourier transforms of $\rho(n,x,y)$ and $A(n,x,y)$ respectively. In (3.9) and (3.10), functions $G_q$, $G^1_q (|\cos q| > 1/2)$ and $\tilde{G}_q (1/2 > |\cos q| > 1/4)$ are defined respectively as unique solutions of functional equations:

$$G_q(x) = \begin{cases} \frac{e^{iq}}{2\cos q} G_q(2x), & 0 \leq x \leq 1/2 \\ \frac{e^{-iq}}{2\cos q} G_q(2x-1) + \frac{e^{iq}}{2\cos q}, & 1/2 \leq x \leq 1 \end{cases}$$  

(3.11a)

$$G^1_q(x) = \begin{cases} \frac{e^{iq}}{2\cos^2 q} G^1_q(2x) + \frac{G_q(x)}{8\cos^2 q} - \frac{e^{-iq}}{2\cos^2 q} \int_0^x dx' G_q(x'), & 0 \leq x \leq 1/2 \\ \frac{e^{iq}}{2\cos^2 q} G^1_q(2x-1) + \frac{G_q(x)-G_q(1/2)}{8\cos^2 q} - \frac{e^{iq}}{2\cos^2 q} \int_{1/2}^x dx' [1 - G_q(x')], & 1/2 \leq x \leq 1 \end{cases}$$

(3.11b)

and

$$\tilde{G}_q(x) = \begin{cases} \frac{e^{-iq}}{4\cos q} \tilde{G}_q(2x), & 0 \leq x \leq 1/2 \\ \frac{e^{-iq}}{4\cos q} \tilde{G}_q(2x-1) + \frac{e^{iq}}{2\cos q} x - \frac{1}{8\cos^2 q}, & 1/2 \leq x \leq 1 \end{cases}$$

(3.11c)

As shown in Fig. 4, the graph of $G_q$ is fractal. The other functions $G^1_q$ and $\tilde{G}_q$ have the similar properties. Hence, the functionals $F^a_{1q}$, $F^b_{1q}$ and $F^b_{1q}$ are singular in $y$, or the contracting direction for the forward evolution, and the functionals $\tilde{F}^a_{1q}$, $\tilde{F}^a_{1q}$ and $\tilde{F}^b_{1q}$ are singular in $x$, or the contracting direction for the ‘backward’ evolution. As in the case

Fig. 4 Singular function $G_q(x)$ for $\cos q = 3/5$. Real part (left) and imaginary part (right).
of the baker map, these singularities can be regarded as reflecting the fragmentation of the
distribution along the contracting direction.

As before, the time dependence of each term of (3.8) suggests that the functionals
$F_{0q}$ and $F_{1q}^j (j = a, b)$ are eigendistributions of the Frobenius-Perron operator $\hat{U}$ with
eigenvalues $\cos q$ and $\cos q/2$ respectively, and that the functionals $\hat{F}_{0q}$ and $\hat{F}_{1q}^j (j = a, b)$
are eigendistributions of its adjoint corresponding respectively to the eigenvalues $\cos q$ and
$\cos q/2$. Indeed, we have, for an arbitrary $A$,

$$
\langle A, \hat{U} F_{0q} \rangle \equiv \langle \hat{U}^\dagger A, F_{0q} \rangle = \cos q \langle A, F_{0q} \rangle, \quad (3.12a)
$$

$$
\langle A, \hat{U} F_{1q}^a \rangle = \frac{\cos q}{2} \langle A, F_{1q}^a \rangle + \frac{1}{8 \cos q} \langle A, F_{1q}^b \rangle, \quad (3.12b)
$$

$$
\langle A, \hat{U} F_{1q}^b \rangle = \frac{\cos q}{2} \langle A, F_{1q}^b \rangle, \quad (3.12c)
$$

and, for an arbitrary $\rho$,

$$
\langle \hat{U}^\dagger \hat{F}_{0q}, \rho \rangle \equiv \langle \hat{F}_{0q}, \hat{U} \rho \rangle = \cos q \langle \hat{F}_{0q}, \rho \rangle, \quad (3.13a)
$$

$$
\langle \hat{U}^\dagger \hat{F}_{1q}^a, \rho \rangle = \frac{\cos q}{2} \langle \hat{F}_{1q}^a, \rho \rangle, \quad (3.13b)
$$

$$
\langle \hat{U}^\dagger \hat{F}_{1q}^b, \rho \rangle = \frac{\cos q}{2} \langle \hat{F}_{1q}^b, \rho \rangle + \frac{1}{8 \cos q} \langle \hat{F}_{1q}^a, \rho \rangle. \quad (3.13c)
$$

### 3.2 Scaling limit and correspondence to diffusion

In the multibaker map, hopping from one square to the other is deterministically
controlled by the baker map, which is a deterministic model of a uniform random generator.
Therefore, the multibaker map can be regarded as a determinisitic model of a random walk.
Indeed, the part of the expectation value (3.8) involving $\cos^q$ precisely corresponds to the
time evolution of the probability distribution for the random walk. To see the relation
with the diffusion more in detail, we consider the scaling limit: $n \to \sqrt{M}X, t \to M\tau$ and
$M \to +\infty$, where the distribution and observable are scaled, in the limit of $M \to +\infty$,
as $\sqrt{M} \rho(\sqrt{M}X, x, y) \to \rho_S(X, x, y)$ and $A(\sqrt{M}X, x, y) \to A_S(X, x, y)$ respectively. Note
that the operation \( n \to \sqrt{M} X \) corresponds to the operation \( q \to k/\sqrt{M} \) for the quasi-momentum. Carrying out the scaling in the expectation value (3.8), one obtains

\[
\langle A \rangle_{\sqrt{M} \tau} = \int_{\cos(k/\sqrt{M}) > 1/2} \frac{dk}{2\pi \cos^2 M} \langle A, F_0, k/\sqrt{M} \rangle \langle \tilde{F}_0, k/\sqrt{M}, \rho \rangle + O\left( \frac{\sqrt{M} \tau}{2\sqrt{M} \tau} \right) .
\]

(3.14)

Because of the factor \( 1/2 \sqrt{M} \tau \), the second term of (3.14) disappears in the limit of \( M \to +\infty \). Since, for \( M \to +\infty \), we have

\[
\cos^M (k/\sqrt{M}) \to \exp\left( -\frac{k^2}{2} \right) ,
\]

\[
\frac{1}{\sqrt{M}} \langle A, F_0, k/\sqrt{M} \rangle = \frac{1}{\sqrt{M}} \sum_{\sqrt{MX} = -\infty}^{+\infty} e^{ikX} \int_{[0,1]^2} dx dy G_{k/\sqrt{M}}(y) A(\sqrt{MX}, x, y) \to \int_{-\infty}^{+\infty} dx e^{ikX} \int_{[0,1]^2} dx dy A_S(X, x, y) = \int_{-\infty}^{+\infty} dx e^{ikX} A_S(X) ,
\]

\[
\langle \tilde{F}_0, k/\sqrt{M}, \rho \rangle = \frac{1}{\sqrt{M}} \sum_{\sqrt{MX} = -\infty}^{+\infty} e^{-ikX} \int_{[0,1]^2} dx dy \rho(\sqrt{MX}, x, y) \to \int_{-\infty}^{+\infty} dx e^{-ikX} \int_{[0,1]^2} dx dy \rho_S(X, x, y) = \int_{-\infty}^{+\infty} dx e^{-ikX} \rho_S(X) ,
\]

with double bar \((=)\) denoting the average with respect to \((x, y)\), the scaling limit of the expectation value finally becomes

\[
\lim_{M \to -\infty} \langle A \rangle_{\sqrt{M} \tau} = \int_{-\infty}^{+\infty} dx A_S(X) \int_{-\infty}^{+\infty} dX_0 \frac{1}{\sqrt{2\pi \tau}} \exp\left( -\frac{(X - X_0)^2}{2\tau} \right) \rho_S(X_0) ,
\]

(3.15)

which agrees precisely with the averaged observable calculated from the diffusion equation with the diffusion coefficient \( D = 1/2 \). Therefore, in the scaling limit, the deterministic dynamics of the multibaker map reduces to the diffusion process. It is worthwhile to note that 1) the intra-square information is averaged out automatically in the scaling limit and 2) the eigenfunctionals \( F_0 q \) and \( \tilde{F}_0 q \) reduce to the eigenfunction \( \exp(-ikX) \) of the diffusion operator (cf. eqs. before (3.15)). From this observation, the eigenfunctionals \( F_0 q \)
and $\tilde{F}_{0q}$ can be regarded as exact decay modes representing the diffusive relaxation. In other words, one can construct diffusive relaxation modes exactly as eigendistributions of the Frobenius–Perron operator with the aid of singular functions with fractal properties.

§4. Nonequilibrium states and eigenvalue problem of evolution operator

- nonequilibrium stationary states with flow in the multibaker map -

4.1 Equation of motion and conservation law

Here we consider nonequilibrium stationary states in the multibaker map, following the argument of Ref. 14. The problem formally corresponds to solving the eigenvalue equation $\hat{U}\rho = \rho$, but, as we have seen before, if one only considers states represented by density functions with respect to the Lebesgue measure, the equation admits the Lebesgue measure as the unique invariant measure. So we consider more general states represented by Borel measures $\mu$. Such states are completely specified by the cumulative function $G$:

$$G(n, x, y) \equiv \mu\left(\{[0, x] \times [0, y]\}_n\right), \quad (4.1)$$

where the subscript $n$ in $\{[0, x] \times [0, y]\}_n$ denotes that the rectangle $[0, x] \times [0, y]$ belongs to the $n$th square.

The equation of motion for the cumulative function is derived from the conservation of the measure (analog to the Liouville theorem):

$$G_{t+1}(n, x, y) = UG_t(n, x, y) \equiv \begin{cases} 
G_t\left(n + 1, \frac{x}{2}, 2y\right), & 0 \leq y < \frac{1}{2}, \\
G_t(n + 1, \frac{x}{2}, 1) + G_t\left(n - 1, \frac{x + 1}{2}, 2y - 1\right) \\
- G_t\left(n - 1, \frac{1}{2}, 2y - 1\right), & \frac{1}{2} \leq y \leq 1,
\end{cases} \quad (4.2)$$

where the subscript $t$ stands for the time. The operator $U$ precisely corresponds to the Frobenius–Perron operator $\hat{U}$.

For the multibaker map, one could introduce the flow of particles across the boundary between the $n$th and $(n + 1)$th unit squares. Under the multibaker map $\tilde{B}$, the half-square
(1/2, 1) × [0, 1) in the $n^{th}$ unit square moves to the right and the half-square $[0, 1/2) × [0, 1)$ in the $(n + 1)^{th}$ unit square moves to the left. Thus, the flow $J_{n|n+1}(t)$ from left to right at the $n$-$(n + 1)$ boundary and at time $t$ is given by

$$J_{n|n+1}(t) = \mu_t\left(\left\{\left[\frac{1}{2}, 1\right] × [0, 1)\right\}_n\right) - \mu_t\left(\left\{[0, 1/2) × [0, 1)\right\}_{n+1}\right)$$

$$= G_t(n, 1, 1) - G_t\left(n, \frac{1}{2}, 1\right) - G_t\left(n + 1, \frac{1}{2}, 1\right). \quad (4.3)$$

As expected, the flow $J_{n|n+1}$ together with $G_t(n, 1, 1)$ satisfy the equation of continuity

$$G_{t+1}(n, 1, 1) - G_t(n, 1, 1) = -\{J_{n|n+1}(t) - J_{n-1|n}(t)\}. \quad (4.4)$$

4.2 Homogeneous stationary states and their properties

Now we turn our attention to the stationary solutions of the equation of motion (4.2). Since $x$- and $y$-directions are mapped onto themselves in the multibaker map and are therefore independent, we can expect the existence of a product invariant measure, for which the cumulative function is a product of a function $F(n, x)$ of $x$ and a function $G(n, 1, y)$ of $y$:

$$G(n, x, y) = G(n, 1, y)F(n, x). \quad (4.5)$$

It then turns out that the equation of motion (4.2) is separable in the sense that it is separated into two distinct equations for $F(n, x)$ and $G(n, 1, y)$, where $F(n, 1/2)$ plays a role of a separation constant. The constant is set to be $\alpha$, which satisfies $0 < \alpha < 1$ because of the positivity of the invariant measure. The separated equations are given by

$$G(n, 1, y) = \begin{cases} \alpha G(n + 1, 1, 2y), & 0 \leq y < \frac{1}{2}, \\ (1 - \alpha)G(n - 1, 1, 2y - 1) + \alpha G(n + 1, 1, 1), & \frac{1}{2} \leq y \leq 1 \end{cases}, \quad (4.6a)$$

$$F(n, x) = \begin{cases} \alpha F(n - 1, 2x), & 0 \leq x < \frac{1}{2}, \\ (1 - \alpha)F(n + 1, 2x - 1) + \alpha, & \frac{1}{2} \leq x \leq 1 \end{cases}. \quad (4.6b)$$

The set of equations admits a unique solution for each $\alpha$ once two values of $G(n, 1, 1)$ are given. Two cases should be distinguished:
$\alpha \neq 1/2$, $0 < \alpha < 1$

In this case,

$$G(n, x, y) = f_\alpha(x) \left[ A_1 \left( \frac{1-\alpha}{\alpha} \right)^n f_{1-\alpha}(y) + A_2 f_\alpha(y) \right], \quad (4.7)$$

where $A_1$ and $A_2$ are constants determined by the boundary condition. The function $f_\alpha$ is defined as the unique solution of deRham's functional equation$^{(9,15)}$:

$$f_\alpha(x) = \begin{cases} \alpha f_\alpha(2x), & 0 \leq x < \frac{1}{2}, \\ (1-\alpha)f_\alpha(2x - 1) + \alpha, & \frac{1}{2} \leq x \leq 1. \end{cases} \quad (4.8)$$

which is a Lebesgue singular function, i.e., a monotonically increasing continuous function with zero derivatives almost everywhere$^{(9,15,16)}$.

As seen in (4.7), the intercell distribution is exponential with respect to the cell coordinate while the intracell distribution is singular since it is expressed by the Lebesgue singular function $f_\alpha$. The inter- and intra-cell distributions are depicted in Fig. 5a and 5b, 5c respectively. The corresponding flow is calculated from (4.3):

$$J_{n|n+1} = (1-\alpha)G(n, 1, 1) - \alpha G(n+1, 1, 1) = (1-2\alpha)A_2. \quad (4.9)$$

In this case, the flow is due to the term of (4.7) which is independent of the cell coordinate $n$. This part of the measure gives a weight $\alpha A_2$ to the left-hand half of each cell and a weight $(1-\alpha)A_2$ to the right-hand half. One iteration of the multibaker map induces a left-to-right flow of $(1-\alpha)A_2$ and a right-to-left flow of $\alpha A_2$, and as a result, a net flow of $(1-2\alpha)A_2$ from left to right. In other words, the difference of the weights of the half-cells is at the origin of the flow. In this sense, the flow (4.9) corresponds to a ballistic motion. On the contrary, the term of (4.7) which depends on the cell coordinate $n$ does not contribute to the net flow as a consequence of the cancellation between the ballistic and diffusive flows.

$(b) \quad \alpha = 1/2$

In this case,

$$G(n, x, y) = x \left\{ B_1 \left[ ny + T(y) \right] + B_2 y \right\}. \quad (4.10)$$
Fig. 5 Cumulative function ($\alpha = 2/5$)  
(a) $G(n,1,1)$ v.s. $n$  
(b) $G(5,x,1)$ v.s. $x$  
(c) $G(5,1,y)$ v.s. $y$

Fig. 6 Cumulative function ($\alpha = 1/2$; Fickian state)  
(a) $G(n,1,1)$ v.s. $n$  
(b) $G(5,x,1)$ v.s. $x$  
(c) $G(5,1,y)$ v.s. $y$
where $B_1$ and $B_2$ are constants determined from the boundary condition, and $T(y)$ is the Takagi function. We remark that the intercell distribution is here linear with respect to the cell coordinates while the intracell distribution is singular in the $y$-direction. The inter- and intra-cell distributions are depicted in Fig.6a and 6b, 6c respectively. The singularity of the distribution is due to the self-similarity of the Takagi function $T(y)$.

In this case, the flow is given by
\[
J_{n|n+1} = -\frac{B_1}{2} = -\frac{1}{2} \left[ G(n+1,1,1) - G(n,1,1) \right],
\]
(4.11)
Contrary to the previous case, the flow is here due to the nonuniformity of the distribution, i.e. to the term of (4.10) which depends on the cell coordinate $n$. The flow is here proportional to the gradient $G(n+1,1,1) - G(n,1,1)$ with a negative constant $-1/2$. As seen in the previous section, this constant gives the diffusion coefficient $D = 1/2$ of the multibaker map $\bar{B}$. Therefore, the relation (4.11) is nothing but Fick's law.

Further stationary states may be obtained by the time-reversal operation since the multibaker map $\bar{B}$ is symmetric under time reversal. It turns out, however, that no new states are obtained in case of $\alpha \neq 1/2$. For $\alpha = 1/2$, we have

(c) Time reversal of $\alpha = 1/2$

The cumulativ function $\bar{G}_{1/2}(n,x,y)$ of the time-reversed state is given by
\[
\bar{G}_{1/2}(n,x,y) \equiv \mu \left( I \{ [0,x] \times [0,y] \} \right)_n = \mu \left( \{ 1-y,1 \} \times (1-x,1) \right)_n
\]
\[
= G_{1/2}(n,1,1) + G_{1/2}(n,1-y,1-x) - G_{1/2}(n,1,y,1) - G_{1/2}(n,1,1-x)
\]
\[
= y \left\{ B_1 [nx - T(x)] + B_2 x \right\},
\]
(4.12)
for which the intercell distribution is identical to the original one. However, the original distribution (4.10) is regular in $x$ and singular in $y$ although the time reversed state (4.12) is singular in $x$ and regular in $y$. Because of the term with the Takagi function, the flow for the time-reversed state obeys an anti-Fick law
\[
\bar{J}_{n|n+1} = \frac{1}{2} B_1 = \frac{1}{2} \left[ \bar{G}_{1/2}(n+1,1,1) - \bar{G}_{1/2}(n,1,1) \right]
\]
\[
= D \left[ \bar{G}_{1/2}(n+1,1,1) - \bar{G}_{1/2}(n,1,1) \right],
\]
(4.13)
where the flow is positively proportional to the concentration difference. It is important to note the role of the intracell distribution in the derivation of this result.

Before closing this subsection, we remark important implications of the appearance of singular functions in the stationary states. Firstly, according to Mandelbrot, self-similar and singular functions like the Takagi function are referred to as fractals. In this respect, an important implication of our results is that nonequilibrium steady states of mechanical systems turn out to be typical fractal objects. Secondly, since the singular functions have no finite derivatives almost everywhere, the corresponding invariant measures (except in the case where $\alpha = 1/2$ and $B_1 = 0$) are not absolutely continuous with respect to the Lebesgue measure. As a consequence, they cannot be expressed in terms of density functions $\rho(n, x, y)$:

$$G(n, x, y) \neq \int_{0}^{x} dx' \int_{0}^{y} dy' \rho(n, x', y').$$

Therefore, it was essential to consider the time evolution of the measure directly represented by its cumulative distribution function rather than by its density function, in contrast with conventional treatments of statistical mechanics.

4.8 Physical states, fractals and irreversibility

The results in the previous section imply that the multibaker map admits uncountably many stationary states for a boundary condition imposed at the level of the intercell distribution. Indeed, uncountably many distributions are possible if we specify two numbers like $G(0, 1, 1)$ and $G(N, 1, 1)$ at both ends of a chain of length $N$. Such boundary conditions may be considered as coarse-grained boundary conditions in which only an averaged value is imposed on the distribution. However, as in the case of several dynamical systems(17–19), every one of these measures is not physically realizable. In order to specify the physical measures, we studied the time evolution of an open multibaker chain of scattering type where measures at the both edges of the chain are fixed as uniform Lebesgue measures with different densities(14). We then found that any initial distribution smooth in $x$-direction asymptotically tends, for $t \to +\infty$, to the stationary distribution with a uniform intercellular gradient and obeys Fick’s law. As time evolves, the distribution first
becomes uniform along the expanding direction on a short kinetic time scale given by the inverse of the Lyapunov exponent (corresponding to a decay rate of $\ln 2$). Thereafter, the linear concentration profile is achieved through diffusion on a longer hydrodynamic time scale given by the rate of escape out of the finite chain (corresponding to the decay rate $-\ln \cos(\pi/(N + 2))$ for the chain of length $N + 1$). It is important to note that the so-obtained stationary state is uniform along the expanding $x$-direction as the state (4.10).

This observation also suggests an important role of fractals in the emergence of irreversibility in the multibaker map. First we note that non-Fickian stationary states are all singular in the expanding direction. On the other hand, the multibaker map $\tilde{B}$ has a tendency to uniformize the distribution along the expanding direction. Therefore, the maintenance of a stationary state which is singular in the expanding direction requires the self-similarity of the initial states along the expanding direction in order to prevent the uniformization. This implies that, except for very special initial states prepared to be self-similar, almost all initial states converge to the one which is uniform in the expanding direction, and which obeys Fick's law. The stationary state with Fick's law is stable in this sense. In other words, it is the necessity of the fractal initial conditions for realizing non-Fickian states that makes those states exceptional and, thus, prevents them from being realized 'naturally'. Note that the singularity along the expanding direction of the anti-Fickian state, i.e., the stationary state obeying anti-Fick's law, is the very consequence of the singularity along the contracting direction of the Fickian state as well as the time-reversal symmetry of the dynamics. Therefore, in a sense, the fractality of the Fickian state automatically prevents the realization of its time-reversed state and, thus, can be regarded as the origin of irreversibility.

We also remark that the similar arguments can be applied to the decay modes discussed in the previous section. The diffusive relaxation mode $F_0q$ for $|\cos q| > 1/2$ corresponds to the cumulative function $G(n, x, y) = e^{i n q x} G_q(y)$. Its time-reversed state is represented by $\tilde{G}(n, x, y) = e^{i n q} G_q^*(x)y$. Then according to the equation of motion (4.2) for the cumulative function, the time-reversed state is found to grow in time:

$$U^t \tilde{G}(n, x, y) = \left( \frac{1}{\cos q} \right)^t \tilde{G}(n, x, y).$$  \tag{4.15}
Since the time-reversed state $\tilde{G}(n, x, y)$ is fractal along the expanding direction, it is exceptional and is not realized 'naturally' as the non-Fickian states. Hence, also in this case, the fractality of the relaxation modes prevents the unphysical growing modes from being realized.

§5. Perspective

We have rigorously constructed decay modes associated with (weak) relaxation processes as well as non-equilibrium stationary states with the aid of fractal functions for the baker and multibaker maps. The results seem to suggest that the fractality of relaxation modes as well as non-equilibrium stationary states is the origin of irreversibility. We believe that this is generally true for mixing systems. The reason is as follows. Suppose a given reversible system $\Sigma$ is mixing with respect to the Liouville measure, then any state described by a density function, i.e., by an absolutely continuous measure with respect to the equilibrium Liouville measure, weakly converges to the equilibrium state and there cannot be any other stationary state. Therefore, if the system $\Sigma$ admits non-equilibrium stationary states, they cannot be described by density functions, but should be described by measures which are singular with respect to the equilibrium Liouville measure. Because of the folding along the contracting direction, any distribution evolves into the one which has a fragmented structure along the contracting direction. Hence, non-equilibrium stationary states obtained as long-time limits are considered to be singular along the contracting direction. Moreover, the singularity can be regarded as the origin of irreversibility from the similar reason to that for the multibaker map. Firstly, since the time-reversal operation interchanges the contracting and expanding directions, the time-reversed non-equilibrium states are singular along the expanding direction. On the other hand, dynamics has a tendency of uniformize the distribution along the expanding direction. Therefore, to realize the time-reversed non-equilibrium states, one needs a fine tuning of the initial states so that they are self-similar along the expanding direction. Since such an initial state is exceptional, the time-reversed non-equilibrium states are not realized 'naturally'.

- 42 -
A similar picture about the appearance of irreversibility has been discussed by Horita and Mori\(^{(20)}\). They studied the distribution of the local Lyapunov exponents, which should be an even function of the argument if the system is time-reversal symmetric. They found an asymmetric distribution for the standard map, which corresponds to the emergence of irreversibility, and considered the instability of the time-reversed motion against errors as its reason. The key point of their arguments is the observation that any error entering into the reversed motion prevents the phase point from going back to its initial value as a result of the chaotic nature of the dynamics.

Moreover, recent studies have shown that certain fractal sets in the phase space, called fractal repellors, play an important role in the transport processes for conservative dynamical systems\(^{(10,21)}\). Let \( C \) be a physical quantity in question, then the fractal repellor consists of trajectories, for which \( C \)-values always fall in the interval \( c_0 \leq C \leq c_0 + \Delta \). Then the relaxation of the physical quantity \( C \) corresponds to the escape from the repellor and its rate can be obtained from the dynamical properties of the trajectories forming the repellor. This and the results discussed in the previous sections seem to show a new picture

\[
(\text{CHAOS}) \Rightarrow (\text{FRACTAL STRUCTURE}) \Rightarrow \text{IRREVERSIBILITY}
\]

of the emergence of irreversibility in conservative mixing dynamical systems.

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**References**