HAMILTONIAN BROWNIAN MOTION
IN GAUSSIAN THERMALLY FLUCTUATING POTENTIAL.
I. EXACT LANGEVIN EQUATIONS,
INVALIDITY OF MARCOVIAN APPROXIMATION,
COMMON BOTTLENECK OF DYNAMIC NOISE THEORIES,
AND DIFFUSIVITY/MOBILITY 1/F NOISE

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ABSTRACT. Dynamical random walk of classical particle in thermodynamically equilibrium fluctuating medium, - Gaussian random potential field, - is considered in the framework of explicit stochastic representation of deterministic interactions. We discuss corresponding formally exact Langevin equations for the particle’s trajectory and show that Markovian kinetic equation approximation to them is inadequate, - even (and especially) in case of spatially-temporally short-correlated field, - since ignores such actual effects of exponential instability of the trajectory (in respect to small perturbations) as scaleless low-frequency diffusivity/mobility fluctuations (and other excess degrees of randomness) reflected by third-, fourth- and higher-order long-range irreducible statistical correlations. We try to catch the latter, - squeezing through typical theoretical narrow bottleneck, - with the help of an exact relationship between the instability and diffusivity statistical characteristics, along with standard analytical approximations. The result is quasi-static diffusivity fluctuations which generally are comparable with mean value of diffusivity and disappear in the limit of infinitely large medium’s correlation length or infinitely small correlation time only, in agreement with the previously suggested theorem on fundamental 1/f noise.

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1. INTRODUCTION

In this paper we shall touch classical analogue of interesting quantum statistical-mechanical problem already touched in [1, 2]. Namely, statistics of dynamical “random walk”, or “Brownian motion”, of (microscopic) particle interacting with thermodynamically equilibrium scalar boson field. For instance, with (harmonic) phonon field (crystal lattice or other medium oscillations).

Key words and phrases. dynamical foundations of kinetics, molecular Brownian motion, random walks and mobility 1/f fluctuations in (infinitely) many-particle Hamiltonian systems, fundamental 1/f-noise.
In [1, 2], basing on the widely known Hamiltonian model of such interaction ("polaron model"), we obtained an exact system of shortened evolution equations for probability distribution of the "Brownian particle" (BP) and its statistical correlations with the "phonon field" ("boson thermostat"), and argued that exact solutions to these equations includes 1/f-type (scaleless) low-frequency fluctuations of BP’s diffusivity and thus mobility. But direct formulations of these solutions, or at least good enough approximation to them (without loss of the diffusivity/mobility 1/f-noise), still are absent. Therefore, for further progress in statistical-mechanical theory of fundamental 1/f-noise, it may be useful to consider classical variant of the mentioned Hamiltonian model.

At that, we can avoid any detailing of "phonon" (thermostat) part of full Hamiltonian, if instead exploit the "stochastic representation" (SR) of dynamical (deterministic) interactions, for the first time suggested and tested in [3, 4] and later generalized, developed and applied in [5, 6, 7, 8, 9]. Thus our consideration will be at once additional probing of old and search of new SR possibilities.

2. Principles of the stochastic representation

Firstly we have to recall main SR statements [3, 4, 5, 7]. Let a Hamiltonian system consists of a “Dynamical subsystem” under our interest, “D”, and some its environment, or “thermal Bath” (thermostat), “B”, and full Hamiltonian of “D+B” has bilinear form

\[ H = H_d + H_b + H_{\text{int}}, \quad H_{\text{int}} = \sum_n D_n B_n, \]

(1)

where operators (or phase functions, in classical mechanics) \( H_d, D_n \) and \( H_b, B_n \) are defined in Hilbert spaces (or phase spaces) of “D” and “B”, respectively. Besides, let initially, somewhen in the past, full density matrix (probability distribution function) of “D+B” \( \rho(t) \) had factored form: \( \rho^{(\text{in})} = \rho(t \to -\infty) = \rho_d^{(\text{in})} \rho_b^{(\text{in})} \). Then marginal density matrix (DM) of “D”, \( \rho_d(t) = \text{Tr}_B \rho(t) \), can be expressed as average value,

\[ \rho_d(t) = \langle \tilde{\rho}(t) \rangle, \]

(2)

of randomly varying DM \( \tilde{\rho}(t) \) satisfying stochastic von Neumann (or Liouville) evolution equation

\[ \frac{d\tilde{\rho}(t)}{dt} = \frac{i}{\hbar} \left[ \tilde{\rho}(t), H_d + \sum_n x_n(t) D_n + \sum_n y_n(t) D_n \circ \tilde{\rho}(t) \right], \]

(3)
where $\circ$ denotes symmetrized (Jordan) product, $A \circ B = (AB + BA)/2$, and $x_n(t)$ and $y_n(t)$ are random processes.

At that, all statistical characteristics of $x_n(t)$ and $y_n(t)$ are unambiguously determined by internal dynamical properties of “B”, along with its initial DM, $\rho_b^{(in)}$. Corresponding formulae can be found in [3, 4, 5, 6, 7] (for most general variants of SR, including non-Hamiltonian dynamics, see [5]). In particular, if “B” is a set (continuum) of harmonic oscillators (wave modes), while $\rho_b^{(in)}$ has canonical Gibbs form, with some temperature $T$, then $x_n(t)$ and $y_n(t)$ are stationary Gaussian random processes representing thermodynamically equilibrium “Gaussian thermostat”.

Below, we confine ourselves by this case, but generalize it to continuous index $n$:

$$\sum_n D_n B_n \Rightarrow \int D(r) B(r) \, dr , \quad (4)$$

$$\sum_n x_n(t) D_n \Rightarrow \int x(t, r) D(r) \, dr , \quad \sum_n y_n(t) D_n \Rightarrow \int y(t, r) D(r) \, dr ,$$

where $r$ marks points of a $d$-dimensional space, and $dr = d^d r$.

3. Random fields of equilibrium thermostat

It is important to remind, firstly, that $x_n(t)$ and hence $x(t, r)$ represent direct dynamical perturbation of “D” by “B”, i.e. thermostat noise, while $y_n(t)$ and $y(t, r)$ inverse perturbation of “B” by “D” and related feedback action of “B” onto “D”, in particular, “friction” or “viscosity”, etc., i.e. thermostat induced dissipation. Therefore $y_n(t)$ or $y(t, r)$ are peculiar (“ghost”) random variables: all their self-correlation are zeros, e.g. $\langle y(t_1, r_1) y(t_2, r_2) \rangle = 0$, although their cross-correlations with $x_n(t)$ or $x(t, r)$ can differ from zero.

Secondly, the generalized fluctuation-dissipation relations (FDR, see e.g. [10, 11, 12, 13, 14, 15, 16, 17, 18, 19] and references therein), resulting from fundamental properties of Hamiltonian dynamics, imply definite mutual correspondence of the “x-y” cross-correlators and “x-x” self-correlators. In particular, for equilibrium and spatially homogeneous thermostat, according to standard recipes from [3, 4, 5, 6], we can write

$$K_{xx}(\tau, r_1 - r_2) \equiv \langle x(t + \tau, r_1) x(t, r_2) \rangle = \int_{-\infty}^{\infty} \cos \omega \tau \, S(\omega, r_1 - r_2) \, \frac{d\omega}{2\pi} ,$$

$$K_{xy}(\tau, r_1 - r_2) \equiv \langle x(t + \tau, r_1) y(t, r_2) \rangle = -\theta(\tau) \frac{2}{\hbar} \int_{-\infty}^{\infty} \sin \omega \tau \, \tanh \frac{\hbar \omega}{2T} \, S(\omega, r_1 - r_2) \, \frac{d\omega}{2\pi} , \quad (5)$$
where \( \theta(\tau) \) is Heaviside step function, thus expressing both “x-x” and “x-y” correlators through one and the same spectral function, \( S(\omega, r_1, r_2) \geq 0 \). Importantly, in accordance with the causality principle, \( y(t,r) \) is only correlated with later \( x(t' > t, r') \). In the classical limit, the FDR (5) reduces to

\[
K_{xy}(\tau, r) = \frac{\theta(\tau)}{T} \frac{\partial}{\partial \tau} K_{xx}(\tau, r)
\]  

(6)

In case of harmonic thermostat, these two correlators completely determine (Gaussian) statistics of \( x(t,r) \) and \( y(t,r) \).

4. Particle in thermal random field

To consider “Brownian particle” (BP) in a thermally fluctuating media, let us model the latter with potential field and choose in (1)-(4)

\[
H_d \Rightarrow \frac{P^2}{2m}, \quad D_n \Rightarrow D(r) = \delta(r-R)
\]  

(7)

with \( P \) and \( R \) being (operators of) BP’s momentum and coordinate and \( B(r) \) (operator of) the fluctuating potential. Then, in the Wigner representation, the “stochastic von Neumann (quantum Liouville) equation” (3) takes form

\[
\frac{\partial \tilde{\rho}}{\partial t} = -\frac{P}{m} \nabla_R \tilde{\rho} + \frac{i}{\hbar} \left[ x(t, R - i\hbar/2 \nabla_P) - x(t, R + i\hbar/2 \nabla_P) \right] \tilde{\rho} + \\
\frac{1}{2} \left[ y(t, R - i\hbar/2 \nabla_P) + y(t, R + i\hbar/2 \nabla_P) \right] \tilde{\rho}
\]  

(8)

with \( \nabla_R \) and \( \nabla_P \) denoting derivatives (gradients). In the classical limit, clearly, it turns to “stochastic Liouville equation” (SLE)

\[
\frac{\partial \tilde{\rho}}{\partial t} = -\frac{P}{m} \nabla_R \tilde{\rho} + \nabla x(t,R) \nabla_P \tilde{\rho} + y(t,R) \tilde{\rho}
\]  

(9)

where \( \nabla x(t,R) = \nabla_R x(t,R) \).

5. Langevin equations

Natural solution to the SLE (9) is

\[
\tilde{\rho}(t,R,P) = \delta(R-R(t)) \delta(P-P(t)) \exp \left[ \int_{t'}^t y(t',R(t')) dt' \right] ,
\]  

(10)

where \( R(t) \) and \( P(t) \) are random processes obeing stochastic ODE

\[
\frac{dR(t)}{dt} = \frac{P(t)}{m}, \quad \frac{dP(t)}{dt} = -\nabla x(t,R(t))
\]  

(11)

Notice that in [3,4] the minus sign in (5) was absent, but this misprint had not penetrated to results of SR applications.
with some (may be random) initial conditions in the past.

These equations do not display dissipative feedback action of the media (i.e. BP’s self-action through media), which however is completely involved by field \( y(t, r) \) and comes apparent after averaging expression (10) to get (2).

At the same time, classical SR allows [7] to perform in (10) separate averaging over “x-y” cross-correlations, in such way removing \( y(t, r) \) from (10) and displaying its effect in (11). As the result, stochastic equations (11) transform to what can be called “Langevin equations” (LE). A general recipe to construct LE is accumulated by Eqs.39-42 in [7]. In case of Gaussian thermostat, it strongly simplifies (see Eqs.44 and following example in [7]), and in application to our present system, as defined by Eqs.7 yields

\[
\begin{align*}
\frac{dR(t)}{dt} &= P(t), \\
\frac{dP(t)}{dt} &= f(t, R(t)) - \int_{t'>t} K(t - t', R(t) - R(t')) dt'.
\end{align*}
\]

(12)

Here, the integral represents medium’s feedback response, introducing friction and dissipation, its (vector-valued) kernel \( K(t, r) \) is expressed by

\[
K(t, r) = \nabla_r K_{xy}(t, r) = \frac{1}{T} \int \int \sin kr \sin \omega \tau \frac{\omega}{k} S(\omega, \vert k \vert) \frac{d\omega}{2\pi} \frac{d^d k}{(2\pi)^d},
\]

(13)

and \( f(t, r) = -\nabla x(t, r) \) is feedback-free “seed” medium’s random force field possessing Gaussian statistics with zero average value,

\[
\langle f(t, r) \rangle = 0,
\]

(14)

and correlation function

\[
\langle f(t_1, r_1) \ast f(t_2, r_2) \rangle = \nabla_{r_1} \ast \nabla_{r_2} K_{xx}(t_1 - t_2, r_1 - r_2)
\]

(15)

( \ast \) denotes tensor product of vectors). Now the random distribution function (DF) to be inserted to (2) is, instead of (10), merely \( \tilde{\rho}(t) = \delta(R - R(t)) \delta(P - P(t)) \).

Of course, BP’s state \( \{ R(t), P(t) \} \) is densely correlated with the force \( f(t, R(t)) \), therefore Gaussianity of the field \( f(t, r) \) in itself does not mean Gaussianity of \( f(t, R(t)) \).

6. Quasi-quantum formulation

Excluding from theory, - in the spirit of quantum mechanics, - BP’s momentum, and considering BP’s coordinate marginal distribution only,

\[
\tilde{W}(t, R) = \int \tilde{\rho}(t, R, P) d^d P,
\]
one can derive for it, instead of (9), equations

\[
\frac{\partial \tilde{W}(t, R)}{\partial t} = -\nabla [V(t, R) \tilde{W}(t, R)] + y(t, R) \tilde{W}(t, R),
\]

(16)

\[
V(t, r) = -\frac{1}{m} \nabla A(t, r),
\]

where \( V(t, r) \) is random velocity field generated by scalar “action” field \( A(t, r) \) which satisfies nonlinear stochastic Hamilton-Jacobi equation:

\[
\frac{\partial A(t, r)}{\partial t} = \frac{1}{2m} (\nabla A(t, r))^2 + x(t, r)
\]

(17)

Then, again performing partial averaging in respect to “x-y” cross-correlations, we can transform this into

\[
\frac{\partial \tilde{W}}{\partial t} = -\nabla [V \tilde{W}] \quad \text{and} \quad V = -\frac{1}{m} \nabla A,
\]

(18)

\[
\frac{\partial A}{\partial t} = \frac{(\nabla A)^2}{2m} + x(t, r) + \int_{t'>t} \int \nabla K_{xx}(t-t', r-r') \tilde{W}(t', r') \, d^d r' \, dt'
\]

(19)

Obviously, the latter stochastic PDE envelopes Eqs.12 and serves as a kind of LE.

7. Concretization of Problem

It is seems reasonable to assume, first, that our fluctuating media is statistically isotropic, therefore functions from (5) are spherically symmetric functions of coordinate differences, and we can write

\[
S(\omega, r) = \int \cos kr \, S(\omega, |k|) \frac{d^d k}{(2\pi)^d}
\]

(with, clearly, \( S(-\omega, \kappa) = S(\omega, \kappa) \)).

Second, the force field is not too singular, so that BP’s momentum diffusivity is finite:

\[
\int_0^\infty \langle f(t, R(t)) \ast f(t-\tau, R(t-\tau)) \rangle \, d\tau \sim \\
\sim \int_0^\infty [ -\nabla \ast \nabla K_{xx}(\tau, R(t) - R(t-\tau)) ] \, d\tau \equiv D^{(P)} \neq \infty
\]

(20)

This condition holds only if

\[
\int k^2 S(Vk, |k|) \, d^d k < \infty
\]

(21)

at any velocity \( V \). Then BP’s momentum and velocity, \( V(t) \equiv dR(t)/dt = P(t)/m \), behave as continuous random processes.
Third, at any \( k \),
\[
\int S(\omega, |k|) \, d\omega < \infty
\]  
(22)

This means that \( f(t, r) \) possesses nonzero correlation time, \( \tau_c \), i.e. is not a “white noise” in time. Evidently, otherwise space-time variations of \( f(t, r) \) would be able to propagate with infinite velocity, which would be rather nonphysical behavior.

Fourth, the spectral function \( S(\omega, |k|) \) is such that
\[
\lim_{\tau \to 0} \nabla K_{xx}(\tau, V\tau)) = 0
\]

Then, using FDR (6) and calculating the feedback integral in Eq. (12) by parts, we can transform Eqs. (12) into
\[
\frac{dR(t)}{dt} = V(t),
\]
\[
\frac{dV(t)}{dt} = f(t, R(t))/m - \int_{t'>t} G(t - t', R(t) - R(t')) V(t') \, dt',
\]  
(23)

where matrix response function
\[
G(\tau, r) = \langle f(\tau, r) \ast f(0, 0) \rangle / mT = -\nabla \ast \nabla K_{xx}(\tau, r)/mT =
\]
\[
= \frac{1}{mT} \int \int \cos kr \cos \omega \tau k \ast k S(\omega, |k|) \frac{d\omega}{2\pi} \, dk
\]  
(24)
determines BP’s viscous friction (here and below \( dk \equiv d^dk/(2\pi)^d \)).

It is interesting task to reveal, under enumerated conditions, long-time statistical properties of BP’s displacement, e.g. \( \Delta R(t) = R(t) - R(0) \).

8. Likely conjectures and Markovian approximation

8.1. Time-local friction approximation. Notice that because of condition (22) the friction always is more (may be highly) or less (may be slightly) nonlinear in respect to BP’s velocity.

If characteristic velocity’s relaxation time,
\[
\tau_v \sim mT/D^{(P)}
\]
(with \( D^{(P)} \)’s diagonal in mind), is large enough in comparison with that of \( G(\tau, V\tau) \) (i.e. the force’s correlation time \( \tau_c \) ), then one can visualize the non-linearity by “time-local approximation” of LE (23),
\[
\frac{dR(t)}{dt} = V(t),
\]
\[
\frac{dV(t)}{dt} = f(t, R(t))/m - g(V(t)) V(t),
\]  
(25)
with time-local relaxation rate

\[ g(V) \equiv \int_{0}^{\infty} G(\tau, V\tau)) d\tau = \frac{1}{2mT} \int k^* k S(Vk, |k|) dk \sim \frac{1}{\tau_v}. \tag{26} \]

8.2. Marcovian approximation. Simultaneously, the above approximation pushes to treat \( f(t, R(t)) \) like delta-correlated (“white”) noise. In order to reasonably determine its characteristics, we have to consider evolution equation for the random DF \( \tilde{\rho}(t) = \tilde{\rho}(t, R, V) \), corresponding to Eqs.25 i.e. SLE

\[ \frac{\partial \tilde{\rho}}{\partial t} = \left\{ -V \nabla_R + \nabla_V \left[ g(V) V - f(t, R) \right] \right\} \tilde{\rho}, \tag{27} \]

and coarsen it into approximate kinetic (Fokker-Planck) equation for actual BP’s DF \( \rho_d(t) = \rho_d(t, R, V) \) \( \text{(2)} \). Quite standard manipulations yield

\[ \frac{\partial \rho_d(t)}{\partial t} = \left\{ -V \nabla_R + \nabla_V \left[ g(V) V - f(t, R) \right] \right\} \rho_d(t) - \nabla_V \left( m^{-1} \left\{ f(t, R) \tilde{\rho}(t) \right\} \right) \approx \]

\[ \approx \left[ \frac{1}{m^2} \int_{0}^{\infty} \langle f(t, R) e^{-\tau V R} f(t, R) \nabla_V \tilde{\rho}(t - \tau) \rangle d\tau \right] \rho_d(t) = \]

\[ \approx \left[ \frac{1}{m^2} \int_{0}^{\infty} \langle f(t, R) f(t - \tau, R - V \tau) \rangle \nabla_V e^{\tau V \nabla_R} \nabla_V \rho_d(t) \right] \]

\[ \approx \left[ \frac{1}{m^2} \int_{0}^{\infty} \langle f(t, R) f(t - \tau, R - V \tau) \rangle \nabla_V \rho_d(t) \right], \tag{31} \]

that is finally, in the simplest “one-loop” approximation,

\[ \frac{\partial \rho_d}{\partial t} = -V \nabla_R \rho_d + \nabla_V g(V) \left[ (T/m) \nabla_V + V \right] \rho_d. \tag{32} \]

Thus, we in fact replaced the force \( f(t, R(t)) \) by BP’s coordinate-independent but instead velocity-dependent Gaussian white noise \( \tilde{f}(t, V(t)) \) with correlator

\[ \langle \tilde{f}(t, V(t)) \star \tilde{f}(t', V(t')) \rangle_V = 2Tm g(V) \delta(t - t') \sim 2D^{(P)} \delta(t - t'), \tag{33} \]

with \( \langle \ldots \rangle_V \) meaning conditional averaging under fixed \( V \).

8.3. Marcovian stochastic equations. To write out an equivalent SE, notice, in view of the \( g(V) \)’s definition \( \text{(26)} \) and condition \( \text{(21)} \), that one always can make single-valued smooth change of variables, \( V \Rightarrow U \), such that

\[ (\partial U/\partial V) g(V) (\partial U/\partial V)^\dagger = \bar{g}, \]
where $\mathbf{g}$ is a constant (unit matrix). It will be good choice if it equals to $g(V)$'s average over equilibrium Maxwell probability distribution of velocity:

$$\mathbf{g} = \int g(V) M(V) \, d^4V , \quad M(V) = \frac{\exp(-mV^2/2T)}{(2\pi T/m)^{d/2}}$$

(34)

(naturally, - as Eq.$\mathbf{32}$ says, - stationary $V$'s distribution is Maxwellian). Then, in terms of $U$, the SE corresponding to Eqs.$\mathbf{32,33}$ looks merely as

$$dR/dt = V(U) , \quad dU/dt = \tilde{f}(t)/m - \gamma(U) ,$$

$$\gamma(U) = \mathbf{g} \nabla_U [V^2(U) - (T/m) \ln \det g(V(U))] / 2,$$

with velocity-independent white noise source:

$$\langle \tilde{f}(t) * \tilde{f}(t') \rangle_U = 2Tm \mathbf{g} \delta(t-t') \quad (36)$$

9. **Inadequacy of Markovian approximation: disclosing of conventional conjectures**

For the first look, we just demonstrated that our problem hides nothing novel, since reduces to quite trivial SE. But this is wrong impression.

The matter is that the Markovian approximation (32)-(36) has qualitative defect: it neglects the above mentioned non-Gaussianity of the force acting onto BP, $f(t, R(t))$, and therefore losses specific non-Gaussian (higher-order) correlations between $f(t, R(t))$ and BP’s path $R(t)$. This loss took beginning in transition from expression (28) to expression (29), which just means replacement of $f(t, R(t))$ by Gaussian white noise. In fact, the resulting Eqs.$\mathbf{32,36}$ may arouse suspicions already because have no essential difference from equations for particle under short-correlated in time but infinitely far-correlated (constant) in space random force!

In order to better feel importance of the loss, let us compare “fidelities” of solutions to SE (35) and LE (25), that is their sensibilities to small perturbations (e.g. that of initial conditions). At that, non-linearity of friction plays no essential role, and for simplicity and visuality we deal with linear friction.

9.1. **Fidelity of solutions to SE in Markovian approximation.** First, consider differential response of Eqs.$\mathbf{35}$'s solutions to infinitesimally small change of (initial) velocity at time $t = 0$, that is

$$v(t) \equiv \partial V(t)/\partial V(0) , \quad r(t) \equiv \partial R(t)/\partial V(0)$$

Notice also that singularity of such change of variables would indicate inapplicability of time-local approximations at all, not speaking about Markovian approximation.
Since the noise source in Eqs.35 is insensible to BP’s state, it disappears under differentiation in respect to $V(0)$ or $U(0)$, that is does not influence on $v(t)$, $r(t)$. For linear friction, when $U = V$ and $\gamma(U) = gV$, with $g = \bar{g} = \text{const}$, we thus have equations

$$
\frac{dr}{dt} = v, \quad \frac{dv}{dt} = -g v,
$$

with initial conditions $v(0) = 1$, $r(0) = 0$. Consequently, at large $t$ velocity’s perturbation certainly tend to zero, while path’s (coordinate’s) one to a constant:

$$
v(t) \to 0, \quad r(t) \to 1/g
$$

(37)

9.2. Fidelity of solutions to LE in time-local friction approximation. Now, turn to the approximate but more adequate LE (23). From them we have, also at linear friction,

$$
\frac{dr}{dt} = v, \quad \frac{dv}{dt} = \left(\nabla f(t, R(t))/m\right) r - g v,
$$

(38)

again with initial conditions $v(0) = 1$, $r(0) = 0$. Thus, now we meet essentially multiplicative “noise source”, $(\nabla f(t, R(t))/m) r$, which can not be made state-independent by a non-singular change of variables. On average, solution to these equations coincides with (37). But in the sense of fluctuations it is much more interesting: naturally, it is statistically unstable.

To see this in most simple way, let us consider 1D case, $d = 1$, - when $v(t)$, $r(t)$, etc., become scalars instead matrices. Introduce random DF

$$
\tilde{\varrho}(t, r, v) = \delta(r - r(t)) \delta(v - v(t))
$$

and derive approximate kinetic equation for its average

$$
\varrho(t, r, v) = \langle \tilde{\varrho}(t, r, v) \rangle,
$$

by treating $f(t, R(t))$ as white noise (like in (29)-(31)). The result is

$$
\frac{\partial \varrho}{\partial t} = [-v \nabla_r + g \nabla_v] \varrho + Q (r \nabla_v)^2 \varrho,
$$

(39)

where parameters are expressed by

$$
g = \bar{g} = \frac{1}{2mT} \int k^2 \bar{S}(|k|) \, dk, \quad Q \equiv \frac{1}{2m^2} \int k^4 \bar{S}(|k|) \, dk, \quad \bar{S}(|k|) \equiv \int S(V k, |k|) M(V) \, dV
$$

(40)
Next, considering evolution of second-order statistical moments, from Eq. 39 (or directly from Eqs. 38 we have

$$\frac{d}{dt} \begin{pmatrix} \langle r^2 \rangle \\ \langle rv \rangle \\ \langle v^2 \rangle \end{pmatrix} = \mathcal{M} \begin{pmatrix} \langle r^2 \rangle \\ \langle rv \rangle \\ \langle v^2 \rangle \end{pmatrix}, \quad \mathcal{M} = \begin{pmatrix} 0 & 2 & 0 \\ 0 & -g & 1 \\ 2Q & 0 & -2g \end{pmatrix}$$

(41)

Eigenvalues, $\mu_j$, of matrix $\mathcal{M}$ are roots of cubic equation

$$\mu (\mu + g) (\mu + 2g) = 4Q$$

(42)

It clearly shows that one of roots, - let be denoted by $\mu_+$, - is real positive, that is solutions of Eqs. 38 are unstable in the sense of second-order (and hence higher-order) moments.

Rate of the instability, $\mu_+$, as compared with velocity relaxation rate $g \sim 1/\tau_v$, is determined by dimensionless parameter $Q/g^3$. From (40) it follows that

$$\frac{Q}{g^3} \sim \frac{T}{m r_c^2 g^2} \sim \frac{\lambda^2}{r_c^2},$$

where $r_c$ is characteristic correlation length of the force field $f(t, r)$, and $\lambda \sim \sqrt{T/m}/g \sim \tau_v \sqrt{T/m}$ characteristic BP’s “free path” length. Hence, if $r_c \ll \lambda$, then $Q/g^3 \gg 1$ and, according to Eq. 42, $\mu_+ \gg g$.

9.3. Fundamental incompleteness of Marcovian approach and typical “bottleneck” of dynamical theory of noises. We just revealed crucial defect of Marcovian approximation: it completely loses exponential instability of BP’s trajectories in respect to their small perturbations. As the consequence, it loses all statistical effects of this instability and therefore, generally speaking, can give only a caricature of real dynamical noise.

Then, how one should avoid the loss? The answer was prompted long ago by critical analysis of “molecular chaos” in fluids [20], crystals [22], under charge transport [19, 23, 24] and generally in transport phenomena [21, 23]. Namely, we have to reject any a priori statements (even very attractive) about “independencies” of “random” variables, - like e.g. “molecular chaos hypothesis” or “marcovianity”, - and allow any statistical dependencies and correlations compatible with equations of statistical mechanics. After that we might find that some of a priori unexpected or neglected dependencies and correlations really take place and are physically important.

Thus, in general there are two variants of approximate theory of transport noise: one (conventional) before the mentioned theoretical “bottleneck” (overcoming usual
instinctive conjectures and another behind the “bottleneck”. Figuratively speaking, that are two different solutions of same approximate equations, “trivial” and “non-trivial”. The latter contains low-frequency fluctuations, - like 1/f-noise, - of transport characteristics which are constants in the former.

10. **First steps to solution of the problem. Exponential instability, higher-order statistics, and scaleless diffusivity fluctuations**

To understand possible consequences of the exponential instability, first it is useful to point out several facts.

10.1. **Some useful formulae and remarks.** 1. Stationary (equilibrium) distribution of BP’s velocity has Maxwellian form, i.e. is Gaussian, regardless of degree of BP-thermostat interaction. This statement follows from the structure of Hamiltonian of our system as defined by (1) and (7). Therefore, in equilibrium statistical ensemble, for any function \( \Phi(V, \ldots) \) of \( V \) and some other random factors independent on \( V \), we can write

\[
\langle V, \Phi(V, \ldots) \rangle = \left( \frac{T}{m} \right) \langle \nabla V \Phi(V, \ldots) \rangle,
\]

\[
\langle V, V, \Phi(V, \ldots) \rangle = \left( \frac{T}{m} \right)^2 \langle \nabla V \nabla V \Phi(V, \ldots) \rangle,
\]

e tc. Here and below, angle brackets with \( n \) commas denote joint cumulant of \( n + 1 \) expressions separated by the commas (the Malakhov’s cumulant brackets). Similarly, since field \( f(t, r) \) is Gaussian,

\[
\langle f(t, r), \Phi(V, f, \ldots) \rangle = \int dt' \int dr' \langle f(t, r), f(t', r') \rangle \left\langle \frac{\delta \Phi(V, f, \ldots)}{\delta f(t', r')} \right\rangle
\]

(so-called Furutsu-Novikov formula).

2. BP’s state \( \{ R(t_0), V(t_0) \} \) at arbitrary chosen (and then fixed) “initial” time moment \( t_0 \) can be considered as statistically independent on the simultaneous medium’s state. Then, any function of later BP’s states \( \{ R(t), V(t) \} \ (t > t_0) \) and BP’s displacement (path) \( \Delta R = R(t) - R(t_0) \) gives an example of the mentioned function

\footnote{“Prejudices” disclosed by N. Krylov in [25].}

\footnote{For more explanations see review-discussion pages in [1, 2, 19, 20, 21, 22, 24] and also [26, 28, 29, 30, 31, 32, 33, 34, 35]. A hidden role of the exponential instability in fundamental 1/f-noise formation was directly demonstrated [22].}
Φ(V, . . .), with \( V = V(t_0) \), and Eq.43 yields, in particular,
\[
\langle V(t), V(t_0) \rangle = \left( \frac{T}{m} \right) \langle \partial V(t)/\partial V(t_0) \rangle,
\]
\[
\langle \Delta R, V_0 \rangle = \left( \frac{T}{m} \right) \langle \partial \Delta R/\partial V_0 \rangle,
\]
\[
\langle \Delta R^2, V_0, V_0 \rangle = \left( \frac{T}{m} \right)^2 \langle \partial^2 \Delta R^2/\partial V_0^2 \rangle,
\]
where for brevity we use \( V_0 \equiv V(t_0) \).

3. Notice that at \( t - t_0 \gg \tau_v \) second of expressions (45) gives BP’s diffusivity, let be denoted by \( D \). According to Eqs.37 \( D \approx T/mg = T/m \bar{f} \). Thus, mean value of the differential response \( \partial \Delta R/\partial V_0 \) is directly connected to the diffusivity.

Similarly, fluctuations of this response are closely connected to BP’s diffusivity fluctuations. The latter, on the other hand, can be adequately characterized by fourth-order BP’s path-velocity cumulants. Namely \([2, 19, 20, 21, 23, 24, 26, 28, 32, 34, 35]\), at \( \tau \equiv t - t_0 \gg \tau_v \), function
\[
K_D(\tau) = \frac{1}{24 \tau^2} \langle \Delta R, \Delta R, \Delta R, \Delta R \rangle = \frac{1}{24} \frac{d^2}{dt^2} \langle \Delta R^{(4)} \rangle = - \frac{1}{24} \frac{d^2}{dt dt_0} \langle \Delta R^{(4)} \rangle
\]
plays role of correlation function of equilibrium BP’s diffusivity fluctuations (and that of BP’s mobility fluctuations in weakly non-equilibrium regime under external force).

Here \( \langle X^{(n)} \rangle \) is short designation for \( X \)'s \( n \)-order cumulant, and we took into account that at \( t - t_0 \gg \tau_v \) the path statistics must depend on time difference \( t - t_0 \) only. We thus have
\[
K_D(t - t_0) = \frac{1}{2} \langle V(t), \Delta R, \Delta R, V(t_0) \rangle,
\]
or equivalently
\[
K_D(t - t_0) = \frac{1}{2} \langle \Delta R, \Delta R, V(t_0), V(t_0) \rangle - \frac{1}{6} \langle \Delta R, \Delta R, \Delta R, dV(t_0)/dt_0 \rangle = \frac{1}{2} \langle V(t), V(t), \Delta R, \Delta R \rangle + \frac{1}{6} \langle dV(t)/dt, \Delta R, \Delta R, \Delta R \rangle
\]

The differential response appears in visual form if we notice that at \( t - t_0 \gg \tau_v \) the two velocity values, \( V(t) \) and \( V(t_0) \), certainly are almost statistically independent and hence mutually Gaussian random quantities. Consequently, formula \(48\) can be transformed as follows,
\[
K_D(t - t_0) \Rightarrow \frac{T^2}{m^2} \left[ \frac{1}{2} \left\langle \frac{\partial^2 \Delta R^2}{\partial V(t) \partial V(t_0)} \right\rangle - \left\langle \frac{\partial \Delta R}{\partial V(t)} \right\rangle \left\langle \frac{\partial \Delta R}{\partial V(t_0)} \right\rangle \right],
\]
Clearly, right-hand side here consists of squared first-order differential response and besides second-order (double-differential) one. Analogously, with the help of Eqs.43-44 and other above formulas, transforms expressions (49).

4. Integrating Eq.47 one in the same fashion obtains relations

$$\int_0^\tau K_D(\tau') d\tau' = \frac{1}{6} \langle \Delta R, \Delta R, \Delta R, V_0 \rangle,$$

$$\frac{1}{\tau} \int_0^\tau K_D(\tau') d\tau' = \frac{1}{\tau} \frac{T}{2m} \left\langle \Delta R, \Delta R, \frac{\partial \Delta R}{\partial V_0} \right\rangle$$  \hspace{1cm} (51)

The latter thus calls for analysis of third-order irreducible correlations (cumulants) which address $K_D(\tau)$ to mutual correlation between “fidelity” and “diffusivity” of BP’s trajectories. In essence, this is particular case of general exact expression for correlation functions of low-signal excess noise and dissipation fluctuations [22] (see also [10]).

10.2. How the instability might work. 1. In the Marcovian approximation, the fourth cumulant $\langle \Delta R^{(4)} \rangle$ certainly is either linear function of $\tau = t - t_0$ at $\tau \gtrsim \tau_v$ or (in linear approximation) identical zero. Hence, $K_D(\tau)$ can appear non-zero at $\tau \gg \tau_v$ due only to what is lost under Marcovian approximation, i.e. the exponential instability of BP’s trajectories. Hence, to calculate some of the $K_D(\tau)$’s expressions (47)-(51), one have to substitute there exact solutions of LE (12) or (23) and then perform necessary averaging over realizations of the field $f(t, r)$.

At present, we do not know a regular method to break away from this “vicious circle” (penetrate through the “bottleneck”). Therefore, it would be quite good if we demonstrated significance of $\langle \Delta R^{(4)} \rangle$ and $K_D(\tau)$ at $\tau \gg \tau_v$ at least under some reasonable approximation of LE.

In this respect, the last of equivalent expressions (47)-(51) appears most suitable, in combination with the approximate time-local Eqs.25 and 38 since this combination most visually highlights statistical interference between BP’s trajectory $\{R(t), V(t)\}$ itself and its fidelity $\{r(t), v(t)\}$.

2. For simplicity, moreover, we apply also linear-friction approximation, - replacing in Eqs.25 $g(V)$ by $g = \overline{g} = \text{const}$ (with $\overline{g}$ from (31)), - and, besides, calculate right-hand side in Eq.51 under $V_0 = V(t_0) = 0$ (for anyway long-time behavior of $K_D(\tau)$ must be indifferent to $V(t_0)$ [1]).

5 At that, we merely omit from solution $\Delta R$ of Eqs.25 additive $V_0$’s contribution, $\exp(-g t) V_0$. 
Then, introducing functions
\[ \xi(t) = f(t, R(t))/m \quad \eta(t) = \nabla f(t, R(t))/m \quad C(\tau) = [1 - \exp(-g\tau)]/g \]
and taking \( t_0 = 0 \) and naturally \( R(0) = 0 \), we can write solution to Eqs.25 as
\[ \Delta R(t) = \int_0^t C(t - t') \xi(t') \, dt' \quad \text{(52)} \]
while solution to Eqs.38 as infinite iteration series
\[ r(t) = C(t) + \int_0^t C(t - t') \eta(t') \, dt' + \]
\[ + \int_0^t C(t - t') \eta(t') \int_0^{t'} C(t' - t'') \eta(t'') \, dt'' \, dt' + \ldots \quad \text{(53)} \]
Next, inserting all this into Eq.51 and imagining, in the spirit of time-local linear approximation, \( \xi(t), \eta(t) \) like white noises, one can see that in fact the only third term of expansion (53) survives after averaging. It produces
\[ \int_0^t K_D(\tau) \, d\tau = \frac{T}{m} \langle \Delta R(t), \Delta R(t), r(t) \rangle \approx \quad \text{(54)} \]
\[ \approx \frac{T}{m} \int_0^t dt' \int_0^{t'} dt'' C^2(t - t') C(t' - t'') C(t - t'') \times \]
\[ \times \int \int \langle I(t_1 - t', R(t_1) - R(t')) I(t_2 - t'', R(t_2) - R(t'')) \rangle \, dt_1 \, dt_2 \]
Here new (tensor) function \( I(\tau, r) \) appears defined by “\( \eta-\xi \)” cross-correlator:
\[ \langle \nabla f(t', R(t')) \ast f(t_1, R(t_1)) \rangle_R/m^2 = I(t_1 - t', R(t_1) - R(t')) , \]
\[ \quad I(\tau, r) = \nabla \ast \nabla \ast \nabla K_{xx}(\tau, r)/m^2 = \quad \text{(55)} \]
\[ = \frac{1}{m^2} \int \int k \ast k \ast k \, \sin kr \, \cos \omega \tau \, S(\omega, |k|) \frac{d\omega}{2\pi} \, dk , \]
with \( \langle \ldots \rangle_R \) standing for conditional average under given BP’s trajectory.

Evidently (and importantly), when performing integrations over \( t_1 \) and \( t_2 \) in Eq.54 we have to make replacement
\[ R(t_1) - R(t') \Rightarrow V(t') \tau - gV(t') \tau^2/2 \quad (\tau \equiv t_1 - t') \quad \text{(56)} \]
and similarly for \( R(t_2) - R(t'') \). At that, we remove from this displacements their parts containing \( f(t, R(t)) \), since contribution of these parts to the average in (54) is
definitely negligible, at least under condition $\tau_v \gg \tau_c$. Accordingly, applying under integral in Eq.55 approximation

$$\sin [k (V\tau - gV\tau^2/2)] \approx \sin kV\tau - k (gV\tau^2/2) \cos kV\tau,$$

we can write

$$\int I(t_1 - t', R(t_1) - R(t')) dt_1 \Rightarrow g\Upsilon(V(t')) V(t'), \quad (57)$$

$$\Upsilon(V) \equiv \frac{1}{m^2} \int k^4 S''(kV, |k|) dk = \frac{2T}{m} \nabla^2 g(V) \quad (58)$$

and analogously for second multiplier under the average (using symbolical scalar notations, instead of tensor ones, or for simplicity taking in mind $d = 1$).

At last, before inserting (57) to (54) let us make simplification as follows,

$$\langle g\Upsilon(V(t')) V(t') g\Upsilon(V(t'')) V(t'') \rangle \Rightarrow g^2\Upsilon^2 \langle V(t') V(t'') \rangle \approx \quad (59)$$

$$\approx \frac{g^2\Upsilon^2 T}{m} \exp \left( -g |t' - t''| \right)$$

and besides notice that at $t \gg \tau_v \sim 1/g$ all functions $C(\ldots)$ in Eq.54, - except $C(t' - t'')$, - can be replaced by constant $1/g$. Then we come to

$$\frac{1}{t} \int_0^t K_D(\tau) d\tau \approx \frac{T^2 \Upsilon^2}{2 m^2 g^4} = \frac{D^2 \Upsilon^2}{2 g^2}, \quad (60)$$

that is non-decaying, infinitely long-range, diffusivity’s correlation function.

3. Let us recall that, by the $K_D(\tau)$’s “microscopic” definition in “macroscopic” (phenomenological) sense

$$K_D(\tau) = \langle \tilde{D}(t + \tau), \tilde{D}(t) \rangle = \langle \tilde{D}(t + \tau) \tilde{D}(t) \rangle - \langle \tilde{D} \rangle^2,$$

where $\tilde{D}(t)$ represents fluctuating diffusivity, and $\langle \tilde{D}(t) \rangle = D$. Hence, our result (60) states that correlation function of BP’s diffusivity fluctuations never decays to zero, as if $\tilde{D}(t)$ were constant in time but randomly different from one BP’s trajectory to another.

Such “quasi-static” fluctuations are typical result of quantitatively rough theoretical approaches to 1/f-type low-frequency fluctuations of diffusivity/mobility or other transport rates. For examples see e.g. [36, 37]. Nevertheless, nothing prevents such

6 Notice also that in place of $\Upsilon^2$ it may be more correct to write $\Upsilon^2 = \int \Upsilon^2(V) M(V) dV$. 
approaches from giving reasonable estimates of 1/f-noise level, and they are rather cor-
rect in prediction of characteristic long-range statistical scale invariance of transport
processes \[19, 23, 24, 20, 21, 22\], i.e. \(\Delta R = R(t) - R(0)\) in the present case.

Indeed, considering higher-order equilibrium cumulants \(\langle \Delta R^{(2n)} \rangle\) by means of obvi-
ous generalization of exact relation (51),

\[
\frac{d}{dt} \langle \Delta R^{(2n)} \rangle = 2n (2n - 1) \frac{T}{m} \left\langle \Delta R^{(2n-2)} , \frac{\partial \Delta R}{\partial V_0} \right\rangle ,
\]

and again approximate expressions (52)-(53), it is not too hard to see that (at \(t \gg \tau_v\))

\[
\langle \Delta R^{(2n)} \rangle \approx (2n - 1)!! c_n \langle \Delta R, \Delta R \rangle^n \propto t^n ,
\]

with some coefficients \(c_n\) which can be obtained from a recursive procedure. Such
the asymptotic law detects essential non-Gaussianity of transport process and inappli-
cability of the “law of large numbers” to it.

At the same time, more accurate theories expectedly must lead to violation of such
literal scale invariance and appearance of some slow-varying, logarithmic or power-
law, factors in the \(K_D(t)\) and higher-order cumulants (62). For examples see e.g.
\[19, 23, 24, 20, 21, 26, 28, 30, 31, 34, 37\].

11. Variance of diffusivity fluctuations. Discussion of the result

1. Testing of more correct self-consistent approaches to our present problem we
leave for future. Now, instead let us discuss our spare but not trivial result (60).

Its above derivation shows that formal “entry point” to the mentioned theoretical
“narrow bottleneck” may be accounting for interplay between the exponential instability
and friction (dissipation) both simultaneously induced by the medium (thermostat).
Indeed, non-zero value of the integrated “\(\eta-\xi\)” correlation in Eq.55 is due to the sec-
ond term of (56) reflecting BP’s “braking” by the friction. Hence, in essence that
is “instability-friction” correlation. It then naturally causes fluctuations in friction-
related characteristics of BP’s motion, first of all in diffusivity, as Eq.51 prompts.

At that, the complete “I-I” correlor in Eq.54 (and its simplification in Eq.59) is
in fact fourth-order cross-correlator (cumulant) of the random force \(f(t, R(t))\) and
its gradient \(\nabla f(t, R(t))\). According to Eqs.51, 54 and finally 60 this correlation im-
plies specific long-range fourth-order (four-point) irreducible BP’s velocity correlations.
They, in turn, in accordance with Eq.61 give rise to an infinite hierarchy of higher-order
(many-point) long-range velocity (and force) cumulants.
2. Physical meaning of all such terrible picture was not once commented and explained in our works during last thirty years (please see above references and that therein).

Our consideration once again demonstrated that diffusivity by its origin never can be quite certain (a priori predictable) quantity. In absence of friction, it would have no definite value at all, because of constant BP’s stochastic acceleration and kinetic energy growth (as if the medium had infinitely large temperature). But when friction takes place, it immediately interferes with the exponential instability (IE) and, - together with BP’s diffusivity, - acquires fluctuations, as unboundedly diverse and unique as IE is in itself in (infinitely) many-particle systems.

In principle, such consequences of IE were predicted already by N. Krylov [25].

3. What is for quantitative meaning of our result (60), there are many different possibilities depending on structure of the medium’s spectral function \( S(\omega, |k|) \). Therefore let us imagine that it possesses some primitive “bell-like” shape and can be characterized by three parameters only, i.e. medium’s correlation time \( \tau_c \) and length \( r_c \) and, besides, magnitude of the force field fluctuations. The latter parameter can be replaced by the velocity relaxation rate \( g \sim 1/\tau_v \).

Then, in view of Eq.58 and under approximation (59), we come to estimate

\[
\frac{K_D}{D^2} \approx \frac{T^2}{2g^2} \sim \left( \frac{T \tau_c^2}{m r_c^2} \right)^2 \sim \left( \frac{T}{m u^2} \right)^2 ,
\]

(63)

where \( u \sim r_c/\tau_c \) can be interpreted as characteristic propagation velocity of the force field. Thus, this estimate well agrees with the reasonings expounded in Sec.7 and 9.

Let us also remind of, firstly, our assumption \( g \ll 1/\tau_c \), which in standard terms means weakness of the field fluctuations. Secondly, conventional opinion that Markovian approximation coincides with exact theory at least in the “infinitely weak interaction (weak noise) limit” \( g\tau_c \to 0 \). In reality, however, - as Eq.63 shows, - variance of relative low-frequency (quasi-static) diffusivity fluctuations, \( \tilde{D}(t)/D \), is insensible to the \( g\tau_c \)'s value, if the ratio \( \tau_c/r_c \) keeps constant. Hence, generally Markovian approximation has no justification even in the weak noise limit (not speaking that anyway it losses any diffusivity fluctuations)!

\[ \]
To improve our estimates of the diffusivity 1/f noise, even in case weak medium’s noise, one should return to formally exact LE (12) or (23) or may be (19) and carefully do with their non-linearities, playing significant role at non-zero ratio $\tau_c/r_c$.

12. Conclusion

To resume, we considered Langevin equations describing random walk of particle in thermodynamically equilibrium fluctuating medium, and showed that the particle’s diffusivity undergoes scaleless (1/f-type) low-frequency fluctuations whose magnitude can be comparable with average value of diffusivity (or even much exceed it) regardless of magnitude of the medium noise.

At that we demonstrated, on one hand, usefulness of traditional “stochastic calculus” in the framework of dynamically based theory. On the other hand, necessity to control stochastic way of thinking, since its seeming completeness may lead to too hasty and wrong conclusions (in particular it by itself automatically losses the diffusivity fluctuations under our interest).

The obtained result confirms rather general “theorem on fundamental 1/f noise” discussed in [35] (and, under more specific conditions, in [2, 32]). I hope it will stimulate further investigations of transport 1/f noises in various many-particle Hamiltonian systems.

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and fallacies [40], which was excellently illustrated in [25] by example of statistical physics. In contrast to poor pure stochastics, dynamics allows for some “free will”.

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