

RANDOM WALK, DIFFUSION AND WAVE EQUATION*

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One-dimensional random walk is analyzed. First, it is shown that the classical interpretation of random walk reaching Lord Rayleigh's analysis should be completed. Further, an attention is called to the fact that the parabolic diffusion is not an unique interpretation, but also the wave (or hyperbolic) equation can be deduced. It depends on the accepted scale of the length of step h and duration of the step τ in the walk, whether Fick–Smoluchowski's diffusion or a wave process is obtained. Only additional arguments, such as positivity of distribution function or positivity of the entropy growth, can help to choose the proper physical model. Also, the infinite diffusion velocity paradox in connection with Einstein's formula is explained.

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1. Introduction

The concept of *random walk* was first introduced by Karl Pearson in 1905 [1]. However, earlier in 1880, Lord Rayleigh applied this process (without naming it) to analyse a certain random vibration problem [2, 3].

Random walk is an idealisation of a path realised by a succession of random steps, and can serve as a model for different stochastic processes. It is discussed in mathematics, physics, biology, economics and finance. It may denote the path traced by a Brownian particle as it travels in a liquid, the search path of a foraging animal and the stock fluctuating price, as well [4–15].

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Below, after summaries of Rayleigh's and Kac's approaches, an analysis of difference scheme realised by the random walk is given. It is shown that, depending on choice of scale of length of path and time needed to perform the path, we obtain either Fickian (parabolic) diffusion or wave (hyperbolic) equation.

Last, some consequences of hyperbolicity of wave diffusion equation are discussed and the source of the infinite speed the paradox is explained. It lies in a mathematical passage to infinitesimal increments in random walk, but is substantiated by Einstein's formula, verified by experiments.

One-dimensional random walk proceeds on the one-dimensional lattice: the integer number line. The walker can only jump to neighbouring sites of the lattice: he starts at 0 and at each step moves $+1$ or -1 with prescribed probability. Below, initially, the discussion is conducted for the symmetrical random walk. In Sections 8–10, the non-symmetrical case is treated.

1.1. Lord Rayleigh's approach

Lord Rayleigh inquired what results from the composition of a large number n of equal vibrations of amplitude unity, of the same period, and of phases accidentally determined [2, 3]. First, he analysed the case in which the possible phases are restricted to two opposite phases, what is equivalent to regarding the amplitudes as at random positive or negative. If there is as many positive as negative, the result is zero.

Adopting the Bernoulli binomial method, Rayleigh considered N independent combinations, each consisting of n unit vibrations. When N is sufficiently large, the statistics become regular and the number of combinations in which the resultant amplitude is found to be x may be denoted by $Nf(n, x)$, where f is definite function of n and x . Let each of the N combinations receives another random contribution of ± 1 . Only those combinations can subsequently possess a resultant x which originally had amplitudes $x - 1$ and $x + 1$. Half of the former, and half of the latter number (symmetrical case of the random walk) will acquire the amplitude x , so that the number required is

$$\frac{1}{2}Nf(n, x - 1) + \frac{1}{2}Nf(n, x + 1).$$

Because this should be identical with the number corresponding to $n + 1$ and x , we obtain

$$f(n + 1, x) = \frac{1}{2}f(n, x - 1) + \frac{1}{2}f(n, x + 1) \quad (1)$$

what can be written in the form

$$f(n + 1, x) - f(n, x) = \frac{1}{2} \{f(n, x - 1) - 2f(n, x) + f(n, x + 1)\}. \quad (2)$$

This can be regarded as a difference counterpart of the differential equation

$$\frac{\partial f}{\partial n} = \frac{1}{2} \frac{\partial^2 f}{\partial x^2} \tag{3}$$

which describes process of diffusion (or heat) propagation [16–18].

1.2. Mark Kac’s approach

Systematic deduction of the diffusion equation from the random walk (the non-symmetric case included) we owe to Kac [19].

Consider a walker which moves along the x -axis by steps. Each step has the length h and time duration τ . The walker in each step can move either h to the right (event R) or h to the left (event L). At each step, the probability of moving to the right and moving to the left is the same, and equals $1/2$.

The probability that among n events the events R are produced in number k and events L in number $n - k$, is given by Bernoulli’s distribution

$$P_n(k) = \frac{n!}{k!(n - k)!} \cdot \frac{1}{2^n} \quad \text{with} \quad \sum_{k=0}^n P_n(k) = 1. \tag{4}$$

Arriving the particle at position $x = mh$ after time $t = n\tau$ needs $m = k - (n - k) = 2k - n$ steps. Notice that $m + n = 2k$ what means that m and n are both simultaneously even or uneven, *cf.* Fig. 1.

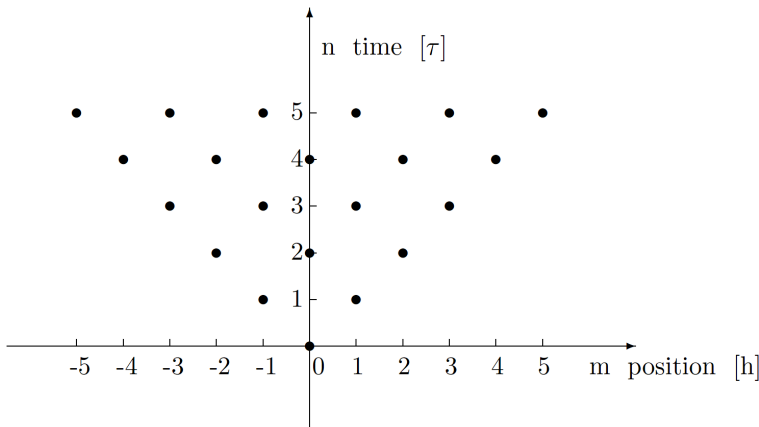


Fig. 1. One-dimensional random walk in successive tosses, numbered by n . All possible random walk position outcomes are denoted by m . Unit of distance is h , unit of time is τ .

Let at time $t = 0$ the particle be at $x = 0$. Let $f_n(m)$ denote the probability of the event that after time $t = n\tau$ the particle will be at $x = mh$. Because $k = (n + m)/2$ and $n - k = (n - m)/2$

$$f_n(m) = \frac{n!}{\frac{n+m}{2}! \frac{n-m}{2}!} \cdot \frac{1}{2^n}. \tag{5}$$

This implies, otherwise obvious iterative relation given by Eq. (1). Equation (2) can be written as

$$\frac{f_{n+1}(m) - f_n(m)}{\tau} = \frac{h^2 f_n(m + 1) - 2f_n(m) + f_n(m - 1)}{h^2} \tag{6}$$

or after substitution

$$D = \frac{h^2}{2\tau} \tag{7}$$

to the form

$$\frac{f_{n+1}(m) - f_n(m)}{\tau} = D \frac{f_n(m + 1) - 2f_n(m) + f_n(m - 1)}{h^2}. \tag{8}$$

Its differential analog takes the form of diffusion (heat) equation

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}. \tag{9}$$

Of course, Eq. (3) is a specific case of Eq. (9), when $h = 1$ and $\tau = 1$.

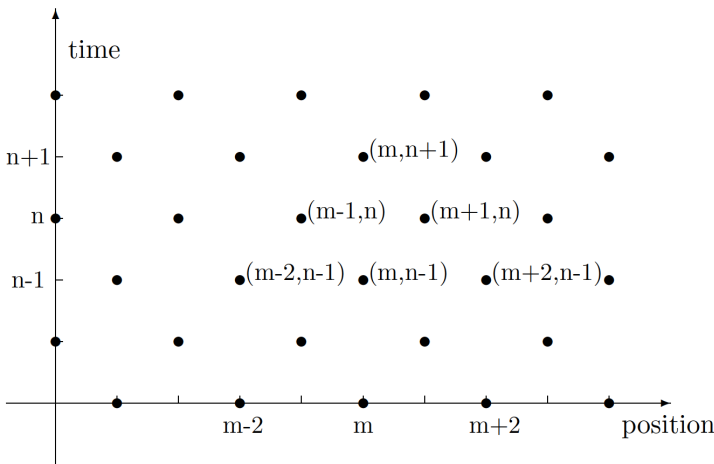


Fig. 2. One-dimensional random walking scheme. Numbers in round brackets are the position-time coordinates of relevant points in $[h, \tau]$ units, respectively.

Be aware, however, that at the given time moment n , the distance between neighbouring positions is $2h$ and that to the given position m , the walker can return from neighbouring position after time 2τ . Thus, the point $(m, n + 1)$ is inaccessible for the walker being in (m, n) in the time period τ , and in Eq. (2) or (8) the subtrahend function $f_n(m)$ is not determined, as the point m, n is omitted in the random walk, cf. Fig. 2.

It is also important to notice that the diffusion Eq. (9) was obtained after the limits $h \rightarrow 0$ and $\tau \rightarrow 0$ were taken in such a way that the coefficient D given by Eq. (7) was kept constant.

2. Random walk and wave equation

As the $f_n(m)$ appearing in (6) does not exist in a real random walk process, cf. Fig. 2, at the end of the previous section, we have indicated an apparent inconsistency of the Rayleigh–Kac scheme. It can be easily verified that the realistic scheme reads

$$\frac{f_{n+1}(m) - f_{n-1}(m)}{2\tau} = \frac{h^2}{2\tau} \frac{f_{n-1}(m + 2) - 2f_{n-1}(m) + f_{n-1}(m - 2)}{4h^2} \quad (10)$$

and differs from Eqs. (2) or (8) by taking as the difference step for the space and time instead h and τ the quantities $2h$ and 2τ , respectively.

Indeed, the iteration (1) written in the form

$$f_{n+1}(m) = \frac{1}{2} \{f_n(m + 1) + f_n(m - 1)\}$$

implies analogical relations

$$f_n(m + 1) = \frac{1}{2} \{f_n(m + 2) + f_n(m)\}$$

and

$$f_n(m - 1) = \frac{1}{2} \{f_{n-1}(m) + f_{n-1}(m - 2)\}$$

what, after combination, gives

$$f_{n+1}(m) = \frac{1}{4} \{f_{n-1}(m + 2) + 2f_{n-1}(m) + f_{n-1}(m - 2)\} . \quad (11)$$

Hence, we get Eq. (10), which can be transformed into Fick’s diffusion equation, after Rayleigh–Kac’s prescription.

However, this prescription is not *a priori* unique. Let us introduce the continuous function $f(x, t)$ which in nodal points $(mh, n\tau)$, m, n — integer, takes values

$$\{f(x, t)\}_{(mh, n\tau)} = f(mh, n\tau) = f_n(m) .$$

Applying Taylor's expansion about the point $(mh, (n-1)\tau)$ and keeping consequently terms including the second order, we get the following approximation of the finite forward difference

$$f_{n+1}(m) - f_{n-1}(m) = 2\tau \frac{\partial f}{\partial t}(mh, (n-1)\tau) + \frac{1}{2}(2\tau)^2 \frac{\partial^2 f}{\partial t^2}(mh, (n-1)\tau). \quad (12)$$

In the similar manner, we get

$$f_{n-1}(m+2) = f_{n-1}(m) + 2h \frac{\partial f}{\partial x}(mh, (n-1)\tau) + \frac{1}{2}(2h)^2 \frac{\partial^2 f}{\partial x^2}(mh, (n-1)\tau)$$

and

$$f_{n-1}(m-2) = f_{n-1}(m) - 2h \frac{\partial f}{\partial x}(mh, (n-1)\tau) + \frac{1}{2}(2h)^2 \frac{\partial^2 f}{\partial x^2}(mh, (n-1)\tau).$$

Addition of two least equations by sides and arranging of terms gives the following expression for the second order central difference

$$f_{n-1}(m-2) - 2f_{n-1}(m) + f_{n-1}(m+2) = (2h)^2 \frac{\partial^2 f}{\partial x^2}(mh, (n-1)\tau). \quad (13)$$

We substitute relations (12) and (13) into (10). Thus, by proceeding in the similar manner as it was done by Rayleigh and Kac, but keeping the second derivatives in both, spatial and temporary variables, we get

$$\tau \frac{\partial^2 f}{\partial t^2} + \frac{\partial f}{\partial t} = \frac{h^2}{2\tau} \frac{\partial^2 f}{\partial x^2} \quad (14)$$

or

$$\frac{\partial^2 f}{\partial t^2} + \frac{1}{\tau} \frac{\partial f}{\partial t} = c^2 \frac{\partial^2 f}{\partial x^2}, \quad (15)$$

where we have denoted

$$c^2 = \left(\frac{h}{\tau}\right)^2. \quad (16)$$

Equation (15) has the form of wave equation of diffusion (or heat) propagating with the velocity c , discussed in [20–25]. We have also

$$\tau = \frac{D}{c^2}. \quad (17)$$

In this derivation, the quantity τ is small but finite, and is known as the *relaxation time* for a phenomenon described by Eq. (15).

Notice also that, as a result of many-body stochastic interactions, the velocity c is $\sqrt{2}$ times smaller then the velocity of singular step equal to h/τ . Analogical diminishing of velocity is presumed in three dimensions [25].

The reason of obtaining different results (9) and (15) based on the same difference algorithm (1) lies in admission of the second time derivative in the substitution of finite difference equation by a differential one.

3. Wave equation of diffusion

Macroscopic derivation of the wave equation of diffusion is based on the assumption that the stream of the particles j is not generated by the density gradient instantaneously (as in process described by the Fick's diffusion equation), but it is delayed by a time τ_0 , called a relaxation time.

The continuity relation links temporal variation of the density of particles $f(x, t)$ with the spatial variation of the particle stream j , and in one dimension it reads

$$\frac{\partial f}{\partial t} = -\frac{\partial j(x, t)}{\partial x}, \tag{18}$$

and if combined with Fick's law of diffusion

$$j = -D \frac{\partial f}{\partial x}, \tag{19}$$

where D stands for the diffusion coefficient, the classical diffusion equation (9) is obtained.

However, if there exists a certain time delay, τ_0 , between change of the density gradient and the stream generated by it

$$j(x, t + \tau_0) = -D \frac{\partial f}{\partial x}$$

then, under assumption of a sufficiently small τ_0 , after expansion of the left-hand side of the last equation into power series of τ_0 , one gets

$$j(x, t) + \tau_0 \frac{\partial j(x, t)}{\partial t} = -D \frac{\partial f}{\partial x}. \tag{20}$$

Hence, after applying the (one-dimensional) divergence operator

$$\frac{\partial j(x, t)}{\partial x} + \tau_0 \frac{\partial}{\partial t} \frac{\partial j(x, t)}{\partial x} = -D \frac{\partial^2 f}{\partial x^2},$$

and after using the continuity equation (18), one obtains

$$\tau_0 \frac{\partial^2 f}{\partial t^2} + \frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2} \tag{21}$$

what is known as the wave or hyperbolic diffusion equation, cf. Eq. (15), in distinction of the parabolic diffusion equation (9).

Equation (21) is the telegrapher's type equation, cf. [26, 27]. It is worth to notice that such an equation was obtained also by Kac [24] after adopting another scheme of interpretation of the non-symmetric random walk. Namely, Kac considered a particle starting from the original $x = 0$ and always moving with the speed v . It can move either in positive direction or in the negative direction. Each time the particle arrives at a lattice point, there is a probability of reversal of direction. With these assumptions, Eqs. (15) or (21) can be obtained.

4. Entropy of the system

To answer which way of interpretation of random walk, either this which leads to parabolic diffusion or to hyperbolic one, the entropy growth of two processes should be compared.

4.1. Entropy

Let us assume that the distribution density f is positive. After [28, 29], for the continuum limit of the Shannon entropy of our problem is accepted

$$S = - \int_{\Omega} f(x, t) \ln f(x, t) dx. \quad (22)$$

Here, Ω denotes the infinite one-dimensional interval in which the diffusion is considered. We find by differentiation

$$\frac{dS}{dt} = - \int_{\Omega} \frac{\partial f(x, t)}{\partial t} \ln f(x, t) dx - \int_{\Omega} \frac{\partial f(x, t)}{\partial t} dx, \quad (23)$$

or after using the continuity relation (18)

$$\frac{dS}{dt} = \int_{\Omega} \ln f(x, t) \frac{\partial j(x, t)}{\partial x} dx + \int_{\Omega} \frac{\partial j(x, t)}{\partial x} dx. \quad (24)$$

By the (one-dimensional) divergence theorem, the second term at right-hand side is zero, if there are no particle flows at infinity, and

$$\frac{dS}{dt} = - \int_{\Omega} \ln f(x, t) \frac{\partial j(x, t)}{\partial x} dx.$$

Once again, the integration by parts gives

$$\frac{dS}{dt} = \int_{\Omega} \frac{1}{f(x, t)} \frac{\partial f(x, t)}{\partial x} j(x, t) dx$$

or

$$\frac{dS}{dt} = \int_{\Omega} \frac{1}{f(x, t)} \frac{1}{D} \left\{ j(x, t) + \tau_0 \frac{\partial j(x, t)}{\partial t} \right\} j(x, t) dx, \quad (25)$$

where the relation (20) was exploited.

4.2. Entropy growth

The last result can be written as

$$\frac{dS}{dt} = \overline{J^2} + \frac{1}{2} \tau_0 \frac{d\overline{J^2}}{dt}, \tag{26}$$

where

$$\overline{J^2} \equiv \int_{\Omega} \frac{1}{f(x, t)D} j(x, t)^2 dx. \tag{27}$$

In the limiting case, when the entropy production rate vanishes ($dS/dt = 0$), we get by Eq. (26)

$$\overline{J^2} = \overline{J_0^2} e^{-2t/\tau_0}. \tag{28}$$

On the other hand, for $\tau_0 = 0$, the entropy production rate according to Eq. (26) is always non-negative. For $\tau_0 \neq 0$, by integration of Eq. (26), we find

$$\overline{J^2} - \overline{J_0^2} e^{-2t/\tau_0} = \frac{2t}{\tau_0} e^{-2t/\tau_0} \int_0^t \frac{dS}{dt'} e^{2t'/\tau_0} dt'. \tag{29}$$

If

$$\overline{J^2} > \overline{J_0^2} e^{-2t/\tau_0}, \tag{30}$$

then also $dS/dt > 0$.

In general, however, the criterion (26) is too weak to judge whether the process is thermodynamically consistent [28]. One can argue that for sufficiently small τ_0 , this inequality may be satisfied, and the wave equation of diffusion seems to be affirmed in some experiments [30, 31].

4.3. Density distribution

Mathematical form of Eq. (21) is identical with the telegrapher’s equation, which describes the voltage or current on an electrical transmission line with distance and time [26, 27]. Its Green’s function reads

$$f(x, t) = 2\pi c e^{-\frac{t}{2\tau_0}} \mathcal{J}_0 \left(\frac{1}{2\sqrt{D\tau_0}} \sqrt{x^2 - c^2 t^2} \right) \eta(ct - x), \tag{31}$$

where

$$c^2 \equiv \frac{D}{\tau_0}$$

denotes square of the velocity of diffusive wave and $\eta(x)$ is the unit step function (equal 1 for x non-negative, and zero for x negative).

This solution achieves non-zero values for finite x only, $x \leq ct$, but, in spite of the definition of probability, it admits also the negative values due to the properties of Bessel function \mathcal{J}_0 , and for this reason it cannot be adequate for the problem of diffusion.

For the same reason, one cannot look for the solution of Eq. (21) in form of a damped wave

$$f = f_0 e^{i(kx - \omega t)}$$

which is typical to the telegrapher's equation.

5. Fick's diffusion

Green's function for the one-dimensional diffusion equation (9) reads

$$f(x, t) = \frac{1}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}}. \quad (32)$$

From this formula, we deduce that if in a region whose dimension is of the order of length ℓ , a non-uniform distribution is introduced, the order of magnitude t_R of the time required for the distribution to become approximately the same throughout the region is

$$t_R \approx \frac{\ell^2}{D}. \quad (33)$$

The time t_R may be called the *relaxation time* for the density equalisation process [17].

The diffusion process described by formula (32) has the property that for any $t > 0$, the function $f(x, t) > 0$ in the whole space, it is the effect of the initial perturbation, is propagated instantaneously through all space. Some authors interpret this property as an admission of the infinite speed of mass distribution and hence, the violation of the rules of physics. To avoid such contradiction, called a paradox, they use a hyperbolic diffusion equation (15), instead of the parabolic (9). For example, they use the hyperbolic diffusion equation to study the transport process of electrolytes in media such as gels and porous media [30, 31].

However, the paradox is only apparent and does not object to the physical reality. The mass of substance which is to be found at time t further from the source, then a is

$$\int_a^\infty f(x, t) dx = \int_a^\infty \frac{1}{2\sqrt{\pi Dt}} e^{-\frac{x^2}{4Dt}} dx \quad (34)$$

and as $a \rightarrow \infty$, it becomes negligibly small.

6. Arising of the paradox

From Bernoulli’s distribution results that the probability of event to achieve after n steps the distance nh is $1/2^n$, and in one-dimensional random walk, the probability density is not zero in the region, $[-nh, +nh]$, while is vanishing outside of it. An example of the progress of diffusion front is shown in Fig. 3. After the time $(n + 1)\tau$, the range of the region is $[-(n + 1)h, +(n + 1)h]$. Thus the front moves with the velocity

$$v_f = \frac{h}{\tau}. \tag{35}$$

If $h = 1$ and $\tau = 1$, $D = 1$ and $v_f = 1$. If $h \rightarrow 0$ and $\tau \rightarrow 0$, one should keep

$$\frac{h^2}{2\tau} = D = \text{constant}. \tag{36}$$

This means that $\tau \rightarrow 0$ one order more quickly than h . We find

$$\frac{h}{\tau} = \frac{2D}{h} \rightarrow \infty \quad \text{if} \quad h \rightarrow 0. \tag{37}$$

Hence, comparing with the definition (35)

$$v_f = \frac{h}{\tau} \rightarrow \infty. \tag{38}$$

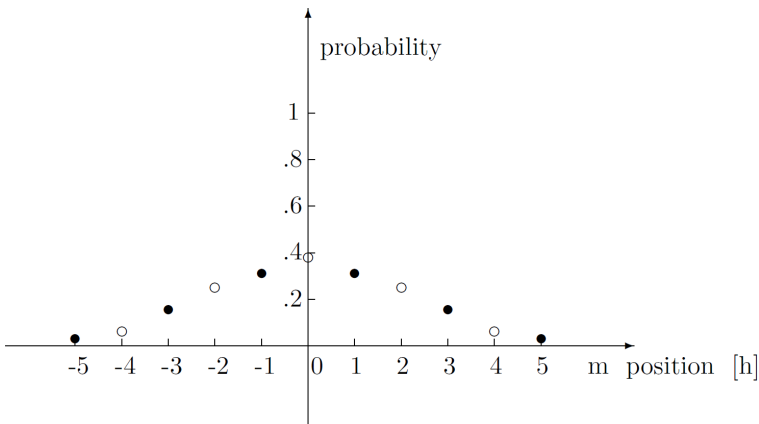


Fig. 3. Probability distribution in one-dimensional random walk after successive tosses. Initial position of the wanderer is $m = 0$ (probability = 1). Position of the diffusion front is visible after 4 (white circles, $|m| = 4$) and after 5 (black circles, $|m| = 5$) tosses. Unit of distance is h , unit of time is τ .

The range of the distribution after n steps is $r = nh$, and the time necessary to build up such range is $t = n\tau$. The height of the diffusion front diminishes, however, with n as $1/2^n$. Hence

$$n = \frac{t}{\tau} \quad \text{and} \quad r = nh = \frac{t}{\tau} h = t v_f.$$

For any finite time t , in the limit of $\tau \rightarrow 0$ and $h \rightarrow 0$, the range $r \rightarrow \infty$, because of (38), the height of the front reduces to zero, and the paradox of instantaneous propagation without front arises.

7. The diffusion coefficient

The diffusion coefficient (7) for the symmetric random walk

$$D = \frac{h^2}{2\tau} \tag{39}$$

is similar to that given by the kinetic theory of gases [32]

$$D = \frac{1}{2} h \frac{h}{\tau}. \tag{40}$$

It reveals also an analogy with Einstein's relation [4, 5]

$$D = \frac{\langle x^2 \rangle}{2t}, \tag{41}$$

where $\langle x^2 \rangle$ is an average squared deviation of a distinct particle in the Brownian movement realised in the time t .

From Eq. (33), we obtain

$$D \approx \frac{\ell^2}{t_R}. \tag{42}$$

It is worth mentioning that the last relation obtained from the macroscopic theory has a similar form to relations (39)–(41), obtained from the microscopical theories. This persistence of the form argues also for the parabolic interpretation of the random walk.

8. Non-symmetric random walk

In this case, at each step, the probability of moving to the right (event R) is p and moving to the left (event L) is $q = 1 - p$. In symmetrical Rayleigh's case $p = q = 1/2$, while the general non-symmetric case of $p \neq q$ was treated by Kac [19].

The probability that among n events the events R are produced in number k and events L in number $n - k$ is given by Bernoulli's distribution

$$P_n(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k} \quad \text{with} \quad \sum_{k=0}^n P_n(k) = 1. \quad (43)$$

As in the symmetrical case, finding the particle at position $x = mh$ after time $t = n\tau$ needs $m = k - (n - k) = 2k - n$ steps, cf. Fig. 1.

Let at time $t = 0$ the particle be at $x = 0$. Then,

$$f_n(m) = \frac{n!}{\frac{n+m}{2}! \frac{n-m}{2}!} p^{\frac{n+m}{2}} (1-p)^{\frac{n-m}{2}} \quad (44)$$

denotes the probability of the event that after time $t = n\tau$ the particle will be at $x = mh$. This implies, otherwise obvious iterative relation

$$f_{n+1}(m) = (1-p)f_n(m+1) + pf_n(m-1) \quad (45)$$

instead of relation (1).

A positive quantity ε may be defined such that

$$p \equiv \frac{1}{2} + \varepsilon \quad \text{and} \quad 1-p = \frac{1}{2} - \varepsilon. \quad (46)$$

Then, Eq. (45) may be written as

$$f_{n+1}(m) = \left(\frac{1}{2} - \varepsilon\right) f_n(m+1) + \left(\frac{1}{2} + \varepsilon\right) f_n(m-1). \quad (47)$$

For $\varepsilon = 0$, we get Rayleigh's case (1).

In a similar manner as Eq. (45), two other iterative relations can be written

$$f_n(m-1) = \left(\frac{1}{2} + \varepsilon\right) f_{n-1}(m-2) + \left(\frac{1}{2} - \varepsilon\right) f_{n-1}(m), \quad (48)$$

and

$$f_n(m+1) = \left(\frac{1}{2} + \varepsilon\right) f_{n-1}(m) + \left(\frac{1}{2} - \varepsilon\right) f_{n-1}(m+2). \quad (49)$$

Substituting (48) and (49) into (45), we get

$$\begin{aligned} f_{n+1}(m) &= \frac{1}{4} [f_{n-1}(m-2) + 2f_{n-1}(m) + f_{n-1}(m+2)] \\ &\quad + \varepsilon [f_{n-1}(m-2) - f_{n-1}(m+2)] \\ &\quad + \varepsilon^2 [f_{n-1}(m-2) - 2f_{n-1}(m) + f_{n-1}(m+2)]. \end{aligned} \quad (50)$$

Similarly, as in the symmetrical case, at the given time n , the distance between neighbouring positions is $2h$ and that the return to the given position m is possible after the time period 2τ , only, cf. Fig. 2.

9. Difference equation of diffusion with drift

We subtract from both sides of (50) the quantity $f_{n-1}(m)$

$$f_{n+1}(m) - f_{n-1}(m) = \left(\frac{1}{4} + \varepsilon^2\right) [f_{n-1}(m-2) - 2f_{n-1}(m) + f_{n-1}(m+2)] \\ + \varepsilon [f_{n-1}(m-2) - f_{n-1}(m+2)], \quad (51)$$

and transform it as follows

$$\frac{f_{n+1}(m) - f_{n-1}(m)}{2\tau} \\ = \left(\frac{1}{4} + \varepsilon^2\right) \frac{(2h)^2}{2\tau} \frac{f_{n-1}(m-2) - 2f_{n-1}(m) + f_{n-1}(m+2)}{(2h)^2} \\ + \varepsilon \frac{4h}{2\tau} \frac{f_{n-1}(m-2) - f_{n-1}(m+2)}{4h}. \quad (52)$$

After introducing the notation

$$D = (1 + 4\varepsilon^2) \frac{h^2}{2\tau} \quad \text{and} \quad \frac{D}{T} \frac{\partial V}{\partial x} = \frac{2h}{\tau} \varepsilon, \quad (53)$$

we get

$$\frac{f_{n+1}(m) - f_{n-1}(m)}{2\tau} = D \frac{f_{n-1}(m-2) - 2f_{n-1}(m) + f_{n-1}(m+2)}{(2h)^2} \\ + \frac{D}{T} \frac{\partial V}{\partial x} \frac{f_{n-1}(m-2) - f_{n-1}(m+2)}{4h}. \quad (54)$$

This can be regarded as a difference counterpart of the differential equation of Smoluchowski's diffusion, known also as the diffusion equation with drift [6, 7]. The exterior force $(-\partial V/\partial x)$ is the cause of the drift. The quantity T is the temperature in units of the energy. Here, in contrast to Kac' results [19], the diffusion coefficient D is modified by the non-symmetry indicator ε .

10. Differential equation of diffusion and wave equation

Despite of formal similitude of equations (52) and (10), the transition $h \rightarrow 0$ and $\tau \rightarrow 0$, necessary to obtain differential equation of diffusion, is in the case of Eq. (52) more difficult. Namely, because according to equation (53)

$$D \propto \frac{h^2}{\tau} \quad \text{while} \quad \frac{D}{T} \frac{\partial V}{\partial x} \propto \frac{h}{\tau}, \quad (55)$$

it is impossible to keep simultaneously the diffusion coefficient

$$D \propto \frac{h^2}{\tau} = \text{constant}, \tag{56}$$

and the drift force

$$-\frac{\partial V}{\partial x} \propto \frac{1}{h} \frac{h^2}{\tau} \tag{57}$$

non-singular. To avoid this singularity, Kac proposed to use the substitution [19]

$$\varepsilon = \beta h \quad \text{with} \quad \beta = \text{constant} \tag{58}$$

which assures the non-singularity of the drift force. But this means, when $h \rightarrow 0$, then also $\varepsilon \rightarrow 0$ and only the very small deviations from symmetry of the random walk, and consequently very small drift forces in Eq. (54) are permitted.

However, if instead of (56) and (57), we accept the following limit relations for $h \rightarrow 0$ and $\tau \rightarrow 0$

$$\frac{h}{\tau} \propto v = \text{constant}, \tag{59}$$

then

$$\frac{h^2}{\tau} \propto D \rightarrow 0, \tag{60}$$

and Eq. (54) becomes

$$\frac{f_{n+1}(m) - f_{n-1}(m)}{2\tau} = v \frac{f_{n-1}(m-2) - f_{n-1}(m+2)}{4h} \tag{61}$$

with

$$v = \varepsilon \frac{4h}{2\tau}. \tag{62}$$

After passing to limit with h and τ , we get

$$\frac{\partial f}{\partial t} = -v \frac{\partial f}{\partial x}. \tag{63}$$

It is, the so-called advection equation, closely related to the wave equation. The constant v is the speed of wave motion.

11. Conclusions

The description of diffusion as a random walking resembles the hopping models proposed in [33], and by Grasselli and Streater [34].

Notice also that for the non-symmetric walk when $\varepsilon \neq 0$, not only the drift force, but also the diffusion coefficient depends on ε . This is conform to the phenomenological description of the two-level diffusion, where the change of the potential for external drift force is accompanied by the change of diffusion coefficient [28].

Random walk is a certain mathematical tool, characterised by the iterative relation (1) for the symmetric coin, and relation (45) for the non-symmetric one. As every mathematical concept, it receives its physical meaning after appropriate attribution of physical quantities to the mathematical terms. In our case, the appropriateness denotes the agreement with the laws of thermodynamics, and we must chose between different proposals of interpretation.

It is widely accepted that the random walk is a simplified picture of diffusion phenomena the most famous example of which is the Brownian movement. However, another hyperbolic interpretations of the random walk are possible.

If one assumes the fraction $h^2/(2\tau)$ to be constant when the limits $h \rightarrow 0$ and $\tau \rightarrow 0$ are taken, then Fick's diffusion equation is obtained, while assumption that the quotient h/τ keeps constant leads to the wave diffusion equation. It seems interesting that the same pattern appears at different levels of the diffusion analysis. This is a strong support for the classical (parabolic) interpretation of the random walk, cf. Section 7.

We indicated the controversies to which the hyperbolic equation of diffusion is leading, especially the possibility of appearing of non-positive density and decreasing entropy. The inconvenience of the classical diffusion manifested in the so-called infinite speed paradox seems to be unimportant in comparison. The infinite range of the classical distribution, for any time $t > 0$, appears as a mathematical effect, in result of limit passage to infinitesimal increments, and corresponds to Einstein's formula for Brownian diffusion.

Between several possible interpretation of the random walk mathematical process, one should choose those which are conform to the physical rules. In our case, this role of Occam's razor is realised by two laws: the positivity of the probability density, and the entropy growth of free system.

REFERENCES

- [1] K. Pearson, *The Problem of the Random Walk*, *Nature* **72**, 294 (1905).
- [2] J.W. Strutt, Lord Rayleigh *On the Resultant of a Large Number of Vibrations of the Same Pitch and of Arbitrary Phase*, *Philos. Mag.* **10**, 73 (1880).

- [3] J.W. Strutt, Lord Rayleigh, *The Theory of Sound*, Volume 1, section 42a, Second edition revised and enlarged, Dover Publications, New York 1945.
- [4] A. Einstein, *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen*, *Ann. Phys.* **322**, 549 (1905).
- [5] A. Einstein, *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen*, J. Barth, Leipzig 1905.
- [6] M. v. Smoluchowski, *Drei Vorträge über Diffusion, Brownsche Molekularbewegung und Koagulation von Kolloidteilchen*, *Physikalische Zeitschrift* **17**, 557 (1916); **17**, 587 (1916).
- [7] S. Chandrasekhar, M. Kac, R. Smoluchowski, *Marian Smoluchowski — His Life and Scientific Work*, ed. R.S. Ingarden, PWN, Warszawa 1999.
- [8] N.W. Goel, N. Richter-Dyn, *Stochastic Models in Biology*, Academic Press, New York 1974.
- [9] P.G. De Gennes, *Scaling Concepts in Polymer Physics*, Cornell University Press, Ithaca, London 1979.
- [10] M. Doi, S.F. Edwards, *The Theory of Polymer Dynamics*, Clarendon Press, Oxford 1986.
- [11] N.G. Van Kampen, *Stochastic Processes in Physics and Chemistry*, revised and enlarged edition, North-Holland, Amsterdam 1992.
- [12] S. Redner, *A Guide to First-passage Process*, Cambridge University Press, Cambridge, UK 2001.
- [13] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 4th edition, World Scientific, Singapore 2004.
- [14] R. Wojnar, *Acta Phys. Pol. A* **114**, 607 (2008).
- [15] R. Wojnar, *Acta Phys. Pol. A* **123**, 624 (2013).
- [16] H.S. Carslaw, J.C. Jaeger, *Conduction of Heat in Solids*, Clarendon Press, Oxford 1948.
- [17] L.D. Landau, E.M. Lifshitz, *Fluid Mechanics*, Vol. 6 of Course of Theoretical Physics, 2nd English ed., translated from Russian by J.B. Sykes, W.H. Reid, Pergamon Press, Oxford–New York–Beijing–Frankfurt–Sao Paulo–Sydney–Tokyo–Toronto 1987.
- [18] R. De Groot, P. Mazur, *Non-Equilibrium Thermodynamics*, North-Holland Publ. Co, Amsterdam 1962.
- [19] M. Kac, *Am. Math. Mon.* **54**, 369 (1947).
- [20] C. Maxwell, *On the Dynamical Theory of Gases*, *Philos. Trans. R. Soc. London* **157**, 49 (1867).
- [21] C.R. Cattaneo, *Sulla conduzione del calore*, *Atti Sem. Mat. Fis. Univ. Modena* **3**, 83 (1948).

- [22] C.R. Cattaneo, *Sur une forme de l'équation de la chaleur éliminant le paradoxe d'une propagation instantanée*, *Comptes Rendus Acad. Sci.* **247**, 431 (1958).
- [23] P. Vernotte, *Les paradoxes de la théorie continue de l'équation de la chaleur*, *Comptes Rendus Acad. Sci* **246**, 3154 (1958).
- [24] M. Kac, *Rocky Mountain J. Math.* **4**, 497 (1974).
- [25] M. Chester, *Phys. Rev.* **131**, 2013 (1963).
- [26] Ph.M. Morse, H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill, New York–Toronto–London 1953, Section 7.4.
- [27] M. Suffczyński, *Elektrodynamika*, PWN, Warszawa 1964, in Polish.
- [28] R.F. Streater, *Rep. Math. Phys.* **40**, 557 (1997).
- [29] Z. Burda, J. Duda, J.M. Luck, B. Waclaw, *Phys. Rev. Lett.* **102**, 160602 (2009).
- [30] J.R. Ramos-Barrado, P. Galan-Montenegro, C. Criado Combon, *J. Chem. Phys.* **105**, 2813 (1996).
- [31] C. Criado, P. Galan-Montenegro, P. Velasquez, J.R. Ramos-Barrado, *J. Electroanal. Chem.* **488**, 59 (2000).
- [32] O.E. Meyer, *De gasorum theoria, Dissertatio inauguralis mathematica–physica*, Maelzer, Vratislaviae 1866.
- [33] R.F. Streater, *Proc. Roy. Soc.* **A456**, 205 (2000).
- [34] M.R. Grasselli, R.F. Streater, *Rep. Math. Phys.* **50**, 13 (2002).