Poincaré cycle of an Ehrenfest multiurn model in a one-dimensional ring

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We study an Ehrenfest multiurn model of a one-dimensional ring, generalizing the directed transport in the previous model to arbitrary transports. We analytically study the evolution of the system and calculate the Poincaré cycle for given transport probabilities. The result shows that the average number of balls in an urn evolves according to the transport probability, but the Poincaré cycle is only related to the initial configuration.

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The Poincaré *ergodic theorem* states that a system having a finite energy and confined to a finite volume will return to the initial state. But the Boltzmann *H theorem* singles out a preferred direction of time; it is the so-called *reversal paradox* for historical interest [1]. Since Ehrenfest brought out his *urn model* to show the process of approaching equilibrium in precise terms, the paradox was apparently resolved. The urn model has played a very important role in fundamental concepts of statistical mechanics [2] (see Fig. 1).

In a previous paper we studied an Ehrenfest multiurn model with directed transport [3] defined for N balls distributed between M urns. In that model the urns are connected sequentially, and the periodic boundary condition is used, i.e., the first and the Mth urns are connected. The dynamics of the model is defined as follows: (i) One of the N balls is selected randomly. (ii) The ball selected from the ith urn is placed into the $(i+1)$th urn determinedly. This model can be exactly solved, and it confirms the ergodic theory in that the entire accessible phase space will be traversed at an explicit Poincaré cycle. However, it is a stringent requirement to place the selected ball into the next urn. Usually, to describe the stochastic motion of a large number of particles one uses a diffusion equation, which implies nonzero outward flux on both the left-hand and right-hand sides of a given urn. Thus it is desirable to relax the original transport model to place the selected ball into any other urn with certain probability.

In general, the direction and the distance between the original and the target urns determine the probability of arriving at a target urn. In this paper we study the system with the new dynamics: (i) One of the balls is selected randomly. (ii) The ball selected from the ith urn is placed into the $(i+j)$th urn with probability p_j. Hereafter we denote $\vec{p} \equiv (p_1, p_2, \ldots, p_M)$ as the *jumping rate*. As before, we number the urns from 1 to M, and define the $(M+1)$th urn as the first urn. The distribution of the N balls in the M urns is given by the *state vector* $|m_1, m_2, \ldots, m_M\rangle \equiv |\mathbf{m}\rangle$, where m_i is the number of balls in the ith urn. At the start, the initial state vector is denoted as $|\mathbf{m}_0\rangle$. After d steps, the system has several possible states. The transition probability defined as the probability from state $|\mathbf{m}_0\rangle$ to state $|\mathbf{m}\rangle$ can be written as $\langle \mathbf{m}|S^d|\mathbf{m}_0\rangle$, where S represents the operation in one step, and these state vectors are orthonormal. Accordingly, the transition probability corresponding to the dth step and the $(d-1)$th step satisfies the recursion relation

$$\langle m_1, m_2, \ldots, m_M|S^d|\mathbf{m}_0\rangle = \sum_{i=1}^{M}\sum_{j=1}^{M} \frac{p_j(m_i+1)}{N} \times \langle \ldots, m_i+1, \ldots, m_{i+j}-1, \cdots |S^{d-1}|\mathbf{m}_0\rangle, \tag{1}$$

where $m_{M+k}=m_k$. In addition, any state must satisfy the conservation of balls and the conservation of total jumping rate

$$\sum_{i=1}^{M} m_i = N, \quad \text{and} \quad \sum_{i=1}^{M} p_i = 1. \tag{2}$$

We first calculate the average number of balls appearing in the kth urn after d steps. According to the definition, we get

$$\langle m_k\rangle_d = \sum_{\{\mathbf{m}\}} m_k \langle \mathbf{m}|S^d|\mathbf{m}_0\rangle, = \left(1-\frac{1}{N}\right)\langle m_k\rangle_{d-1} + \sum_{j=1}^{M} \frac{p_j \langle m_{k-j}\rangle_{d-1}}{N}. \tag{3}$$

Here we have used the constraint as spelled out by Eq. (2). For solving Eq. (3), we define an $M\times 1$ column vector $\mathcal{M}_d$ as

$$[\mathcal{M}_d]_k \equiv \langle m_k\rangle_d, \quad \{k=1,\ldots,M\}, \tag{4}$$

and an $M\times M$ matrix S_{av} as

$$[S_{av}]_{i,j} \equiv \delta_{i,j}\left(1-\frac{1}{N}\right) + \frac{p_{i-j}}{N}, \quad \{i,j=1,\ldots,M\}. \tag{5}$$

Then Eq. (3) can be calculated recursively:

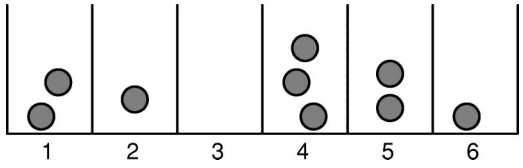

FIG. 1. An example of the urn model: a configuration for a system with six urns and nine balls. The state vector for this configuration is $|\mathbf{m}\rangle = |2,1,0,3,2,1\rangle$.

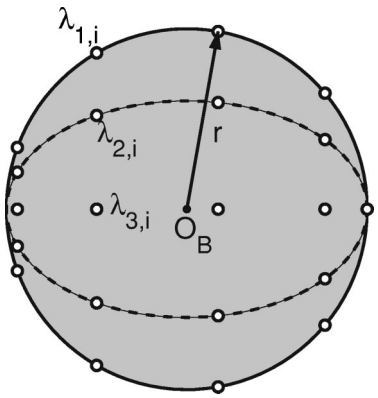

FIG. 2. Eigenvalues $\{\lambda_{k,i}\}$ of the matrix $S_{k,av}$. Here $r=1/N$ is the radius of the reference circle, and $O_B(1-1/N,0)$ is its center.

$$\mathcal{M}_d = S_{av}\mathcal{M}_{d-1} = S_{av}^d \mathcal{M}_0, \tag{6}$$

where $\mathcal{M}_0$ represents the initial state.

Under the rotation symmetry, we found Eq. (6) has same transformation matrix with Ref. [3]. For convenience, we define

$$\theta \equiv \frac{2\pi}{M}, \quad q_m \equiv \exp(im\theta), \quad \{m=1,2,\ldots,M\}, \tag{7}$$

vectors $\vec{q}_m$ and an $M\times M$ matrix Q:

$$\vec{q}_m \equiv (q_m, q_m^2, \ldots, q_m^M), \quad \text{and} \quad Q_{m,n} \equiv (q_m)^n. \tag{8}$$

The transformation matrix R of S_{av} is given by

$$R = R^{-1*} = \frac{Q}{\sqrt{M}}. \tag{9}$$

The eigenvalues of S_{av} (see Fig. 2) are

$$\lambda_m = 1 - \frac{1}{N} + \frac{1}{N}\sum_{i=1}^{M} p_i q_m^{i*} = 1 - \frac{1-\vec{p}\cdot\vec{q}_m^*}{N}, \tag{10}$$

and the components of the eigenvalue matrix Λ are

$$\Lambda_{m,n} = \delta_{m,n}\lambda_m. \tag{11}$$

Thus we can get the average number of balls in k urn after d steps as

$$\langle m_k\rangle_d = (S_{ave}^d \mathcal{M}_0)_k = (R\Lambda^d R^{-1}\mathcal{M}_0)_k = \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M} q_i^{(k-j)}\lambda_i^d m_{j,0}. \tag{12}$$

Considering a specific jumping rate,

$$\{p_i | p_1 = p, \quad p_{M-1} = q = (1-p), \quad p_i = 0 \quad (\text{others})\}, \tag{13}$$

we name it the *pq model*. The urn model in Ref. [3] has $p=1$. For the $N=1$ case, the problem is reduced to the random walk in a one-dimensional ring. Figure 2 shows the eigenvalues for the $M=9$ case: $\{\lambda_{1,i}\}$, $\{\lambda_{2,i}\}$, and $\{\lambda_{3,i}\}$ correspond to the cases of $p=1$, $p=0.8$, and $p=0.5$, respectively. In general, the eigenvalues are all distributed inside the gray circle region.

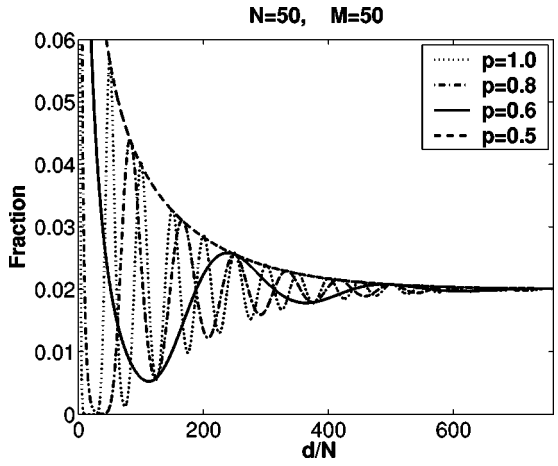

FIG. 3. In the pq model, some examples of the average number of balls evolve from all balls in the last urn. Here we plot "fraction"$=\langle m_M\rangle_d/N$.

Let us now consider a simple example. Suppose initially all balls are in the last urn, that is,

$$m_{1,0} = m_{2,0} = \cdots = m_{M-1,0} = 0, \quad m_{M,0} = N. \tag{14}$$

Then according to Eq. (12),

$$\langle m_M\rangle_d = \frac{N}{M}\sum_{j=1}^{M}\lambda_j^d. \tag{15}$$

The behavior of $\langle m_M\rangle_d/N$ is a universal function for a fixed M in the large N limit, that is, Eq. (15) can be approximated by

$$\lim_{N\to\infty}\frac{1}{N}\langle m_M\rangle_d = \frac{1}{M}\sum_{j=1}^{M}\exp[-\tau(1-\vec{p}\cdot\vec{q}_j^*)], \tag{16}$$

where we have defined the time τ as

$$\tau \equiv \frac{d}{N}. \tag{17}$$

In the long run, the system will approach equilibrium by $\langle m_k\rangle_\infty = N/M$, when every urn has reached its stationary state.

Figure 3 shows several cases for different p values of the pq model at $N=50$, $M=50$. In each case we observe that before the system arrives at its equilibrium, $\langle m_k\rangle_d$ undergoes several times of oscillation, which seems to have different behavior for different jumping rate. However, in all cases we observe the same damping rate, which means they have the same relaxation time before they approach the equilibrium.

These phenomena can be understood in a global sense. We define the center-of-mass (COM) as

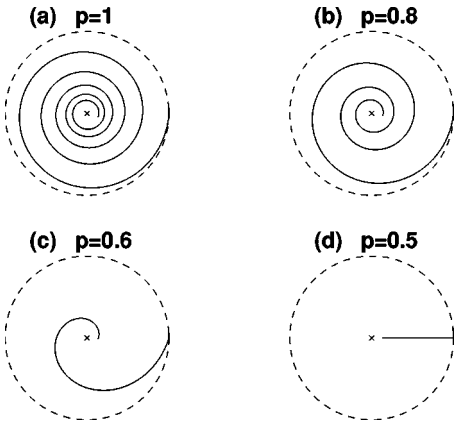

FIG. 4. Four COM curves in the pq model.

$$\mathrm{COM} \equiv \frac{1}{N} \sum_{k=1}^{M} e^{i\phi_k} \langle m_k \rangle_d , \tag{18}$$

where $\phi_k = -k\theta$ is the "phase angle" of the kth urn.

In general $\mathrm{COM} \equiv re^{i\phi}$ is a complex number, with $r = |\mathrm{COM}|$ satisfying $0 \leqslant r \leqslant 1$. ϕ is the phase angle of COM, and $d\phi/d\tau$ ($\tau = d/N$) represents the angular velocity of COM. The norm r here gives us the information of the distribution of the N balls. Substituting Eq. (12) into Eq. (18), we get

$$\mathrm{COM} = \lambda_1^d . \tag{19}$$

In the pq model, we get

$$\mathrm{COM} \approx e^{-\tau\theta^2/2} e^{-i(2p-1)\tau\theta}, \tag{20}$$

hence $r = \exp(-\tau\theta^2/2)$, and $\phi = -(2p-1)\tau\theta$.

The COM curve is approximately described by a spiral circulating inside a unit circle with an angular frequency (with respect to $\tau = s/N$) $-(2p-1)\theta = -2\pi(2p-1)/M$ (clockwise), consistent with the oscillation behaviors of the $\langle m_M \rangle_d / N$ curve discussed before.

When

$$\tau > \frac{M^2}{2\pi^2}, \tag{21}$$

the balls become widely distributed. $M^2/2\pi^2$ is the *relaxation time* of the pq model. Figure 4 plotted the pq model from $d=0$ to $d = M^2 N/\pi^2$ at $M=50$, $N=50$ for $p = (1.0, 0.8, 0.6, 0.5)$.

We now derive $\langle \mathbf{m} | S^d | \mathbf{m}_0 \rangle$—the transitional probability from $|\mathbf{m}_0\rangle$ to $|\mathbf{m}\rangle$ after d steps. We define the matrix S with components

$$S_{\mathbf{m}\mathbf{m}'} = \langle \mathbf{m} | S | \mathbf{m}' \rangle . \tag{22}$$

Here S is a $H_N^M \times H_N^M$ matrix, we name it as *state matrix*, and $|\mathbf{m}\rangle$ is a H_N^M column vector. According to Eq. (1), the matrix S has components

$$S_{\mathbf{m}\mathbf{m}'} = \sum_{i=1}^{M} \sum_{j=1}^{M} \frac{p_j m_i'}{N} \times \delta_{m_1, m_1'} \cdots \delta_{m_i, m_i'-1} \cdots \delta_{m_{i+j}, m_{i+j}'+1} \cdots \delta_{m_M, m_M'} . \tag{23}$$

The eigenvalue equation can be written as

$$\sum_{\{\mathbf{m}'\}} S_{\mathbf{m}\mathbf{m}'} \phi_{\mathbf{m}'}(\mathbf{n}) = \gamma_{\mathbf{n}} \phi_{\mathbf{m}}(\mathbf{n}), \tag{24}$$

where $\mathbf{n}$ characterizes the eigenvalue $\gamma_{\mathbf{n}}$. Here we have set $\phi_{\mathbf{m}}(\mathbf{n}) = 0$ for those $|\mathbf{m}\rangle = |m_1, m_2, \ldots, m_M\rangle$ that do not satisfy constraint (2).

To diagonalize S, we construct a generating function for $\phi_{\mathbf{m}}(\mathbf{n})$ and transform the matrix eigenvalue Eq. (24) to its differential equation form.

Defining the generating function as

$$f_{\mathbf{n}}(x_1, \ldots, x_M) \equiv \sum_{\{\mathbf{m}\}} \phi_{\mathbf{m}}(\mathbf{n}) x_1^{m_1} x_2^{m_2} \cdots x_M^{m_M}, \tag{25}$$

multiplying $x_i^{m_i}$ over all i on both sides of Eq. (24), and summing over all $\{\mathbf{m}\}$, we get the desired differential equation

$$\sum_{i=1}^{M} \sum_{j=1}^{M} p_j \frac{x_{i+j}}{N} \partial_{x_i} \ln[f_{\mathbf{n}}(x_1, \ldots, x_M)] = \gamma_{\mathbf{n}} . \tag{26}$$

Define

$$x_{q_k} \equiv x_1 q_k + x_2 q_k^2 + \cdots + x_M q_k^M ; \tag{27}$$

then the complete solution of $f(x_1, \ldots, x_M)$ can be written as

$$f_{\mathbf{n}}(x_1, \ldots, x_M) = \prod_{k=1}^{M} (x_{q_k})^{n_k} . \tag{28}$$

Here $f_{\mathbf{n}}(x_1, \ldots, x_M)$ is a homogeneous Nth power function. The vector $\mathbf{n} = [n_1, n_2, \ldots, n_M]$ satisfies

$$\sum_{k=1}^{M} n_k = N, \tag{29}$$

thus the eigenvalue is

$$\gamma_{\mathbf{n}} = \frac{1}{N} \sum_{j=1}^{M} \sum_{k=1}^{M} n_k q_k^{j*} p_j = \frac{\mathbf{n} \cdot Q^* \cdot \vec{p}}{N} . \tag{30}$$

The $\mathcal{S}$ matrix can be expressed as

$$U^{-1} S U = \Gamma , \tag{31}$$

where Γ is the eigenvalue matrix with components $\Gamma_{\mathbf{m}\mathbf{m}'} = \gamma_{\mathbf{m}} \delta_{\mathbf{m}\mathbf{m}'}$. The matrix elements of the transformation matrix U and its inverse U^{-1} are

$$U_{\mathbf{mn}}=\phi_{\mathbf{m}}(\mathbf{n}),\quad U^{-1}_{\mathbf{nm}}=\frac{1}{M^N}\phi_{\mathbf{n}}(\tilde{\mathbf{m}}), \tag{32}$$

where $\phi_{\mathbf{m}}(\mathbf{n})$ according to Eq. (25) is the coefficient of $\Pi x_i^{m_i}$ that appears in the expansion of Eq. (28), and $\tilde{\mathbf{m}}$ is defined as

$$\tilde{\mathbf{m}}\equiv[m_{M-1},m_{M-2},m_{M-3},\ldots,m_1,m_M]. \tag{33}$$

Finally we obtain the desired solution of $\langle\mathbf{m}|S^d|\mathbf{m}_0\rangle$

$$\langle\mathbf{m}|S^d|\mathbf{m}_0\rangle=(U\Gamma^sU^{-1})_{\mathbf{mm}_0}$$

$$=\frac{1}{M^N}\sum_{\mathbf{m}'}\gamma^d_{\mathbf{m}'}\phi_{\mathbf{m}}(\mathbf{m}')\phi_{\mathbf{m}'}(\tilde{\mathbf{m}}_0). \tag{34}$$

The *Poincaré cycle* is defined as the expected number of steps of a system to first return to the initial state. Now, giving an initial state $\mathbf{m}_0$, the transition probability for the system to return to this state after d steps is

$$\langle\mathbf{m}_0|S^d|\mathbf{m}_0\rangle=\frac{1}{M^N}\sum_{\mathbf{m}}\gamma^d_{\mathbf{m}}\phi_{\mathbf{m}_0}(\mathbf{m})\phi_{\mathbf{m}}(\tilde{\mathbf{m}}_0)\equiv\mathcal{P}(d). \tag{35}$$

Note that $\mathcal{P}(d)$ does not preclude the possibility that the initial state has already been rearrived at before.

Define a function $\mathcal{Q}(d)$ as the probability for the first return to the initial state at the dth step, which relates to $\mathcal{P}(d)$ via

$$\mathcal{P}(d)=\mathcal{Q}(d)+\sum_{k=1}^{d-1}\mathcal{Q}(k)\mathcal{P}(d-k), \tag{36}$$

and hence the Poincaré cycle can be obtained,

$$\mathcal{C}_P=\sum_{d=0}^{\infty}d\,\mathcal{Q}(d). \tag{37}$$

In a previous paper [3] we got the relation of the Poincaré cycle with components of the state vectors as

$$\mathcal{C}_P=\frac{M^N}{\phi_{\mathbf{m}_0}(\mathbf{m}_{\gamma=1})\phi_{\mathbf{m}_{\gamma=1}}(\tilde{\mathbf{m}}_0)}. \tag{38}$$

Now since

$$\phi_{\mathbf{m}_0}(\mathbf{m}_{\gamma=1})=\binom{N}{\mathbf{m}_0},\quad \phi_{\mathbf{m}_{\gamma=1}}(\tilde{\mathbf{m}}_0)=1, \tag{39}$$

we have

$$\mathcal{C}_P=\frac{M^N}{\binom{N}{\mathbf{m}_0}}. \tag{40}$$

Here the factor

$$\binom{N}{\mathbf{m}_0}=\frac{N!}{m_{1,0}!m_{2,0}!\cdots m_{M,0}!}$$

is the degeneracy of the configuration $\mathbf{m}_0$. The Poincaré cycle implies that the fluctuations in the noise range repeat themselves. This result shows that the period of the fluctuation is inversely proportional to the degeneracy of its configuration, but independent of the jumping rate. In nature, systems are not always really ergodic; examples are glasses, folding proteins and harmonic crystals.

Finally, we would like to mention the applications of various urn models. They provide very good descriptions of granular and glass systems [4–7]. Lipowski *et al.* studied an urn model that characterized by a parameter T as the temperature [8–10]. It was shown to undergo a symmetry-breaking transition at critical temperature T_c. Our paper corresponds to the case of $T=0$. Recently, Shim *et al.* solved the Lipowski urn model analytically in the two urn cases [11]. It would be of interest to extend this to the multiurn models.

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