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To cite this article: Tetsuro Konishi 2006 J. Phys.: Conf. Ser. 31 43

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Dynamical order in Hamiltonian systems with long-range interaction

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Abstract. In this paper we introduce several systems which have ordered structure such as clusters by its own dynamics. The systems consist of particles with long-range interaction, just like many-body systems in astrophysics. Since the systems are Hamiltonian systems, the spatial structures thus formed are not “attractors” or asymptotic states we observe in the infinite future. Rather the states are observed in transiency or in the course of itinerancy among several quasi-stationary states.

1. Introduction
Spatial order and structure formation is important and interesting subject in various fields of physics. Crystals or lattice structure of solid is a traditional example. Formation of solar systems or galaxies are interesting examples in astrophysics. In addition, shapes of proteins are important when considering their biological functions (it is said that enzymes work correctly when their shape match the “target” molecules), and their shapes or forms (called “protein folding problem”) should be explained from physics.

One way to analyze this problem of is to use of statistical physics, where the spatial order which is realized is determined as what minimizes free energy.

However, this approach has fundamental limitation. That is, the order or structure have to be stationary and should be realized in asymptotically infinite future in time. On the other hand, transient behavior of systems are more and more of importance with the increase of time resolution in experimental situation, and traditional approach fails to cope with the situation.

For example, hydrogen bonding in liquid water molecules changes its network connection structure from time to time [1, 2]. Their dynamics is characterized by 1/f-type large fluctuation. Small cluster of metal atoms changes its shape [3]. Also it is known that large molecules (such as protein) in biological systems functions by transforming to appropriate shape in appropriate situation. All these examples suggests that we need some concept and methods to understand dynamic structure change beyond thermal fluctuation around equilibrium.

In this paper we introduce an alternative approach with the use of a concept “dynamical order”. Dynamical order is a kind of spatial structure shown in dynamical system with many degrees of freedom. It is not obtained as global minimum of free energy.

Since the symposium is interdisciplinary, the paper is intended to be eligible to non-specialist of dynamical systems. For that purpose, before introducing a definition of dynamical order and results, we add some words about some preliminaries. For more detailed and precise description for the introductory part please refer to reference textbooks [4, 5, 6].
This paper is organized as follows. First we give some definitions and preliminaries for Hamiltonian systems in sections 2 and 3. In section 4 we briefly introduce dynamical order, and some examples are shown in section 5.

2. Hamiltonian systems
Dynamical order can be found in many types of dynamical systems, and in this paper we focus on Hamiltonian systems.

Here we define “Hamiltonian systems” as a dynamical system \( \phi (\vec{q}, \vec{p}) \mapsto (\vec{q}', \vec{p}') \) whose temporal evolution is always a canonical transformation. That is,

\[
\sum_{i=1}^{n} dq_i \wedge dp_i = \sum_{i=1}^{n} dq_i' \wedge dp_i',
\]

where the symbol \( \wedge \) represents exterior product. Exterior product has bilinear property and anti-commutation property:

\[
dx \wedge (\alpha dy + \beta dz) = \alpha dx \wedge dy + \beta dx \wedge dz \quad (\alpha, \beta \in \mathbb{R}),
\]

\[
dx \wedge dy = -dy \wedge dx
\]

The relation (1) is equivalent to the invariance of Poisson bracket.

**example 1:** Systems which have Hamiltonian \( H(q,p) \) are Hamiltonian systems:

\[
\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.
\]

**example 2:** Symplectic mappings (defined later) are also included in this definition of Hamiltonian systems.

This definition is wider than usual definition of Hamiltonian systems (example 1). Here we adopt this extended definition because by doing so we can treat systems with Hamiltonian \( H(q,p) \) and symplectic mapping in parallel.

2.1. Poincaré mapping

![Figure 1](image.png)

**Figure 1.** left: schematic representation of Poincaré mapping. right: actual Poincaré mapping for Henon-Heiles model [7].

Before describing what is a symplectic mapping, let us introduce “Poincaré mapping”. Suppose one has a dynamical system \( \phi \) defined on continuous time. An orbit of the system is a continuous curve in the phase space (except for fixed points)

\[
P(t) \equiv (q_1(t), q_2(t), \cdots, q_n(t), p_1(t), p_2(t), \cdots, p_n(t))
\]
Suppose a hypersurface $\Pi$ in the phase space (say, $q_1 = 0$) and consider the intersection of the surface $\Pi$ and the orbit. Suppose the orbit crosses the surface at time $t = t_1, t_2, \cdots$. Then one has a sequence of points $P(t_1) \mapsto P(t_2) \mapsto \cdots$. Then, for any point $P$ on the surface $\Pi$ there is a point $P'$ uniquely defined for the original dynamical system such that

$$P' \equiv \text{the first point of the orbit start from } P \text{ which crosses } \Pi.$$  \hspace{1cm} (4)

Then the mapping $P \mapsto P'$ is called the **Poincaré mapping** (or Poincaré map) for the original dynamical system $\phi$. See Fig.1

Plotting Poincaré mapping we can distinguish regular orbits and chaotic orbits. In the phase space, regular orbits are confined on smooth low-dimensional manifold. Hence on Poincaré mapping regular orbits constitute smooth curves. On the other hand, chaotic orbits spread in the whole dimension of the phase space, hence on Poincaré mapping also chaotic orbits are shown as scattered points.

### 2.2. symplectic mapping

**Symplectic mapping** is a dynamical system which satisfies (1). It is important because

- If one make a Poincaré mapping from a Hamiltonian $H(q,p)$, then it can be proved that the resulting mapping is a symplectic mapping. Note that this property holds even when the temporal interval between the crossing varies from time to time.

- In some cases it is easy to analyze symplectic mappings, and of course they are numerically tractable than continuous time Hamiltonian systems.

**example 1: standard mapping**

$$\begin{align*}
(q, p) &\mapsto (q', p') , \; q, p \in \mathbb{R} , \; p' = p + \frac{K}{2\pi} \sin(2\pi q) \; (K > 0) , \; q' = q + p'.
\end{align*}$$  \hspace{1cm} (5)

Note that the rhs of the last equation includes $p'$, not $p$. (This ensures the symplectic property.) Symplectic property (1) of this mapping can easily be checked as follows:

$$\begin{align*}
dq' & = dq + dp' , \; dp' = dp + 2\pi K \cos(2\pi q) dq \\
 dq' \wedge dp' & = (dq + dp') \wedge dp' = dq \wedge dp' + dp' \wedge dp' = dq \wedge dp' = dq \wedge dp + 2\pi K \cos(2\pi q) dq \\
 & = dq \wedge dp + 2\pi K \cos(2\pi q) dq \wedge dq = dq \wedge dp
\end{align*}$$  \hspace{1cm} (6)

**Figure 2.** Phase space of standard map (5). $K = 0.85$. A stable fixed point at $(q, p) = (1/2, 0)$ (and $(1/2, 1)$, which is equivalent). Unstable fixed point at $(0, 0)$ and $(0, 1), (1, 0)$ and $(1, 1)$ (all are equivalent). Stable period-2 points exist at $(0, 1/2)$ and $(1/2, 1/2)$. Closed curves are quasi-periodic orbits. They surround periodic points. Scattered points are chaotic orbits. right: blow up of the left figure. Hierarchical structure is seen.

$$\begin{align*}
 dq' & = dq + dp' , \; dp' = dp + 2\pi K \cos(2\pi q) dq \\
 dq' \wedge dp' & = (dq + dp') \wedge dp' = dq \wedge dp' + dp' \wedge dp' = dq \wedge dp' = dq \wedge dp + 2\pi K \cos(2\pi q) dq \\
 & = dq \wedge dp + 2\pi K \cos(2\pi q) dq \wedge dq = dq \wedge dp
\end{align*}$$  \hspace{1cm} (7)
As one may have noticed, symplectic condition for 1-degrees of freedom system is equivalent to preservation of area element. Hence symplectic mapping of 1-degrees of freedom is often called as “area preserving mapping”.

Phase space portrait (orbits generated from many different initial conditions) is shown in the Fig. 2.

2.3. Importance of Hamiltonian systems
Thinking of the fact that most situations in nature is accompanied with dissipation, what is the advantage and use of considering Hamiltonian systems? Is it physically legitimate?

Dissipation occurs when one neglects some degrees of freedom, e.g., neglecting gas while describing point masses for stellar systems, neglecting water while describing molecules for biological systems, etc. Still it is effective to consider Hamiltonian model for not so long-time description.

2.4. conserved systems
Readers may have found a phrase “conserved systems” on papers or textbooks. The definition of “conserved systems” varies on the context, but in most cases the phrase “conserved systems” are used in the same meaning as “Hamiltonian systems”.

For some cases a “conserved system” is defined as a dynamical system where phase space volume element is conserved in the course of temporal evolution \((x_1, \ldots, x_n) \mapsto (x'_1, \ldots, x'_n)\):

\[
dx_1dx_2\cdots dx_n = dx'_1dx'_2\cdots dx'_n. \tag{8}\]

In Hamiltonian systems (8) is satisfied as “Liouville’s theorem”:

\[
dq_1dq_2\cdots dq_Ndp_1dp_2\cdots dp_N = dq'_1dq'_2\cdots dq'_Ndp'_1dp'_2\cdots dp'_N, \tag{9}\]

which can be derived by taking \(n\)-th power of symplectic property (1).

2.5. Dissipative systems
Opposite to Hamiltonian system there is a class of dynamical systems called dissipative systems. A damped linear oscillator is a simple example of dissipative system: \(\ddot{x} + \gamma \dot{x} + \omega^2 x = 0, \gamma > 0\).

Another example is the famous Lorentz equation [8]: \(\dot{X} = -\sigma X + \sigma Y, \dot{Y} = -XZ + rX - Y, \dot{Z} = XY - bZ\). This equation originates from model equation of thermal convection of fluids. \(X\) represents amplitude of velocity, \(Y\) and \(Z\) represent Fourier coefficient of thermal profile. In this case volume element of phase space shrinks by a rate \(- (\sigma + 1 + r)\).

In dissipative systems volume element of phase space is not conserved.

Note that the conserved systems is called “conserved” not because it has a conserved quantity. In fact, it is possible to think of an abstract dynamical system which has a conserved system and at the same time whose phase space volume element decays in time: \(\dot{x} = -\lambda x, \lambda > 0, \dot{y} = 0\).

Here the system shrinks in \(x\)-direction while keeping \(y\) = const..

2.6. Attractor
Attractor is, roughly speaking, a subset of phase space where orbits asymptotically converges. Typical attractors are shown in Fig.3.

If a system has attractors, then at first we focus on the attractors for understanding the system, because the system spend most of the time near or on the attractors.

Since phase space volume shrinks in approaching an attractor, Hamiltonian systems do not have attractor. (Remember that volume element is conserved in Hamiltonian systems.)

Hence we need another way to understand dynamics of Hamiltonian systems.
3. Typical behavior of Hamiltonian systems: traditional viewpoint

In this section we show some typical behavior of Hamiltonian systems.

3.1. Ergodicity, mixing, and relaxation

Hamiltonian systems with many degrees of freedom are, in other words, “isolated many body systems”. Although Hamiltonian systems do not have attractors, most of them are usually considered to relax to a specific state, called “thermal equilibrium”.

Dynamical explanation of thermal equilibrium is as follows:

(a) The system we are interested in is attached to a large system called “a heat bath”. (b) The whole system (the system we observe and the heat bath) is isolated, that is, a Hamiltonian system. (c) In the whole system microcanonical distribution is established. Every part on the energy surface (the surface $H(q, p) = E$ in the phase space of the whole system) is realized. (d) Then the probability distribution of the system we observe obeys canonical distribution.

Condition (c) is equivalent to that ergodicity is established in the whole system. That is, for most physical quantity $A$, time average $\overline{A}$ and phase space average $\langle A \rangle$ equals: $\overline{A} = \langle A \rangle$.

Note that a system is not always ergodic just because it is a Hamiltonian system. In fact, only a few systems are proved to be ergodic (an example is the infinite-particle ideal gas). Nonetheless thermal equilibrium were believed to hold for most Hamiltonian systems.

Mixing is another important property of dynamical systems. If, for any two regions A and B, $\mu(A \cap \phi^t(B))/\mu(B) \to \mu(A)$ for $t \to \infty$ holds, then the dynamical system is said to have mixing. ($\mu(A)$ is relative “volume” of the region A, and $\phi^t(B)$ is the image of the region B after time $t$.) Mixing is a kind of relaxation.

3.2. Long-time correlation, (also known as “1/f-type fluctuation”)

Another typical feature of Hamiltonian systems is that they often have strong temporal correlations. If the fluctuation is of thermal nature, they are naturally independent and temporal correlation of physical quantity of the system decays exponentially: $\langle A(t_0)A(t_0 + t) \rangle \propto e^{-t/\tau}$. (Average value of $A$ is subtracted.) In this case correlation is effectively negligible after finite time $\tau$, and $\tau$ is called the characteristic time for relaxation (of $A$). However, for many Hamiltonian systems we can observe another type of temporal correlation [9, 10, 11, 12, 13, 14, 15, 16]: $\langle A(t_0)A(t_0 + t) \rangle \propto (t/\tau)^{-\alpha}$. (Average value of $A$ is subtracted.) In this case the system has no characteristic time and the effect of initial condition remains forever. In this sense the system is called to have strong temporal correlation.

This power-law behavior in time domain is considered to be related with another power-law behavior, that is, self-similar hierarchical structure in the phase space, which is common in Hamiltonian systems [13, 14, 15, 16]. It is also seen in Fig.2.
4. Dynamical order
Dynamical order is a kind of spatial structure shown in dynamical system with many degrees of freedom. Now we will see some examples in the following section.

5. Examples of dynamical order
5.1. Formation and decay of cluster in globally coupled symplectic map
Here we introduce an example where we find a cluster of particles is dynamically formed and decays in globally coupled symplectic map [17, 18]. The map is defined as

\[
(x_i, p_i) \mapsto (x'_i, p'_i), \quad i = 1, 2, \ldots, N, \quad p'_i = p_i + K \sum_{j=1}^{N} \sin 2\pi (x_j - x_i), \quad x'_i = x_i + p'_i. \quad (10)
\]

(K > 0.) We have \( N \) particles with equal mass on a unit circle. \( x_i \) represents phase (divided by \( 2\pi \)) of \( i \)-th particle and \( p_i \) its conjugate momentum. This model has only one parameter \( K \). With the same value of parameter \( K \), this model shows two distinct phases of motion: clustered state and non-clustered (random) state just by changing initial condition.(Fig.4)

![Figure 4. clustered state(left) and non-clustered state for the map (10).](image)

Both states are chaotic, and so the system can go from one state to the other state within one orbit. That is, cluster is formed and decays and formed again, and so on.

Detailed analysis on Lyapunov exponents and vectors and phase space structure revealed that the clustered state is supported by hierarchical structure commonly found in chaos in Hamiltonian systems [17, 18].

5.2. Itinerant behavior in the mass sheet model
Next example is found in what is called “mass sheet model”, also known as 1-dimensional self gravitating system.

Creation and decay of clustered state we saw in the previous subsection (10) suggests that non-uniformity (heterogeneity) of the phase space is important for existence of dynamical order. Then what about gravitational systems or some similar physical models?

This problem is inspired from a problem in astrophysics. Equilibrium shape of self-gravitating system is spherically symmetric. However, observed shape of elliptical galaxies are, as the name tells, not spherical, but mostly they are triaxial. How can we explain this difference?

Previous studies tried to solve this problem by constructing regular orbit without spherical symmetry. But it is quite unlikely that many-body system interacting with non-linear potential with (almost surely) irregular initial condition run on some special exact solution. They should behave rather chaotically. Hence we may understand the spatial structure as “dynamically supported”, or as dynamical order, not in equilibrium.

Going back to mathematical model, we start with the Hamiltonian

\[
H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + 2\pi G m^2 \sum_{i \neq j} |x_i - x_j|, \quad -\infty < x_i < \infty. \quad (11)
\]
This model is schematically represented by Fig.5.

**Figure 5.** left: A schematic picture of the model (11). right: a schematic representation of itinerant behavior of the model.

In this model thermal equilibrium is considered to be what is known as “isothermal state”. In the course of numerical time evolution we found that for some orbits the system once relaxes to equilibrium but then goes back to some other “quasi-equilibrium” state [20, 21, 22, 23]. We found that the system has many quasiequilibria and the system moves from one quasi-equilibrium to another by emitting and swallowing particles with extremely high energy. The process is summarized in Fig.5. This is also an example of “chaotic itinerancy” [24].

5.3. Emergence of spatial power-law correlation in the mass sheet model

In the same model we see in the previous subsection (eq.(11) and Fig.5), another interesting dynamical order is discovered. By choosing a “cold initial state” (initial kinetic energy is set to zero) with random spatial configuration, the system spontaneously creates power-law spatial correlation, instead of just monotonically relaxing to thermal equilibrium [25, 26, 27]. See Fig.6.

**Figure 6.** Formation of structure with power-law correlation. left: $\mu$-space, right: spatial 2-point correlation function. Power-law behavior $\xi(r) \propto r^{-\alpha}$ is seen. Initial condition : $x_i$: uniformly random in $[0,1]$, $v_i = 0$, $N = 2^{15}$, $t = 9.375$.

6. Summary

We have seen three examples of dynamical order where spatial structure is constructed in non-equilibrium situation in Hamiltonian dynamical systems. Origin of dynamical order comes from
inhomogeneity of phase space. Dynamical order will be of much importance when we adventure into the world of non stationary systems.

Acknowledgments
I would like to thank the organizers for this excellent symposium. Thanks are also due to active collaborators, Hiroko Koyama, Toshio Tsuchiya, Naoteru Gouda, Yoshiyuki Y. Yamaguchi and Kunihiko Kaneko. Working with them is pleasant and stimulating experience.

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