

Drifting diffusion on a circle as continuous limit of a multiurn Ehrenfest model

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We study the continuous limit of a multibox Ehrenfest urn model proposed before by the authors. The evolution of the resulting continuous system is governed by a differential equation, which describes a diffusion process on a circle with a nonzero drifting velocity. The short time behavior of this diffusion process is obtained directly by solving the equation, while the long time behavior is derived using the Poisson summation formula. They reproduce the previous results in the large M (number of boxes) limit. We also discuss the connection between this diffusion equation and the Schrödinger equation of some quantum mechanical problems.

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In a previous study [1] we proposed a generalized Ehrenfest urn model [2] with N balls and M urns that arranged periodically along a circle. The evolution of the system is governed by a directed stochastic operation. Using the standard matrix diagonalization procedures together with a multivariable generating function method, we have solved the problem completely. We found that for a generic $M > 2$ case the average number of balls in a certain urn oscillates several times before it reaches a stationary value. We also obtained the Poincaré cycle [3], i.e., the average time interval required for the system to return to its initial configuration. The result is simply given by M^N , which indicates that the fundamental assumption of statistical mechanics holds in this system. Taking $M = 2$, our model reproduces all the results of the original Ehrenfest urn model [2].

In this paper, we further study the continuous limit (the large M and N limit) of the proposed multiurn model. We show that by defining a density function ρ as the continuous limit of the fraction $f_i = \langle m_i \rangle / N$, i.e., the average number of balls in the i th urn divided by N , the continuous limit of the model exists if we also define the drifting velocity and diffusion constant appropriately. The evolution of ρ in space-time is then governed by a differential equation, which can be solved under proper initial condition and boundary conditions. The results obtained in this paper are in agreement with those obtained before by the standard matrix diagonalization method. Since for even a generic M -urn and N -ball case the Poincaré cycle M^N is too huge to be experienced, the evolution of the system can in practice be treated as unrepeatable, thus the average quantities considered here become more important than those of microstate details.

We start from the Eq. (4) of Ref. [1]:

$$\langle m_i \rangle_s = \left(1 - \frac{1}{N} \right) \langle m_i \rangle_{s-1} + \frac{1}{N} \langle m_{i-1} \rangle_{s-1}, \quad (1)$$

where $\langle m_i \rangle_s$ denotes the number of balls in the i th urn after s steps, and N is the total number of the balls. This result can be understood as follows. At each time step a certain ball has the probability $1/N$ of being chosen and thrown into the next urn, thus the increment of $\langle m_i \rangle_s$ in one step caused by the

positive contribution $\langle m_{i-1} \rangle_{s-1} / N$ coming from the last urn, and the negative contribution $-\langle m_i \rangle_{s-1} / N$ leaking out into the next urn.

Equation (1) can be rewritten as

$$f_i(s) - f_i(s-1) = -\frac{1}{N} [f_i(s-1) - f_{i-1}(s-1)], \quad (2)$$

where $f_i(s) \equiv \langle m_i \rangle_s / N$. Adding $[f_{i+1}(s-1) - f_{i-1}(s-1)] / 2N$ to both sides of Eq. (2), we get

$$\begin{aligned} \frac{f_i(s) - f_i(s-1)}{\Delta t} + \frac{\Delta x}{N \Delta t} \left[\frac{f_{i+1}(s-1) - f_{i-1}(s-1)}{2 \Delta x} \right] \\ = \frac{(\Delta x)^2}{2N \Delta t} \left[\frac{f_{i+1}(s-1) - 2f_i(s-1) + f_{i-1}(s-1)}{(\Delta x)^2} \right], \end{aligned} \quad (3)$$

where Δt represents the time interval in one step, and Δx stands for the center-center distance between two neighboring urns. Taking the continuous limit, we obtain

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial x} = D \frac{\partial^2 \rho}{\partial x^2}, \quad (4)$$

where we have used the substitutions

$$f_i(s) \rightarrow \rho(x, t), \quad \frac{\Delta x}{N \Delta t} \rightarrow v, \quad \frac{(\Delta x)^2}{2N \Delta t} \rightarrow D. \quad (5)$$

It is clear that Eq. (4) is a diffusion equation. Since the model is defined on a circle, we replace x by ϕ , v by ω , Δx by θ , and the diffusion equation becomes

$$\frac{\partial \rho}{\partial t} + \omega \frac{\partial \rho}{\partial \phi} = D \frac{\partial^2 \rho}{\partial \phi^2}. \quad (6)$$

Before further exploring Eq. (6), here we give a simple and general derivation of the diffusion equation. Note that the conservation of probability implies

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}, \quad (7)$$

where $\rho(\mathbf{r}, t)$ is the probability density and $\mathbf{J}(\mathbf{r}, t)$ is the probability current density. Now, the probability current can be written as the sum of two terms, one for the “diffusion part,” and the other for the “drifting part” of the probability carriers (the balls), that is,

$$\mathbf{J} = -D\nabla\rho + \rho\mathbf{v}, \quad (8)$$

where D is the diffusion constant and \mathbf{v} is the drifting velocity caused by some pumping force.

Substitute Eq. (8) into Eq. (7), we obtain

$$\frac{\partial \rho}{\partial t} = D\nabla^2\rho - \nabla \cdot (\rho\mathbf{v}). \quad (9)$$

We further assume that $\nabla \cdot \mathbf{v} = 0$ (incompressible fluid; one special case is that $\mathbf{v} = \text{constant}$), then we have

$$\frac{\partial \rho}{\partial t} = D\nabla^2\rho - \mathbf{v} \cdot \nabla\rho, \quad (10)$$

which is the desired diffusion equation and has the same form as Eq. (4) and (6).

On a straight line, the above equation becomes Eq. (4), and we adopt the boundary condition

$$\rho(\infty, t) = \rho(-\infty, t) = 0. \quad (11)$$

On a circle, Eq. (10) becomes Eq. (6), with boundary condition

$$\rho(\phi, t) = \rho(\phi + 2\pi, t). \quad (12)$$

Now we find the solutions ρ for the one-dimensional (1D) diffusion equations on a straight line (4) and on a circle (6), respectively. Assuming the initially condition

$$\rho(x, 0) = \delta(x), \quad (13)$$

the solution on a line can be obtained by Fourier transform method [4]:

$$\rho(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x-vt)^2}{4Dt}\right]. \quad (14)$$

Similarly, for the circle problem, given the initial condition

$$\rho(\phi, 0) = \delta(\phi), \quad (15)$$

we obtain

$$\rho(\phi, t) = \frac{1}{\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \exp\left[-\frac{(\phi - \omega t + 2n\pi)^2}{4Dt}\right]. \quad (16)$$

In deriving Eq. (16), we have used the identity

$$\int_{-\infty}^{\infty} f(x) dx = \sum_{n=-\infty}^{\infty} \int_0^{2\pi} f(x + 2n\pi) dx \quad (17)$$

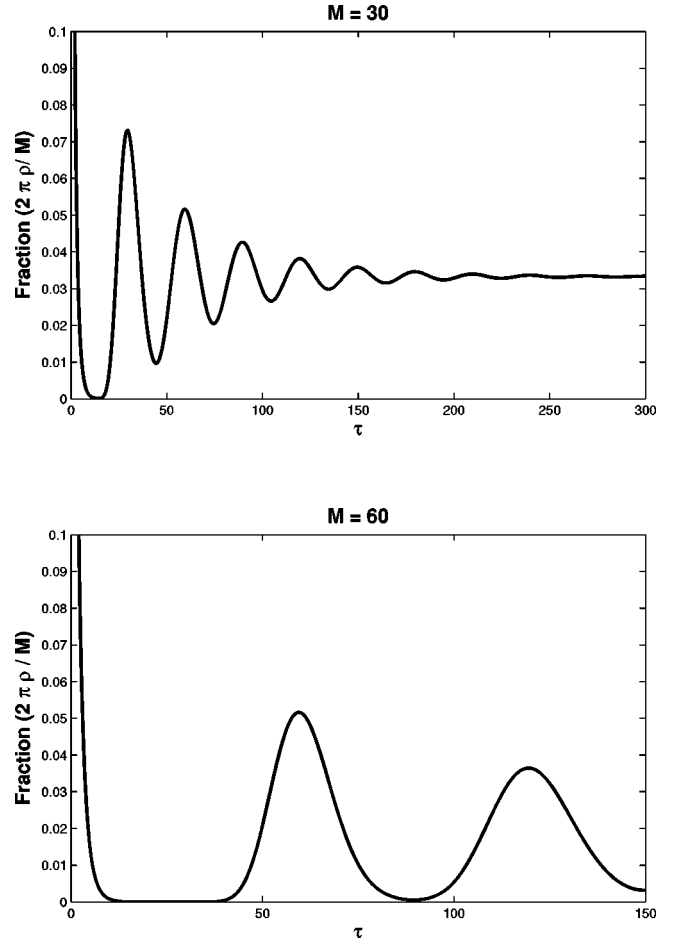


FIG. 1. Fraction curves calculated from the exact solution of the diffusion equation.

for a localized function $f(x)$, and we have treated the “circle problem” as an “infinite-folded line problem.”

As such, the “center of mass” can be written by

$$\begin{aligned} \text{COM} &= \int_0^{2\pi} d\phi \rho(\phi, t) \exp(i\phi) \\ &= \frac{1}{\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \int_0^{2\pi} d\phi e^{-[(\phi + 2n\pi - \omega t)^2/4Dt] + i(\phi + 2n\pi)} \\ &= \exp(-Dt + i\omega t), \end{aligned} \quad (18)$$

which is equivalent to Eq. (32) of Ref. [1] if we define

$$Dt = \frac{\theta^2}{2} \tau = \frac{2\pi^2}{M^2} \tau, \quad \omega t = \theta \tau = \frac{2\pi}{M} \tau. \quad (19)$$

Here τ and θ are defined as

$$\tau \equiv \frac{t}{N\Delta t} = \frac{s}{N}, \quad \theta = \Delta x = \frac{2\pi}{M}. \quad (20)$$

Now we compare the results with those in Ref. [1]. Figure 1 shows the results from Eq. (16), (19), and (20) for the cases $M=30$ and $M=60$. As one can see, the present equation

indeed reproduce the results of Ref. [1] in the large M limit. The parameter N does not appear here because the motion of each particle is independent in our model.

Note that although for a small t the expression (16) is good enough to be a fast convergent series, however, when t becomes large, Eq. (16) converges slowly. In this situation we use a more accurate expression for ρ :

$$\begin{aligned}\rho(\phi, t) &= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{-n^2 D t + i n (\phi - \omega t)} \\ &= \frac{1}{2\pi} + \frac{1}{\pi} \sum_{n=1}^{\infty} e^{-n^2 D t} \cos[n(\phi - \omega t)],\end{aligned}\quad (21)$$

which can be derived from Eq. (16) using the *Poisson summation formula* [5]

$$\sum_{n=-\infty}^{\infty} f(na) = \frac{2\pi}{a} \sum_{n=-\infty}^{\infty} g\left(\frac{2n\pi}{a}\right).\quad (22)$$

Here $f(x)$ is a localized function, and

$$g(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx\quad (23)$$

is its Fourier transform.

We now consider some solvable generalizations of Eq. (4) and (6). Note that the ratio between D and ω in our model is fixed

$$\frac{D}{\omega} = \frac{\theta}{2} = \frac{\pi}{M}.\quad (24)$$

To relax this restriction, we modify our urn model by assuming that at each time step the picked ball can have probability p to be put into the next urn and probability $q = 1 - p$ to be put into the previous urn. Hereafter we call this modified model the pq model. The pq model is also solvable [6] by using methods like those used in Ref. [1]. The continuous limit of the pq model can be derived from the recurrence relation for f_i :

$$f_i(s) = \left(1 - \frac{1}{N}\right) f_i(s-1) + \frac{p}{N} f_{i-1}(s-1) + \frac{q}{N} f_{i+1}(s-1),\quad (25)$$

where

$$p + q = 1,$$

and

$$0 \leq p, q \leq 1.\quad (26)$$

Adding

$$\frac{(p-q)}{2N} [f_{i+1}(s-1) - f_{i-1}(s-1)]$$

to both sides of Eq. (25), it becomes

$$\begin{aligned}\frac{f_i(s) - f_i(s-1)}{\Delta t} + \frac{2(p-q)\Delta x}{2N\Delta t} \left[\frac{f_{i+1}(s-1) - f_{i-1}(s-1)}{2\Delta x} \right] \\ = \frac{(\Delta x)^2}{2N\Delta t} \left[\frac{f_{i+1}(s-1) - 2f_i(s-1) + f_{i-1}(s-1)}{(\Delta x)^2} \right].\end{aligned}\quad (27)$$

Now define

$$f_i(s) \rightarrow \rho(x, t), \quad \frac{(p-q)\Delta x}{N\Delta t} \rightarrow v, \quad \frac{(\Delta x)^2}{2N\Delta t} \rightarrow D,\quad (28)$$

then we get a continuous equation of the form (4), without the restriction (24). One special case is $p = q = 1/2$, which has a zero drifting velocity, and the evolution of the system is governed by pure diffusion process—the random walk.

For another generalization we assume that the drifting velocity v varies with time, that is,

$$\frac{\partial \rho}{\partial t} + v(t) \frac{\partial \rho}{\partial x} = D \frac{\partial^2 \rho}{\partial x^2}.\quad (29)$$

Defining $x(t)$ as the time integral of $v(t)$:

$$x(t) = \int_0^t v(t') dt',\quad (30)$$

and adopting the initial condition (13), then

$$\rho(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - x(t))^2}{4Dt}\right].\quad (31)$$

Similarly, for the diffusion equation on a circle with a time-dependent $\omega(t)$ and initial condition (15)

$$\frac{\partial \rho}{\partial t} + \omega(t) \frac{\partial \rho}{\partial \phi} = D \frac{\partial^2 \rho}{\partial \phi^2},\quad (32)$$

and the solution is

$$\rho(\phi, t) = \frac{1}{\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} \exp\left[\frac{-(\phi - \phi(t) + 2n\pi)^2}{4Dt}\right].\quad (33)$$

Here

$$\phi(t) = \int_0^t \omega(t') dt'.\quad (34)$$

The reason why v and ω can freely vary with time relies on Eq. (28). Recall that in our original multiurn Ehrenfest model or the pq model both the time interval between two steps and the distance (angle difference) between two urns are undefined. Thus in deriving the continuous limit of these models we do not have to adopt a constant Δt at each step or a fixed Δx ($\Delta \theta$) between two neighboring urns. If we relax the restriction in Eq. (28) and modify them to Δt_s and Δx_i ($\Delta \theta_i$), then the continuous limit of these quantities lead to $v(t)$ or $\omega(t)$.

It is interesting to note that the solutions for the diffusion equation (10) can be used to find the wave function or

Green's function of some time-dependent quantum mechanical problems [7]. The main idea is to define a transformation appropriately between the parameters used in the diffusion equation (10) or (4) and (6) and those used in the corresponding Schrödinger equations. For instance, consider a quantum point particle of charge q and mass m moving under the influence of a vector potential $\mathbf{A}(t)$ [8]:

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} \left(-i\hbar \nabla - \frac{q\mathbf{A}(t)}{c} \right)^2 \psi, \quad (35)$$

here we have assumed that $\mathbf{A}(t)$ is a function of time t only. Executing the transformation

$$\psi = \exp \left[\frac{1}{2i\hbar m} \int_0^t \left(\frac{qA(t')}{c} \right)^2 dt' \right] \tilde{\psi}, \quad (36)$$

then Eq. (35) can be rewritten as

$$\frac{\partial \tilde{\psi}}{\partial t} = \frac{i\hbar}{2m} \nabla^2 \tilde{\psi} + \left(\frac{q\mathbf{A}}{mc} \right) \cdot \nabla \tilde{\psi}. \quad (37)$$

Comparing Eq. (37) with (10), we find that they can be transformed to each other by the substitution

$$D \leftrightarrow \frac{i\hbar}{2m}, \quad \mathbf{v} \leftrightarrow - \left(\frac{q\mathbf{A}}{mc} \right), \quad \rho \leftrightarrow \tilde{\psi}. \quad (38)$$

To be more specific, consider the case where the particle is moving on a circle of radius 1. Suppose the circle is lying on the xy plane and centered at $(x, y) = (0, 0)$. The vector potential can be chosen as $\mathbf{A}(t) = A(t) \hat{e}_\phi$ and is generated by a time-dependent magnetic flux $\Phi(t)$ tube going through the origin and pointing along the z axis

$$\mathbf{A}(t) = A(t) \hat{e}_\phi = \frac{\Phi(t)}{2\pi} \hat{e}_\phi. \quad (39)$$

Choosing the initial condition as

$$\tilde{\psi}(\phi, 0) = \psi(\phi, 0) = \delta(\phi), \quad (40)$$

then

$$\psi(\phi, t) = \frac{U(t)}{\sqrt{2\pi i\hbar t/m}} \sum_{n=-\infty}^{\infty} \exp \left[\frac{-(\phi - \phi(t) + 2n\pi)^2}{(2i\hbar t/m)} \right]. \quad (41)$$

Here

$$U(t) = \exp \left[\frac{1}{2i\hbar m} \int_0^t \left(\frac{qA(t')}{c} \right)^2 dt' \right], \quad (42)$$

and

$$\phi(t) = - \frac{q}{mc} \int_0^t A(t') dt'. \quad (43)$$

Note that the ψ in Eq. (41) is nothing but the Green's function $G(\phi, \phi_0; t, t_0)$ for the quantum particle with $\phi_0 = t_0 = 0$. If $A(t) = 0$, Eq. (41) gives the well known results [9]:

$$G(\phi; t) = \frac{1}{\sqrt{2\pi i\hbar t/m}} \sum_{n=-\infty}^{\infty} \exp \left[- \frac{(\phi + 2n\pi)^2}{(2i\hbar t/m)} \right], \quad (44)$$

and

$$G(\phi; t) = \frac{1}{2\pi} + \frac{1}{\pi} \sum_{n=1}^{\infty} e^{-n^2(i\hbar/2m)t} \cos n\phi \quad (45)$$

for small and large t , respectively.

In conclusion, we have derived the continuous limit of a mutium Ehrenfest model, which is a diffusion equation with a drifting velocity term. Solving the equation gives us the correct time evolution behavior of the ball distribution. A transformation was introduced, which changes the solution of the diffusion equation to the corresponding solution for the problem of a quantum particle moving under the influence of a time-varying magnetic field.

Note added. After submission of the present report we noticed another paper concerning diffusion equation [10], where the dynamics of the breakdown of granular clusters was investigated using a multiurn Ehrenfest model. In their model the evolution of particle concentration in one urn depends on both the local concentration and the concentration in the neighboring urns, and the transition probabilities to the two neighboring urns are equal. For a broken cluster they found both the normal and anomalous diffusion behaviors depending on the form of flux function they choose. Now, if one modifies the transition probability to an asymmetric form as our pq model (their model in the $T \rightarrow \infty$ limit is our pq model with $p = q = 1/2$), then other features such as concentration oscillation might appear. However, we expect that the diffusion exponent has nothing to do with the asymmetry, since it contributes only a drift velocity in the continuous limit.

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- [1] Y.M. Kao and P.G. Luan, Phys. Rev. E **67**, 031101 (2003).
 [2] P. Ehrenfest and T. Ehrenfest, Phys. Z. **8**, 311 (1907).
 [3] K. Huang, *Statistical Mechanics* (Wiley, New York, 1987).
 [4] J. Mathews and R. L. Walker, *Mathematical Methods of Physics*, 2nd ed. (Addison-Wesley, Reading, MA, 1971).
 [5] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, New York, 1953).
 [6] Yee-Mou Kao and Pi-Gang Luan, Phys. Rev. E (to be published).

- [7] J. Bauer, Phys. Rev. A **65**, 036101 (2002).
 [8] R. P. Feynman, R. B. Leighton, and M. L. Sands, *The Feynman Lectures on Physics* (Addison-Wesley, Reading, 1989), Vol. III.
 [9] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics*, 2nd ed. (World Scientific, Singapore, 1995).
 [10] F. Coppex, M. Droz, and A. Lipowski, Phys. Rev. E **66**, 011305 (2002).