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Invalidity of the spatiotemporal white noise assumption for a stochastic diffusion-type equation

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I point out that the Gaussian white noise assumption, where the random variables have the spatiotemporal δ-function-type correlation, for the Edwards-Wilkinson equation with periodic boundary condition is not valid in dimensions higher than two, because it leads to divergent fluctuation of surface height. It is stressed that the physical solution should be irrelevant to the choice of the cutoff. One finds through exploring a continuum limit that the correlation should be less singular than the δ function and we have a finite solution with the vanishing roughness exponent. [S1063-651X(97)50402-8]

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The purpose of this paper is to call attention to the probabilistic property of random variables in stochastic diffusion-type equations (SDEs). In these cases a set of stochastic variables depending on both position and time is a subject of study. What I would like to emphasize here is that the spatiotemporal Gaussian white noise assumption occasionally is not valid in dimensions higher than two. Indeed for the growing surface problem described by a SDF [1–5] the divergent fluctuation of surface height results from this assumption. Introducing a cutoff length presenting an underlying microscopic unit such as a lattice constant may avoid outwardly the divergence, though the surface fluctuation depends strongly on the cutoff. However, the variance above is a macroscopic quantity irrelevant to the choice of cutoff, so that it should take a finite value in the vanishing limit of the cutoff, insofar as the SDE describes properly a physical phenomenon as a continuum model. In order to resolve the contradiction, the stochastic property of the random variables is examined through exploring a continuum limit of a stochastic difference equation to the SDE. Then we find, through a linear theory, that the correlation between the stochastic variables must be less singular than the δ function in dimensions higher than two.

The Langevin equations including a diffusion term have been often studied as a tool to describe mathematically physical phenomena in wide fields [6]. However, the careless use of the spatiotemporal white noise assumption may run the risk of leading to errors. The fact mentioned in the preceding paragraph has rarely been recognized in the physical community, so that misleading descriptions are found in the literature. Simultaneously we will also propose the question of how to carry out numerical integrations of the SDEs. A naive integration is pointed out to bring about mistakes occasionally. If one attempts to study more interesting equations such as the Kardar-Parisi-Zhang equation [7], careful examination of the random variables is required, because the nonlinearity does not always guarantee to counterbalance the failure of the assumption.

Our subject is to study exhaustively the following simple but basic equation,

$$\partial h(\mathbf{r},t)/\partial t = \nu \nabla^2 h(\mathbf{r},t) + \eta(\mathbf{r},t), \tag{1}$$

which models in the simplest way the dynamics of growing surfaces with self-affine symmetry [1–5]. This is often called the Edwards-Wilkinson (EW) equation [8]. The height of the surface, $h(\mathbf{r},t)$, is measured at t from a position $\mathbf{r}$ of a d-dimensional substrate with linear size of L ($\mathbf{r} \in [0,L]^d$). The periodic boundary condition, that is, $h(\mathbf{r}+L\mathbf{e}_l,t) = h(\mathbf{r},t)$ with a unit vector $\mathbf{e}_l$ along the lth axis, is assumed, which meets the growing surface problem. The first term of the right hand side of Eq. (1) describes the effect of surface

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tension smoothing the surface. The noise $\eta(\mathbf{r},t)$ has zero mean, $\langle \eta(\mathbf{r},t)\rangle = 0$, and its correlation is given as

$$\langle \eta(\mathbf{r},t)\,\eta(\mathbf{r}',t')\rangle = 2D\,\delta^d(\mathbf{r}-\mathbf{r}')\,\delta(t-t'), \qquad (2)$$

that is, we usually assume for $\eta(\mathbf{r},t)$ the δ-function-type correlated noise with respect to space and time. The roughness of the surface is estimated by height fluctuation $w(L,t) \equiv \langle \{h(\mathbf{r},t) - \langle h(\mathbf{r},t)\rangle\}^2\rangle^{1/2}$. Our purpose is to derive a scaling form of $w(L,t)$ expressed for large L and t as [9]

$$w(L,t) = L^{\alpha}\Psi(t/L^z) \qquad (3)$$

and to calculate the roughness exponent α (or the Hurst exponent for self-affine fractals) and the dynamic exponent z as functions of d. The scaling function $\Psi(x)$ increases as x^{β} for sufficiently small x and approaches a saturation value as x is increased beyond a crossover $x_c \simeq 1$. The temporal scaling exponent β is given by $\beta = \alpha/z$. Hereafter the cases of $d < 1$ will be abandoned due to their unphysical situation.

Since Eq. (1) is a linear equation, we have easily

$$w^2(L,t) = (D/\nu)\int_{2\pi/L \leqslant k} \frac{d^d\mathbf{k}}{(2\pi)^d}\{1-\exp(-2\nu k^2 t)\}/k^2 \qquad (4)$$

for an initial condition $h(\mathbf{r},0)=0$, which seems to satisfy the scaling form of Eq. (3) with $\alpha = (2-d)/2$ and $z=2$.

In dimensions higher than two, $d>2$, however, a divergence of Eq. (4) is brought out from modes with very short wavelength (ultraviolet divergence). Of course infinitesimal short modes should be considered to have no meaning from a physical point of view, because Eq. (1) is constructed in a coarse-grained sense. In order to avoid the divergence, we may then take into account the cutoff wave vector Λ, proportional inversely to underlying microscopic size such as a lattice constant [3,5,10]. However, we recall that introducing Λ is valid only if the results eventually obtained do not depend on the choice of Λ. Nevertheless $w(L,t)$ in Eq. (4), as a macroscopic quantity, depends strongly on Λ in cases of $d>2$. Anyway a finite integration in Eq. (4) estimated in any conventional way gives a negative value of α for $d>2$ [3–5,10], which is not acceptable because $0 \leqslant \alpha \leqslant 1$ is required from a mathematical sense [11]. As far as I know, no one has yet obtained the correct exponents for $d>2$.

Now we examine the probabilistic property of the random variables. In order to give them definitely, we start with a discrete version, where the continuum limit should be studied carefully. We divide the substrate into $(2N)^d$ cells with linear size of a. The positions of lattice points are denoted by $\mathbf{x}_i = a\mathbf{i}$ using d-dimensional integers $\mathbf{i} = (i_1, i_2, \ldots, i_d)$ with $i_l = 0, \pm 1, \ldots, \pm N$ $(l=1,2,\ldots,d)$. The time is also discretized as $t_j = j\tau$ $(j=0,1,\ldots)$ with time step τ. The difference for Eq. (1) is written in the Euler formula as

$$h(\mathbf{x}_i,t_{j+1}) = h(\mathbf{x}_i,t_j) + (\nu\tau/a^2)\sum_{l=1}^{d}\{h(\mathbf{x}_i + a\mathbf{e}_l,t_j) - 2h(\mathbf{x}_i,t_j) + h(\mathbf{x}_i - a\mathbf{e}_l,t_j)\} + B(\mathbf{x}_i,t_j), \qquad (5)$$

where $\mathbf{e}_l$ is a unit vector along the lth axis [12]. The random variables $B(\mathbf{x}_i,t_j)$ are supposed to be Gaussian and they are distributed independently on each space-time lattice point. Their correlation is then expressed as

$$\langle B(\mathbf{x}_i,t_j)B(\mathbf{x}_{i'},t_{j'})\rangle = 2Da^{-\phi}\tau^{2-\psi}\delta_{i_1,i_1'}\delta_{i_2,i_2'}\cdots\delta_{i_d,i_d'}\delta_{j,j'}. \qquad (6)$$

For convenience below we have introduced two exponents, ϕ and ψ. Keep in mind that Eq. (2) corresponds to $\phi = d$ and $\psi = 1$. Although we have here assumed the random variables to be of Ito type, the conclusion remains unchanged for those of Stratonovich type in linear problems.

The discretization of Eq. (1) is not restricted to the Euler formula above. Since our purpose is to see how the stochastic variables can be defined in a continuum limit, however, it is enough for our purpose to consider only the Euler formula (5) as a prototype. To make sure of it, I have examined that the *implicit* Euler method for discretization, written as [12]

$$h(\mathbf{x}_i,t_{j+1}) = h(\mathbf{x}_i,t_j) + (\nu\tau/a^2)\sum_{l=1}^{d}\{h(\mathbf{x}_i + a\mathbf{e}_l,t_{j+1}) - 2h(\mathbf{x}_i,t_{j+1}) + h(\mathbf{x}_i - a\mathbf{e}_l,t_{j+1})\} + B(\mathbf{x}_i,t_j), \qquad (7)$$

leads to the same conclusion obtained below.

The spatial Fourier transformation of $h(\mathbf{x}_i,t_j)$,

$$\hat{h}(\mathbf{k}_n,t_j) = (2N+1)^{-d}\sum_{\{\mathbf{i}\}} e^{-i\mathbf{k}_n\cdot\mathbf{x}_i}h(\mathbf{x}_i,t_j), \qquad (8)$$

is useful to solve Eq. (5) under the periodic boundary condition. The discrete wave vectors $\mathbf{k}_n = (k_{n_1}, k_{n_2}, \ldots, k_{n_d})$ are defined by $k_{n_l} = 2\pi n_l/(L+a)$, using $n_l = 0, \pm 1, \ldots, \pm N$ $(l=1,2,\ldots,d)$. The solution of Eq. (5) for the initial condition $h(\mathbf{x}_i,0) = \hat{h}(\mathbf{k}_n,0) = 0$ can be immediately obtained as

$$\hat{h}(\mathbf{k}_n,t_{j+1}) = \sum_{j'=0}^{j}[1 - Y(\mathbf{k}_n)]^{j-j'}\hat{B}(\mathbf{k}_n,t_{j'}), \qquad (9)$$

using $Y(\mathbf{k}_n) = (4\nu\tau/a^2)\Sigma_{l=1}^{d}\sin^2(k_{n_l}a/2)$ for abbreviation. Substituting Eq. (9) with Eq. (6) gives

$$w^2(L,t_{j+1}) = 2Da^{-\phi}\tau^{2-\psi}(2N+1)^{-d} \times \sum_{\{\mathbf{n}\}}{}' \left[\frac{1-\{1-Y(\mathbf{k}_n)\}^{2j}}{1-\{1-Y(\mathbf{k}_n)\}^2}\right]. \qquad (10)$$

$\Sigma'_{\{\mathbf{n}\}}$ stands for $\Sigma_{n_1=-N}^{N}\Sigma_{n_2=-N}^{N}\cdots\Sigma_{n_d=-N}^{N}$, excluding the $\mathbf{n} = \mathbf{0}$ mode.

The continuum limit of Eq. (10) is taken through $a,\tau \to 0$ with L and t fixed, then Eq. (5) returns back to Eq. (1). To estimate Eq. (10) it is useful that the $\Sigma'_{\{\mathbf{n}\}}$ is divided into two parts;

$$\sum_{\{\mathbf{n}\}}{}' = \sum_{n_1=-N_c}^{N_c}\sum_{n_2=-N_c}^{N_c}\cdots\sum_{n_d=-N_c}^{N_c} + \text{(other terms)}, \qquad (11)$$

N_c being such an integer that $1 \ll N_c \ll N$ with a fixed ratio to N, $b = N_c/N \ll 1$. Once again the first sum is noted not to include the $\mathbf{n}=\mathbf{0}$ term.

In the first sum of Eq. (11) we can approximate $Y(\mathbf{k}_n)$ to $\nu\tau k_n^2$, which leads to

$$(D/\nu)a^{d-\phi}\tau^{1-\psi}\int \cdots \int_{\Omega}\{1-\exp[-2\nu k^2 t]\}/k^2 \times \prod_{l=1}^{d} (dk_l/2\pi), \tag{12}$$

using $\{1-Y(\mathbf{k}_n)\}^{2t/\tau} \to \exp(-2\nu k_n^2 t)$ as $\tau \to 0$. Here the integration region is $\Omega = \{\cap_{l=1}^{d}\{k_l;|k_l| \leq 2\pi b/a\}\} \cap \{\cap_{l=1}^{d}\{k_l;|k_l| \leq 2\pi/L\}\}^c$, where $\{\cdots\}^c$ is a complement set of $\{\cdots\}$. This is the most dominant contribution to $w^2(L,t)$ arisen from the first sum in the limit. Note that the above procedure fails for $d>2$ because the integration in Eq. (12) diverges as a tends to zero.

In the other sums of Eq. (11), we put $y_{n_l} = \pi n_l/(2N+1)$. Since $Y(\mathbf{k}_n)$ is finite there $[Y(\mathbf{k}_n) \geq (4\nu\tau/a^2)\sin^2(\pi b/2)]$, $\{1-Y(\mathbf{k}_n)\}^{2t/\tau}$ vanishes through taking the limit of $\tau \to 0$ under fixed conditions:

$$\sigma \equiv \tau/a^2 < (2\nu d)^{-1}. \tag{13}$$

The latter condition ensuring $|1-Y(\mathbf{k}_n)|<1$ appears whenever we integrate numerically partial differential equations of parabola type in the Euler formula [12]. Using the implicit Euler formula, the condition is not necessary [12]. Then we have for the second contribution to $w^2(L,t)$,

$$(D/4\nu)\sigma^{1-\psi}a^{4-\phi-2\psi}\int \cdots \int_{\bar{\Omega}}\left[\sum_{l=1}^{d}\sin^2 y_l - 2\nu\sigma \times\left(\sum_{l=1}^{d}\sin^2 y_l\right)^2\right]^{-1}\prod_{l=1}^{d}(dy_l/\pi). \tag{14}$$

$\bar{\Omega}$ is a peripheral region of Ω scaled appropriately or

$$\bar{\Omega} = \left\{\bigcap_{l=1}^{d}\{y_l;|y_l| \leq \pi/2\}\right\} \bigcap \left\{\bigcap_{l=1}^{d}\{y_l;|y_l| \leq \pi b/2\}\right\}^c.$$

The integration in Eq. (14) is always bounded.

From Eqs. (12) and (14), we see that the condition resulting in a finite $w(L,t)$ for $d<2$ through the continuum limit is satisfied if and only if

$$\phi = d \quad \text{and} \quad \psi = 1, \tag{15}$$

while Eq. (14) vanishes in this limit. For $d<2$ we could recover Eq. (4) with $\alpha=(2-d)/2$ and $z=2$, which has been obtained by the direct integration of Eq. (1) with Eq. (2), that is, under the spatiotemporal white noise assumption.

For $d>2$, an infrared divergence does not occur. We have then immediately Eq. (14), where the integration region is replaced with $\tilde{\Omega} = \cap_{l=1}^{d}\{y_l;|y_l| \leq \pi/2\}$. In order to let $w(L,t)$ be finite, the condition

$$4-\phi-2\psi=0 \tag{16}$$

must be satisfied. If the spatiotemporal white noise assumption is adopted $(\phi=d,\psi=1)$, $w(L,t)$ no longer has physical meaning because of its infiniteness. The resulting $w(L,t)$ is independent of L and t, indicating $\alpha=\beta=0$.

Keeping the continuum version of Eq. (1), we can also derive the same conclusion above [13]. To this end we study the noise correlation, instead of Eq. (2),

$$\langle \eta(\mathbf{r},t)\eta(\mathbf{r}',t')\rangle = 2D[R(a)\Delta_a(\mathbf{r}-\mathbf{r}')][T(\tau)\Delta_\tau(t-t')], \tag{17}$$

where $\Delta_a(\mathbf{r})[\Delta_\tau(t)]$ is a sharply localized function of $\mathbf{r}$ $[t]$ around the origin with narrow width a (τ), which corresponds to some microscopic size existing in phenomena under consideration such as a lattice constant. For example, $\Delta_a(\mathbf{r}) = \exp[-r^2/(2a^2)]$ and $\Delta_\tau(t) = \exp[-t^2/(2\tau^2)]$. As the microscopic sizes a and τ are decreased, the respective magnitude is assumed to grow as

$$R(a) \propto a^{-\phi}, \quad T(\tau) \propto \tau^{-\psi}. \tag{18}$$

Notice again that Eq. (2) corresponds to $\phi=d$ and $\psi=1$. Requiring $w(L,t)$ to be finite in the limits of $a \to 0$ and $\tau \to 0$ under fixed $\sigma=\tau/a^2$ gives the relations (15) and (16) between the exponents, ϕ and ψ, for $1 \leq d<2$ and $d>2$, respectively. The reader may consult Ref. [13] about the details.

Apart from the growing surface problem, I remark here on a property of the function $R(a)\Delta_a(\mathbf{r})$. If we consider for simplicity the case of $\psi=1$ [stochastic process of the Wiener (Markov) type], $\phi=2$ should be selected irrespective of spatial dimensions whenever $d>2$. Thereby when $d>2$, $\int d^d\mathbf{r}\, R(a)\Delta_a(\mathbf{r}) \propto a^{d-\phi}$ goes to zero in the limit of $a \to 0$. $\lim_{a\to 0} R(a)\Delta_a(\mathbf{r})$ is considered as a new type of distribution (functional), which is less singular than $\delta^d(\mathbf{r})$. Mathematical establishment is eagerly expected.

Now let us imagine that we try to integrate Eq. (1) numerically. In this task we usually calculate Eq. (10) under the condition that $L,t \to \infty$ with a and τ fixed. We expect that an asymptotic form of $w(L,t)$ is identical with one obtained through the continuum limit. I will emphasize below, however, that the two approaches do not always reach the same goal.

The estimation of $w(L,t)$ in Eq. (10) is also carried out by dividing $\Sigma'_{\mathbf{n}}$ into two parts as in Eq. (11). The first sum yields Eq. (12) by replacing $\{1-Y(\mathbf{k}_n)\}^{2t/\tau}$ with $\exp(-2\nu k^2 t)$ because $Y(\mathbf{k}_n) \simeq \nu\tau k_n^2 \leq \nu\tau d(\pi b)^2/a^2 \ll 1$. Even when $d>2$, however, the divergence of the integral does not occur in the limit due to the finitely discretized unit a. While Eq. (12) is proportional to L^{2-d} for $d<2$, its most dominant term is a constant [14] independent of L and t for $d>2$. On the other hand, the other sums in Eq. (11) yield Eq. (14) for $t \gg \tau/[2|\ln\{1-Y(\mathbf{k}_n)\}|](\geq a^2/[2\nu(\pi b)^2])$, giving L^0 order term for any dimensions. The condition (13) is also necessary for the Euler formula to keep $|1-Y(\mathbf{k}_n)|$ less than unity.

It is concluded therefore that through the latter limit (L and $t \to \infty$ with fixed a and τ) we have the same exponents for α and z as obtained through the continuum limit (a and $\tau \to 0$ with fixed L and t). Remember, however, that the above can be obtained without specifying the values of ϕ

and ψ. Even if we put $\phi = d$ and $\psi = 1$ (the spatiotemporal Gaussian white noise) for $d > 2$, the finite value of $w(L,t)$ is realized, contradicting the result of the continuum limit. This suggests in general that we must reconsider carefully whether the naive numerical integration of SDEs gives the continuum limit result.

In summary we have clarified the following:

(1) The scaling exponents of the EW model are

$$\alpha = (2-d)/2, \quad \beta = (2-d)/4, \quad z=2 \qquad \text{for} \quad 1 \leqslant d < 2,$$

$$\alpha = \beta = 0, \quad z=2 \qquad \text{for} \quad d > 2.$$

There should appear logarithmic corrections when $d=2$. Negative α for $d>2$ cannot be justified [3–5,10].

(2) In spaces with dimension higher than two, the correlation between the random variables should be weakened infinitesimally to obtain the physical solution irrelevant to the choice of the cutoff. The exponents satisfying the relation (16) correspond to the less singular correlation than the δ function. Nevertheless the random noises are indispensable to exclude a simply decaying solution. This is understandable from an intuitive argument; while in lower dimensions fluctuations induced by the spatiotemporal Gaussian white noise are crucial in that they keep accumulating to yield the rough surface solution; they are too strong to form the surface in higher dimensions due to the fluctuation accumulation from surroundings. If one continues to add the noise to the system, the solution may become the sum of δ functions.

(3) We have given an example that the two limits (a, $\tau \to 0$ with fixed L,t and $L,t \to \infty$ with fixed a, τ) do not lead to the same results. For $d>2$, the latter approach results in providing a finite $w(L,t)$ even in the case of being inherently infinite. I would like to conjecture that there exist such SDEs elsewhere. For these cases, in order to be consistent with an original continuum model, the numerical integration should be carried out by taking limits of a, $\tau \to 0$ for given L and t, however it looks troublesome.

(4) There are a lot of discrete versions converging in the Edwards-Wilkinson equation through continuum limits. In the present paper I have taken into account three routes from Eqs. (5), (7), and (1) with Eq. (17). For $d<2$, we have the same result of $w(L,t)$ through all routes, while for $d>2$ the value of $w(L,t)$ (=const) depends on how to approach the continuum model due to different microscopic situations. However, the exponents including zero themselves remain unchanged irrespective to the routes.

The above conclusions have been obtained within a linear theory. However, the assertion that the spatiotemporal white noise assumption turns out valid due to some nonlinear effect is necessary to be proved. For the Kardar-Parisi-Zhang equation [7], therefore, careful reconsideration of random variables must be required for $d>2$. Work on this problem is planned for the near future.

I would like to refer mathematical literature, where the related problems have been treated. In Ref. [15] the theorem that a heat equation with a noisy force, equivalent to the Kardar-Parisi-Zhang equation, has a unique distribution-valued solution for $d>2$ has been proved. Unfortunately the solution belongs to the L^2 class, being inappropriate for the growing surface problem. In addition Walsh showed in Ref. [16] that the stochastic wave equation has only a solution as a distribution valued stochastic process for $d \geqslant 2$.

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