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FUNCTIONAL EQUATION FOR THE CROSSOVER IN THE MODEL OF ONE-DIMENSIONAL WEIERSTRASS RANDOM WALKS

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We consider the problem of one-dimensional symmetric diffusion in the framework of Markov random walks of the Weierstrass type using two-parameter scaling for the transition probability. We construct a solution for the characteristic Lyapunov function as a sum of regular (homogeneous) and singular (nonhomogeneous) solutions and find the conditions for the crossover from normal to anomalous diffusion.

Keywords: normal diffusion, anomalous diffusion, Markov process, fractal dimension, functional pressure, Weierstrass function

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1. Introduction

The problem of diffusion (both normal and anomalous) remains one of the central issues in modern physical chemistry and other applications (see, e.g., [1]–[3] where the formalism of fractional derivatives, which is not well known to physicists, is used). Moreover, this problem is interesting from the mathematical standpoint as one of the sections of analytic probability theory (see, e.g., [4]–[7]). The connection between these fields of study is based on modeling diffusion processes in the framework of one-dimensional (on the continuous spatial coordinate axis $-\infty < x < \infty$) and symmetric Markov random walks (RWs) with the transition probability $P(x)$.

Of special interest are, for example [8], [9], where arbitrarily large (even infinite) values of the effective radius $R_{\text{eff}} = \sigma$ are allowed for a symmetric function $P(-x) = P(x)$. Here, $\sigma^2 = m_2$ is the dispersion or a second central moment $P(x)$. Moreover, in the symmetric case, all even central moments coincide with the simple moments, and all odd ones are equal to zero.

It is essential that the transition function $P(x)$ in [8], [9] is equipped with one or two control values that allow varying R_{eff} over a wide range and hence passing from normal diffusion (ND) with a finite value of R_{eff} and an exponential front to anomalous diffusion (AD) with an infinite R_{eff} and a polynomial front. If the initial distribution is $p_0(x) = \delta(x)$, then according to [4]–[7], the sought distribution $p_N(x)$ after $N \geq 1$ steps (hops) is an N-fold convolution of $P(x)$, and it is hence feasible to pass from the function $P(x)$ to its Fourier image $G(k)$, the characteristic Lyapunov function for which convolution becomes multiplication. Moreover, the function $G(k)$ smooths all singularities of $P(x)$, and by the Tauber theorems, the sought asymptotic forms $p_N(x)$ both in discrete time (for $N \gg 1$) and in space (for large values of $x \gg 1$) is defined by the values $G(k)$ for small values of k near $k = 0$.

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This problem is complex because for the functions $P(x)$ that are interesting from the physical standpoint, the functions $G(k)$ are often quite "exotic," for example, generalized Riemann theta function for the Riemann RW in [8] or the Weierstrass function[1] for the Weierstrass RW in [9]. Of outstanding interest is the fact that depending on the control values, these functions can yield both analytic ($\sim k^2$) and nonanalytic ($\sim k^\alpha$, $0 < \alpha < 2$) behaviors of $G(k)$ as $k \to 0$.

It is essential that the analytic behavior of $G(k)$ is universal for all $P(x)$ with a *finite* value of $R_{\text{eff}} = \sigma = \sqrt{m_2}$. Moreover, according to [4]–[7], $p_N(x)$ also has an asymptotically universal form, namely, the normal (Gaussian) form, and describes Gauss–Einstein–Wiener ND where $p_N(x) \sim e^{-x^2/2\sigma_N^2}$, $\sigma_N^2 \sim N$. In a nutshell, this claim is just one of the forms of the central limit theorem [4].

For infinite R_{eff}, in contrast, the value α is specific for each $P(x)$ and depends differently on the parameters of $P(x)$; hence, the diffusion front $p_N(x)$ has a polynomial form $C_\alpha N x^{-(1+\alpha)}$ indicative of AD (sometimes called the Levy–Khintchine AD). It is clear that using the control values, we can adjust $R_{\text{eff}} = \sigma = \sqrt{m_2}$ and thus realize the *crossover* between the two modes ND and AD of the general phenomenon of diffusion. We discussed this issue in detail in [12] based on similarity of the diffusional crossover and the magnetic phase transition.

To conclude this section, we note that even the explicit form of $G(k)$ given, for example, by an infinite power of trigonometric series, does not fix α. It seems that the most adequate approach for finding α is to obtain and solve the functional equation for $G(k)$ using the properties of *generalized homogeneity* (self-similarity, scale invariance) of this function. This approach is widely used, for example, in the renormalization group method (see, e.g., [11]).

One of the advantages of this approach is the possibility of avoiding the fractional derivatives, which are unknown to many physicists [1]–[3]. As an illustrative example, we consider the Weierstrass RW model formulated by Montroll et al. in [9].

2. Markov random walks of the Weierstrass type

A simple yet substantial model of the transition probability $P(x)$ with double power scaling (sometimes called Bernoulli scaling) was studied in [9]:

$$P(x,\lambda) = p\sum_{j=0}^{\infty} \lambda^{-j}[\delta(x-b^j)+\delta(x+b^j)]. \tag{1}$$

In this model, the *radii* of one-dimensional steps and the corresponding *probabilities* form two unbounded geometric progressions: an increasing one (with respect to the step length) $\pm 1, \pm b, \dots, \pm b^j, \dots,$ where $1 < b < \infty$, and a decreasing one (with respect to the probability value) $p, p/\lambda, \dots, p/\lambda^j, \dots,$ where $1 < \lambda < \infty$, $0 < p < 1$. The number of nodes ($j = 0, 1, \dots$) is assumed to be unbounded, and we choose the value $b > 1$ to be fixed ($b = \text{const}$) for simplicity. It is clear that as λ decreases, the distribution $P(x,\lambda)$ becomes wider (slowly decaying), but the values of $\lambda \le 1$ are omitted in view of violation of the normalization condition, by virtue of which $2[p + (p/\lambda) + \cdots + (p/\lambda^j) + \cdots] = 1$, whence we easily find $p = p(\lambda) = (1 - 1/\lambda)/2$.

We note that in the limit $\lambda \to \infty$ in series (1), only the first summand with $j = 0$ is preserved, and hence $P(x,\lambda) \to P(x,\infty) = P(\pm 1) = p(\infty) = 1/2$ in this limit, which coincides with the standard definition of the Gauss–Einstein–Wiener RW [4]–[7]. In this case, the distribution $P(x,\infty)$ is the narrowest, and $R_{\text{eff}} = \sigma = \sqrt{m_2}$ takes the minimum value equal to unity. Obviously, as λ decreases, the distribution $P(x,\lambda)$ widens because the value $R_{\text{eff}} = \sigma = \sqrt{m_2}$ increases until it diverges, defining the crossover between ND and AD. For a precise numerical estimate and to specify this point, we need an explicit expression for the dispersion $\sigma^2(b,\lambda)$, and always $\partial\sigma^2(b,\lambda)/\partial\lambda < 0$ for all λ.

[1] We note that this year is exactly 100 years since Hardy investigated this function in great detail in [10].

The technique of the characteristic function $G(k,\lambda)$ is convenient for solving this problem; for $P(x,\lambda)$ in (1), this function is the Weierstrass function:

$$G(k,\lambda) = 2p(\lambda)\sum_{j=0}^{\infty} \lambda^{-j}\cos(kb^j), \tag{2}$$

where $G(0,\lambda) \equiv 1$ by the normalization condition and $G'(0,\lambda) = 0$ by the symmetry. Expression (2) is a trigonometric series with omissions (lacunas), which allows finding formal expressions for all even moments $m^{(2s)}(\lambda)$, which are by definition equal to the derivatives $G^{(2s)}(k,\lambda)$ with respect to k of the order $2s$ at $k = 0$:

$$|m_{2s}(\lambda)| = 2p(\lambda)\sum_{j=0}^{\infty}\left(\frac{\lambda_{\rm cr}^{(s)}}{\lambda}\right)^j, \qquad \lambda_{\rm cr}^{(s)} = (\lambda_{\rm cr})^s, \qquad \lambda_{\rm cr} = b^2. \tag{3}$$

If all values of moments (3) were finite for all values of λ, then we could pass from Fourier expansion (2) to the Taylor expansion of $G(k,\lambda)$ valid for all values of $1 < \lambda < \infty$ (at least close to $k = 0$),

$$G(k,\lambda) = 1 + \sum_{s=1}^{\infty}\frac{1}{(2s)!}(i^{2s})m_{2s}(\lambda)k^{2s}. \tag{4}$$

But each moment (3) of the order $2s$ has the form of an infinite geometric progression with the denominator $\lambda_{\rm cr}^{(s)}/\lambda$, where the threshold values $\lambda_{\rm cr}^{(s)}$ form an unbounded geometric increasing progression (as the order s increases from 1 to ∞) with the denominator $\lambda_{\rm cr}^{(s)} = (\lambda_{\rm cr})^s$, $\lambda_{\rm cr} = b^2 > 1$.

Hence, each series (3) for the moment $m_{2s}(\lambda)$ converges only for $\lambda_{\rm cr}^{(s)}/\lambda < 1$, i.e., for sufficiently large values of λ; the moments have finite values $m_{2s}(\lambda) = 2p(\lambda)[1-(\lambda_{\rm cr}^{(s)}/\lambda)]^{-1}$ only in this case, where $p(\lambda) = (1-1/\lambda)/2$. Obviously, in infinite series (4), there always are infinitely many divergent (singular) summands for each finite λ. We use this fact below in Sec. 3, where we construct the solution of the functional equation for $G(k,\lambda)$ for each λ.

Therefore, Taylor series (4) converges only in the limit $\lambda \to \infty$ considered above. Moreover, with the obvious equality $m_{2s}(\infty) = 2p(\infty) \equiv 1$ for all values of s from 1 to ∞, the sum of series (4) is equal to $\cos k$ for all values of k. The same result, of course, also follows from expansion (2), where only the first summand $G(k,\infty) = \cos k$ (for $j = 0$) remains as $\lambda \to \infty$, the ND mode is hence unique for the diffusion, and the AD mode (and hence the AD–ND crossover) is absent in principle.

For arbitrary λ in the general case, Taylor expansion (4) loses its applicability and cannot describe all modes of diffusion. In other words, the function $G(k,\lambda)$ for finite λ is not analytic in the neighborhood of $k = 0$, and its expansion has only odd orders k. For example, the summand of the lowest order in this expansion has the form k^α, where $0 < \alpha < 2$, and then $m_2(\lambda) \equiv G^{(2)}(k=0,\lambda)$, as expected, diverges for $\lambda < \lambda_{\rm cr}^{(1)}$.

Precisely these values of the parameter λ define the AD mode, but we must also consider that as λ varies from infinitely large values to the minimum (equal to unity), there is in fact an infinite cascade of "crossovers" similar to the so-called devil's staircase of phase transitions (see, e.g., [7]). We gave a detailed analysis of the corresponding phase diagram of the analogue of the magnetic phase transition with a logarithmic order parameter in [12], but we are here interested in the interrelation of expansions (2) and (4).

3. Functional equations for the Weierstrass function

Because Taylor expansion (4) cannot be applied for all finite λ, we must propose an approach that allows finding the nonanalytic part of the expansion of the original function (2) for small k. For this, Montroll et al. [9] used the representation depending on the kth factor $\cos(kb^j)$ in the form of the inverse

Mellin transform with the following application of the residue theorem. As expected, in the interval of values $1 < \lambda < \lambda_{\rm cr}^{(1)} = b^2$, the expansion $G(k, \lambda) \approx 1 - C_\alpha k^\alpha + \ldots$ holds, where $\alpha = 2\log\lambda/\log\lambda_{\rm cr}^{(1)} = \log\lambda/\log b$, hence $0 < \alpha < 2$ in this interval, and $G''(0, \lambda) = m_2(\lambda)$ obviously diverges. According to [7], [9], the parameter α determines the fractal dimension of the cluster diffusion.

Nevertheless, the approach for finding the result in [9] is not very clear physically and requires additional mathematical proof. Therefore, we below propose an alternative approach based on the existence of a functional equation for $G(k, \lambda)$, whose form follows directly from definition (2):

$$G(k, \lambda) = \frac{1}{\lambda}\, G(bk, \lambda) + 2p(\lambda)\cos k. \tag{5}$$

Equation (5) is a linear nonhomogeneous functional equation that holds in the whole interval $1 < \lambda < \infty$, and the nonhomogeneous summand $2p(\lambda)\cos k$ in the right-hand side of (5) is regular in k in a neighborhood of $k = 0$ for all possible values of λ. It follows that this summand can only contribute to the ND mode, and the AD mode (existing only for $1 < \lambda < b^2$) is hence fully determined by the homogeneous summand $(1/\lambda)G(bk, \lambda)$. This fully agrees with the fact that the summand $(1/\lambda)G(bk, \lambda)$ disappears in the limit case[2] $\lambda \to \infty$, where, as shown above, only the ND mode exists (we take into account that $G(bk, \infty) = \cos(bk)$ is always finite).

Based on these observations, we can easily obtain a particular (singular) solution $G_{\rm sing}(k, \lambda)$ of functional equation (5) describing AD for $1 < \lambda \le \lambda_{\rm cr} = b^2$ and completely omitting the nonhomogeneous regular summand. It is natural to seek $G_{\rm sing}(k, \lambda)$ in the form[3]

$$G_{\rm sing}(k, \lambda) = C(\lambda) k^{\alpha(\lambda)} Q(k), \qquad Q(bk) = Q(k). \tag{6}$$

Substituting (6) in reduced (homogeneous) equation (5), we easily obtain

$$1 = \left(\frac{1}{\lambda}\right) b^{\alpha(\lambda)}, \qquad \alpha(\lambda) = \frac{\log\lambda}{\log b}, \quad 0 < \alpha(\lambda) \le 2, \quad 1 < \lambda \le \lambda_{\rm cr} = b^2. \tag{7}$$

It is therefore reasonable to seek a complete solution of (5) in the additive form

$$G(k, \lambda) = G_{\rm reg}(k, \lambda) + G_{\rm sing}(k, \lambda). \tag{8}$$

We return to formal Taylor expansion (4), which is completely regular only in the limit $\lambda \to \infty$. For each finite λ, it is reasonable to seek a regular (analytic) part of the solution $G(k, \lambda)$ in the form (see below about the choice $S = S(\lambda)$; we now only note that $S \to \infty$ as $\lambda \to \infty$)

$$G_{\rm reg}(k, \lambda(S)) = 1 + \sum_{s=1}^{S-1} (-1)^s \frac{1}{(2s)!} m_{2s}[\lambda(S)] k^{2s}. \tag{9}$$

The rest of expansion (4) is singular or completely nonanalytic because of the divergences of the m_{2s} for $s \ge S$ considered above:

$$G_{\rm sing}(k, \lambda(S)) = 1 + \sum_{s=S}^{\infty} (i)^{2s} \frac{1}{(2s)!} m_{2s}[\lambda(S)] k^{2s}. \tag{10}$$

Similarly to (6), infinite sum (10) over the (even) integer powers k can then be replaced with only one summand but of a fractional order in k:

$$G_{\rm sing}(|k|, \lambda(S)) = C[\lambda(S)] |k|^{\alpha[\lambda(S)]} Q(|k|), \tag{11}$$

[2]This circumstance opens the possibility of an iterative solution of functional equation (5) in powers of $1/\lambda$.
[3]As we later show, the factor $Q(k)$ contains only corrections that are logarithmic in k.

where the coefficient $C[\lambda(S)]$ and the anomalous value $\alpha[\lambda(S)]$ are independent of k (see below about the amplitude function $Q(|k|)$). We note that the representation of solution (8) as a sum of (9) and (11) is very similar to the Taylor formula frequently used in applications in the form of a sum of Taylor polynomial (9) and a residual term in a form (11) similar to the Peano form,[4] but with reverse ordering relative to the order symbol o, and hence $G_{\rm reg}(k,\lambda(S)) = o[G_{\rm sing}(k,\lambda(S))]$. In other words, in some interval of values of $\lambda(S)$ (for a given value of S) in the limit $k \to 0$ that is of interest to us, the residual term exceeds the main term and hence determines the asymptotic behavior of the whole function $G(k,\lambda)$ and therefore of the function $P(x,\lambda)$ in the limit $x \to \infty$.

The actual construction of expansions (9) and (11) is based on the fact that for each finite value of λ in the open interval $(1,\infty)$, there always exists a value $S(\lambda)$ (also finite) in the half-open interval $[1,\infty)$ and there correspondingly exists an inverse function $\lambda(S)$ for which the inequalities $\lambda_{\rm cr}^{(S-1)} < \lambda(S) < \lambda_{\rm cr}^{(S)}$ are satisfied and, moreover, $\lambda_{\rm cr}^{(1)} = 1$ $\lambda_{\rm cr}^{(2)} = b^2$, etc. The moments $m_{2s}(\lambda)$ then exist and are finite only for $s = 1, 2, \ldots, S-1$ and diverge for $s \geq S$, and expansion (9) is hence truncated on the summand of the order $k^{2(S-1)}$.

The greatest interest is presented by the parameter $\alpha[\lambda(S)]$ satisfying the strict inequality $2(S-1) < \alpha[\lambda(S)] < 2S$ because all derivatives $G_{\rm sing}^{(2s)}(k,\lambda)$ with $s \geq S$ are singular for $k = 0$ only in this case. Indeed, let $2S - \alpha = \varepsilon$ with $0 < \varepsilon < 2$ and $s = S + r$, $r = 0, 1, \ldots$. Then $G_{\rm sing}^{(2s)}(|k|,\lambda) \sim |k|^{-(\varepsilon+2r)} \to \infty$ for $k = 0$ and arbitrarily small $\varepsilon > 0$. There is no need to differentiate the factor $Q(|k|)$ (see footnote 3).

The parameter $\alpha[\lambda(S)]$ can be calculated exactly, similarly to how it was calculated in relation (8), using only the homogeneous part $G(|k|,\lambda) = (1/\lambda)G(b|k|,\lambda)$ of functional equation (6), which is sometimes called the *scaling* or self-similar part. According to this equation, $G(|k|,\lambda)$ is a generalization of the notion of a homogeneous function in the sense of Euler. Assuming the additional functional equation $Q(b|k|) = Q(|k|)$ for the amplitude function $Q(|k|)$, from (9), we obtain

$$1 = \left[\frac{1}{\lambda(S)}\right] b^{\alpha[\lambda(S)]}, \qquad \alpha[\lambda(S)] = \frac{\log\lambda(S)}{\log b}. \tag{12}$$

We then apply the monotonic logarithm operation to the chain of inequalities $\lambda_{\rm cr}^{S-1} < \lambda(S) < \lambda_{\rm cr}^{S}$ (all terms in this chain are greater than unity, and their logarithms are therefore positive) and divide each term by $\log\lambda_{\rm cr} > 0$ to obtain the inequality $S - 1 < \log\lambda(S)/\log\lambda_{\rm cr} < S$. Taking into account that $\lambda_{\rm cr} = b^2$, we finally obtain the inequality $2(S-1) < \alpha[\lambda(S)] < 2S$, which yields the nonanalyticity of the singular part of solution (11). Dividing this inequality by S, we note that $2(1 - 1/S) < \alpha[\lambda(S)]/S < 2$ and hence $\alpha/S \to 2$ as $S \to \infty$ and $\lambda(S) \to \infty$, when the nonanalytic part of solution (11) (and the AD together with it) strictly vanish (as shown in Sec. 2).

The coefficient $C[\lambda(S)]$ in (11) can be determined using "heuristic" considerations, and the result coincides completely with the result more rigorously obtained in [9] using the Mellin integral transformation. The transition from the first divergent summand of the order $2S$ in $G_{\rm reg}(k,\lambda)$ given by (9) to the corresponding summand in $G_{\rm sing}(|k|,\lambda)$ consists in the transition between powers of k, namely, from $2S$ to $\alpha < 2S$. Similar substitutions are performed for the coefficient $1/(2S)!(i)^{2S}$ transforming into the coefficient $C(\alpha)$: $1/(2S)! \equiv 1/\Gamma[1 + (2S)!]$ transforms into $1/\Gamma[1+\alpha] = -(1/\pi)\Gamma(-\alpha)$, while the factor $(i)^{2S} \equiv e^{[i(\pi/2)]^{2S}}$ transforms into $e^{[i(\pi/2)]^{\alpha}}$, preserving only the even part $\cos[(\pi/2)\alpha]$, which vanishes for each even value of α.

With regard to the amplitude function $Q(|k|)$, for the functional equation $Q(b|k|) = Q(|k|)$, there exists a constant solution $Q = {\rm const}$ (which is independent of k). In the more general case, this functional equation defines a log-periodic function in the class of slowly varying functions (in the Karamata sense).

[4]We note that none of the forms of the residual term (Lagrange, Cauchy, Schloemilch–Roche) is suitable because they all imply that the higher-order derivative $G^{(2S)} = m_{2S}$ is finite while this condition is violated in our case for all $s \geq S$.

Indeed, performing the "logarithmic" change of variables $|k| \to \log(|k|)$, $b \to \log b$ (with the condition $b > 1$ taken into account), we transform the functional equation for Q into a more usual functional equation for the periodic function $\mathbb{Q}(\log(|k|)) = \mathbb{Q}(\log(|k|) + \log b)$.

The solution of the last equality has the form of a trigonometric Fourier series in $\log(|k|)$ with the period $\log b$:

$$Q(|k|) = \frac{2}{\log b} \sum_{m=0}^{\infty} q_m \cos\left[2\pi m \frac{\log(|k|)}{\log b} + \varphi_m\right], \tag{13}$$

where the amplitudes q_m and the initial phases φ_m remain undefined. Series (13) contains only the corrections $\sim [\log(|k|)]^n$ logarithmic in $|k|$, where n are natural numbers, which justifies the statement in footnote 4.

4. Conclusions

We have considered the problem of one-dimensional symmetric diffusion including a crossover between the ND (Gauss–Einstein–Wiener) and AD (Levy–Khintchine) modes based on the Markov RW approach. We showed that in the framework of the model of Montroll et al. [9] with two-parameter scaling of the transitional probability for the Weierstrass RW, we can first find the characteristic Lyapunov function and then, using the Tauber theorems, the asymptotic distribution of probabilities (or, in other words, the diffusion front). We proposed a constructive and purely physical approach for constructing the solution of the linear nonhomogeneous functional equation, and the results completely coincide with the rigorous result previously obtained in [9] using the Mellin integral transformation.

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